生物物理

SEIBUTSU BUTSURI

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SUPPLEMENT 1-2

Vol.62

第60回年会プログラム集

主催　一般社団法人　日本生物物理学会

The Biophysical Society of Japan

一般社団法人　日本生物物理学会　https://www.biophys.jp

第 60 回日本生物物理学会年会

The 60th Annual Meeting of the Biophysical Society of Japan

目 次

Contents

開催概要／General Information

The 60th Annual Meeting of the Biophysical Society of Japan
第60回日本生物物理学会年会（2022年度）

会期／Period
2022年9月28日（水）－30日（金）
28 (Wed.) – 30 (Fri.), September, 2022

会場／Venue
函館アリーナ、函館市民会館
Hakodate Arena, Hakodate Citizen Hall

年会長・実行委員長／Chair of the Organizing Committee
金城 政孝（北海道大学大学院先端生命科学研究院）
Masataka Kinjo（Faculty of Advanced Life Science, Hokkaido University）

年会ウエブサイト／Website of the Annual Meeting
https://www2.aeplan.co.jp/bsj2022

年会長挨拶

第60回年会 年会長・実行委員長
金城 政孝
(北海道大学大学院先端生命科学研究院)

日本生物物理学会の第60回年会を、2022年9月28日から30日までの3日間、北海道の南に位置します、函館市の函館アリーナ並びに函館市民会館を中心に開催予定です。

生物物理学は生物を対象として生物、物理、化学、情報、宇宙までを含む非常に幅広い研究者が参画して展開する学問です。そのために会員が一堂に参加する年会は最新の情報を持ちより、議論する一番重要なイベントと考えています。

以上のことを基本としてこの第60回年会は、オンサイト、つまり対面での開催を目指しています。但し、会員の皆様には現地でのご参加を第一にお考え頂きますが、 ウイルス感染状況その他により、現地へお越し頂けない方には、オンラインでご発表 ・ ご参加頂けるように、同時にハイブリッド形式で開催すべく準備を進めております。

本年会では、 会員によるポスター発表と、 口頭発表となるシンポジウムを中心に、 研究を支えて頂いている企業との交流を目指して、 バイオフィジックスセミナー（BPセミナー）その他の企画も実施いたします。

例年参加者が多く、たいへん楽しみにしています懇親会の実施は見送りますが、その代わりにポスター・展示会場でのミキサーを開催できるように準備を進めております。

また今回も高校生・高専生の参加を広く募集しましたので、学会員の一般ポスター発表に交じって、自由な意見交換ができるよう、希望しています。

ポスター発表・シンポジウムともハイブリッドの特徴の一つ、オンラインを利用したオンデマンドによる聴講もおこないます。しかし、一方でハイブリッドでの開催準備となり、参加者の皆様にも多大な準備や協力を必要と考えています。この点、何卒、ご理解を頂きますと幸いです。

年会の会場で、多くの皆様と御会いできることを心から楽しみにしています。これまでの年会と同じように、生物物理学の交流を楽しむ第60回大会に、ぜひご参加ください。

年会実行委員会
Organizing Committee

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相沢 智康　（北海道大学）

プログラム

菊川 峰志　（北海道大学）

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角五 彰　（北海道大学）
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櫻沢 繁　（公立はこだて未来大学）
高木 清二　（公立はこだて未来大学）
塚本 卓　（北海道大学）
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徳楽 清孝　（室蘭工業大学）
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西村 有香子（北海道大学）
芳賀 永　（北海道大学）
日比野 政裕（室蘭工業大学）
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眞山 博幸　（旭川医科大学）

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Masataka Kinjo　(Hokkaido Univ.)

Vice Chair

Tomoyasu Aizawa　(Hokkaido Univ.)

Program

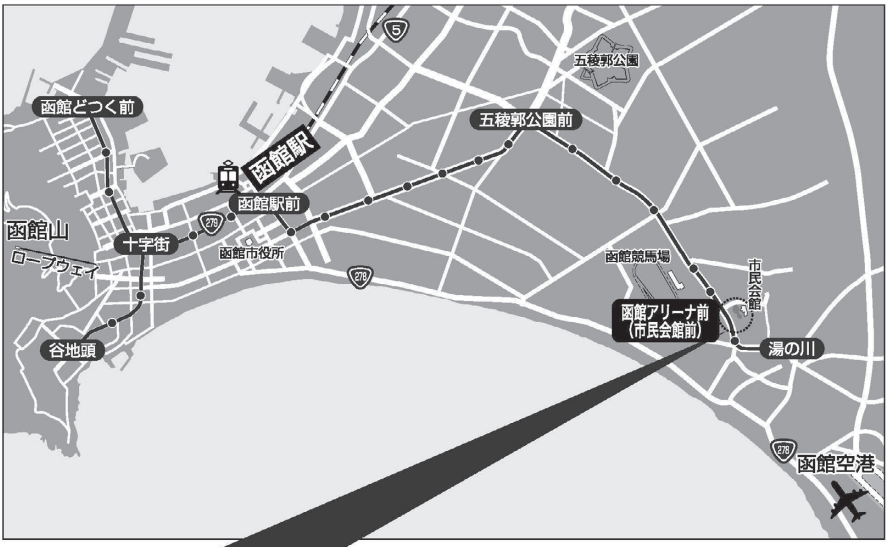
Takashi Kikukawa　(Hokkaido Univ.)

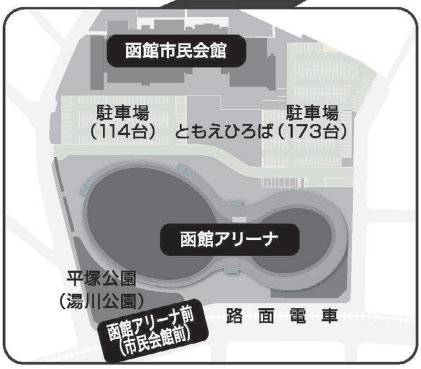
Members

Tatsuo Akitaya　(Asahikawa Med. Univ.)
Koichiro Ishimori　(Hokkaido Univ.)
Akira Inoue　(Hokkaido Univ.)
Takeshi Uchida　(Hokkaido Univ.)
Tsutomu Uchida　(Hokkaido Univ.)
Takaharu Okajima　(Hokkaido Univ.)
Toyoyuki Ose　(Hokkaido Univ.)
Akira Kakugo　(Hokkaido Univ.)
Shunsuke Kita　(Hokkaido Univ.)
Akira Kitamura　(Hokkaido Univ.)
Hiromi Kimura　(CIST)
Tamiki Komatsuzaki　(Hokkaido Univ.)
Hidemasa Kondo　(AIST)
Takashi Saitoh　(Hokkaido Univ. of Sci.)
Shigeru Sakurazawa　(Future Univ. Hakodate)
Seiji Takagi　(Future Univ. Hakodate)
Takashi Tsukamoto　(Hokkaido Univ.)
Makoto Demura　(Hokkaido Univ.)
Kiyotaka Tokuraku　(Muroran Inst. Tech.)
Shinji Nakaoka　(Hokkaido Univ.)
Toshiyuki Nakagaki　(Hokkaido Univ.)
Masafumi Nagayama　(Hokkaido Univ. Edu.)
Yukinori Nishigami　(Hokkaido Univ.)
Yukako Nishimura　(Hokkaido Univ.)
Hisashi Haga　(Hokkaido Univ.)
Masahiro Hibino　(Muroran Inst. Tech.)
Katsumi Maenaka　(Hokkaido Univ.)
Hiroyuki Mayama　(Asahikawa Med. Univ.)

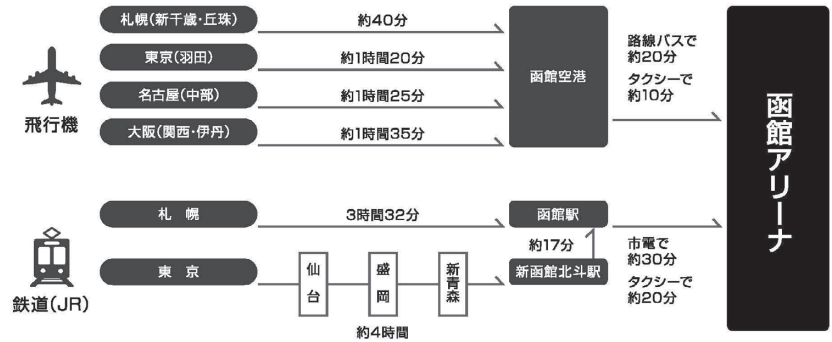
三上 秀治　（北海道大学）　Hideharu Mikami　(Hokkaido Univ.)
水谷 武臣　（北海学園大学）　Takeomi Mizutani　(Hokkai-Gakuen Univ.)
茂木 文夫　（室蘭工業大学）　Fumio Motegi　(Muroran Inst. Tech.)
姚 閔　（北海道大学）　Min Yao　(Hokkaido Univ.)
横山 泰範　（函館工業高等専門学校）　Yasunori Yokoyama　(Natl. Inst. Tech., Hakodate Col.)

交通案内


函館どつく前
函館駅
函館駅前
五稜郭公園
五稜郭公園前
函館山
ロープウェイ
十字街
函館市役所
函館競馬場
市民会館
函館アリーナ前
(市民会館前)
谷地頭
湯の川
函館空港


函館市民会館
駐車場
(114台)
駐車場
ともえひろば(173台)
函館アリーナ
平塚公園
(湯川公園)
路面電車
函館アリーナ前
(市民会館前)


Sapporo
札幌
Hakodate
函館
Aomori
青森
Tokyo
東京
Osaka
大阪
Nagoya
名古屋


飛行機
札幌(新千歳・丘珠)
約40分
東京(羽田)
約1時間20分
名古屋(中部)
約1時間25分
大阪(関西・伊丹)
約1時間35分
函館空港
路線バスで
約20分
タクシーで
約10分
函館アリーナ
鉄道(JR)
札　幌
3時間32分
函館駅
約17分
東　京
仙台
盛岡
新青森
新函館北斗駅
市電で
約30分
タクシーで
約20分
約4時間

＜駐車場＞

※ 会場には有料駐車場がありますが、原則として公共交通機関をご利用ください。

＜函館市電＞

※ 「湯の川」駅行にご乗車いただき、「函館アリーナ前（市民会館前）」で下車してください。

※ 交通系のICカードの使用が可能です。

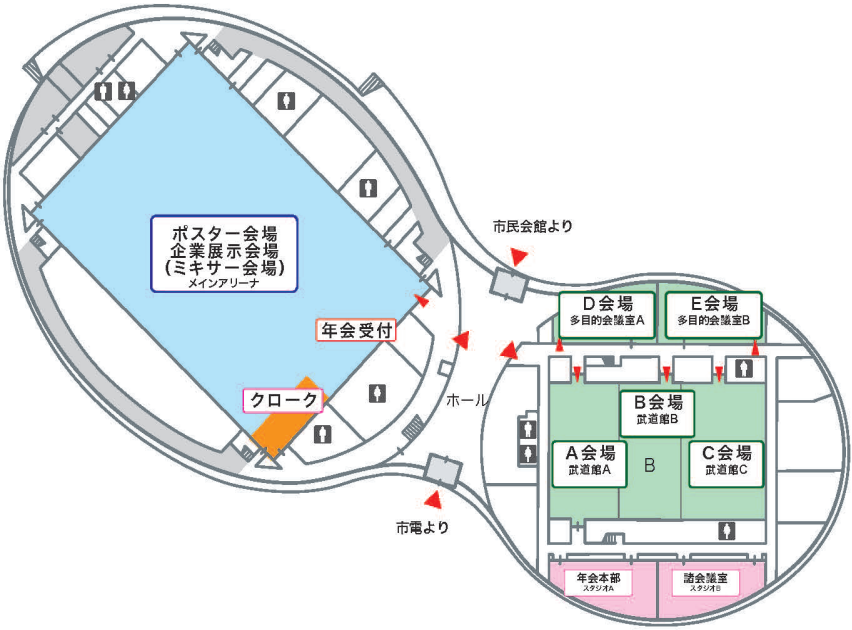
※ 函館駅前 始発（6:53）から、6分間隔で運行しています。なお、7:41から8:05までは、3分間隔に増車しております。

＜路線バス＞

※ 函館駅前4番乗り場から五稜郭経由函館アリーナ行の路線バスを2台運行いたします（有料）。

函館アリーナ

1F

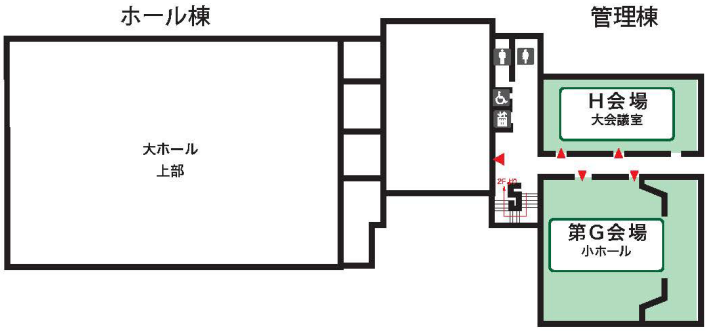


※ メインアリーナの2F観客席もご利用可能です。

※ 函館アリーナ内は、全会場飲食可能ですが、黙食等にご協力ください。

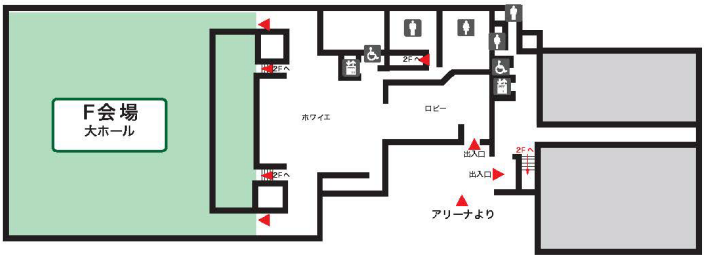
函館市民会館

3F



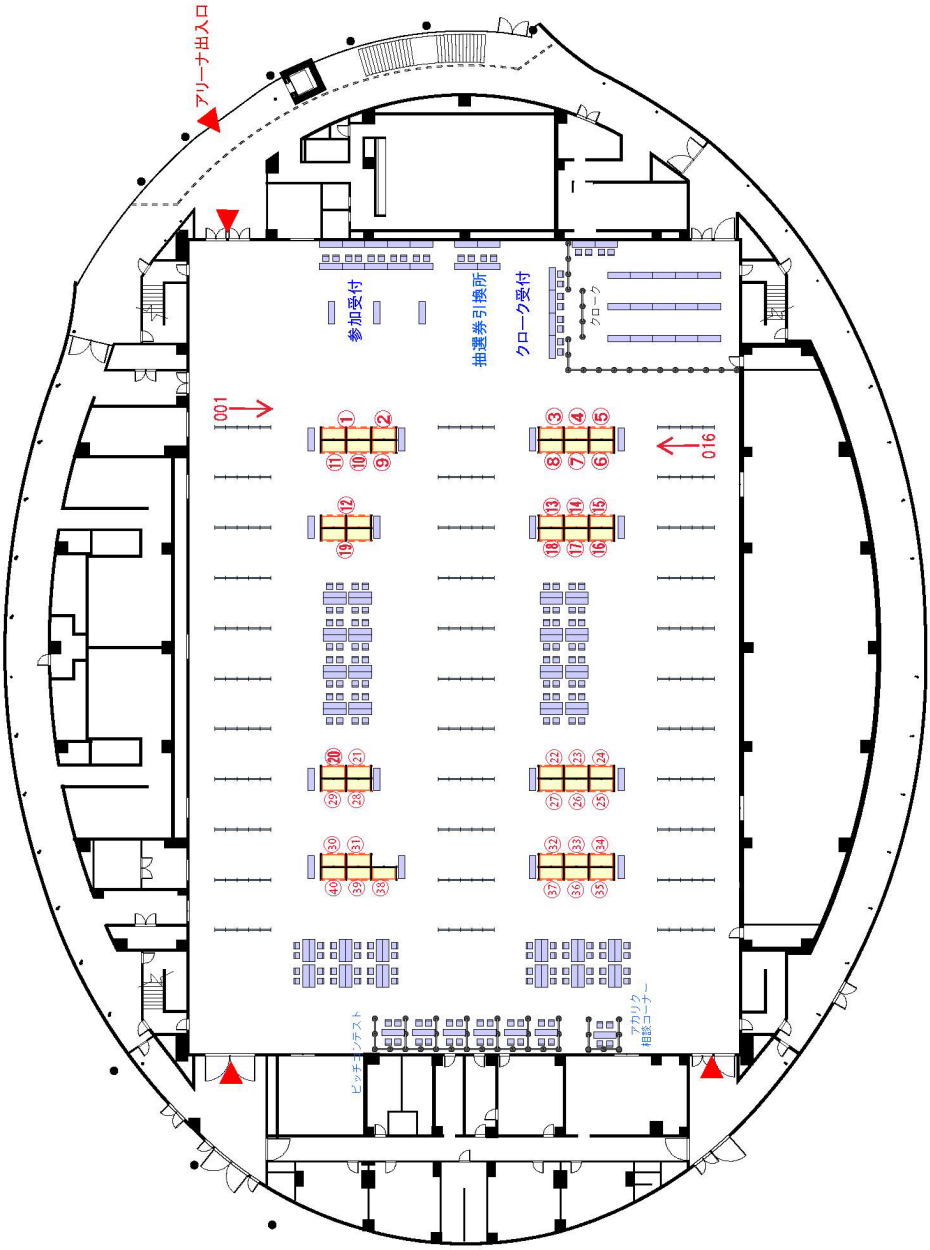
2F

1F



※ F会場（大ホール）は飲食物の持ち込み禁止です。

ポスター・展示会場（メインアリーナ）



出展企業一覧

① （株）エビデント
② 中山商事（株）
③ 三井情報（株）
④ オリシロジェノミクス
⑤ （株）オプトライン
⑥ アイリックス（株）
⑦ コスモ・バイオ（株）
⑧ （株）モルシス
⑨ キーストンサイエンティフィック（株）
⑩ 生体分子計測研究所
⑪ 日本電子（株）
⑫ ソーラボジャパン（株）
⑬ （株）日本レーザー
⑭ 正晃テック（株）
⑮ ブルカージャパン（株）
⑯ 浜松ホトニクス（株）
⑰ ナニオンテクノロジーズ ジャパン合同会社
⑱ （株）セルフリーサイエンス
⑲ クロマテクノロジ ジャパン合同会社
⑳ シグマ光機（株）
㉑ キコーテック（株）
㉒ オックスフォード・インストゥルメンツ（株）
㉓ （株）ビジコムジャパン
㉔ タイテック（株）
㉕ （株）NanoAndMore ジャパン
㉖ ヨダカ技研（株）
㉗ 東京応化工業（株）
㉘ （株）ナックイメージテクノロジー
㉙ レフェイン・ジャパン（株）
㉚ （株）ニコンソリューションズ
㉛ ヘルツ（株）
㉜ 東ソー（株）
㉝ （株）エムエステクノシステムズ
㉞ 横河電機（株）
㉟ （公財）高輝度光科学研究センター
㊱ （公財）中谷医工計測技術振興財団
㊲ 日本蛋白質構造データバンク（PDBj）
㊳ 大陽日酸（株）
㊴ SPT Labtech Japan（株）
㊵ （株）堀場製作所

2022年７月31日現在

■ 2022年 9 月 27 日（火）

	部屋名	会場	8	9	10	11	12	13
函館アリーナ	多目的室A	D会場						
	スタジオB	諸会議						

■ 2022年 9 月 28 日（水）

	部屋名	会場	8	9	10	11	12	13
函館アリーナ	武道館A	A会場		**1SAA** 動的溶液環境が駆動するタンパク質凝集（吉田 紀生, 菅瀬 謙治）		企業展示ブース訪問推奨時間	**BPセミナー1** シグマ光機（株）	日本蛋白質構造データバンク
	武道館B	B会場		**1SBA** 量子ビームでひも解くタンパク質の大きな構造変化−タンパク質ダイナミクス理解の新潮流−（山本 直樹, 関口 博史）			**BPセミナー2** サーモフィッシャーサイエンティフィック	
	武道館C	C会場		**1SCA** 生命金属のライブセルイメージング（石森 浩一郎、平山 祐）			**BPセミナー3** 浜松ホトニクス（株）	
	多目的室A	D会場		**1SDA** 糖鎖の動的構造から機能へ −実験・理論解析の最先端（李 秀栄、山口 芳樹）			キャリア支援説明会	
	多目的室B	E会場		**1SEA** 先端赤外光の利用による生物物理学研究（古谷 祐詞、村越 秀治）				
函館市民会館	大ホール	F会場		若手招待講演シンポジウム				BPPB論文賞受賞講演
	小ホール	G会場		**1SGA** 再構築実験によってアプローチするプロトセル研究と生命の起源への探求（車 兪澈、Tony Z. Jia）			**BPセミナー4** （株）リバネス	
	大会議室	H会場		**1SHA** 分子集団，細胞集団が織りなす自律特性: 生命機能の理解を目指して（茅 元司、島本 勇太）			理事会	
函館アリーナ	メインアリーナ	ポスター	貼付	ポスター掲示				
		展示		機器・試薬展示				
	スタジオB	諸会議		BPPB委員会	出版委員会			

※「企業展示ブース訪問推奨時間」は、特に企業展示ブースの訪問を積極的に行っていただきたい時間帯です。
年会運営には企業等からの支援をいただいております。
これ以外の時間帯にも積極的に企業ブース等へ訪問いただき、製品情報等のご収集にお役立てください。

14	15	16	17	18	19	20
			臨時社員総会			
	WEBサイト 編集委員会					

14	15	16	17	18	19	20
1SAP スーパーコンピューター「富岳」による 創薬・医療の革新 （荒木 望嗣, 池口 満徳）	企業展示ブース訪問推奨時間				企業参画型ピッチコンテスト	
1SBP 細胞内メゾ複雑体の構造と機能 （杉田 有治, 山本 林）						
1SCP 複雑システムの振る舞いの解明に向けたトポロジカルアプローチ （望月 敦史, 岡田 崇）						
1SDP 生体高分子による液液相分離： 基礎と応用 （北原 亮, 亀田 倫史）						
1SEP 微細制御技術を用いた フィジコケミカルバイオロジーへの展開 （北村 朗, 飯塚 怜）						
1SFP 生体膜の生物物理呼応と細胞機能制御への化学的利用 （中瀬 生彦, 広瀬 久昭）						
1SGP 高次構造体を自在に操る （宮﨑 牧人, 小杉 貴洋）						
1SHP "肉"のイマとミライ （鈴木 団, 大山 廣太郎）						
		ポスター発表 （奇数）	ポスター発表 （偶数）	ポスター 発表 (Zoom)	ミキサー	
		若手奨励賞 選考委員会				

■ 2022年 9 月 29 日（木）

	部屋名	会場	8	9	10	11	12	13
函館アリーナ	武道館A	A会場		**2SAA** NMRで迫る膜とペプチドの生物物理 （川村 出, 相沢 智康）		企業展示ブース訪問推奨時間	**BPセミナー5** 日本電子（株）	
	武道館B	B会場	レフェイン・ジャパン	**2SBA** 先端技術と理論で迫るクロマチン機能の理解 （伊藤 由馬, 木村 宏）				
	武道館C	C会場		**2SCA** 発動分子科学への若手研究者による挑戦 （小杉 貴洋, 大友 章裕）			**BPセミナー6** 中山商事（株）	
	多目的室A	D会場		**2SDA** 先端的ラベルフリーナノポア計測による生物物理学への展開と応用 （山崎 洋人, 庄司 観）				
	多目的室B	E会場		**2SEA** 100nm サイズの分子集団で顕在化する非凡な時空アロステリー （成田 哲博, 秋山 修志）				
函館市民会館	大ホール	F会場		**2SFA** Japan-US symposium on motor proteins and associated single-molecule biophysics （Kumiko Hayashi, Jakia Jannat Keya）			会員総会・総会シンポジウム	
	小ホール	G会場		**2SGA** シンギュラリティ生物学を導くイメージング技術 （蛭田 勇樹, 渡邉 朋信）			分野別専門委員会	
	大会議室	H会場		**2SHA** 生体分子工学と低物理エネルギーロジスティックスで切り拓く新たな生体操作学 （井上 圭一, 今村 博臣）			**BPセミナー7** レフェイン・ジャパン（株）	
函館アリーナ	メインアリーナ	ポスター	貼付	ポスター掲示				
		展示		機器・試薬展示				
	スタジオB	諸会議						

※ 「企業展示ブース訪問推奨時間」は、特に企業展示ブースの訪問を積極的に行っていただきたい時間帯です。
年会運営には企業等からの支援をいただいております。
これ以外の時間帯にも積極的に企業ブース等へ訪問いただき、製品情報等のご収集にお役立てください。

14	15	16	17	18	19	20
2SAP 多細胞系の情報物理学 （小林 徹也, 川口 喬吾, 石島 秋彦）						
2SBP 富岳を用いた高性能計算による生物物理 （松永 康佑, 信夫 愛）						
2SCP 生体分子の人工設計：タンパク質、RNA、DNA （古賀 信康, 神谷 由紀子）						
2SDP 金属イオン制御による酵素の動態 （織田 昌幸, 森川 耿右）						
2SEP ダイナミックな翻訳 その開始から終わりまで （丹澤 豪人, 楊 偉皓）						
2SFP 生物物理学による脳の理解と化学的再生 （村岡 貴博, 齋尾 智英）						
2SGP 物理化学的解析から探るアミロイド・ゲルの構造ダイナミクス （田中 元雅, 真板 宣夫）						
2SHP マルチファセット・プロテインズへの生物物理アプローチ （渡邉 力也, 太田 元規）						
		ポスター発表（奇数）	ポスター発表（偶数）	ポスター発表（Zoom）	ミキサー	

企業展示ブース訪問推奨時間

■ 2022年 9 月 30 日（金）

	部屋名	会場	8	9	10	11	12	13
函館アリーナ	武道館A	A会場		**3SAA** 発光・蛍光計測と光学顕微鏡の標準化を目指して（佐々木 章, 近江谷 克裕）		企業展示ブース訪問推奨時間	男女共同参画・若手支援委員会企画シンポジウム	
	武道館B	B会場		**3SBA** 様々な先端的手法で挑む生体分子の構造ダイナミクスの可視化（梅名 泰史, 清水 伸隆）			科研費説明会	
	武道館C	C会場		**3SCA** 自主・自発の階層と適応：冗長性を行動力(健康)につなげる分子-細胞-筋-身体-脳連携（跡見 順子, 岩城 光宏）			**BPセミナー8**（株）ニコンソリューションズ	
	多目的室A	D会場		**3SDA** 硫黄のタンパク質科学の最前線（増田 真二, 中林 孝和）				
	多目的室B	E会場		**3SEA** 生物を利用したゼロエミッション・CO_2資源化技術の可能性（加藤 創一郎, 近藤 英昌）				
函館市民会館	大ホール	F会場		**3SFA** クライオ電子顕微鏡が魅せる生命の未知なる動的なメカニズム（濡木 理, 西増 弘志）				
	小ホール	G会場		**3SGA** 自己組織化で超分子生体膜を創る：材料科学と生物物理学の接点（安原 主馬, 森垣 憲一）				
	大会議室	H会場		**3SHA** 高次機能性分子システム～創る方法の解明に向けて～（松浦 友亮, 川野 竜司, 鈴木 雄太）				
函館アリーナ	メインアリーナ	ポスター		貼付	ポスター掲示			ポスター発表（奇数）
		展示			機器・試薬展示			
	スタジオB	諸会議			企業との意見交換会			

※「企業展示ブース訪問推奨時間」は、特に企業展示ブースの訪問を積極的に行っていただきたい時間帯です。
年会運営には企業等からの支援をいただいております。
これ以外の時間帯にも積極的に企業ブース等へ訪問いただき、製品情報等のご収集にお役立てください。

14	15	16	17	18	19	20
ポスター発表（偶数）	ポスター発表（Zoom）	閉会式				

参加者へのご案内

1．参加方法

本年会はハイブリッド方式（現地開催＋オンライン開催）で開催いたしますが、感染症対策等での問題が無い場合、可能な限り、現地での参加をご検討ください。
ただし、緊急事態宣言などによるイベントの開催に対する制限の要請の状況等に応じて、参加制限、プログラムや実施内容の変更があり得ること、あらかじめご了承ください。

＜オンライン参加＞

年会ウエブサイトから、Confitにログインしてください。ログインには、ID（参加登録に使用したメールアドレス）、PW（bsj2022）が必要です。Confitへのログインは、9月15日（木）頃から可能です（予定）。

2．新型コロナウイルス感染対策について

本年会では下記の通り、新型コロナウイルス感染対策を実施いたします。皆様ご協力いただきますようお願いいたします。

◇下記に該当する方は現地参加をお控えください

1）37.5度以上の発熱がある場合
2）咳、のどの痛み、息苦しさ、疲労倦怠感、味覚・嗅覚異常の症状がある場合
3）感染の疑いがある場合

◇現地での感染対策

1) 会場内でマスクは必ずご着用ください。
2) 会場入口で検温を実施します。37.5度以上の方は、参加をお断りいたします。
3) 会場入口等に、消毒液を設置いたしますので、こまめな手指消毒をお願いいたします。
4) 講演会場への参加人数を制限いたします（立ち見不可）。
5) 講演会場内の換気を実施します。
6) 飲食時（バイオフィジックスセミナー等）は黙食でお願いします。

3．参加登録

◇事前登録

「事前登録（前期）」期間内に参加登録をしていただいた方には参加証（領収証）を事前送付いたします。申込時に同意いただいた方の参加証には、氏名・所属・E-mailアドレスの情報を含む QRコード が印刷されております。参加者間や企業展示ブースでの情報交換の際にご活用ください。

「事前登録（後期）」期間内に参加登録をしていただいた方には参加証は当日受付にてお渡しいたしますので、参加登録完了メールを印刷してお持ちください。

なお、名札ホルダーは会場入口付近で、当日配布します。会場内では必ず参加証をご着用ください。

◇当日登録

事前登録が完了していない方は当日受付でご登録ください。なお、お支払いは現金のみとなります。

場　所：函館アリーナ メインアリーナ

日　時：9月28日（水）・29日（木）8:15-17:00 / 30日（金）8:15-13:30

◇学会デスク

参加受付に学会デスクを設けております。新入会や年度会費の支払いを受付けております。

◇プログラム集 / 予稿集 / Confit Web版･アプリ版（オンライン予稿集）

プログラム集は、日本生物物理学会会員および事前登録（前期）された非会員に事前に送付しております。非会員の事前登録（後期）の方には、会場受付にてお渡しいたします。

予稿本文（PDF版）は、年会WEBサイトに掲載いたします（9月上旬予定）ので、ダウンロードしてください。また、予稿本文は、Confit Web版およびアプリ版（無料）からも閲覧可能です。

予稿集（PDF版）：
https://www2.aeplan.co.jp/bsj2022/program.html
ダウンロードID: ambsj2022
Password: 60hakodate

Confit（Web版 プログラム/予稿集）：
年会Webサイトに掲載します。
ログインID：参加登録に使用したメールアドレス
Password:bsj2022

Confit（アプリ版 プログラム/予稿集）
App Store / Google Playよりダウンロード（無料）
（「生物物理」、「bsj2022」などで検索）
ログインID、Passwordは、Confit（Web版）と同じです。

※ プログラムと予稿集は、年会終了後に日本生物物理学会ウエブサイトの年会の記録および J-STAGEの「生物物理誌」において、パスワードなしで公開されます。

◇Confitの活用について

Confit　Web版･アプリ版からは、「Webポスターの閲覧」や「コメント」機能を利用した質疑応答が可能です。また、参加者の「プロフィール」の公開や「ダイレクトメッセージ」機能を利用した交流も可能です。公開･配布開始後（9月15日頃を予定）は早めにログインいただき、「マイプロフィール」への情報登録にご協力ください。

また、「マッチングフラグ機能」により、会場ポスター掲示やZoomポスター発表の有無なども確認できます。

詳細については、年会ウエブサイトでご案内いたします。

４．年会当日のご案内

◇使用言語

使用言語は原則英語です。ただし、総会シンポジウム、男女共同参画・若手支援委員会企画シンポジウム、キャリア支援説明会、科研費説明会、企業参画型ピッチコンテストなどの企画は日本語で実施します。

◇PC/タブレット/スマホ・ヘッドセット等の活用

ハイブリッド開催となるため、当日会場にWiFi接続可能なPC等お持ちいただき、ご活用ください。特にシンポジウムやZoomポスター発表へのネットからの参加では、イヤホンマイク等が必要となります。メイン アリーナにはWiFi環境が整備されているため、2階観客席等からの接続が可能ですが、他の参加者の声などが気になる場合に備え、ヘッドセット等をお持ちいただくことを推奨いたします。

◇インターネット（WiFi）接続

ポスター・展示会場（メインアリーナ）ではWiFi接続が可能です。
なお、ハイブリッド開催に伴い、各シンポジウム会場への接続を優先いたしますので、回線容量の関係で、接続状況が悪くなる可能性がありますので、なにとぞご了承ください。

※SSID、パスワードは現地でお知らせいたします。

また、メインアリーナ２Fの観客席には電源コンセントがありますので、ご利用ください。

◇Zoomでの参加

来場が不可能な場合等は、シンポジウム及びポスターセッションにZoomから参加することが可能です。
各会場のZoomへはConfit上のプログラムからアクセスすることができます。Zoomで参加する場合には、名前は、原則として英語で「姓　所属」を表示ください。
（例）「Yamada　Hokkaido Univ.」。
質疑応答時以外は、カメラ、マイクはオフで参加ください。

◇シンポジウムへの参加

会場でのシンポジウムへ参加の場合には、コロナウイルス対策のため、各会場に人数制限がありますのでご注意ください。立ち見はできません。定員で入場できない場合は、アリーナ2階観客席等かZoomで参加するか、後日、オンデマンド配信で視聴ください。
会場のスクリーンには、発表時は「発表者のスライド」、質疑応答時は「発表者」、「座長」、「会場全景」、「Zoom参加の質問者」の映像等が投影されます。Zoom参加者のPCへは、「発表者のスライド」、「発表者」、「座長」、「会場全景」、「Zoom参加の質問者」の映像等が表示されます。
会場での質疑応答は、Zoom参加者の視聴のために、必ずマイクを使用して行ってください。Zoom参加者から質問がある場合には、「手を挙げる」機能を使い、座長から指名された時のみ、マイクと画像をオンにして口頭で質問を行ってください。チャットでの質疑応答は原則として受け付けませんが、座長から別途指示があるシンポジウムではこの限りではありません。

◇ポスター発表への参加

会場のポスターは毎日張り替えになります。対面での参加者のポスター発表義務時間は下記の通りです。

ポスターの前での討論にご参加ください。

28日（水）・29日（木） 奇数 16:30-17:30、偶数 17:30-18:30

30日（金） 奇数 13:10-14:10、偶数 14:10-15:10

Zoomポスター発表時間は下記の通りです。Zoomポスター発表に参加される際は、ポスター番号により指定されたZoomのブレイクアウトルームを使用してください。

詳細については、年会ウエブサイトでご案内いたします。

28日（水）・29日（木） 18:30-19:00

30日（金） 15:10-15:40

Webポスターへの質問は、Confitの「コメント」機能を用いて、随時可能です。コメントを書き込むことで、ポスター発表者のメールアドレスに通知が送信されます。発表者は適宜コメント機能を用いて、返答をお願いいたします。ただし、発表者からの回答の書き込みの通知はありませんので、ご了承ください。

◇会員総会・総会シンポジウム

一般社団法人日本生物物理学会第9回会員総会・総会シンポジウムを29日（木）12:35-13:35にF会場（市民会館・大ホール）で開催いたしますのでご出席ください。

◇若手招待講演シンポジウム

第18回若手奨励賞の選考会である若手招待講演シンポジウムを28日（水）9:00 -11:30にF会場（市民会館・大ホール）で開催いたします。授賞式は、29日のミキサー内で行います。

◇クローク

貴重品、コンピュータなどについては、紛失、破損などの責任を負いかねますのでお預かりできません。また、傘もお預かりできません。

場　所：函館アリーナ メインアリーナ

日　時：9月28日（水）・29日（木）8:15-20:30 / 30日（金）8:15-16:30

◇昼食

バイオフィジックスセミナー（28日-30日）、キャリア支援説明会（28日）、男女共同参画・若手支援シンポジウム（30日）、科研費説明会（30日）については、お弁当とお茶が無料で提供されます。なお、お弁当は当日配布する整理券が必要となります。整理券は下記の通り発行いたします。

時　間：各日 8:15～

場　所：函館アリーナ ホール

※整理券は当日開催される分のみ配布いたします。枚数がなくなり次第終了となります。

※開始時間までにご来場されない場合、整理券は無効となりお弁当はチケットをお持ちでない参

加者に提供されますことをご了承ください。

※バイオフィジックスセミナーは企業、団体等の支援による共催セミナーです。参加される場合は最後までご聴講いただくとともに、共催者のアンケート等には必ず所属・氏名を記入して回答くださるよう、ご協力をお願いいたします。

※お弁当数に限りがあるため、当日はお弁当の販売を行う予定です。

◇駐車場

会場には有料駐車場がありますが、原則として公共交通機関をご利用ください。

◇託児所

託児所を設置いたします。詳しくは年会ウエブサイトをご覧ください。

◇ミキサー

懇親会の代わりに、28日・29日（19:00-20:30）にポスター・企業展示会場（メインアリーナ）にて、ミキサーを行います。ビール又はソフトドリンクとおつまみのセット（一人一日1セット）を無料で提供する予定です。なお、会話の際は必ずマスクをご着用ください。

29日のミキサー内で、若手奨励賞及び若手招待講演賞の授賞式を行います。

◇企業展示

メインアリーナでは企業展示を行います。なお、「企業ブース訪問推奨時間」も設けておりますので、積極的に企業展示ブースにお立ち寄りください。 また、スタンプラリーを実施いたしますので、ぜひご参加ください。スタンプラリーの抽選は閉会式で行います。

◇閉会式

30日のポスター発表終了後、ポスター・企業展示会場（メインアリーナ）で閉会式を開催します。閉会式では学生発表賞の受賞者を発表します。ぜひ、皆様ご参加ください。

５．禁止事項

１）種々のパスワードやURLを第三者に伝えることを禁止します。

２）会場内及び講演画面のカメラ、ビデオ、携帯電話などによる撮影や講演音声の録音などを禁止します。またPC画面のスクリーンショット保存も厳禁とします。

座長、発表者へのご案内

◇シンポジウムのオーガナイザーの方へ

受付：セッション開始の15分前までに各会場の「座長席」にお越しの上、係りの者に来場された旨をお伝えください。

感染症対策等で座長の来場ができない場合：万が一来場いただけない場合には、Zoomからの進行が可能ですが、来場できないことが判った時点で、至急年会運営事務局へご連絡ください。※年会運営事務局（jbp2022@aeplan.co.jp）

座長席：座長用のPCが1台備え付けてあります。進行を行う座長はこの席に交代でお座りください。進行を進める座長の映像がカメラによりZoom上に表示されます。

進行：オーガナイザーに一任いたしますので、講演者の講演時間を厳守し、円滑な運営にご協力ください。 講演中は事前に事務局に連絡いただいた時間に従って、計時が表示されます。講演者の講演時間に変更が生じた場合は、会場内の進行スタッフにご連絡ください。
全ての講演は録画され、会期後約2週間、年会への参加登録者に限定してオンデマンド視聴が可能な形で公開されます。開始時にその旨講演者及び参加者に周知ください。

質疑応答：会場からの質問は、Zoom参加者の視聴のために、必ずマイクを使用するように指示してください。 Zoom参加者からの質問がある場合には、「手を挙げる」機能を使って受付、座長の指名により、マイクと画像をオンにして口頭で質問していただくようにしてください。質問は、チャットではなく、口頭で行っていただくことを原則としますが、シンポジウムによって座長の指示によりチャットで質疑応答を受け付けることも妨げませんので、その場合には参加者へその旨を明確に指示するようにご協力をお願いいたします。

◇シンポジウムの講演者の方へ

受付：セッション開始の15分前までに発表用のご自身のPCをお持ちになり、各会場の「PC受付」にお越しください。
PCの映像出力端子はHDMIのみです。端子の形状が異なる場合は変換コネクタをご準備ください。また、バッテリー切れに備え、電源アダプターをお持ちください。
発表スライドをご確認いただいた後、会場スタッフがパソコンを接続いたします。 スライドチェック用の試写室はございません。

講演時間：シンポジウムの時間配分はオーガナイザーに一任しております。 若手招待講演シンポジウムの講演時間は、発表10分、討論3分、パソコン交換2分です。

来場しての講演が出来ない場合：来場できない場合には、Zoomからの発表が可能です。来場できないことが判った時点で、オーガナイザーへご連絡ください。発表会場のZoomには、Confitからアクセスすることが可能です。オーガナイザーの指示に従って登壇ください。

◇ポスター（一般講演）発表者の方へ

発表要項：ポスターは英語で作成してください。ただし、タイトル、所属、著者名は、可能であれば日本語の併記もお願いいたします。発表者の氏名には○印を付けてください。

Webポスター：会場へのポスター掲示の有無にかかわらず、Confit上へのWebポスターファイルのアップロードは必ず行ってください。原則として会場に掲示のポスターと同じファイルを使用し、9月上旬に発表者本人に連絡される専用のサイトからアップロードしてください。アップロードの集中を避けるため、会期1週間前の9月21日（水）をアップロード期限としますが、それ以降も発表当日まで自由に再アップロードして、書き換えいただくことが可能です。Webポスターのアップロードをもって、発表の成立となります。

会場ポスター：ポスターパネルは幅900mm x 高さ2,100mmです。ポスターは毎日張り替えになりますので、発表日当日は可能な限り会場にお越しいただき、貼付時間（28日（水）・30日（金）8:30-9:00、29日（木）8:10-8:45）にポスターを貼り付けください。貼り付けに必要な押しピンは会場に用意します。また発表義務日のポスター発表時間終了後、ミキサーが実施されます。ミキサーに参加される方は、ミキサー終了後にポスターを撤去ください。ミキサーに参加されない方は、発表時間終了後適宜撤去ください。撤去されていないポスターは、年会事務局にて破棄いたしますので、ご了承ください。

また、やむを得ず来場できず、ポスター掲示が困難な場合、以下の対応をお願いします。

・Confitのその発表演題の「コメント」に、ポスター掲示が出来ない旨
（例　会場へのポスター掲示はありません　等）のコメントを入力
・Confitの「マイプロフィール」の「マッチングフラグ」から「会場に居りません」を選択

発表義務時間：対面での参加者は、ポスター発表義務時間にはポスターの前で説明をしてください。やむを得ず来場できない場合は、可能な範囲で以下のZoomでのポスター発表を行ってください。

Zoomポスター発表：Zoomによるポスター発表をされる際は、Zoomポスター発表時間に「ポスター番号により指定されたZoomのブレイクアウトルーム」を使用して説明をしてください。説明に使用する資料は、原則としてWebポスターファイルを用いてください。

Zoomポスター発表を行う場合には、Confitの「マイプロフィール」の「マッチングフラグ」から「Zoom発表を実施します（X日目）」を選択することで、参加者にZoomポスター発表が行われることを明示してください。

なお、来場して対面で参加している場合でも希望により、ご自身の発表義務日にZoomポスター発表をしていただくことも可能です。この場合は、ポスター・企業展示会場（メインアリーナ）の2階観客席などからのWiFi接続等により参加ください。

コメント機能での質疑応答：Confitの「コメント」機能を用いた質疑応答が可能です。コメントが書き込まれた場合、発表者のメールアドレスに通知がきますので、コメント機能を用いた応答をお願いいたします。ただし、返答を書き込んだ旨の質問者への通知はありませんのでご了承

下さい。

ポスター発表タイムテーブル：

		9月28日（水）	9月29日（木）	9月30日（金）
貼付		8:30-9:00	8:15-8:45	8:30-9:00
説明・討論	奇数番号	16:30-17:30	16:30-17:30	13:10-14:10
	偶数番号	17:30-18:30	17:30-18:30	14:10-15:10
	Zoom(任意)	18:30-19:00	18:30-19:00	15:10-15:40
撤去		19:00-20:45	19:00-20:45	15:40-16:45

謝 辞

本年会の開催・運営にあたり，以下の団体よりご協力・ご援助いただきました。関係者一同より御礼を申し上げます。

第60回日本生物物理学会年会
年会長　金城 政孝

助成

函館市、北海道

共催

新学術領域研究「生命金属科学」
新学術領域研究「遺伝子制御の基盤となるクロマチンポテンシャル」
新学術領域研究「発動分子科学」
新学術領域研究「シンギュラリティ生物学」
新学術領域研究「情報物理学でひもとく生命の秩序と設計原理」
新学術領域研究「高速分子動画」
学術変革領域研究（A）「クロススケール新生物学」
学術変革領域研究（A）「マルチファセットプロテインズ」
学術変革領域研究（A）「新興硫黄生物学が拓く生命原理変革」
学術変革領域研究（A）「超越分子システム」
学術変革領域研究（B）「SPEED」
学術変革領域研究（B）「筋肉トランススケール熱シグナリング」
学術変革領域研究（B）「遅延制御超分子化学」
学術変革領域研究（B）「生体分子工学と低物理エネルギーロジスティクスの融合による次世代非侵襲 深部生体操作」
CREST「新たな光機能や光物性の発現・利活用を基軸する次世代フォトニクスの基盤技術」
JST さきがけ「細胞の動的高次構造体」
文部科学省「富岳」成果創出加速プログラム「プレシジョンメディスンを加速する創薬ビッグデータ統合システムの推進」
文部科学省「富岳」成果創出加速プログラム「全原子・粗視化分子動力学による細胞内分子動態の解明」
NEDO ムーンショット型研究開発事業

Greeting

The 60th Annual Meeting of the Biophysics Society of Japan
Chair of the Organizing Committee
Masataka Kinjo
(Hokkaido University)

The 60th Annual Meeting of the Biophysical Society of Japan (BSJ) will be held from September 28 to 30, 2022, at the Hakodate Arena and Hakodate Citizen Hall, Hakodate City, located in the south of Hokkaido.

Biophysics is involved a very wide range of researchers in biology, physics, chemistry, information, and even astronomy. For this reason, the annual meeting is the most important event for members to gather and discuss the latest research progress.

Based on the above, the 60th Annual Meeting of BSJ aims to be held on-site, that is, face-to-face. However, for those who cannot come to the Hakodate due to COVID-19 infection or other reasons, we are preparing to hold the meeting in a hybrid format so that you can present and participate online.

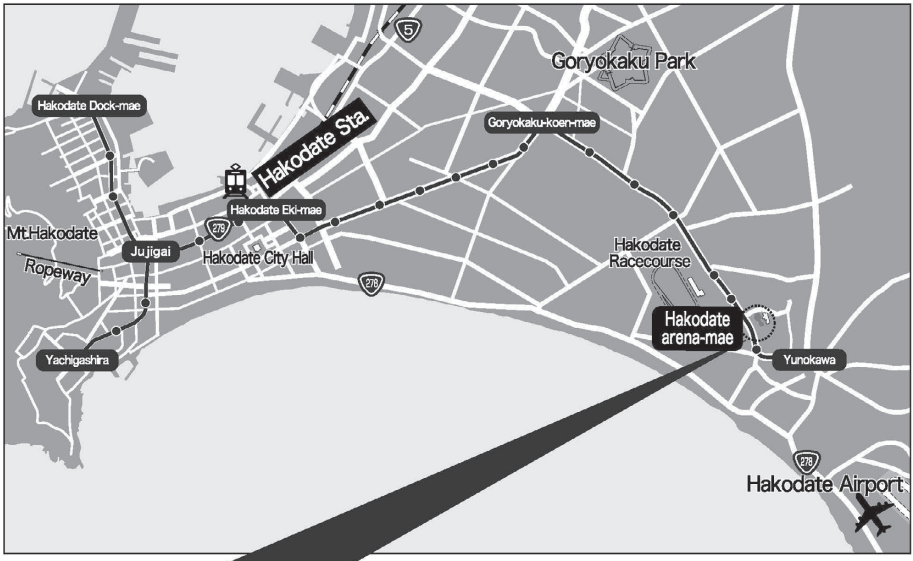
In this annual meeting, we are planning to have poster presentations by members and symposia with oral presentations, as well as a Biophysics Seminar (BP seminar) and other events to promote interaction with companies that support our research.

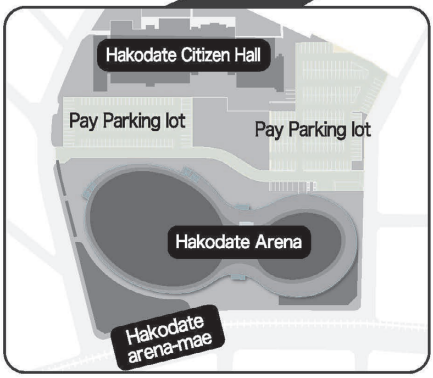
We are considering to hold some form of a banquet, which is always well attended and much looked forward to. We are also looking for high school and technical college students to present their researches. We hope that they will be able to freely exchange their research with the general poster presentations by the conference members.

One of the features of the hybrid format, both the poster presentation and the symposium, is that we are also planning to offer on-demand participating via online. On the other hand, the preparation for the hybrid presentation will require a great deal of preparation and cooperation from the participants. We would be grateful for your understanding in this situation.

I am sincerely looking forward to seeing many of you at the Annual Meeting. We hope you will join us for the 60th Annual Meeting to enjoy the exchange of biophysics as you have done in the past.

Access Information





Plane

Sapporo(New Chitose/Okadama)	Approx. 40min.	Hakodate Airport	By Bus: Approx. 20min. / By Taxi: Approx. 10min. → Hakodate arena-mae
Tokyo(Haneda)	Approx. 1hr. 20min.		
Nagoya(Chubu)	Approx. 1hr. 25min.		
Osaka(Itami)	Approx. 1hr. 35min.		

Train

Sapporo	Approx. 3hr. 32min.	Hakodate Sta.	→ Hakodate arena-mae
Tokyo	Approx. 4hr.	Shin-Hakodate-Hokuto (Approx. 17min. → Hakodate Sta.)	By City Tram: Approx. 30min. / By Taxi: Approx. 20min. → Hakodate arena-mae

[Parking]

* Please use public transportation as there is no free parking at the venue.

[Hakodate's trams]

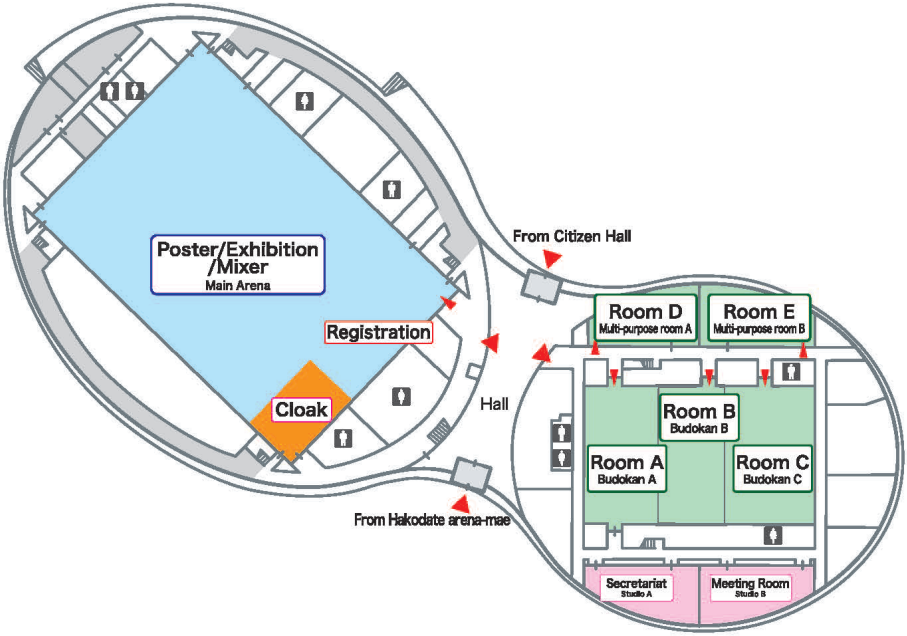
* Take a trams bound for "Yunokawa" and get off at "Hakodate arena-mae"
* Traffic IC cards are accepted.
* The Trams run every 6 minutes from the first departure (6:53) from Hakodate Ekimae. From 7:41 to 8:05, the frequency will be increased to every 3 minutes.

[Bus]

* Two buses will run from platform 4 in front of Hakodate Station to Hakodate Arena via Goryokaku (for a fee).

Hakodate Arena

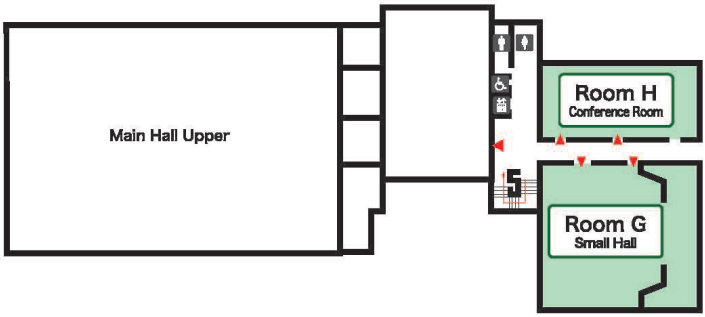
1F



* The 2nd floor spectator seating in the main arena is also available.
* Food and beverages are allowed in Hakodate Arena.
  Please help us eat silently!

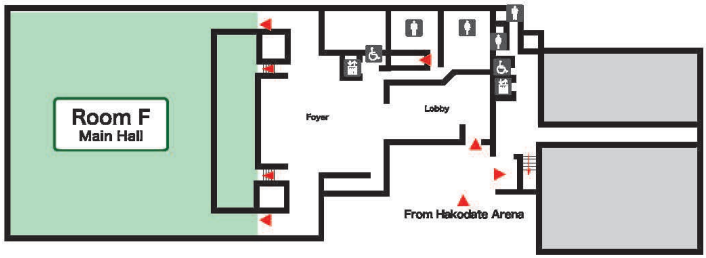
Hakodate Citizen Hall

3F



2F

1F



* Food and beverages are not allowed in Hall F (Main Hall).

■ 27(Tue.) September, 20222

	Room	Venu	8	9	10	11	12	13
Hakodate Arena	Multi-purpose room A	Room D						
	Studio B	Meeting Room						

■ 28(Wed.) September, 2022

	Room	Venu	8	9	10	11	12	13
Hakodate Arena	Budokan A	Room A		**1SAA** Protein aggregation driven by dynamic solution environments (Norio Yoshida, Kenji Sugase)		Exhibition Booths Recommended Visit Time	**BP Seminar 1** Shigmakoki	PDBj / Exhibition Booths Recommended Visit Time
	Budokan B	Room B		**1SBA** Protein large-scale motions revealed by quantum beams -a new era in understanding protein dynamics- (Naoki Yamamoto, Hiroshi Sekiguchi)			**BP Seminar 2** Thermo Fischer Scientific	
	Budokan C	Room C		**1SCA** Live-cell imaging of bio-metal species (Koichiro Ishimori, Tasuku Hirayama)			**BP Seminar 3** Hamamatsu Photonics	
	Multi-purpose room A	Room D		**1SDA** Unveil glycans' function from their dynamical structures. – Cutting-edge Challenges (Suyong Re, Yoshiki Yamaguchi)			Career Support Events	
	Multi-purpose room B	Room E		**1SEA** Utilization of Advanced Infrared Sources for Biophysical Studies (Yuji Furutani, Hideji Murakoshi)			The 10th Award Seminar of Outstanding Biophysics and Physicobiology Paper	
Hakodate Citizen Hall	Main Hall	Room F		The 18th Early Career Award in Biophysics Candidate Presentations				
	Small Hall	Room G		**1SGA** Frontiers of Protocell Research: Exploring the Origin of Life through a Constructivist Approach (Yutetsu Kuruma, Tony Z. Jia)			**BP Seminar 4** Leave a Nest	
	Conference Room	Room H		**1SHA** Autonomous Characteristics of Molecular and Cellular Ensembles: Toward an Understanding of Biological Functions (Motoshi Kaya, Yuta Shimamoto)			Board Meeting	
Hakodate Arena	Main Arena	Poster	Set Up	Poster Display				
		Exhibition			Exhibition			
	Studio B	Meeting Room			BPPB Committee / Publications Committee			

* [Exhibition Booths Recommended Visit Time] is a time when you are especially encouraged to visit company exhibition booths. The Annual Meeting is supported by companies and other organizations. We encourage you to visit company booths during other times of the year to gather information on their products.

14	15	16	17	18	19	20
			Extraordinary General Meeting of Members			
	Web Site Editorial Board					

14	15	16	17	18	19	20
1SAP Innovation of drug discovery and medical treatment using supercomputer Fugaku (Mitsugu Araki, Mitsunori Ikeguchi)					Pitch contest	
1SBP Structure and function of "meso-entangled bodies" in the cell (Yuji Sugita, Hayashi Yamamoto)						
1SCP Topological approaches to understand behaviours of complex biological systems (Atsushi Mochizuki, Takashi Okada)						
1SDP Phase Separation by Biopolymers: Basics and Applications (Ryo Kitahara, Tomoshi Kameda)						
1SEP Physico- and chemical biology using nanomanipulation and micromanipulation Technologies (Akira Kitamura, Ryo Iizuka)						
1SFP Biophysical responses and biochemical/chemical controlling of membranes for cellular regulation and future therapy (Ikuhiko Nakase, Hisaaki Hirose)						
1SGP Uncovering the design principles of supramolecular assemblies through manipulation of the structures, dynamics, and functions (Makito Miyazaki, Takahiro Kosugi)						
1SHP The Future of *Muscle* is Now (Madoka Suzuki, Kotaro Oyama)				Poster Presentation Zoom		
		Poster Presentation Odd num.	Poster Presentation Even num.		Mixer	
		Early Research in Biophyscs Award Selection Meeting				

Exhibition Booths Recommended Visit Time

■ 29(Thu.) September, 2022

	Room	Venu	8	9	10	11	12	13
Hakodate Arena	Budokan A	Room A		**2SAA** NMR Studies in Membrane and Peptide Biophysics (Izuru Kawamura, Tomoyasu Aizawa)		Exhibition Booths Recommended Visit Time	**BP Seminar 5** JEOL	
	Budokan B	Room B	Refeyn Japan	**2SBA** Chromatin function as revealed by cutting-edge technique and theory (Yuma Ito, Hiroshi Kimura)				
	Budokan C	Room C		**2SCA** ackle “Molecular Engine” by Early-career Researchers (Takahiro Kosugi, Akihiro Otomo)			**BP Seminar 6** Nakayama	
	Multi-purpose room A	Room D		**2SDA** Innovative label-free nanopore sensing toward biophysical studies and applications (Hirohito Yamazaki, Kan Shoji)				
	Multi-purpose room B	Room E		**2SEA**Unique Spatiotemporal Allostery Emerges in 100nm-Sized Molecular Systems (Akihiro Narita, Shuji Akiyama)				
Hakodate Citizen Hall	Main Hall	Room F		**2SFA** Japan-US symposium on motor proteins and associated single-molecule biophysics (Kumiko Hayashi, Jakia Jannat Keya)			General Assembly Symposium	
	Small Hall	Room G		**2SGA** Advanced Imaging Technologies Leading the Way to “Singularity Biology” (Yuki Hiruta, Tomonobu Watanabe)			Sectoral Specialties Committee Meeting	
	Conference Room	Room H		**2SHA** Next-generation biological manipulation pioneered by biomolecular engineering and low-physical energy logistics (Keiichi Inoue, Hiromi Imamura)			**BP Seminar 7** Refeyn Japan	
Hakodate Arena	Main Arena	Poster	Set Up	Poster Display				
		Exhibition		Exhibition				
	Studio B	Meeting Room						

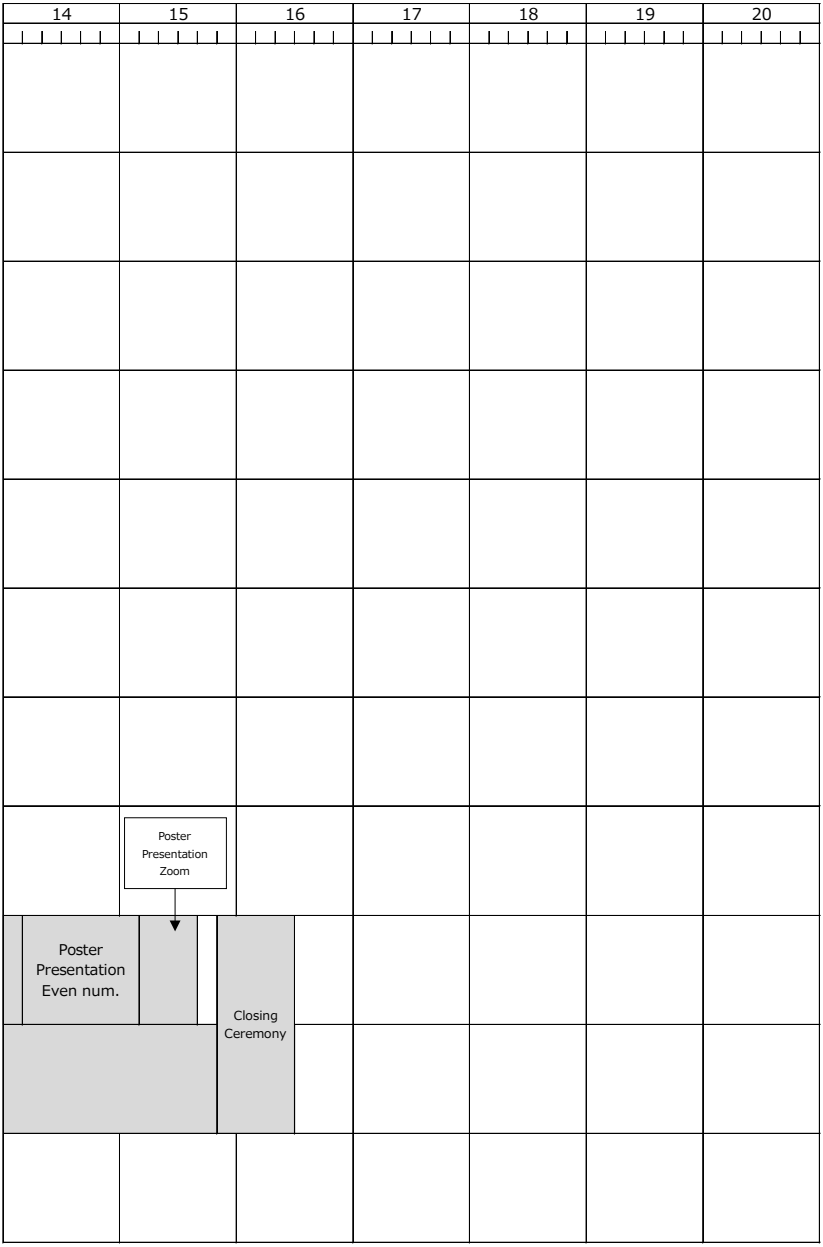
* [Exhibition Booths Recommended Visit Time] is a time when you are especially encouraged to visit company exhibition booths. The Annual Meeting is supported by companies and other organizations. We encourage you to visit company booths during other times of the year to gather information on their products.

14	15	16	17	18	19	20
2SAP Information Physics of multi-cellular systems (Tetsuya J. Kobayashi, Kyogo Kawaguchi, Akihiko Ishijima)		Exhibition Booths Recommended Visit Time				
2SBP High-performance computational biophysics with supercomputer Fugaku (Yasuhiro Matsunaga, Ai Shinobu)						
2SCP Design of biomolecules, protein, RNA, and DNA (Nobuyasu Koga, Yukiko Kamiya)						
2SDP Metal-ion regulation of enzyme dynamics (Masayuki Oda, Kosuke Morikawa)						
2SEP Dynamic translation: from initiation to the end (Takehito Tanzawa, Zhuohao Yang)						
2SFP Biophysical elucidation of neural network and chemical regeneration of neural tissue (Takahiro Muraoka, Tomohide Saio)						
2SGP Physicochemical analyses of structural dynamics for amyloid and gel (Motomasa Tanaka, Nobuo Maita)						
2SHP Biophysical approach for multifaced protein world (Rikiya Watanabe, Motonori Ota)				Poster Presentation Zoom		
		Poster Presentation Odd num.	Poster Presentation Even num.		Mixer	

■ 30(Fri.) September, 2022

	Room	Venu	8	9	10	11	12	13
Hakodate Arena	Budokan A	Room A		**3SAA** Toward a standardization of luminescence, fluorescence measurements and light microscopy (Akira Sasaki, Yoshihiro Ohmiya)		Exhibition Booths Recommended Visit Time	Japanese Session Gender Equality and Young Researchers Support Symposium	
	Budokan B	Room B		**3SBA** Visualization of structural dynamics of biomolecules using a variety of advanced techniques (Yasufumi Umena, Nobutaka Shimizu)			KAKENHI Guide Meeting	
	Budokan C	Room C		**3SCA** Hierarchies of autonomy and spontaneity and adaptation: Molecular-cell-muscle-body□brain linkage of redundancy to action (health) (Yoriko Atomi, Mitsuhiro Iwaki)			**BP Seminar 8** Nikon Solutions	
	Multi-purpose room A	Room D		**3SDA** New implications of sulfur in protein science (Shinji Masuda, Kazutaka Nakabayashi)				
	Multi-purpose room B	Room E		**3SEA** Potential of zero-emission and CO_2-utilizing biotechnologies (Souichiro Kato, Hidemasa Kondo)				
Hakodate Citizen Hall	Main Hall	Room F		**3SFA** Unexpected dynamic mechanisms of life uncovered by Cryo-EM (Osamu Nureki, Hiroshi Nishimasu)				
	Small Hall	Room G		**3SGA** Creation of supramolecular biomembrane by the bottom-up self-assembly: Where material science meets biophysics (Kazuma Yasuhara, Kenichi Morigaki)				
	Conference Room	Room H		**3SHA** Construction of Higher-ordered Molecular Systems - How to Create Them? (Tomoaki Matsuura, Ryuji Kawano, Yuta Suzuki)				
Hakodate Arena	Main Arena	Poster	Set Up	Poster Display				Poster Presentation Odd num.
		Exhibition		Exhibition				
	Studio B	Meeting Room			Opinion meeting with Companies			

* [Exhibition Booths Recommended Visit Time] is a time when you are especially encouraged to visit company exhibition booths. The Annual Meeting is supported by companies and other organizations. We encourage you to visit company booths during other times of the year to gather information on their products.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Poster Presentation Zoom
Poster Presentation Even num.
Closing Ceremony

Information for Participants

1. How to participate

This annual meeting will be held in a hybrid format (on-site and online), but if there are no problems with infection prevention measures etc., please consider participating on-site as far as possible.

However, please note that participation may be restricted or the program may be changed in response to restriction requests by the declaration of a state of emergency or other reasons.

<Online participation>

Please log in to Confit from the annual meeting website. ID [E-mail address used when you registered] and Password [bsj2022] are required to log in. Login to Confit will be available around September 15 (tentative).

2. COVID-19 infection prevention measures

At this annual meeting, COVID-19 infection prevention measures will be implemented as follows. We appreciate your cooperation.

◇If you have any of the following symptoms or conditions, please refrain from participating on-site.

1) Fever of 37.5℃ or higher
2) Cough, sore throat, shortness of breath, fatigue, or loss of taste/smell
3) Suspicion of infection

◇Infection prevention measures in the venue

1) Please be sure to wear a mask in the venue.
2) Temperature will be checked at the entrance of the venue. Those with a fever of 37.5 ℃ or higher will not be allowed to participate on-site.
3) Please disinfect your hands frequently with hand sanitizers placed at theentrance etc.
4) The number of participants allowed into each lecture room will be limited (no standing allowed).
5) Lecture rooms will be ventilated.
6) Please refrain from talking while eating and drinking (except for Luncheon seminars etc.) .

3. Registration

◇Advance registration

For those who have registered during the “early registration” period: A name badge and a receipt will be sent in advance. If you agreed at the time of registration, a QR code containing the information about your name, affiliation,

and e-mail address is printed on the name badge. Please use it to exchange information among participants or with exhibitors.
For those who have registered during the "late registration" period: Please print out a confirmation e-mail of your registration and bring it to the registration desk on the day of the meeting to receive a name badge.
Name badge holders will be distributed on the day of the event near the venue entrance. Please be sure to wear your participation card at the venue.

◇On-site registration
On-site registration is available at the registration desk for those who have not completed advance registration. Only cash payment is accepted.
Location: Main arena, Hakodate arena
Open hours: Sep.28 & 29: 8:15-17:00 / Sep.30: 8:15-13:30

◇The Biophysical Society of Japan desk
Application for membership and payment of the annual membership fee can be made at the Biophysical Society of Japan desk located at the registration area.

◇Program booklet / Proceedings / Online proceedings (Confit Web ver. & App ver.)
Program booklet has been sent in advance to members of the Biophysical Society of Japan and non-members who have registered during the early registration period. Non-members who have registered during the late registration period will receive it at the registration desk on-site.
Proceedings (PDF) will be posted on the meeting website (scheduled in early September), please download it. It can also be viewed on Confit Web ver. and App ver. (free of charge).

Proceedings (PDF):
https://www2.aeplan.co.jp/bsj2022/en-program.html
Download ID: ambsj2022
Password: 60hakodate

Program/Proceedings - Confit (Web ver.):
To be posted on the meeting website.
Login ID: E-mail address used when you registered
Password:bsj2022

Program/Proceedings - Confit (App ver.):
Download from App Store / Google Play (free of charge)
(Search for "biophysics", "bsj2022", etc.)
Login ID and Password are the same as Confit (Web ver.).

* Program and proceedings will be made available without password on the website of the Biophysical Society of Japan and in “Seibutsu Butsuri “ on J-STAGE after the annual meeting.

◇Utilization of Confit

Viewing e-posters and asking/answering questions through the “comments” function are available on Confit Web ver. and App ver.. Also, you can post your “my profile” and interact with other participants using the “direct message” function. Please log in and register your “my profile” as soon as it is released (scheduled on Sep.15).

You can also check if a poster is displayed at the venue, if there will be a poster presentation via Zoom, etc. using the “matching flag” function.

More details will be posted on the annual meeting website.

4．On the day of the annual meeting

◇Language

As a general rule, English is the language used. However, Assembly symposium, Gender equality promotion and young researchers support symposium, Career support event, KAKENHI guide meeting, etc. will be held in Japanese.

◇Utilization of PC/tablet/smartphone, headset, etc.

As this meeting will be held in a hybrid format, please bring and utilize your own Wi-Fi-equipped PC etc. In particular, earphones and microphone are required for online participation in symposia or poster presentations via Zoom. We recommend that you bring a headset or other device in case you are uncomfortable with voices of other participants.

◇Internet access (Wi-Fi)

Wi-Fi is available in the poster/exhibition hall (main arena).

However, please note that the connection might be unstable because the connection to the symposium rooms will be prioritized.

* SSID and password will be provided on-site.

Also, power outlets are available at the audience seats on the 2nd floor of main

arena.

◇Online participation (via Zoom)

If you cannot come to the venue, you can participate in symposia and poster sessions via Zoom.

You can access Zoom for each session from the program on Confit. When participating via Zoom, please indicate your family name and affiliation in English.

(e.g.) Yamada Hokkaido Univ.

Also, please turn off your camera(video) and microphone except during Q&A sessions.

◇Symposia

The number of participants allowed into each room is limited for infection prevention measures. No standing is allowed. When it reaches the capacity, please join the symposium at the audience seats on the 2nd floor of arena or via Zoom, or watch it on demand at a later date.

The following will be projected on the screen at the venue.

During presentations: Presenter's slides

During Q&A sessions: Presenter, Organizers, Panoramic view of the venue, Online questioner

The following will be displayed on PCs of online participants.

Presenter's slides, Presenter, Organizers, Panoramic view of the venue, Online questioner

For online participants, please make sure to use a microphone when asking / answering questions at the venue. If you are participating online and have any questions, please use the "raise hand" function. If the organizer calls on you, please turn on your camera(video) and microphone, and ask a question verbally. As a general rule, Q&A via chat is not accepted, but this does not apply to symposia where the organizer provides separate instructions.

◇Poster presentation

Posters at the venue will be changed each day. The mandatory presentation times at the venue are as follows.

Please join the discussion in front of the posters.

Sep.28 & 29 : Odd numbers 16:30-17:30 / Even numbers 17:30-18:30

Sep.30 : Odd numbers 13:10-14:10 / Even numbers 14:10-15:10

Poster presentation times via Zoom are as follows. Please enter a breakout room

designated by poster number.
More details will be released on the meeting website.
Sep.28 & 29: 18:30-19:00
Sep.30: 15:10-15:40

Questions about e-posters can be posted using the “comments” function on Confit at any time. Presenters will be notified by e-mail when a comment is posted, please reply to it. Please note that responses from presenters will not be notified to questioners.

◇General assembly / Assembly symposium
Please join the 9th general assembly / assembly symposium of the Biophysical Society of Japan which will be held in Room F (Big hall, Citizen hall) on September 29 from 12:35 to 13:35.

◇Early Career Award in Biophysics Candidate Presentation Symposium
Early Career Award in Biophysics Candidate Presentation Symposium, which is the selection for the 18th early career award, will be held in Room F (Big hall, Citizen hall) on September 28 from 9:30 to 11:30. The award ceremony will be held in the mixer on the next day.

◇Cloakroom
Please be advised that valuables, computers etc. are not accepted as we are not responsible for any loss or damage. Umbrellas are also not accepted.
Location: Main arena, Hakodate arena
Open hours: Sep.28 & 29: 8:15-20:30 / Sep.30: 8:15-16:30

◇Lunch
Free box lunch and tea will be provided at Biophysics seminar (Sep.28-30), Career support event (Sep.28), Gender equality promotion and young researchers support symposium (Sep.30), and KAKENHI guide meeting (Sep.30). To receive it, a numbered ticket which is to be distributed on the day is required. Numbered tickets will be distributed as follows.
Time: 8:15～ each day
Location : Hall, Hakodate arena
*Only numbered tickets for sessions scheduled for the day will be distributed. Ticket distribution will be closed when all the tickets are distributed.
*Numbered tickets will be invalid if you do not show up by the start time, and lunch will be provided to other participant who does not have a ticket.
*Biophysics seminars are co-sponsored seminars supported by companies

and organizations. If you attend the seminar, please attend to the end and be sure to answer a questionnaire with your name and affiliation. We kindly ask for your cooperation.

*As the number of box lunch is limited, it will be available for sale.

◇Parking

Paid parking is available at the venue, but please use public transportation as a general rule.

◇Child care

Day care service will be available. Please visit the annual meeting website for more information.

◇Mixer

Instead of a banquet, a mixer will be held in the poster/exhibition hall (main arena) on September 28 and 29 from 19:00 to 20:30. A set of beer/soft drink and snacks (1 set per person per day) will be provided free of charge. Please be sure to wear a mask when having a conversation.

The award ceremony for the early career award and young scientists invited lecture award will be held during the mixer on September 29.

◇Exhibition

An exhibition will be held in main arena. "Recommended time to visit company booths" is scheduled, please stop by company booths. Also, please enjoy a stamp rally at the exhibition.

◇ Closing ceremony

Closing ceremony will be held in the poster/exhibition hall (main arena) after the poster presentations on September 30. The winners of the student presentation award will be also announced at the ceremony. We look forward to your participation.

5. Prohibitions

1) Giving password and URL to a third party is prohibited.
2) Photography and audio/video recordings with any devices are prohibited in the lecture rooms. Saving screenshots of your PC is also strictly prohibited.

Information for Organizers and Presenters

◇**For symposium organizers**

Arrival:

Please come to the organizers' desk at each room and let the staff know of your arrival at least 15 minutes before the session.

If you cannot come to the venue:

You can proceed with the session via Zoom. Please contact the meeting secretariat as soon as you know you will not be able to come.

Organizers' desk:

One PC is prepared for organizers to proceed with the session. The organizer proceeding with the session will be displayed on Zoom.

Process:

Please start and finish all presentations as scheduled for smooth operation. During presentations, remaining time will be displayed according to the time allocation informed to the secretariat in advance. If there are any changes, please let the staff know.

All presentations will be recorded and made available for on-demand streaming for about two weeks after the meeting (available to registered participants only). Please announce this at the start of the session.

Q&A:

[On-site] Please make sure to instruct the questioner to use the microphone.

[Online] Please tell the participants to use the "raise hand" function to ask questions. Also, please ask the questioner to turn on the camera(video) and microphone before asking a question. Basically, questions should be asked verbally not in chat, but it is up to the organizers whether to accept questions in chat. If so, please inform the participants.

◇**For symposium speakers**

Arrival:

Please come to the PC desk at each room with your own PC at least 15 minutes before the session.

PC must be capable of outputting images via HDMI. If you connector is a differen, please bring a conversion connector. Also, please bring an AC adapter in case the battery runs out.

After checking your presentation slides, the staff will connect your PC. There is no preview room for slide check.

Presentation time:
Time allocation is left to the organizers.
[Early Career Award in Biophysics Candidate Presentation Symposium]
10 min for presentation / 3 min for discussion / 2 min for PC exchange

If you cannot come to the venue:
You can give a presentation via Zoom. Please contact the organizers as soon as you know you will not be able to come. Zoom for the presentation can be accessed from Confit. Please follow the organizers' instructions.

◇**For poster presenters (General presentations)**

Poster preparation:
Posters should be prepared in English. If possible, please write title, affiliations, and authors' names in Japanese as well. Also, please put a circle for the presenting author's name.

e-poster:
Regardless of whether or not your poster is displayed at the venue, please make sure to upload your e-poster to Confit. As a general rule, please upload the same file as the poster displayed at the venue. A dedicated site for uploading will be informed to the presenters in early September. The deadline for uploading is September 14, but you can replace the file by uploading again even after that date. Uploading your e-poster is required to complete your presentation.

Poster at the venue:
The size of poster panel is 900mm wide x 2,100mm high. Posters will be changed every day. Please come to the venue on the day of your presentation as far as possible and put up your poster during the posting time (Sep.28 & 30: 8:30-9:00 / Sep.29: 8:10-8:45). Pushpins will be provided at the venue.
If you participate in the mixer which will be held after the poster presentation time, please remove your poster after the mixer. If you do not participate, please remove your poster after the presentation time. Please note that posters remaining after the removal time will be discarded by the secretariat.

If you cannot come to the venue:
Please do the following.
・Enter a comment in the "comments" section of Confit
(ex. No poster is displayed at the venue, etc.)
・Choose "not at the venue" from "matching flag" in "my profile" of Confit

Presentation mandatory time:

[On-site presenters] Please make a presentation in front of your poster in the mandatory presentation time.

[Online presenters] Please make a presentation via Zoom as follows within the realm of possibility.

Poster presentation via Zoom:

Please use a breakout room designated by poster number. As a general rule, please use e-poster as explanation materials.

Also, please choose "I will present via Zoom (Day X)" from the "matching flag" in "my profile" of Confit.

Even if you are at the venue, you can make a presentation via Zoom on the mandatory presentation day if you wish. Please use Wi-Fi at the audience seats on the 2nd floor of the poster/exhibition hall (main arena).

Q&A by comment function:

“Comments” function of Confit is available for Q&A. When a comment is posted, it will be notified by e-mail to the presenter. Please reply using the comment function. Please note that responses from presenters will not be notified to questioner.

Timetable for poster presentation:

		Sep. 28	Sep. 29	Sep. 30
Put up		8:30-9:00	8:15-8:45	8:30-9:00
Presentation & Discussion	Odd numbers	16:30-17:30	16:30-17:30	13:10-14:10
	Even numbers	17:30-18:30	17:30-18:30	14:10-15:10
	Zoom (optional)	18:30-19:00	18:30-19:00	15:10-15:40
Removal		19:00-20:45	19:00-20:45	15:40-16:45

第 9 回会員総会シンポジウム：内藤記念科学振興賞受賞報告

オーガナイザー：日本生物物理学会　理事会
日　時：9 月 29 日（木）12:35 〜 13:35
場　所：函館市民会館（大ホール）F 会場
演　者：安藤敏夫氏（金沢大）「液中生物ナノメーター世界の高速観察の実現」
司　会：田端和仁（東大院・工）
※このイベントは日本語で開催します。
* This event will be presented in Japanese language.

概　要：本年度の総会シンポジウムでは，2021 年度に内藤記念科学振興賞を受賞された，金沢大学の安藤敏夫氏に講演をいただく。安藤氏はタンパク質の「動き」を直接観察することを目標に，1993 年より高速原子間力顕微鏡の開発を一貫しておこなってきた。そして，2010 年に世界で初めてミオシン V がアクチンフィラメント上を動く様子を捉えることに成功し，世界を震撼させた。それ以降もセルロース表面上のセルラーゼの加水分解を伴うスライディング運動の可視化や，回転軸を持たない F_1-ATPase の構造変化の回転伝播，バクテリオロドプシンの光による構造変化など多数のタンパク質の動きを高速 AFM で可視化している。現在では，タンパク質の動きを直接可視化する唯一の技術として認知されている。これら成果により，2021 年度の内藤記念科学振興賞が授与された。また，本賞以外にも多くの賞を受賞していることから，本技術の世界的な評価も高いことがわかる。今回のシンポジウムは安藤氏の受賞をお祝いするとともに，総会シンポジウムでの講演を通して，会員の皆様とともに受賞の喜びを分かち合いたいと企画された。
学会員へのメリットの一つとして，このような賞への推薦がある。学会員が様々な分野で活躍し，成果を上げることは生物物理学会としても大変うれしいことであり，そのような会員に対して受賞の機会を提供していきたい。その一環として，学会からの推薦があり，多くの会員に利用していただきたいと考えている。

一般社団法人日本生物物理学会　第 11 回 Biophysics and Physicobiology 論文賞受賞講演会
The 11th Award Seminar for outstanding Biophysics and Physicobiology paper

オーガナイザー：日本生物物理学会 Biophysics and Physicobiology 論文賞選考委員会
Organizers: Award committee for outstanding Biophysics and Physicobiology paper
日　時：9 月 28 日（水）12:50 ～ 13:30 ／ Sep. 28 Wed.
場　所：函館市民会館（大ホール）F 会場／ Hakodate Citizen Hall (Big Hall) Room F
形　式：講演会／ Lecture

第 11 回 Biophysics and Physicobiology 論文賞受賞者

北村　朗
Akira Kitamura
北大・先端生命
Faculty of Advanced Life Science, Hokkaido University

FRAP 法を用いた拡散係数測定―夏休みの自由研究―
Diffusion coefficient measurement using fluorescence recovery after photobleaching―a homework during summer vacation with refreshment―

Fluorescence recovery after photobleaching (FRAP) enables the characterization of quantitative dynamic properties such as diffusion coefficients of fluorescent molecules in live cells by analyzing the recovery of fluorescence intensity after photobleaching in a specific cellular compartment or area. Here, to quantify the diffusion coefficient of rapidly diffusing fluorescent molecules such as tandemly oligomerized green fluorescent proteins (GFPs), we propose a procedure that makes use of an epi-fluorescence microscope with a photobleaching laser in combination with established models for diffusion analysis. Photobleaching times shorter than the diffusion speed are not necessarily the only way to obtain appropriate diffusion coefficients of fast-moving molecules. Our results also showed that the apparent spreading of the effective radius of the photobleached area acts as a correction factor for determining the appropriate diffusion coefficients of fast-moving molecules such as monomeric GFPs. Our procedure provides a useful approach for the quantitative measurement of diffusion coefficients in live cells. Furthermore, this research was conducted using the equipment loaned to me by a microscope manufacturer for product evaluation, and is, so to speak, published as an achievement of my summer vacation homework. Consequently, I guess that even so busy professional researchers sometimes need to perform “research with refreshment”.

男女共同参画・若手支援委員会企画シンポジウム

ありったけの夢をかきあつめ，いざふたたび世界へ！
オーガナイザー：日本生物物理学会　男女共同参画・若手支援委員会
Organizers: Promotion of Gender Equality and Young Researchers Committee
日　時：9 月 30 日（金）12:00 〜 13:30
会　場：函館アリーナ A 会場
昼　食：お弁当とお茶を無料で提供いたします。ただし，数に限りがあります。
形　式：プレゼンテーション
司　会：今田勝己（大阪大学）
発表者：船引宏則（ロックフェラー大学），服部素之（復旦大学），御手洗菜美子（ニールスボーア研究所 / 京都大学）
※このイベントは日本語で開催します。
*This event will be presented in Japanese language.

概　要：過去 2 年間，新型コロナウィルスが猛威をふるい，その影響は今でも続いています。コロナ禍で, 海外進出に難しさを感じてきた若手研究者も多いのではないでしょうか。ただ，今年度の年会はハイブリッド開催になるなど，復調の兆しも見えてきました。2024 年度には，国際生物物理会議（International Biophysics Congress）が日本（京都）で開催されることもあり，日本生物物理学会としても国際化に力を入れています。いまこそ，若手研究者は再び世界に目を向けて，キャリアアップを図る時ではないでしょうか。
本シンポジウムでは，アメリカ，アジア，ヨーロッパの各地域で研究室を運営する発表者の方に，「どのようにして海外で研究室を運営するにいたったか」，「海外で研究室を運営することの利点・欠点」，そして「海外の言語事情や科研費事情」などについてお話していただきます。また，海外での生活や言語事情についてもお話いただきます。
船引様は，1995 年に京都大学で博士号取得後，アメリカでのポスドクを経て，2002 年からアメリカ・ロックフェラー大学で研究室を主宰し，現在は教授として染色体構造・機能を研究されています。服部様は，2009 年に東京工業大学で博士号取得後，アメリカでのポスドクを経て，2015 年から中国・復旦大学で研究室を主宰するにいたりました。今年で 40 歳となり, 1 児のパパでもあります。御手洗様は, 2003 年に九州大学で博士号取得後，日本でのポスドク・助教を経て，2009 年からデンマーク・ニールスボーア研究所で研究室を主宰するにいたりました。生物と物理の間を行ったり来たりできる環境を楽しんでいるそうです。
本シンポジウムでは，多様なバックグラウンドのもと，それぞれの地域で研究室を運営するに至った 3 名の方に各人 30 分程度お話いただきます。ターニングポイント，重要だった選択など経験談をお話していただくとともに，海外でキャリアアップしていく上での現在の問題点などについてお話していただきます。各講演の後には質疑応答の時間を設けます。キャリアアップしていく上での難しい点や問題点，経験談などを共有することによって，今後に生かしていただければ幸いです。学生，若手研究者の方の参加を歓迎します。また，海外でのキャリアアップに興味を持つ，幅広い年齢の研究者の方の参加も歓迎いたします。

キャリア支援説明会

オーガナイザー：日本生物物理学会 男女共同参画・若手支援委員会
日　時：9 月 28 日（水）11:50 〜 12:50
会　場：函館アリーナ（多目的室 A）D 会場
形　式：ランチョンセミナーと個別キャリア相談会
※このイベントは日本語で開催します。
* This event will be presented in Japanese language.

概　要：若手研究者や学生の今後のキャリア構築の一助となるように，今年度も「キャリア支援説明会」を開催します。昨年の反響を受けて本年会は，（株）アカリクから講師を迎えて大学院生やポストドクター向けの就職支援活動セミナーを実施します。また，昨年度と同様に今年度も個別キャリア相談会を実施いたしますので，是非ご活用ください。博士課程出身のアカリク社員が何でも質問に答えます！

講師プロフィール

神中 俊明（かみなか としあき）
東京理科大学大学院理学研究科物理学専攻で博士（理学）を取得後，博士研究員を経て 2018 年 10 月より株式会社アカリクに所属しています。博士課程 2 年秋に所属研究室が解散した経験や博士研究員としての活動を元に現在，大学院生を始めとする研究に接する人のキャリア支援を行っています。研究を志すキャリアの見通しを良くし，研究環境をより良くすることが目標です。

平田 佐智子（ひらた さちこ）
神戸大学大学院人文学研究科社会動態専攻（心理学）で博士（学術）を取得後，4 年間のポスドク生活を経て民間企業へ就職しました。研究コンサル，データサイエンティストを経て 2021 年 2 月より株式会社アカリク経営企画部に所属しています。現在はアカデミア・民間企業での経験を活かし，博士号所持者がさまざまな場で活躍するための情報提供（セミナー企画運営）や，キャリアマガジン Acaric Journal の編集に従事しています。

アカリクについて
株式会社アカリクは「知恵の流通の最適化」を目指している企業です。大学院を修了・中退され企業へ就職を希望される方，ポスドクや助教の方のキャリア支援や，専門職転職をされる方のサポートをしています。また, ジョブ型インターンシップ対応やセミナー, キャリアマガジン発行を通じて大学院生のキャリアがより良いものとなることを目指し，各種事業を展開しております。事業を通して研究者，大学院の環境，企業との関係をより良いものにしていきたいと考えています。

プログラム：理系大学院生や研究者の就活･転職について,「専門外就職」や「博士人材向け」の情報も交えてお話しいたします。

【Part 1】11:50 ～ 12:10　博士課程・PD の方向けの就職情報
企業の採用対象として存在感を増している博士人材ですが，いつ，どのような準備をして就職活動を行うのが適切かはあまり知られていません。また，研究実績があっても状況の把握や伝え方を誤れば機会を逃してしまいます。そこで，①産業界から見た博士，②博士や PD の就職活動の実態，面接における注意点，③博士課程を中退・単位取得退学する場合の就職活動についてご紹介します。

【Part 2】12:10 ～ 12:30　活躍できる博士になるには
現在博士進学を考えている，または現在博士課程に在籍していて，数年後に民間・アカデミアを問わず就職活動を行う場合，進路決定までの間にどのような情報収集の必要，方法があるかについてご紹介します。

【Part 3】12:30 ～ 12:50　ライフ・リサーチ・バランス
パートナーや家族がサポートを必要としている場合，研究生活に 100% のリソースを費やすことが難しくなります。ときには，自身が家庭を支えるために，研究活動を諦めなければならない場合もあるかもしれません。そのような場合，どのように自身と折り合いをつけていくか，どのような手段が利用可能なのか，についてご紹介します。

個別キャリア相談会：就職活動・キャリアに関する悩みや不安を気軽にご相談ください。本大会では，現地（メインアリーナ・ポスター・企業展示会場）での相談会を開催いたします。就活ノウハウや企業での待遇面など，分からないことがあれば遠慮なくお尋ねください。

【ブースオープン時間】
9/28（水）　14:00–18:00
9/29（木）　10:00–12:00，14:00–19:00
9/30（金）　10:00–15:00
※直接ブースにお越し下さい。空いている場合はすぐご案内できますが，混み合っている場合は，お手数ですが時間を空けて再度お越し下さい。

オンラインでの参加を希望される方は受付フォーム［https://forms.gle/EMnEj2kdSRGjfJUL8］より事前の登録をお願いいたします。

科学研究費助成事業について
Reorganization of KAKENHI: Current Activities of JSPS

世話人：原田慶恵（大阪大学蛋白質研究所，日本学術振興会学術システム研究センター主任研究員）

Organizer：Yoshie Harada (Institute for Protein Research, Osaka University; Program Officer, Research Center for Science Systems, JSPS)

日　時：9 月 30 日（金）12:00 ～ 13:00

会　場：函館アリーナ B 会場

昼　食：お弁当とお茶を無料で提供いたします。

形　式：プレゼンテーション

※このイベントは日本語で開催します。

*This event will be presented in Japanese language.

概　要：今，日本が将来にわたって卓越した研究成果を持続的に生み出し続け，世界の中で存在感を保持できるかが問われています。こうした中，科学技術･学術審議会において，学術研究への現代的要請として，「挑戦性・総合性・融合性・国際性」の四つを挙げ，科研費制度の抜本的改革が提言されました。これを踏まえ，文部科学省では「科研費改革の実施方針」を策定し，科研費の研究種目・枠組みの見直しや審査システムの見直し（「審査システム改革 2018」）が行われ，平成 30 年度科研費（平成 29 年 9 月公募）において，新たな審査システムによる審査を実施しました。今回は，このシステム改革の内容のほか，その他の改善や充実を図った点等について，ご説明をいただきます。

企業参画型ピッチコンテスト

主　催：株式会社リバネス
共　催：日本生物物理学会
日　時：9 月 28 日（水）19:00 ～ 20:30
会　場：A 会場（武道館 A）
※このイベントは日本語で開催します。
* This event will be presented in Japanese language.

概　要：ピッチコンテストとは，新しいアイデアを元に起業したい人たちが，それを支援しようとする企業やファンドの人たちに向けてショートプレゼンテーション（5 分間程度）を行うものです。学会員と企業の交流を促進し，さらに起業や共同研究の発起点となることを狙い，初めての試みとして開催することにしました。コンテスト参加の募集は既に別途ご案内の通り，株式会社リバネスのサイトから行っておりますので，ここではこのイベントへの聴講のご案内となります。

ピッチコンテストの審査は，この企画に賛同をいただいている企業各社と学会からお願いした方に行っていただき，参加者および優秀発表者には参画企業からの賞金が出ます。その様子も含めましてぜひ直接会場でご覧ください。

なお，年会の中のミキサーと同時刻に行われますので，ビール片手の聴講も歓迎いたします。※発表中はお静かにお願いいたします。

第 18 回 若手奨励賞招待講演　The 18th Early Career Award in Biophysics Candidate Presentations

1 日目（9 月 28 日（水））／Day 1（Sep. 28 Wed.）

09:00〜11:30
1YF　日本生物物理学会若手奨励賞選考会
Early Research in Biophysics Award Candidate Presentations

オーガナイザー：男女共同参画・若手支援委員会
Organizer: Promotion of Gender Equality and Young Researchers Committee

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Biophysical Society of Japan (BSJ) grants “Early Career Award in Biophysics” and “Early Career Presentation Award” to young BSJ members for their excellent presentations that show great potential to contribute to the progress of biophysics. In this 18th year, we received 56 highly qualified applications. After the first round of competitive screening based on submitted documents, the following ten applicants were selected as candidates for Early Career Award in Biophysics. In this symposium, each speaker will give a 10-minute presentation followed by a 3-minute discussion as the second round of screening. Up to five awardees of the Early Career Award in Biophysics will be selected. The best presenter will also be awarded IUPAB award from International Union of Pure and Applied Biophysics. The Early Career Presentation Award will be given to the rest of the excellent invited speakers. We welcome all the BSJ members to attend this symposium to foresee the future of biophysics in Japan through the speakers and their research.

9:00　Chiba　Kyoko　3Pos134
1YF0900
KIF5A の ALS 関連遺伝子変異は KIF5A のオリゴマー化と凝集を促進し神経毒性を引き起こす
An ALS-associated KIF5A mutant forms oligomers and aggregates and induces neuronal toxicity
○千葉 杏子 [1], 中野 朱莉 [2], 丹羽 伸介 [1]（[1] 東北大・学際研, [2] 東北大・院生命）
Kyoko Chiba[1], Juri Nakano[2], Shinsuke Niwa[1] ([1]*FRIS, Tohoku Univ.*, [2]*Grad. Sch. of Life Sci., Tohoku Univ.*)

9:15　Furuike　Yoshihiko　2Pos013
1YF0915
原子分解能でみた概日時計の朝夕昼夜
Visualizing a Day of Circadian Clock at Atomic Resolution
○古池 美彦 [1,2], 向山 厚 [1,2], 山下 栄樹 [3], 近藤 孝男 [4], 秋山 修志 [1,2]（[1] 分子科学研究所　協奏分子システム研究センター, [2] 総合研究大学院大学, [3] 大阪大学 蛋白質研究所, [4] 名古屋大学大学院 理学研究科）
Yoshihiko Furuike[1,2], Atsushi Mukaiyama[1,2], Eiki Yamashita[3], Takao Kondo[4], Shuji Akiyama[1,2] ([1]*Research Center of Integrative Molecular Systems (CIMoS), Institute for Molecular Science (IMS)*, [2]*The Graduate University for Advanced Studies (SOKENDAI)*, [3]*Institute for Protein Research (IPR), Osaka University*, [4]*Graduate School of Science, Nagoya University*)

9:30　Hanazono　Yuya　1Pos024
1YF0930
高分解能中性子構造解析によるペプチド結合の平面性の再検討
Revisiting the peptide bond planarity by high-resolution neutron structure
○花園 祐矢 [1,2,3], 平野 優 [2,4], 竹田 一旗 [1], 日下 勝弘 [5], 玉田 太郎 [2], 三木 邦夫 [1]（[1] 京大・院理, [2]QST・量子生命, [3] 東京医科歯科大・難治疾患, [4]JST・さきがけ, [5] 茨城大・フロンティア）
Yuya Hanazono[1,2,3], Yu Hirano[2,4], Kazuki Takeda[1], Katsuhiro Kusaka[5], Taro Tamada[2], Kunio Miki[1] ([1]*Grad. Sch. Sci., Kyoto Univ.*, [2]*Inst. Quant. Lif. Sci., QST*, [3]*Med. Res. Inst., Tokyo Med. Dent. Univ.*, [4]*PRESTO, JST*, [5]*Front. Res. Cent. for Appl. Atom. Sci., Ibaraki Univ.*)

9:45 Jia Tony Z 1Pos238

1YF0945 Cationic Polyester Microdroplets as RNA-containing Protocells

Tony Z Jia[1,2], Niraja V. Bapat[1,3], Ajay Verma[3], Irena Mamajanov[1], H. James Cleaves II[1,2], Kuhan Chandru[4] ([1]*Earth-Life Science Institute, Tokyo Institute of Technology*, [2]*Blue Marble Space Institute of Science*, [3]*Department of Biology, Indian Institute of Science Education and Research*, [4]*Space Science Centre (ANGKASA), Institute of Climate Change, National University of Malaysia*)

10:00 Katoh Takanobu A 2Pos131

1YF1000 **マウスノード不動繊毛は変形の向きを感知して左右軸を決定する: 非対称性を生み出すメカニカルな機構**

Mouse nodal immotile cilia sense bending direction for left-right determination: Mechanical regulation in initiation of symmetry breaking

○加藤 孝信 [1], 大森 俊宏 [2], 水野 克俊 [3], 板橋 岳志 [1], 岩根 敦子 [1], 石川 拓司 [2], 岡田 康志 [1,4], 西坂 崇之 [5], 濱田 博司 [1]（[1] 理研・BDR, [2] 東北大・院・工学, [3] 福井大・医, [4] 東大・院・医, 院・理, UBI, WPI-IRCN, [5] 学習院大・理）

Takanobu A Katoh[1], Toshihiro Omori[2], Katsutoshi Mizuno[3], Takeshi Itabashi[1], Atsuko H. Iwane[1], Takuji Ishikawa[2], Yasushi Okada[1,4], Takayuki Nishizaka[5], Hiroshi Hamada[1] ([1]*BDR, Riken*, [2]*Grad. Sch. Eng., Tohoku Univ.*, [3]*Fac. Med. Sci., Univ. of Fukui*, [4]*Grad. Sch. Med., Grad. Sch. Sci., UBI, WPI-IRCN, The Univ. of Tokyo*, [5]*Fac. Sci., Gakushuin Univ.*)

10:15 Kobayashi Hotaka 1Pos118

1YF1015 **microRNA の機能発現を 1 細胞 1 分子レベルで可視化する新規技術の開発**

In situ single-molecule imaging of microRNA function

○小林 穂高 [1,2]（[1]JST さきがけ, [2] 東京大学 定量生命科学研究所）

Hotaka Kobayashi[1,2] ([1]*JST PRESTO*, [2]*IQB, The University of Tokyo*)

10:30 Motomura Haruka 2Pos216

1YF1030 **全身を周回する神経回路が腸の脂質含量を調節する**

Whole-body neural circuit regulates intestinal fat storage

○本村 晴佳 [1,2], 五百藏 誠 [1,2], 村上 一寿 [1,2], 久原 篤 [1,2,3], 太田 茜 [1,2]（[1] 甲南大・院自然科学, [2] 甲南大学統合ニューロバイオロジー研究所, [3]PRIME, AMED）

Haruka Motomura[1,2], Makoto Ioroi[1,2], Kazutoshi Murakami[1,2], Atsushi Kuhara[1,2,3], Akane Ohta[1,2] ([1]*Grad. Sch of Nat. Sci., Konan Univ.*, [2]*Ins. integrative Neurobio., Konan Univ., Japan*, [3]*PRIME, AMED*)

10:45 Okimura Chika 3Pos146

1YF1045 **魚類ケラトサイトのストレスファイバ直動回転変換メカニズム**

Linear contraction of stress fibers kicks the substratum for their rotation

○沖村 千夏 [1], 秋山 珠祐 [1], 櫻井 建成 [2], 岩楯 好昭 [1]（[1] 山口大・理, [2] 武蔵野大・工）

Chika Okimura[1], Shu Akiyama[1], Tatsunari Sakurai[2], Yoshiaki Iwadate[1] ([1]*Dept.Biol., Yamaguchi Univ.*, [2]*Dept.Math.Eng., Musashino Univ.*)

11:00 Yamagishi Jumpei 2Pos280

1YF1100 **ミクロ経済学としての代謝制御の理解：ワールブルク効果とギッフェン財を例として**

Microeconomics of Metabolism: The Warburg effect as Giffen behavior

○山岸 純平, 畠山 哲央（東京大・院総合文化）

Jumpei Yamagishi, Tetsuhiro Hatakeyama (*Grad. Sch. of Arts and Sci., Univ. Tokyo*)

11:15　Yoneda　Yusuke　1Pos223

1YF1115　**励起子電荷分離混成が酸素発生型光合成を駆動する**

Exciton-charge transfer mixing drives oxygenic photosynthesis

○米田 勇祐[1,2,3], Arsenault Eric A.[1,2], Yang Shiun-Jr[1,2], Orcutt Kaydren[1,2], Iwai Masakazu[1,2], Fleming Graham R.[1,2]（[1] カリフォルニア大学バークレー校, [2] ローレンスバークレー国立研究所, [3] 分子科学研究所）

Yusuke Yoneda[1,2,3], Eric A. Arsenault[1,2], Shiun-Jr Yang[1,2], Kaydren Orcutt[1,2], Masakazu Iwai[1,2], Graham R. Fleming[1,2] ([1]*University of California, Berkeley*, [2]*Lawrence Berkeley National Laboratory*, [3]*Institute for Molecular Science*)

09:00〜11:30　A 会場（函館アリーナ 武道館 A）／Room A（Hakodate Arena Budokan A）

1SAA　動的溶液環境が駆動するタンパク質凝集
Protein aggregation driven by dynamic solution environments

オーガナイザー：吉田 紀生（九州大学），菅瀬 謙治（京都大学）
Organizers: Norio Yoshida (Kyusyu Univ.), Kenji Sugase (Kyoto Univ.)

In cells, the solution environment is constantly changing due to varying concentrations of chemicals, mechanical stimuli, and electric fields. In recent years, it has become evident that intrinsically disordered proteins, which do not have specific conformations, undergo liquid-liquid phase separation and amyloid fibrillization in response to the 'dynamic' solution environment. This series of self-condensation processes is controlled by the protein-protein and protein-solvent interactions of intrinsically disordered proteins, which have dynamic conformations and solvation states. In this workshop, we will discuss the latest research on the self-condensation process of intrinsically disordered proteins and their future development.

はじめに
Opening Remarks

1SAA-1　TIA-1 プリオン様ドメインの ALS 変異は高度に凝縮した病原性構造体を形成する
ALS mutations in the TIA-1 prion-like domain trigger highly condensed pathogenic structures
○関山 直孝 [1], 高場 圭章 [2], 眞木 さおり [2], 赤木 謙一 [3], 大谷 寧子 [1], 今村 香代 [1], 寺川 剛 [1], 山下 恵太郎 [4], 米倉 功治 [2], 児玉 高志 [1], 杤尾 豪人 [1]（[1] 京大・理・生物物理, [2] 理研・放射光科学研究センター, [3] 医薬基盤・健康・栄養研究所, [4]MRC 分子生物学研究所）
Naotaka Sekiyama[1], Kiyofumi Takaba[2], Saori Maki-Yonekura[2], Ken-ichi Akagi[3], Yasuko Ohtani[1], Kayo Imamura[1], Tsuyoshi Terakawa[1], Keitaro Yamashita[4], Koji Yonekura[2], Takashi Kodama[1], Hidehito Tochio[1] ([1]*Dept. of Biophysics, Grad Sch. of Science, Kyoto Univ.*, [2]*RIKEN SPring-8 Center*, [3]*NIBIO*, [4]*MRC Laboratory of Molecular Biology*)

1SAA-2　流れが駆動するタンパク質のアミロイド線維化機構
Mechanism of amyloid fibrillation of a protein driven by a flow
○菅瀬 謙治 [1], 森本 大智 [2], Erik Walinda[3]（[1] 京都大学大学院農学研究科 応用生命科学専攻, [2] 京都大学大学院工学研究科分子工学専攻, [3] 京都大学大学院医学研究科細胞機能制御学）
Kenji Sugase[1], Daichi Morimoto[2], Erik Walinda[3] ([1]*Division of Applied Life Sciences, Graduate School of Agriculture, Kyoto University*, [2]*Department of Molecular Engineering, Graduate School of Engineering, Kyoto University*, [3]*Department of Molecular and Cellular Physiology, Graduate School of Medicine, Kyoto University*)

1SAA-3　生体分子のための動的溶媒和理論の開発
Development of Dynamic Solvation Theory for Biomolecules
○吉田 紀生（名古屋大・院情報）
Norio Yoshida (*Grad. Sch. Info., Nagoya Univ.*)

1SAA-4 リン酸化による HP1α の液-液相分離機構の解明
Phase separation mechanism of HP1α by phosphorylation
○古川 亜矢子 [1], 米澤 健人 [2,3], 根上 樹 [4], 吉村 ゆり子 [5], 林 亜紀 [5], 中山 潤一 [5,6], 安達 成彦 [2], 千田 俊哉 [2], 清水 謙多郎 [4], 寺田 透 [4], 清水 伸隆 [2], 西村 善文 [1,7]（[1] 横市大・生命医科学, [2] 高エネ機構・物構研, [3] 奈良先端大・CDG, [4] 東大・院農, [5] 基生研, [6] 総研大・生命科学研究科, [7] 広島大・統合生命）
Ayako Furukawa[1], Kento Yonezawa[2,3], Tatsuki Negami[4], Yuriko Yoshimura[5], Aki Hayashi[5], Jun-ichi Nakayama[5,6], Naruhiko Adachi[2], Toshiya Senda[2], Kentaro Shimizu[4], Tohru Terada[4], Nobutaka Shimizu[2], Yoshifumi Nishimura[1,7] ([1]*Grad. Sch. Med. Life Sci., Univ. Yokohama City*, [2]*IMSS, KEK,*, [3]*NAIST, CDG*, [4]*Grad. Sch. Agr. Life Sci., Univ. Tokyo*, [5]*NIBB*, [6]*SOKENDAI*, [7]*Grad. Sch. Integ. Sci. Life, Univ. Hiroshima*)

1SAA-5 タンパク質の変性状態における構造ダイナミクスと溶媒環境依存性の理論的解析
Theoretical study on the conformational dynamics of proteins in disordered states under different solvent environments
○森 俊文（九大・先導研）
Toshifumi Mori (*Inst. Mat. Chem. Eng., Kyushu Univ.*)

1SAA-6 ポリマーコートされたダイヤモンドナノ粒子によるバイオセンシング
Biosensing Using Diamond Nanoparticles Coated with Polymers
○外間 進悟, 原田 慶恵（阪大・蛋白研）
Shingo Sotoma, Yoshie Harada (*IPR, Osaka Univ.*)

1SAA-7 (2Pos051) 蝶々型金ナノデバイスが可能にするタンパク質液液相分離過程の制御
(2Pos051) Control of protein condensation by butterfly-shaped gold nanodevices
○延山 知弘 [1], 高田 耕児 [2], 村上 達也 [2], 白木 賢太郎 [1,2]（[1] 筑波大・応用理工, [2] 富山県立大・院工）
Tomohiro Nobeyama[1], Koji Takata[2], Tatsuya Murakami[2], Kentaro Shiraki[1,2] ([1]*Pure and Appli.Sci., Univ.Tsukuba*, [2]*Grad. Sch. Sci. Toyama Pref. Univ*)

1SAA-8 (1Pos054) GGGGCC-RNA は、TDP43 およびそのカルボキシ断片の凝集を抑制する
(1Pos054) GGGGCC-RNA prevents aggregation of TDP43 and its carboxy terminal fragments
○藤本 愛 [1], 金城 政孝 [2], 北村 朗 [2]（[1] 北大・院・生命, [2] 北大・先端生命）
Ai Fujimoto[1], Masataka Kinjo[2], Akira Kitamura[2] ([1]*Grad. Sch. of Life Sci., Hokkaido. Univ*, [2]*Fac. Adv. Life Sci., Hokkaido. Univ*)

おわりに
Closing Remarks

09:00〜11:30　B 会場（函館アリーナ 武道館 B）／Room B（Hakodate Arena Budokan B）

1SBA　量子ビームでひも解くタンパク質の大きな構造変化 –タンパク質ダイナミクス理解の新潮流
Protein large-scale motions revealed by quantum beams -a new era in understanding protein dynamics

オーガナイザー：山本 直樹（自治医科大学），関口 博史（高輝度光科学研究センター）
Organizers: Naoki Yamamoto (Jichi Med. Univ.), Hiroshi Sekiguchi (JASRI)

Biological systems function by constantly changing their hierarchical and inter-hierarchical interactions among molecules, cells, and individuals. In order to visualize these dynamics, it is effective to approach them using penetrating quantum beams such as X-rays and neutron beams. This symposium will introduce recent advances in quantum beam techniques for biophysical research, mainly focusing on large structural changes within and between protein molecules. Furthermore, molecular dynamics simulation studies combined with the experimental researches, which deepen the knowledge on molecular mechanisms of the complexed protein systems, will also be shown.

はじめに
Opening Remarks

1SBA-1　X 線 1 分子追跡法によるヘモグロビン・アロステリーの再検討
Allosteric Transition Dynamics in Hemoglobin Reconsidered by Diffracted X-ray Tracking
○関口 博史 [1], 山本 直樹 [2], 柴山 修哉 [2], 佐々木 裕次 [1,3]（[1] 高輝度光科学研究センター, [2] 自治医科大・医, [3] 東大・新領域）
Hiroshi Sekiguchi[1], Naoki Yamamoto[2], Naoya Shibayama[2], Yuji Sasaki[1,3] ([1]*JASRI/SPring-8*, [2]*Dept. Physiology, Jichi Med. Univ.*, [3]*Grad. Sch. Front. Sci., Univ. Tokyo*)

1SBA-2　Internal dynamics of intrinscially disordered protein as studied by neutron scattering
Rintaro Inoue (*Institute for Integrated Radiation and Nuclear Science, Kyoto University*)

1SBA-3　(2Pos050) タンパク質ケージ内における芳香環相互作用ネットワークの熱力学・分子動力学的解析
(2Pos050) Thermodynamic and Molecular Dynamic Analysis of Aromatic Interaction Networks in Protein Cages
○菱川 湧輝 [1], 野谷 大樹 [1], 浅沼 明日香 [1], Maity Basudev[1], 長門石 曉 [2], 津本 浩平 [2,3], 安部 聡 [1], 上野 隆史 [1]（[1] 東工大・生命理工, [2] 東大・医科研, [3] 東大・院工）
Yuki Hishikawa[1], Noya Hiroki[1], Asuka Asanuma[1], Basudev Maity[1], Satoru Nagatoishi[2], Kouhei Tsumoto[2,3], Satoshi Abe[1], Takafumi Ueno[1] ([1]*Sch. Life Sci. Technol., Tokyo Inst. Technol.*, [2]*Inst. Med. Sci., Univ. Tokyo*, [3]*Sch. Eng., Univ. Tokyo*)

1SBA-4　(1Pos076) 3D structural determination of proteins from fluctuation X-ray scattering data
Wenyang Zhao[1], Osamu Miyashita[1], Florence Tama[1,2] ([1]*Center for Computational Science, RIKEN*, [2]*Grad. Sch. Sci., Univ. Nagoya*)

1SBA-5　Microscopic Mechanisms of Stable Amyloid β (1-42) Oligomer Formation
Ikuo Kurisaki, Shigenori Tanaka (*Graduate School of System Informatics, Kobe University*)

1SBA-6 **非干渉性中性子散乱で観測するアミロイド構造多形体及びリン脂質分子のサブナノ秒ダイナミクス**
Sub-nanosecond dynamics of amyloid polymorphs and phospholipid molecules observed by incoherent neutron scattering
○松尾 龍人 [1,2,3], Francesco Alessio De[2], Cissé Aline[2,3], Bicout Dominique[2,3], Peters Judith[2,3,4] ([1] 量研・量子生命科学研究所, [2]Institut Laue-Langevin, France, [3]Université Grenoble Alpes, France, [4]Institut Universitaire de France)
Tatsuhito Matsuo[1,2,3], Alessio De Francesco[2], Aline Cissé[2,3], Dominique Bicout[2,3], Judith Peters[2,3,4] ([1]*iQLS, QST*, [2]*Institut Laue-Langevin, France*, [3]*Université Grenoble Alpes, France*, [4]*Institut Universitaire de France*)

1SBA-7 **アミロイド線維前駆中間体の構造発達とその阻害**
Structural development of amyloid prefibrillar intermediates and its inhibition
○山本 直樹（自治医大・医）
Naoki Yamamoto (*Sch. Med. Jichi Med. Univ.*)

おわりに
Closing Remarks

09:00〜11:30　C 会場（函館アリーナ 武道館 C）／Room C（Hakodate Arena Budokan C）
1SCA　**【共催：新学術研究領域「生命金属科学」】**

生命金属のライブセルイメージング
Live-cell imaging of bio-metal species

オーガナイザー：石森 浩一郎（北海道大学），平山 祐（岐阜薬科大学）
Organizers: Koichiro Ishimori (Hokkaido Univ.), Tasuku Hirayama (Gifu Pharm. Univ.)

The inorganic ions are essential for life despite their small amounts, in addition to organic macromolecules such as proteins, DNA, carbohydrates, and lipids. The dysfunction of the homeostasis of these inorganic ion species is involved in various pathologies. To understand the dynamics and functions of the inorganic species in living things, the observation of their existence and fluctuation in living cells is necessary. In this symposium, up-and-coming researchers will give talks on innovative methods for imaging inorganic species in living cells. This symposium is a collaborative symposium with Integrated Metal-bioscience.

1SCA-1 **遊離鉄およびヘム蛍光プローブのライブセルイメージングへの応用**
Fluorescence probes for labile iron and heme and their applications to live-cell imaging
○平山 祐（岐阜薬科大学薬化学研究室）
Tasuku Hirayama (*Lab. Pharm. Med. Chem., Gifu Pharm. Univ.*)

1SCA-2 **細胞内遊離亜鉛イオンの定量解析を可能とする小分子蛍光プローブの開発**
Development of small-molecule fluorescent probes for the quantitative analysis of labile Zn^{2+} in cells
○小和田 俊行（東北大学多元物質科学研究所）
Toshiyuki Kowada (*Institute of Multidisciplinary Research for Advanced Materials, Tohoku University*)

1SCA-3 **コンディショナルプロテオミクスによる金属関連タンパク質のイメージングとプロファイリング**
Imaging and profiling of metal-related proteins by conditional proteomics strategies
○田村 朋則（京大院工）
Tomonori Tamura (*Grad. Sch. Eng., Univ. Kyoto*)

1SCA-4 量子ビームによる生命金属シングルセルイメージング
Single cell imaging by quantum beam elemental analyses for dynamics of cellular distribution of bio-metals
○武田 志乃（国立研究開発法人量子科学技術研究開発機構　放射線医学研究所）
Shino Takeda (*National institute of Radiological Sciences, National Institutes for Quantum Science and Technology*)

1SCA-5 蛍光イメージングで解き明かす細胞内マグネシウムイオンの役割
The roles of intracellular magnesium ion revealed by fluorescence imaging
○新藤 豊（慶大・理工・生命情報）
Yutaka Shindo (*Dept. Biosci. Info., Keio Univ.*)

1SCA-6 H_2S 検出蛍光プローブの開発とそれを用いた活性イオウ分子産生酵素の阻害剤スクリーニングへの応用
Development of a fluorescence probe for H_2S and its application to the inhibitor screening of reactive sulfur species-producing enzymes
○花岡 健二郎（慶應大・院薬）
Kenjiro Hanaoka (*Grad. Sch. Pharm. Sci., Keio Univ.*)

09:00〜11:30　D 会場（函館アリーナ 多目的室 A）／Room D（Hakodate Arena Multipurpose Room A）
1SDA　糖鎖の動的構造から機能へ – 実験・理論解析の最先端
Unveil glycans' function from their dynamical structures. – Cutting-edge challenges

オーガナイザー：李 秀栄（医薬基盤・健康・栄養研究所），山口 芳樹（東北医科薬科大学）
Organizers: Suyong Re (NIBIOHN), Yoshiki Yamaguchi (Tohoku Med. and Pharm.l Univ.)

Glycosylation of proteins is a ubiquitous biomolecular process. It adds extra functions or modulates existing functions of proteins, thereby affecting a range of cellular processes and diseases. Despite of the complex and dynamical nature of glycan structures, the recent advances both in experiment and computation enable us to investigate their functions based on the dynamical structures at atomic resolution, as exemplified in the "glycan-shield" of SARS-CoV-2 spike protein. In this symposium, we would like to share the cutting-edge challenges in determining functional structures and dynamics of glycans and discuss the potential future collaborations.

はじめに
Opening Remarks

1SDA-1 Viral glycosylation: HIV-1 to SARS-CoV-2
Max Crispin (*School of Biological Sciences, University of Southampton, UK*)

1SDA-2 Integrative methods in structural glycobiology
Jon Agirre (*University of York*)

1SDA-3 GLYCO: a tool to quantify glycan shielding of glycosylated proteins
Myungjin Lee (*National Institutes of Health*)

1SDA-4 Psme3 の部位特異的な *O*-GlcNAc 修飾は、P-body の恒常性の阻害を介してマウス ES 細胞の多能性維持に関与する
Site-specific *O*-GlcNAcylation of Psme3 maintains mouse embryonic stem cell pluripotency by impairing P-body homeostasis
○西原 祥子（創価大学・糖鎖生命システム融合研究所）
Shoko Nishihara (*Glycan & Life System Integration Center (GaLSIC), Soka University*)

1SDA-5 Description of the dynamic conformation of oligosaccharides by combining NMR spectroscopy and molecular simulation

Takumi Yamaguchi[1,2] ([1]*School of Materials Science, Japan Advanced Institute of Science and Technology*, [2]*Graduate School of Pharmaceutical Sciences, Nagoya City University*)

1SDA-6 病原性細菌における付着因子の糖鎖認識機構

Analyses of recognition mechanism and structure of bacteria FimH adhesin

○能登 香（北里大学・一般教育）

Kaori Ueno-Noto (*Coll. Lib. Arts Sci., Kitasato Univ.*)

09:00〜11:30　E 会場（函館アリーナ 多目的室 B）／Room E（Hakodate Arena Multipurpose Room B）

1SEA 【共催：CREST 「新たな光機能や光物性の発現・利活用を基軸とする次世代フォトニクスの基盤技術」】

先端赤外光の利用による生物物理学研究

Utilization of Advanced Infrared Sources for Biophysical Studies

オーガナイザー：古谷 祐詞（名古屋工業大学），村越 秀治（生理学研究所）

Organizers: Yuji Furutani (NITech), Hideji Murakoshi (NIPS)

Infrared (IR) light has been widely utilized for analyzing molecular structure and interaction in biological and organic materials. Nowadays, new infrared light sources have been developed, such as ultrafast pulsed IR lasers, quantum cascade lasers, and fiber lasers. These lasers are applicable not only to vibrational spectroscopy on biological molecules but also to microscopic imaging of biological systems such as tissues and cells. Multi-photon microscopy is one of the most important applications, which can shed light on deep inside brains. In this symposium, we would like to discuss the possibility of new infrared light sources in biophysical studies.

はじめに

Opening Remarks

1SEA-1 1800 nm フェムト秒ファイバーレーザーを用いた多光子蛍光顕微鏡

Multi-photon fluorescence microscopy using a 1800 nm femtosecond fiber laser system

○藤 貴夫 [1], 村越 秀治 [2,3], 植田 大海 [2,3], 濱田 航輔 [1], 後藤 龍一郎 [4]（[1] 豊田工業大学, [2] 生理学研究所, [3] 総合研究大学院大学, [4] ファイバーラボ株式会社）

Takao Fuji[1], Hideji Murakoshi[2,3], Hiromi Ueda[2,3], Kosuke Hamada[1], Ryuichiro Goto[4] ([1]*Toyota Technological Institute*, [2]*National Institute for Physiological Sciences*, [3]*The Graduate University for Advanced Studies*, [4]*Fiberlabs Inc.*)

1SEA-2 高機能超短パルスファイバレーザーを用いた第 3 の生体の窓における生体深部イメージング

Deep tissue imaging using highly functional ultrashort pulse fiber laser in the third NIR optical tissue window

○西澤 典彦 [1], 山中 真仁 [2]（[1] 名古屋大学工学研究科電子工学専攻, [2] 大阪大学工学研究科応用物理学専攻）

Norihiko Nishizawa[1], Masahito Yamanaka[2] ([1]*Department of Electronics, Nagoya University*, [2]*Department of Applied Physics, Osaka University*)

1SEA-3 非線形光学過程を利用した 2 種類の赤外超解像顕微鏡による生体試料の観察

Selective IR super-resolution imaging of biological samples by micro-spectroscopies based on non-linear optical process

○高橋 広奈, 酒井 誠（岡山理大・理）

Hirona Takahashi, Makoto Sakai (*Faculty of Sci., Okayama Univ. of Sci.*)

1SEA-4 ロドプシンをモデルとした膜タンパク質の表面増強赤外分光計測による構造変化解析
Structural changes of rhodopsin studied by surface-enhanced infrared spectroscopy as a model system of membrane proteins
○古谷 祐詞 [1,2]（[1] 名工大・院工, [2] 名工大・オプトバイオ）
Yuji Furutani[1,2] ([1]*Grad. Sch. Eng., Nagoya Inst. Tech.*, [2]*OptoBio, Nagoya Inst. Tech.*)

1SEA-5 高速中赤外分光および顕微鏡
High-speed mid-infrared spectroscopy and microscopy
○井手口 拓郎（東京大学・フォトンサイエンス研究機構）
Takuro Ideguchi (*IPST, Univ. Tokyo*)

おわりに
Closing Remarks

09:00〜11:30　G 会場（函館市民会館 3F 小ホール）／Room G（Hakodate Citizen Hall 3F Small Hall）
1SGA　再構築実験によってアプローチするプロトセル研究と生命の起源への探求
Frontiers of Protocell Research: Exploring the Origin of Life through a Constructivist Approach

オーガナイザー：車 兪澈（海洋研究開発機構），Tony Z. Jia（東京工業大学）
Organizers: Yutetsu Kuruma (JAMSTEC), Tony Z. Jia (Tokyo Tech)

The search for the origin of life (OoL) is now entering a new phase, involving researchers from various fields and incorporating new scientific findings. Especially, the study of artificial cells by a constructivist approach and assembly of protocells by liquid-liquid phase separation or other non-“traditional” physical processes have been advocating a new interpretation in OoL studies. This symposium will focus on the frontiers of the construction and assembly of protocells and artificial cells with novel emergent structures and functions relevant to the origins of life.

はじめに
Opening Remarks

1SGA-1 DNA ナノテクノロジーを軸に挑む人工分子システム構築
Toward the construction of cell-like molecular systems based on DNA nanotechnology
○佐藤 佑介（九工大・院情報工）
Yusuke Sato (*Fac. Comp. Sci. and Sys. Eng., Kyushu Inst. Tech.*)

1SGA-2 (2Pos120) 人工核酸 PNA を用いた DNA の液ー液相分離制御
(2Pos120) Regulation of liquid-liquid phase separation of DNA using peptide nucleic acid (PNA)
○相馬 陸杜, 愛場 雄一郎, 柴田 将成, 有安 真也, 荘司 長三（名古屋大学大学院理学研究科）
Rikuto Soma, Yuichiro Aiba, Masanari Shibata, Shinya Ariyasu, Osami Shoji (*Graduate School of Science, Nagoya University.*)

1SGA-3 Investigating the role of membrane biophysical properties on protein folding and sorting
Neha Kamat[1,2] ([1]*Department of Biomedical Engineering, Northwestern University*, [2]*Center of Synthetic Biology, Northwestern University*)

1SGA-4 脂質を合成する人工細胞
Lipid synthesis in artificial cell
Yutetsu Kuruma[1,2], Yasuhiro Shimane[1], Rumie Matsumura[1] ([1]*JAMSTEC*, [2]*JST PRESTO*)

1SGA-5 RNA 複製と進化のための区画構造
Compartmentalization for RNA replication and evolution
○水内 良 [1,2]（[1] 東大・先進科学, [2]JST・さきがけ）
Ryo Mizuuchi[1,2] ([1]*Komaba Inst. Sci., Univ. Tokyo*, [2]*JST, PRESTO*)

1SGA-6 エクソソームが司る、がん転移の新しいストーリー
Exosomes, new players in the field of metastasis
○星野 歩子（東京工業大学）
Ayuko Hoshino (*Tokyo Institute of Technology*)

おわりに
Closing Remarks

09:00〜11:30　H 会場（函館市民会館 3F 大会議室）／Room H（Hakodate Citizen Hall 3F Conference Room）

1SHA　分子集団，細胞集団が織りなす自律特性: 生命機能の理解を目指して
Autonomous Characteristics of Molecular and Cellular Ensembles: Toward an Understanding of Biological Functions

オーガナイザー：茅 元司（東京大学），島本 勇太（国立遺伝学研究所）
Organizers: Motoshi Kaya (The Univ. of Tokyo), Yuta Shimamoto (NIG)

The autonomous characteristics of molecular and cellular assemblies are of a higher order than can be imagined from the characteristic of a single molecule or cell, and are the essence of various biological functions. In this symposium, we will invite researchers who are working on the mechanisms of cell motility, tissue formation, etc., using a variety of advanced approaches. We will discuss how understanding the autonomous characteristics of molecular and cellular ensembles can advance our understanding of biological functions.

1SHA-1 骨格筋ミオシン，心筋ミオシン分子集団の自律特性が骨格筋，心臓収縮を作り出す
Autonomous characteristics of skeletal and cardiac myosin ensembles are essential for contractile functions of skeletal muscle and heart
○茅 元司（東大・院理）
Motoshi Kaya (*Grad. Sch. Sci., Univ. Tokyo*)

1SHA-2 人工細胞による細胞動態の再構築：自発運動から波動現象の力学的理解へ向けて
Artificial cells: Reconstruction of cell-like behaviors from spontaneous migration to wave dynamics toward understanding cell mechanics
Ryota Sakamoto[1,2], Ziane Izri[3], Yuta Shimamoto[4], Makito Miyazaki[5,6,7,8], Yusuke Maeda[2] ([1]*Dept. Biomed. Engr., Yale Univ.*, [2]*Dept. Phys., Kyushu Univ.*, [3]*Dept. Phys., Minessota Univ.*, [4]*Natl. Inst. Genetics*, [5]*Hakubi Ctr., Kyoto Univ.*, [6]*Dept. Phys., Kyoto Univ.*, [7]*Institut Curie*, [8]*JST PRESTO*)

1SHA-3 紡錘体の自己組織化ダイナミクスと微小管の集団運動メカニクス
Morphological growth dynamics and active microtubule mechanics underlying spindle self-organization
○島本 勇太（国立遺伝学研究所）
Yuta Shimamoto (*National Institute of Genetics*)

1SHA-4 時計回りの組織形成を支える集団細胞移動の作動原理
Mechanical perspective of collective cell movement in epithelial morphogenesis
○倉永 英里奈（東北大・院生命科学）
Erina Kuranaga (*Grad. Sch. Life Sci., Tohoku Univ.*)

1SHA-5 魚類表皮ケラトサイト集団ではリーダー細胞とフォロワー細胞が協調的かつ強制的にフォロワーをリーダーに昇進させる
Cooperative but forcible promotion of follower cells to leaders in collective migration of fish keratocytes
○岩楯 好昭（山口大・理）
Yoshiaki Iwadate (*Dept. Biol., Yamaguchi Univ.*)

1SHA-6 Interaction rules within multicellular dynamics and biological condensates
Kawaguchi Kyogo (*RIKEN CPR/BDR*)

13:50〜16:20　A 会場（函館アリーナ 武道館 A）／Room A（Hakodate Arena Budokan A）
1SAP　【共催：文部科学省「富岳」成果創出加速プログラム
「プレシジョンメディスンを加速する創薬ビッグデータ統合システムの推進」】

スーパーコンピューター「富岳」による創薬・医療の革新
Innovation of drug discovery and medical treatment using supercomputer Fugaku

オーガナイザー：荒木 望嗣（京都大学），池口 満徳（横浜市立大学）
Organizers: Mitsugu Araki (Kyoto Univ.), Mitsunori Ikeguchi (Yokohama City Univ.)

Drug discovery and medical technologies are being innovated by development of high performance computing (HPC). Large-scale molecular dynamics simulations performed on supercomputer Fugaku permit atomic-level observation of "slow" biomolecular processes such as protein conformational transition and protein-drug interaction processes, providing deeper insight into molecular mechanisms of disease and drug design to overcome it. In this symposium, we will discuss about the forefront of next-generation molecular simulation techniques for drug discovery and medical treatment.

はじめに
Opening Remarks

1SAP-1 超高周波超音波照射下での分子動力学シミュレーションによるタンパク質-医薬品結合プロセスの加速
Hypersound-perturbed molecular dynamics to accelerate slow protein-ligand binding processes
○荒木 望嗣, 奥野 恭史（京大・院医）
Mitsugu Araki, Yasushi Okuno (*Grad.Sch.Med., Kyoto Univ.*)

1SAP-2 スーパーコンピューター「富岳」による創薬へ向けた自由エネルギー摂動法の開発
Development of the free-energy perturbation method toward drug discovery on supercomputer Fugaku
○尾嶋 拓 [1], 杉田 有治 [1,2,3]（[1] 理研・BDR, [2] 理研・R-CCS, [3] 理研・CPR）
Hiraku Oshima[1], Yuji Sugita[1,2,3] ([1]*RIKEN BDR*, [2]*RIKEN R-CCS*, [3]*RIKEN CPR*)

1SAP-3 Binding Kinetics of Kinase Complexes by PaCS-MD/MSM
Kazuhiro Takemura, Akio Kitao (*SLST, TokyoTech*)

1SAP-4 MD シミュレーションで考える抗原-抗体界面：合理的な抗体医薬品設計に向けて
A molecular dynamics study on the antigen-antibody interface: Toward rational antibody drug design
○山下 雄史（東京大学）
Takefumi Yamashita (*The University of Tokyo*)

1SAP-5 大規模分子動力学シミュレーションを用いた上皮成長因子受容体キナーゼの活性化メカニズムの研究
A study of activation mechanism of epidermal growth factor receptor kinase using large-scale molecular dynamics simulations
○井上 雅郎 [1], 浴本 亨 [1], 山根 努 [2], 池口 満徳 [1,2]（[1] 横浜市大・院生命医科学, [2] 理研・計算科学研究センター）
Masao Inoue[1], Toru Ekimoto[1], Tsutomu Yamane[2], Mitsunori Ikeguchi[1,2] ([1]*Grad. Sch. Med. Life Sci., Yokohama City Univ.*, [2]*RIKEN R-CCS*)

1SAP-6 Extracting protein dynamics from experimental cryo-EM maps using a machine learning technique combining with MD simulations
Shigeyuki Matsumoto[1], Shoichi Ishida[2], Kei Terayama[2], Yasushi Okuno[1,3] ([1]*Grad. Sch. Med., Kyoto Univ.*, [2]*Grad. Sch. Med. Life Sci., Yokohama City Univ.*, [3]*RIKEN R-CCS*)

おわりに
Closing Remarks

13:50〜16:20　B 会場（函館アリーナ 武道館 B）／Room B（Hakodate Arena Budokan B）
1SBP　【共催：学術変革領域研究（A）「クロススケール新生物学」】

細胞内メゾ複雑体の構造と機能
Structure and function of “meso-entangled bodies” in the cell

オーガナイザー：杉田 有治（理化学研究所），山本 林（東京大学）
Organizers: Yuji Sugita (RIKEN), Hayashi Yamamoto (The Univ. of Tokyo)

Proteins often assemble to form "mesoscopic" complexes – some ordered and some disordered – to exert their functions in the cell. Therefore, elucidating their architectures and physical properties is necessary to understand the molecular mechanisms underlying life phenomena and diseases. In this research area "Cross-Scale Biology", we particularly focus on mesoscopic structures in the range of 20–500 nm (including LLPS condensates), which we define as "meso-entangled bodies (MEBs)", because MEBs are thought to be key factors that determine the fate of organisms through the transition from disordered to ordered states at the mesoscale. In this symposium, researchers working on the MEBs will gather to discuss the latest technologies and findings, including In-cell AFM, cryo-EM, chemical biology, and LLPS.

1SBP-1 ナトリウムポンプのつくりかた
How to make a sodium pump
○阿部 一啓（名古屋大・細胞生理）
Kazuhiro Abe (*CeSPI, Nagoya Univ*)

1SBP-2 光可逆的蛋白質ラベル化システムによる細胞内蛋白質動態と細胞機能の光制御
Optical control of intracellular protein dynamics and cellular functions using a photoreversible protein labeling system
○水上 進（東北大・多元研）
Shin Mizukami (*IMRAM, Tohoku Univ.*)

1SBP-3 分離した RNP ミセルとしてのパラスペックル核内構造体の構築機構
Construction mechanism of nuclear paraspeckle as an isolated RNP micell
○廣瀬 哲郎 [1,2], 高桑 央 [1,3], 山本 哲也 [4], 山崎 智弘 [1]（[1] 阪大・院生命機能, [2] 阪大・先導学際機構, [3] 北大・院医, [4] 北大・化学反応拠点）
Tetsuro Hirose[1,2], Takakuwa Hiro[1,3], Yamamoto Tetsuya[4], Yamazaki Tomohiro[1] ([1]*Grad. Sch. Front. Biosci., Osaka Univ*, [2]*OTRI, Osaka Univ*, [3]*Grad. Sch. Med., Hokkaido Univ*, [4]*ICReDD, Hokkaido Univ*)

1SBP-4 細胞内における酵母プリオン伝播のクロススケール解析
Cross-scale analyais of yeast prion propagation in cells
Motomasa Tanaka (*RIKEN Center for Brain Science*)

1SBP-5 原子間力顕微鏡を用いた生きた細胞のメゾスケール表面構造体及び内部構造体観察方法の開発
Development of the method for observing mesoscale structures outside and inside living cells using atomic force microscopy
○市川 壮彦 [1], Penedo Marcos[2], 宮澤 佳甫 [1,3], 古庄 公寿 [1], Alam Mohammad Shahidul[1], 宮田 一輝 [1,3], 中村 史 [4], 福間 剛士 [1,3]（[1] 金沢大・ナノ研, [2]EPFL・生物工, [3] 金沢大・フロンティア工, [4]AIST・細胞工）
Takehiko Ichikawa[1], Marcos Penedo[2], Keisuke Miyazawa[1,3], Hirotoshi Furusho[1], Mohammad Shahidul Alam[1], Kazuki Miyata[1,3], Chikashi Nakamura[4], Takeshi Fukuma[1,3] ([1]*NanoLSI, Kanazawa Univ.*, [2]*Inst. Bioeng., EPFL*, [3]*Frontier Eng., Kanazawa Univ.*, [4]*CMB, AIST*)

1SBP-6 Structure modeling of protein complex from experimental data using molecular dynamics simulation
Takaharu Mori (*RIKEN CPR*)

1SBP-7 Ferritin phase separation driven by NCOA4 promotes two types of ferritin autophagy, macro-autophagy and endosomal micro-autophagy
Hayashi Yamamoto (*Grad. Sch. Med., Univ. Tokyo*)

13:50〜16:20　C 会場（函館アリーナ 武道館 C）／Room C（Hakodate Arena Budokan C）
1SCP　複雑システムの振る舞いの解明に向けたトポロジカルアプローチ
Topological approaches to understand behaviours of complex biological systems

オーガナイザー：望月 敦史（京都大学），岡田 崇（理化学研究所）
Organizers: Atsushi Mochizuki (Kyoto Univ.), Takashi Okada (RIKEN)

It is considered that biological functions emerge from dynamics of complex systems consisting from interactions of many biomolecules. Obtaining logical understandings for behaviors of network systems is strongly required in life sciences. To meet it, a series of mathematical methods have been developed, by which important aspects of dynamical behaviors are determined from the topology of networks alone. They have been applied to real biological systems and have made unique achievements. Recently, we see a series of technical or theoretical progresses, which broaden the scope of applications of the methods. In this symposium, we will introduce topological approaches to the network system, and discuss future perspectives of them.

はじめに
Opening Remarks

1SCP-1 ネットワーク構造に基づく細胞運命の制御
Controlling cell fate specification system based on network structure
○望月 敦史（京都大・医生研）
Atsushi Mochizuki (*Inst. Life Med. Sci, Kyoto Univ.*)

1SCP-2 **摂動後の発現時系列データを用いた遺伝子制御ネットワーク推定法**
Estimating gene regulatory network using time-series expression data following gene perturbation
○石川 雅人[1], 永樂 元次[2], 遊佐 宏介[2], 山内 悠平[2], 木立 尚孝[1], 望月 敦史[2]（[1] 東京大・院新領域, [2] 京都大・医生研）
Masato Ishikawa[1], Mototsugu Eiraku[2], Kosuke Yusa[2], Yuhei Yamauchi[2], Hisanori Kiryu[1], Atsushi Mochizuki[2] ([1]*Grad. Sch. Front. Sci., UTokyo*, [2]*Inst. Life Med. Sci., Kyoto Univ.*)

1SCP-3 **ネットワーク構造から生化学反応の摂動応答を決める**
Network architecture determines sensitivity of biochemical reaction systems
Takashi Okada[1], Je-Chiang Tsai[2], Atsushi Mochizuki[1] ([1]*Inst. Life Med. Sci, Kyoto Univ.*, [2]*National Tsing Hua University, Taiwan*)

1SCP-4 **複雑な化学反応ネットワークを単純化する**
Simplifying complex chemical reaction networks
Yuji Hirono (*Asia Pacific Center for Theoretical Physics*)

1SCP-5 **開放系トポロジカル相**
Topological phases in open systems
○佐藤 昌利（京都大学基礎物理学研究所）
Masatoshi Sato (*Yukawa Institute for Theoretical Physics, Kyoto University*)

13:50〜16:20　D 会場（函館アリーナ 多目的室 A）／Room D（Hakodate Arena Multipurpose Room A）

1SDP　生体高分子による液液相分離: 基礎と応用
Phase Separation by Biopolymers: Basics and Applications

オーガナイザー：北原 亮（立命館大学），亀田 倫史（産業技術総合研究所）
Organizers: Ryo Kitahara (Ritsumeikan Univ.), Tomoshi Kameda (AIST)

Although cells organize many biochemical processes in membrane-less compartments via liquid-liquid phase separation (LLPS), physicochemical properties and molecular details of LLPS consisting of proteins and nucleic acids are still largely unknown. This symposium contains lectures on the physicochemical basis of biomolecular LLPS and some recent experimental and theoretical developments to elucidate its structure and dynamics. For example, pressure perturbation spectroscopy, single-molecule fluorescence microscopy, Raman microscopy, and molecular dynamics simulations for protein LLPS will be introduced.

はじめに
Opening Remarks

1SDP-1 **圧力ジャンプ法による液液相分離の速度論解析：RNA 結合タンパク質 FUS**
Pressure-jump kinetics of liquid-liquid phase separation (LLPS) : The RNA-binding protein fused in sarcoma (FUS)
○北原 亮[1,2], 李 書潔[2], 吉澤 拓也[3]（[1] 立命館大・薬, [2] 立命館大院・薬, [3] 立命館大・生命）
Ryo Kitahara[1,2], Shujie Li[2], Takuya Yoshizawa[3] ([1]*Coll. Pharm. Sci., Ritsumeikan Univ.*, [2]*Grad. Sch. Pharm. Sci., Ritsumeikan Univ.*, [3]*Coll. Life Sci., Ritsumeikan Univ.*)

1SDP-2 **アミノ酸の溶解性に基づくタンパク質の液- 液相分離**
Liquid-liquid phase separation of proteins based on the solubility of amino acids
○野本 晃, 白木 賢太郎（筑波大院・数理）
Akira Nomoto, Kentaro Shiraki (*Pure and Appl. Sci., Univ. Tsukuba*)

1SDP-3 Raman and Brillouin microscopy as a tool for quantitative study of LLPS
Shinji Kajimoto[1,2] ([1]*Grad. Sch. Pharm. Sci., Tohoku University*, [2]*JST PRESTO*)

1SDP-4 液–液相分離会合体の分子取り込みと並進拡散運動に関する分子文法解析
Molecular grammar characterization of recruitment and translational dynamics of guest proteins in liquid droplets
○鎌形 清人（東北大多元研）
Kiyoto Kamagata (*IMRAM, Tohoku Univ.*)

1SDP-5 分子動力学シミュレーションと機械学習を組み合わせたペプチド凝集予測
Prediction of peptide aggregation by combining molecular dynamics simulation and machine learning
○亀田 倫史（産総研・人工知能）
Tomoshi Kameda (*AIRC, AIST*)

おわりに
Closing Remarks

13:50〜16:20　E 会場（函館アリーナ 多目的室 B）／Room E（Hakodate Arena Multipurpose Room B）
1SEP　微細制御技術を用いたフィジコケミカルバイオロジーへの展開
Physico- and chemical biology using nanomanipulation and micromanipulation technologies

オーガナイザー：北村 朗（北海道大学），飯塚 怜（東京大学）
Organizers: Akira Kitamura (Hokkaido Univ.), Ryo Iizuka (The Univ. of Tokyo)

Various nano- and micromanipulation technologies provide novel strategies to elucidate nature in many scientific fields such as biophysics, physicobiology, and chemical biology. Here, we introduce the cutting-edge topics using nanomanipulation and micromanipulation technologies with a single molecule sensitivity, chemical biology, optogenetics, and mechanistic measurements for understanding and controlling cells and organisms. Furthermore, research topics in molecular and cellular biology from physicochemical perspectives will be discussed.

はじめに
Opening Remarks

1SEP-1 マイクロ・ナノ加工技術を用いた 3D 腫瘍組織構築と新しいがん創薬開発にむけて
Construction of 3D tumor tissue using micro/nano processing technology and toward to development of new drug discovery
○繁富（栗林） 香織（北大・高等推進）
Kaori Kuribayashi-Shigetomi (*Inst. Adv. High. Edu., Hokkaido Univ.*)

1SEP-2 Crosstalk between myosin II and formin in the regulation of force generation and actomyosin dynamics in stress fibers
Yukako Nishimura[1,2], Shidong Shi[2], Virgile Viasnoff[2,3], Alexander Bershadsky[2,4] ([1]*IGM, Hokkaido Univ.*, [2]*MBI, NUS, Singapore*, [3]*Dept.of Biol.Sci., NUS*, [4]*Dept. of Mol. Cell Biol., Weizmann Inst.*)

1SEP-3 (3Pos312) Triple-color photothermal dye-based nanoheaters to generate multiple heat spots within a single cell
Md Monir Hossain, Takeru Yamazaki, Kayoko Nomura, Satoshi Arai (*Grad. Sch. NanoLS., Kanazawa Univ.*)

1SEP-4 Evaluation of the physicochemical properties of biomolecules using microdroplets
Ryo Iizuka (*Dept. of Biol. Sci., Grad. Sch. of Sci., The Univ. of Tokyo*)

1SEP-5 (3Pos093) Control of small G-protein Ras using calmodulin-based ionochromic molecular device.
Yassine Sabek, Nobuyuki Nishibe, Kazunori Kondo, Shinsaku Maruta (*Graduate school of science and engineering , department of biosciences , soka university, Hachioji TOKYO*)

1SEP-6 (1Pos283) Centromere-kinetochore structures revealed by 12x modified expansion microscopy
Yasuhiro Hirano[1], Aussie Suzuki[2], Yasushi Hiraoka[1], Tatsuo Fukagawa[1] ([1]*Graduate School of Frontier Biosciences, Osaka University*, [2]*McArdle Laboratory for Cancer Research, University of Wisconsin-Madison*)

1SEP-7 ボトムアップポリマーナノテクノロジーを用いたミクロレベル・マクロレベルの液液相分離制御
Control of the microscopic and macroscopic liquid-liquid phase separation based on bottom-up polymer nanotechnology
○岸村 顕広（九州大学大学院工学研究院応用化学部門）
Akihiro Kishimura (*Department of Applied Chemistry, Faculty of Engineering, Kyushu University*)

1SEP-8 発色団補助光不活化法 (CALI) の基礎と利用
Basics and applications of chromophore-assisted light inactivation (CALI)
○北村 朗（北大・先端生命）
Akira Kitamura (*Fac. Adv. Life Sci., Hokkaido Univ.*)

おわりに
Closing Remarks

13:50～16:20　F 会場（函館市民会館 1F 大ホール）／Room F（Hakodate Citizen Hall 1F Main Hall）
1SFP　生体膜の生物物理呼応と細胞機能制御への化学的利用
Biophysical responses and biochemical/chemical controlling of membranes for cellular regulation and future therapy

オーガナイザー：中瀬 生彦（大阪公立大学），広瀬 久昭（京都大学）
Organizers: Ikuhiko Nakase (Osaka Metropolitan Univ.), Hisaaki Hirose (Kyoto Univ.)

Biological membranes participate in responses for acceptance/rejection of stimulation and environmental changes from outside/inside cells, leading to signal transduction and cellular responses including e.g., cellular uptake, migration, proliferation, and cell death. The biophysical responses/mechanisms-based membrane controlling systems are highly anticipated to be next-generation therapeutic methodologies for further achievements of disease regulation such as cancers. In this proposal symposium, advanced research technologies and achievements of visualizing and controlling membrane traffic, structures, penetration, and shape-dependent cellular signaling from the fusion viewpoints of biophysics, molecular cell biology, chemistry, and chemical biology will be presented, and membrane-based therapeutic methodology will be discussed.

はじめに
Opening Remarks

1SFP-1 Uptake mechanisms of cell-penetrating peptides
Christian Widmann (*University of Lausanne, Switzerland*)

1SFP-2 Roles of membrane lipids in the organization of cell-cell adhestion structure
Junichi Ikenouchi (*Grad. Sch. Sci., Kyushu Univ.*)

1SFP-3 (2Pos198) Mechanism study of antimicrobial peptide synergistic effects at the molecular level by combining spectroscopy and electrochemical methods
Yuge Hou, Kaori Sugihara (*Institute of Industrial Science, The University of Tokyo,*)

1SFP-4 Biofunctional peptide-modified exosomes for intracellular delivery
Ikuhiko Nakase (*Grad. Sch. Sci., Osaka Metropolitan Univ.*)

1SFP-5 Membrane shaping by the BAR domain superfamily proteins and the extracellular vesicles by the shedding of filopodia
Shiro Suetsugu[1,2,3] ([1]*Biological Science, Nara Institue of Science and Technology*, [2]*Data Science Center, Nara Institue of Science and Technology*, [3]*Digital Green-Innovation, Nara Institue of Science and Technology*)

1SFP-6 Investigating the mechano-osmotic regulation of cell membrane tension using fluorescent membrane tension probes
Aurelien Roux[1,2] ([1]*Department of Biochemistry, CH-1211, University of Geneva*, [2]*NCCR Chemical Biology, CH-1211, University of Geneva*)

おわりに
Closing Remarks

13:50〜16:20　G 会場（函館市民会館 3F 小ホール）／Room G（Hakodate Citizen Hall 3F Small Hall）

1SGP　【共催：JST さきがけ「細胞の動的高次構造体」】

高次構造体を自在に操る
Uncovering the design principles of supramolecular assemblies through manipulation of the structures, dynamics, and functions

オーガナイザー：宮﨑 牧人（京都大学），小杉 貴洋（分子科学研究所）
Organizers: Makito Miyazaki (Kyoto Univ.), Takahiro Kosugi (IMS)

Cells contains various types of supramolecular assemblies ranging from nanometer-scale structures such as protein complexes and RNA-protein complexes to micrometer-scale structures such as organelles and liquid droplets. A growing body of evidence suggests that these ordered and dynamic structures regulate various key functions of the cell which were previously unknown or unnoticed. To uncover the design principles of the supramolecular assemblies, not only identification of the molecular components and observation of the dynamics, but also manipulation of their structures, dynamics, and functions will be of crucial importance. In this symposium, we will invite talented early-career researchers in various research fields who are developing cutting-edge technologies to manipulate the supramolecular assemblies.

はじめに
Opening Remarks

1SGP-1 高次構造体の協奏的機能を合理的に制御することを目指して
Toward rational control of concerted functions by supramolecular assemblies
○小杉 貴洋 [1,2,3,4]（[1] 分子研, [2] 総研大, [3] 生命創成探究センター, [4]JST・さきがけ）
Takahiro Kosugi[1,2,3,4] ([1]*IMS*, [2]*SOKENDAI*, [3]*ExCELLS*, [4]*PRESTO, JST*)

1SGP-2　タンパク質合成を司る高次構造体を操る：リボソームの光制御
Controlling a supra-assembly dedicated to protein synthesis: optogenetic control of ribosomes in the cell
○横山 武司 [1,2,3]（[1] 東北大・生命科学, [2] 東北大・INGEM, [3]JST さきがけ）
Takeshi Yokoyama[1,2,3] ([1]*Grad. Sch. Lif. Sci., Tohoku Univ.*, [2]*INGEM, Tohoku Univ.*, [3]*JST PRESTO*)

1SGP-3　両親媒性 α ヘリックスが操るオートファジー関連分子 ATG3 の機能
Amphipathic α-helix Manipulates ATG3 Function
○西村 多喜 [1,2,3], Lazzeri Gianmarco[4], 水島 昇 [2], Covino Roberto[4], Tooze Sharon[3]（[1]JST さきがけ専任研究員, [2] 東大・医・分子生物, [3] フランシス・クリック研究所, [4] フランクフルト高等研究所）
Taki Nishimura[1,2,3], Gianmarco Lazzeri[4], Noboru Mizushima[2], Roberto Covino[4], Sharon Tooze[3] ([1]*JST PRESTO Researcher*, [2]*Dept. of Biochem & Mol. Biol., Faculty of Med., The Univ. of Tokyo*, [3]*The Francis Crick Institute*, [4]*Frankfurt Institute for Advanced Studies*)

1SGP-4　ヘテロクロマチン形成高次構造体の解明と制御
Understanding and reconstructing small RNA mediated heterochromatin formation
○岩崎 由香（慶大・医）
Yuka Iwasaki (*Keio Univ. Sch. Med.*)

1SGP-5　操ることで見えてきた細胞内相分離現象の時空間デザイン原理
Spatio-temporal design principles of intracellular phase separation
○下林 俊典（京都大学 iPS 細胞研究所）
Shunsuke Shimobayashi (*CiRA, Kyoto University*)

1SGP-6　合成生物学で生きた細胞内の動的構造体を操り、デザインし、理解する
Manipulation, design, and analysis of dynamic intracellular structures with synthetic biology tools
○中村 秀樹 [1,2]（[1] 京大・白眉センター, [2] 京大・院工学研究科）
Hideki Nakamura[1,2] ([1]*Hakubi Center, Kyoto University*, [2]*Grad. Sch. Eng., Kyoto University*)

おわりに
Closing Remarks

13:50〜16:20　H 会場（函館市民会館 3F 大会議室）／Room H（Hakodate Citizen Hall 3F Conference Room）
1SHP　【共催：学術変革領域（B）「筋肉トランススケール熱シグナリング」】

“肉”のイマとミライ
The Future of Muscle is Now

オーガナイザー：鈴木 団（大阪大学），大山 廣太郎（量子科学技術研究開発機構）
Organizers: Madoka Suzuki (Osaka Univ.), Kotaro Oyama (QST)

Muscle is one of the main subjects that have been studied extensively in the field of Biophysics. We can now explain how the force is produced and assembled at all levels of the hierarchy in muscle; single protein molecule, molecular assembly (sarcomere), myofibril, cell (fiber) and tissue. Is the end of muscle study approaching? In this symposium, we will review the current status with senior researchers, and foresee the future advances with researchers at their early- and mid-carriers who demonstrate originalities and creativities in new methods.

はじめに
Opening Remarks

1SHP-1　筋収縮・制御機構に関する研究の現在と将来について
About the present and future of research on muscle contraction/regulation mechanism
○石渡 信一（早稲田大・理工学術院）
Shin'ichi Ishiwata (*Fac. Sci. & Engn., Waseda Univ.*)

1SHP-2　高輝度シンクロトロン放射光に照らされる筋肉研究の明るい未来
Rosy future of muscle research illuminated by bright synchrotron radiation X-rays
○岩本 裕之（高輝度光科学研究センター）
Hiroyuki Iwamoto (*SPring-8, JASRI*)

1SHP-3　局所熱パルスによる横紋筋の細いフィラメントの活性化
Microscopic heat pulses induce activation of striated muscle thin filaments
○石井 秀弥 [1], 福田 紀男 [2]（[1] 量研, [2] 慈恵医科大・細胞生理）
Shuya Ishii[1], Norio Fukuda[2] ([1]*QST*, [2]*Dept Cell Physiol, Sch Med, Jikei Univ.*)

1SHP-4　3 次元バイオプリントで作られた和牛ステーキ：未来の肉？
3D-Bioprinted Wagyu Steak: Meat of the future?
○松崎 典弥（阪大院工）
Michiya Matsusaki (*Grad. Sch. Eng., Osaka Univ.*)

1SHP-5　光熱変換を利用した局所熱パルス法による筋肉の熱暴走メカニズムの解明
Thermal runaway in muscles studied using a local heat pulse method
○鈴木 団（阪大・蛋白研）
Madoka Suzuki (*Inst. Protein Res., Osaka Univ.*)

おわりに
Closing Remarks

2 日目（9 月 29 日（木））／Day 2（Sep. 29 Thu.）

08:45〜11:15　A 会場（函館アリーナ 武道館 A）／Room A（Hakodate Arena Budokan A）
2SAA　NMR で迫る膜とペプチドの生物物理
NMR Studies in Membrane and Peptide Biophysics

オーガナイザー：川村 出（横浜国立大学），相沢 智康（北海道大学）
Organizers: Izuru Kawamura (Yokohama National Univ.), Tomoyasu Aizawa (Hokkaido Univ.)

Biomembranes and peptides have always been important research targets in the field of biophysics. In particular, their interactions and dynamic properties have not yet been fully elucidated, and many cutting-edge studies have been conducted by applying NMR techniques, which provide information at atomic resolution that is difficult to obtain by other spectroscopic methods. In this symposium, researchers in these fields are invited as speakers to discuss the results of their research using NMR methods.

はじめに
Opening Remarks

2SAA-1　Solid-State NMR spectroscopic approaches to investigate membrane-bound peptide structure
Izuru Kawamura (*Grad. Sch. Eng. Sci., Yokohama Natl. Univ.*)

2SAA-2 Mobility, location, and kinetics of membrane binding and cell entry of peptides by solution-state ^{19}F and ^{1}H NMR
Emiko Okamura (*Faculty Pharm. Sci., Himeji Dokkyo Univ.*)

2SAA-3 Sec 非依存性膜蛋白質膜挿入における大腸菌由来糖脂質 MPIase の役割解明
Role of a bacterial glycolipid MPIase in Sec-independent membrane protein integration
○野村 薫（公益財団法人サントリー生命科学財団）
Kaoru Nomura (*Suntory Foundation for Life Sciences*)

2SAA-4 Solid-state NMR measurements of amphotericin B, a natural product that interacts with lipid bilayers
Yuichi Umegawa (*Grad. Sch. Sci., Osaka Univ.*)

2SAA-5 Revealing Novel Polymorphs and Cross Propagation for 42-residue Amyloid beta by Solid-state NMR
Yoshitaka Ishii[1,2] ([1]*Tokyo Institute of Technology, School of Life Science and Technology*, [2]*RIKEN, BDR*)

08:45〜11:15　B 会場（函館アリーナ 武道館 B）／Room B（Hakodate Arena Budokan B）
2SBA　【共催：新学術領域研究「遺伝子制御の基盤となるクロマチンポテンシャル」】

先端技術と理論で迫るクロマチン機能の理解
Chromatin function as revealed by cutting-edge technique and theory

オーガナイザー：伊藤 由馬（東京工業大学），木村 宏（東京工業大学）
Organizers: Yuma Ito (Tokyo Tech), Hiroshi Kimura (Tokyo Tech)

Recent advance in genomics and imaging technologies have contributed to understanding the function of chromatin for gene regulation beyond the canonical role in genomic DNA packaging. To understand the principles of highly organized and dynamic chromatin architecture, the integrated approaches using various experimental techniques and theoretical modeling are essential. In this symposium, we aim to promote discussion by sharing the latest research on measuring and modeling the biophysical properties of chromatin and the relevance to gene regulation using state-of-the-art techniques.

2SBA-1 Chromatin mobility of X-linked loci and its epigenetic regulation
Yuko Sato[1,2], Yuma Ito[2], Satoshi Uchino[2], Makio Tokunaga[2], Hiroshi Kimura[1,2] ([1]*IIR, Tokyo Tech*, [2]*Sch. Life Sci. Tech., Tokyo Tech*)

2SBA-2 (2Pos303) ヒト生細胞の局所クロマチン動態は細胞周期を通して一定である
(2Pos303) Single-nucleosome imaging reveals steady-state motion of interphase chromatin in living human cells
○飯田 史織 [1,2], 新海 創也 [3], 伊藤 優志 [1], 田村 佐知子 [1], 鐘巻 将人 [2,4], 大浪 修一 [3], 前島 一博 [1,2]
([1] 遺伝研・ゲノムダイナミクス研究室, [2] 総研大・生命・遺伝, [3] 理研 BDR, [4] 遺伝研・分子細胞工学研究室)
Shiori Iida[1,2], Soya Shinkai[3], Yuji Itoh[1], Sachiko Tamura[1], Masato Kanemaki[2,4], Shuichi Onami[3], Kazuhiro Maeshima[1,2] ([1]*Genome Dynamics Lab., Natl. Inst. of Genet.*, [2]*Dept. of Genet., Sch. of Life Sci., SOKENDAI*, [3]*RIKEN BDR*, [4]*Mol. Cell Eng. Lab., Natl. Inst. of Genet.*)

2SBA-3 DNA の量とクロマチン構造による核のサイズ制御機構
DNA quantity and chromatin structure contribute to nuclear size control in *Xenopus laevis*
○原 裕貴（山口大・理）
Yuki Hara (*Fac. Sci., Yamaguchi Univ.*)

2SBA-4 (2Pos116) 細胞核内における underwound DNA の蛍光イメージング
(2Pos116) Fluorescence imaging of underwound DNA in the cell nucleus
○福手 淳平[1,2], 牧 功一郎[1,3], 安達 泰治[1,2,3]（[1] 京大・医生研, [2] 京大・院生命科学, [3] 京大・院工学）
Jumpei Fukute[1,2], Koichiro Maki[1,3], Taiji Adachi[1,2,3] ([1]*Inst. Life & Med. Sci., Kyoto Univ.*, [2]*Grad. Sch. Biostudies, Kyoto Univ.*, [3]*Grad. Sch. Eng., Kyoto Univ.*)

2SBA-5 (3Pos305) High-resolution mapping of chromatin compaction and dynamics in live cells by label-free interference microscopy
Yi-Teng Hsiao, Chia-Ni Tsai, Fasih Bintang Ilhami, Chia-Lung Hsieh (*Institute of Atomic and Molecular Sciences (IAMS), Academia Sinica / Taiwan*)

2SBA-6 (3Pos301) 細胞内の一分子を三次元でナノレベルの分解能で観察できる「クライオ三次元ナノスコピー」の開発
(3Pos301) Cryo-3D Nanoscopy to localize three-dimensional position of individual fluorophore with nanometer precision in the cell
○成瀬 寛太[1], 松田 剛[1], 溝内 雄太[1], 志見 剛[2], 木村 宏[2], 中田 栄司[3], 森井 孝[3], 松下 道雄[1], 藤芳 暁[1]（[1] 東京工業大学理学院物理学系物理学コース, [2] 東京工業大学科学技術創成研究院細胞制御工学研究センター, [3] 京都大学エネルギー理工学研究所）
Kanta Naruse[1], Tsuyoshi Matsuda[1], Yuta Mizouchi[1], Takeshi Shimi[2], Hiroshi Kimura[2], Eiji Nakata[3], Takashi Morii[3], Michio Matsushita[1], Satoru Fujiyoshi[1] ([1]*Department of physics, Tokyo institute of technology*, [2]*Cell Biology Center, Institute of Innovative Research, Tokyo institute of technology*, [3]*Institute of Advanced Energy, Kyoto University*)

2SBA-7 新しいクロマチン基盤ユニットである H3-H4 オクタソームのクライオ電子顕微鏡解析
Cryo-electron microscopic analysis reveal a novel structural unit of chromatin
○野澤 佳世[1], 滝沢 由政[2], 七種 和美[3], 明石 知子[4], 胡桃坂 仁志[2]（[1] 東京工業大学・生命理工学院, [2] 東京大学・定量生命科学研究所, [3] 産業技術総合研究所, [4] 横浜市立大学・生命医科学研究科）
Kayo Nozawa[1], Yoshimasa Takizawa[2], Kazumi Saikusa[3], Satoko Akashi[4], Hitoshi Kurumizaka[2] ([1]*Tokyo Institute of Technology, School of Life Science and Technology*, [2]*The University of Tokyo, Institute for Quantitative Biosciences*, [3]*National Institute of Advanced Industrial Science and Technology*, [4]*Yokohama City University, Graduate School of Medical Life Science*)

2SBA-8 斥力相互作用する溶質混合系における相分離：クロマチン高次構造の視点から
Phase separation in soft-repulsive mixtures: implication for chromatin organization
Takahiro Sakaue, Naoki Iso, Yuki Norizoe (*Dep. Phys. Aoyama Gakuin Univ.*)

2SBA-9 1 細胞全ゲノム DNA 複製解析からゲノム三次元構造動態を探る
Unraveling the dynamic 3D genome architecture through single-cell DNA replication profiling
○平谷 伊智朗（理化学研究所　生命機能科学研究センター　発生エピジェネティクス研究チーム）
Ichiro Hiratani (*Laboratory for Developmental Epigenetics, RIKEN Center for Biosystems Dynamics Research (RIKEN BDR)*)

08:45〜11:15　C 会場（函館アリーナ 武道館 C）／Room C（Hakodate Arena Budokan C）
2SCA　【共催：新学術領域研究 「発動分子科学」】

発動分子科学への若手研究者による挑戦
Tackle “Molecular Engine” by Early-career Researchers

オーガナイザー：小杉 貴洋（分子科学研究所），大友 章裕（分子科学研究所）
Organizers: Takahiro Kosugi (IMS), Akihiro Otomo (IMS)

“Molecular Engine”, design of autonomous functions through energy conversion, has bud by the orchestration of chemists, biologists, and physicists in the last five years. This scientific concept should be passed down to the next generations for further development. To this end, early-career researchers in various research fields are trying to elucidate the energy conversion mechanism of molecular machines and to design novel ones. In this symposium, budding researchers who will lead this field related to biophysics in the future will give a talk about their latest exciting research results by developing cutting-edge technologies and future prospects.

はじめに
Opening Remarks

2SCA-1　アクティブマターが示す秩序形成の幾何的設計原理
Geometric design principle for active ordering
Kazusa Beppu[1], Yusuke T. Maeda[2] ([1]*Appl. Phys., Aalto Univ. Sch. of Sci.*, [2]*Phys., Kyushu Univ.*)

2SCA-2　(1Pos217) Conversion of light-driven outward proton pump rhodopsin into inward proton pump
Maria Del Carmen Marin Perez[1], Masae Konno[1,2], Himoru Yawo[1], Keiichi Inoue[1] ([1]*ISSP, Univ. Tokyo*, [2]*PRESTO, Japan Science and Technology Agency*)

2SCA-3　フッ素化人工チャネルによる膜間物質輸送
Transmembrane material transport by fluorinated channels
○佐藤 浩平（東工大・生命理工）
Kohei Sato (*Sch. Life Sci. Tech., Tokyo Tech.*)

2SCA-4　(3Pos128) 1 分子回転操作実験によって解明されたミトコンドリア由来 ATP 合成酵素における阻害因子 IF_1 の一方向制御機構
(3Pos128) Unidirectional regulation of ATPase factor 1 in mitochondrial ATP synthase studied by single-molecule manipulation experiments
○小林 稜平 [1,2], 上野 博史 [1], 岡崎 圭一 [2], 野地 博行 [1]（[1] 東大・院工・応化, [2] 分子研）
Ryohei Kobayashi[1,2], Hiroshi Ueno[1], Kei-ichi Okazaki[2], Hiroyuki Noji[1] ([1]*Appl. Chem., Grad. Sch. Eng., Univ. Tokyo*, [2]*Inst. for Mol. Sci.*)

2SCA-5　1 分子計測・活性測定・タンパク質工学による回転型 V-ATPase の統合的研究
Integrated research on rotary V-ATPase approached by single-molecule observation, biochemical assay, and protein engineering
○大友 章裕 [1,2], 飯野 亮太 [1,2]（[1] 分子科学研究所, [2] 総合研究大学院大学）
Akihiro Otomo[1,2], Ryota Iino[1,2] ([1]*Institute for Molecular Science*, [2]*The Graduate University for Advanced Studies*)

2SCA-6 ミトコンドリア呼吸鎖における熱産生の物理化学的メカニズム
Physicochemical mechanism of heat generation in mitochondrial respiratory chain
○武安 光太郎 [1,2,3], Namari Nuning[4], 中村 潤児 [2,5]（[1] 筑波大・数理物質系, [2] 筑波大・TREMS, [3] 筑波大・ゼロ CO2, [4] 筑波大・院理工情報生命, [5] 九州大・I2CNER）
Kotaro Takeyasu[1,2,3], Nuning Namari[4], Junji Nakamura[2,5] ([1]*Fac. Pure and Appl. Sci., Unive. Tsukuba*, [2]*TREMS, Univ. Tsukuba*, [3]*Zero-CO2, Univ. Tsukuba*, [4]*Grad. Sch. Sci. Technol., Univ. Tsukuba*, [5]*I2CNER, Kyushu Univ.*)

2SCA-7 キラル液晶の自己組織化ナノ構造を利用した力学センシングと応答速度設計
Mechanical sensor using chiral liquid crystals with self-organized nanostructures and tuning of molecular recovery response
○久野 恭平 [1,2], 宍戸 厚 [2], 堤 治 [1]（[1] 立命館大・生命科学, [2] 東工大・化生研）
Kyohei Hisano[1,2], Atsushi Shishido[2], Osamu Tsutsumi[1] ([1]*Col. of Life Sci., Ritsumeikan Univ.*, [2]*Lab. for Chem. & Life Sci., Tokyo Tech*)

2SCA-8 Structural stability and dynamics of de novo designed transmembrane peptide barrels
Ai Niitsu[1], Jaewoon Jung[2], Yuji Sugita[1,2] ([1]*Wako Inst., Riken*, [2]*Kobe Inst., Riken*)

おわりに
Closing Remarks

08:45〜11:15　D 会場（函館アリーナ 多目的室 A）／Room D（Hakodate Arena Multipurpose Room A）
2SDA　先端的ラベルフリーナノポア計測による生物物理学への展開と応用
Innovative label-free nanopore sensing toward biophysical studies and applications

オーガナイザー：山崎 洋人（東京大学），庄司 観（長岡技術科学大学）
Organizers: Hirohito Yamazaki (The Univ. of Tokyo), Kan Shoji (Nagaoka Univ. of Tech.)

The understanding of the biomolecule structural and dynamic properties has provided a plethora of information about the roles of various molecules, and leads to the development of innovative industrial enzymes and pharmaceuticals. Among technologies uncovering biological molecules, nanopore sensing has become attractive since it can study single molecule properties, such as surface charge, molecular size, shape, chain length, chemical structures and so on. In this symposium, we will organize the session to present the latest nanopore research for biophysics studies and applications.

2SDA-1 Toward broadly accessible, highly scalable solid-state nanopore research
Kyle Briggs (*University of Ottawa, Department of Physics*)

2SDA-2 プローブ型人工細胞システムの応用展開
Application of Probe-Type Artificial Cell Membrane Systems
○庄司 観（長岡技大）
Kan Shoji (*Nagaoka Univ. Tech.*)

2SDA-3 ナノポアシーケンサと nanoDoc を用いた DNA/RNA 修飾解析
Detection of DNA/RNA modification using nanopore sequencer and nanoDoc
○上田 宏生（東京大・先端研・生命データサイエンス）
Ueda Hiroki (*Biological Data Science, RCAST, Univ. of Tokyo*)

2SDA-4 (2Pos290) Nanopore direct determination of DNA methylation and demethylation intermediates
Ping Liu[1], Masayuki Honda[1], Ryuji Kawano[2] ([1]*Department of Food and Energy Systems Science, Tokyo University of Agriculture and Technology*, [2]*Institute of Engineering, Tokyo University of Agriculture and Technology*)

2SDA-5 (2Pos315) ATP を検出可能な DNA ナノポアセンサの開発
(2Pos315) ATP-detectable DNA nanopore sensor
○赤井 大夢, 庄司 観（長岡技術科学大学）
Hiromu Akai, Kan Shoji (*Nagaoka University of Technology*)

2SDA-6 Integrating nanopore sensing and artificial intelligence for multiplex single-virus identification
Akihide Arima (*IIFS, Nagoya Univ.*)

2SDA-7 Probing the Effect of Ubiquitinated Histone on Mononucleosomes through solid-state nanopores
Hu Rui, Wei Guanghao, Wang Zhan, **Qing Zhao** (*Peking University, School of Physics*)

2SDA-8 Light Enhanced Solid-state Nanopore for Single Molecule Sensing
Yamazaki Hirohito (*The University of Tokyo, Department of Biological Science*)

08:45〜11:15　E 会場（函館アリーナ 多目的室 B）／Room E（Hakodate Arena Multipurpose Room B）

2SEA　100nm サイズの分子集団で顕在化する非凡な時空アロステリー
Unique Spatiotemporal Allostery Emerges in 100nm-Sized Molecular Systems

オーガナイザー：成田 哲博（名古屋大学），秋山 修志（分子科学研究所）
Organizers: Akihiro Narita (Nagoya Univ.), Shuji Akiyama (IMS)

Is it possible to explain biological phenomena occurring at the cellular level on the basis of the physicochemical properties of molecules? Observations focused on the cellular scale provide little information about molecules, while investigations of molecular structure and dynamics with high spatiotemporal resolution require handling isolated and purified samples in vitro. However, how and what kind of connections do we need in order to understand biological phenomena? In modern life science research, the initial selection of the most suitable model organism has a great impact on the success or failure of later research. In the same way, the selection of an appropriate spatiotemporal scale is important for cutting into the logic of "cross-scale causality". From this perspective, we realize that the smallest unit of the molecular system that shows some correlation with physiological properties at the tissue or cellular level is exclusively concentrated in the 100 nm scale (or several hundred molecules). In this symposium, we will examine the spatiotemporal hierarchy of the 100 nm scale from multiple perspectives of biophysics, structural biology, and computational science, and discuss strategies for the evolution of correlation into causation.

はじめに
Opening Remarks

2SEA-1 アクチン線維において顕在化する時空アロステリー
Spaciotemporal allostery in the actin filament
○成田 哲博（名古屋大、理学）
Akihiro Narita (*Grad. Sci, Nagoya Univ.*)

2SEA-2 細菌べん毛モーター回転制御機構の理解の進展
Recent understanding of the control mechanism of the bacterial flagellar motor rotation
○今田 勝巳（阪大・院理）
Katsumi Imada (*Grad. Sch. Sci., Osaka Univ.*)

2SEA-3 膜と細胞骨格の動態制御におけるダイナミンのヘクトスケール分子集団のアロステリー変化
Allosteric changes of hecto-scale population of dynamin GTPases provide in dynamic regulation of membranes and cytoskeletons
○竹居 孝二, 阿部 匡史, 竹田 哲也, 山田 浩司（岡山大・院医歯薬）
Kohji Takei, Tadashi Abe, Tetsuya Takeda, Hiroshi Yamada (*Fac. Med. Dent. Pharma. Sci., Okayama Univ.*)

2SEA-4 夜明けに自律離散する概日時計システム
Autonomous Disassembly of Circadian Clock System at Dawn
○秋山 修志 [1,2]（[1] 協奏分子システム研究センター・分子研, [2] 総研大）
Shuji Akiyama[1,2] ([1]*CIMoS, IMS, NINS*, [2]*SOKENDAI*)

2SEA-5 高速 AFM による 100-nm サイズの分子集団の直接観察
Direct observation of 100 nm-sized molecular systems by high-speed AFM
○古寺 哲幸（金沢大・WPI-NanoLSI）
Noriyuki Kodera (*WPI-NanoLSI, Kanazawa Univ.*)

2SEA-6 長距離アロステリーの物理基盤としてのクーロン結合ネットワーク
Coulomb bond network as a physical basis for long-range allostery
○高野 光則（早大・先進理工）
Mitsunori Takano (*Grad. Sch. Sci. Eng., Waseda Univ*)

2SEA-7 (3Pos013) Optineurin の E50K 緑内障変異はオリゴマー粒径を増大させる
(3Pos013) The E50K mutation of optineurin increases the oligomer size
○河村 綸太郎 [1], 植月 聡也 [1], 丹澤 豪人 [2], 加藤 貴之 [2], 金城 政孝 [3], 北村 朗 [3]（[1] 北大・院生命科学, [2] 阪大・蛋白研, [3] 北大・院先端生命）
Rintaro Kawamura[1], Soya Uetsuki[1], Takehito Tanzawa[2], Takayuki Kato[2], Masataka Kinjo[3], Akira Kitamura[3] ([1]*Grad. Sci. Life Sci., Hokkaido Univ.*, [2]*Inst., for Proteins Res., Osaka Univ.*, [3]*Fac. Adv. Life sci., Hokkaido Univ.*)

おわりに
Closing Remarks

08:45〜11:15　Room F（Hakodate Citizen Hall 1F Main Hall）
2SFA　Japan-US symposium on motor proteins and associated single-molecule biophysics

Organizers: Kumiko Hayashi (Tohoku Univ.), Jakia Jannat Keya (NINS)

This is the second symposium between Japan and USA on motor proteins as a continuation of the first one held in 2021 BSJ meeting. Speakers in this symposium are internationally recognized as experts in the field of motor proteins, and their associated proteins. We are planning to prepare enough time to have a deep and detailed discussion among the speakers and audience on these subjects. The symposium topics cover multidisciplinary applications of genetics, bio-engineering, bio-chemistry, medical science, and physics, which will give us new insights into motor proteins, as well as interesting applications of existing single-molecule techniques.

Opening Remarks

2SFA-1 Torque Generation Mechanism of F_1-ATPase
Hiroyuki Noji, Hiroshi Ueno (*Grad. Sch. Eng., Univ. Tokyo*)

2SFA-2 Regulation of Motors by Microtubule-Associated Proteins
Ahmet Yildiz (*University of California Berkeley*)

2SFA-3 Cholesterol in the cargo membrane amplifies the inhibitory effects of tau on kinesin-1-based transport
Qiaochu Li[1], James Ferrare[2], Jonathan Silver[2], John Wilson[1], Luis Arteaga-Castaneda[1], Weihong Qiu[3], Michael Vershinin[4], Stephen King[5], Keir Neuman[2], **Jing Xu[1]** ([1]*Physics, University of California, Merced, CA, USA*, [2]*Laboratory of Single Molecule Biophysics, National Heart, Lung and Blood Institute, National Institutes of Health, Bethesda, MD, USA*, [3]*Physics, Oregon State University, Corvallis, OR, USA*, [4]*Physics and Astronomy, University of Utah, Salt Lake City, UT, USA*, [5]*Burnett School of Biomedical Sciences, University of Central Florida, Orlando, FL, USA*)

2SFA-4 Ultralong-Term, Real-Time Tracking of Single Cargoes in Living Neurons
Sam Peng (*Stanford University*)

2SFA-5 (1Pos137) Plus and minus ends of microtubules respond asymmetrically to kinesin binding by a long-range directionally driven allosteric mechanism
Huong T Vu[1], Zhechun Zhang[2], Riina Tehver[3], Dave Thirumalai[4] ([1]*University of Warwick*, [2]*Harvard University*, [3]*Denison University*, [4]*University of Texas*)

2SFA-6 (3Pos143) SLC26 ion transporters act as electricity-driven motor proteins
Tomohiro Shima (*Grad. Sch. Sci., Univ. Tokyo*)

Closing Remarks

08:45〜11:15　G 会場（函館市民会館 3F 小ホール）／Room G（Hakodate Citizen Hall 3F Small Hall）
2SGA　【共催：新学術領域研究「シンギュラリティ生物学」】

シンギュラリティ生物学を導くイメージング技術
Advanced Imaging Technologies Leading the Way to “Singularity Biology”

オーガナイザー：蛭田 勇樹（慶應義塾大学），渡邉 朋信（理化学研究所）
Organizers: Yuki Hiruta (Keio Unv.), Tomonobu Watanabe (RIKEN)

In order to study the processes that “singularity cells”, considered as minority entities, causing criticality to a multi-cellular system, comprehensive development of imaging technologies is essential because of its necessary for multi-layer and multi-modal observation of the dynamics and functions of the cells and the multi-cellular system. To do the end, the research project “Singularity Biology” have developed a trans-scale microscopy system, AMATERAS, as a basis for imaging. This symposium introduces the microscopy technologies, including AMATERAS, and advanced probe technologies to visualize singularity phenomena. We hope that this symposium will lead to the creation of effective collaboration projects on Singularity Biology.

はじめに
Opening Remarks

2SGA-1 シンギュラリティ現象を直接観るトランススケールスコープ AMATERAS
Trans-scale scope AMATERAS for direct observation of singularity phenomena
○市村 垂生 [1], 垣塚 太志 [2], 橋本 均 [1,3], 永井 健治 [1,2] ([1] 大阪大学・先導, [2] 大阪大学・産研, [3] 大阪大学・薬学)
Taro Ichimura[1], Taishi Kakizuka[2], Hitoshi Hashimoto[1,3], Takeharu Nagai[1,2] ([1]*OTRI, Osaka Univ.*, [2]*SANKEN, Osaka Univ.*, [3]*Grad. Sch. Pharm., Osaka Univ.*)

2SGA-2 Chemical probes for detecting enzyme activities in living cells with single cell resolution
Mako Kamiya (*Dep. Life Sci. Tech., Tokyo Tech.*)

2SGA-3 (3Pos277) Decoding single-cell transcriptomic phenotypes from cell images enabled by robotic data acquisition and deep learning
Jianshi Jin[1], Taisaku Ogawa[1], Nozomi Hojo[1], Kirill Kryukov[2], Kenji Shimizu[3], Tomokatsu Ikawa[4], Tadashi Imanishi[2], Taku Okazaki[3], Shiroguchi Katsuyuki[1] ([1]*BDR, RIKEN*, [2]*Dept. of Mol. Life Sci., Tokai Univ. Sch. of Med.*, [3]*Inst. for Quant. Biosci., Univ. of Tokyo*, [4]*Res. Inst. for Biomed. Sci., Tokyo Univ. of Sci.*)

2SGA-4 局所かつ任意のタイミングで摂動を与える光操作技術 CALI 法とその応用
A light manipulation technology by CALI that provides localized and arbitrarily timed perturbations
○竹本 研（三重大学大学院医学系研究科生化学分野）
Kiwamu Takemoto (*Mie University, Graduate School of Medicine*)

2SGA-5 最小の発光酵素「picALuc」の開発とその応用
Development of the smallest luciferase “picALuc” and its applications
○大室 有紀 [1], 金 誠培 [2], 松井 勇人 [1], 叶井 正樹 [1], 古田 忠臣 [3]（[1] 島津製作所, [2] 産総研, [3] 東工大・生命理工）
Yuki Ohmuro[1], Sung Bae Kim[2], Hayato Matsui[1], Masaki Kanai[1], Tadaomi Furuta[3] ([1]*Shimadzu Corporation*, [2]*AIST*, [3]*Sch. Life Sci. Tech., Tokyo Tech*)

2SGA-6 時空間トランススケールイメージングを可能にするケージドルシフェリンの開発
Development of caged luciferin enabling spatiotemporal trans-scale imaging
○蛭田 勇樹（慶應大・理工）
Yuki Hiruta (*Fac. Sci. Tech., Keio Univ.*)

08:45〜11:15　H 会場（函館市民会館 3F 大会議室）／Room H（Hakodate Citizen Hall 3F Conference Room）
2SHA　【共催：学術変革領域研究（B）
「生体分子工学と低物理エネルギーロジスティクスの融合による次世代非侵襲深部生体操作」】

生体分子工学と低物理エネルギーロジスティックスで切り拓く新たな生体操作学
Next-generation biological manipulation pioneered by biomolecular engineering and low-physical energy logistics

オーガナイザー：井上 圭一（東京大学），今村 博臣（京都大学）
Organizers: Keiichi Inoue (The Univ. of Tokyo), Hiromi Imamura (Kyoto Univ.)

Optogenetics enabled us precisely and noninvasively manipulate a variety of biological events in vivo such as neural firing, gene expression, cellular morphological change and so on. To expand the concept of optogenetics toward biological events in deep tissue which are difficult by using visible light, further paradigm shift of manipulation technology is required. To achieve this goal, we are focusing on using photothermal effect, ultrasound and magnetic field as novel external-field technologies to manipulate biological responses even in deep tissues by combining biomolecular engineering of new molecular systems and low-physical energy logistics. In this symposium, we will introduce cutting-edge researches for next generation biological manipulation.

はじめに
Opening Remarks

2SHA-1 **光熱変換を利用した細胞操作に向けた試み**
Toward cell manipulation through photothermal conversion
○今村 博臣（京都大学生命科学研究科）
Hiromi Imamura (*Graduate School of Biostudies, Kyoto University*)

2SHA-2 **高効率光熱変換タンパク質ヒーター創出に向けた分子内熱伝導機構の解明**
Elucidation of intramolecular heat transfer mechanism for construction of highly effective photothermal protein heaters
○水野 操（阪大・院理）
Misao Mizuno (*Grad. Sch. Sci., Osaka Univ.*)

2SHA-3 **BMI のための高密度皮質脳波電極の開発**
Development of high-density ECoG array for BMI
○鈴木 隆文 [1], 海住 太郎 [1], 平田 雅之 [1,2]（[1] 脳情報通信融合研究センター（情報通信研究機構、大阪大学）, [2] 大阪大学大学院医学系研究科）
Takafumi Suzuki[1], Taro Kaiju[1], Masayuki Hirata[1,2] ([1]*Center for Information and Neural Networks (CiNet), NICT & Osaka Univ.*, [2]*Osaka Univ. graduate school of medicine*)

2SHA-4 **深部神経活動磁場操作に向けた新規分子ツール開発**
Development of molecular tools for magnetic manipulation of neural activity in the deep tissue
○井上 圭一（東大・物性研）
Keiichi Inoue (*Inst. Solid State Phys., Univ. Tokyo*)

2SHA-5 **生体内磁性粒子を操るための磁気力場の設計と最適化**
Design and optimization of magnetic force field for manipulating magnetic particles in living bodies
○関野 正樹 [1], 吉岡 輝 [1], 中川 桂一 [1], 井上 圭一 [2]（[1] 東大・工, [2] 東大・物性研）
Masaki Sekino[1], Hikaru Yoshioka[1], Keiichi Nakagawa[1], Keiichi Inoue[2] ([1]*Grad. Sch. Eng., Univ. Tokyo*, [2]*ISSP, Univ. Tokyo*)

おわりに
Closing Remarks

13:50〜16:20　A 会場（函館アリーナ 武道館 A）／Room A（Hakodate Arena Budokan A）
2SAP　**【共催：新学術研究領域「情報物理学でひもとく生命の秩序と設計原理」】**

多細胞系の情報物理学
Information Physics of multi-cellular systems

オーガナイザー：小林 徹也（東京大学），川口 喬吾（理化学研究所），石島 秋彦（大阪大学）
Organizers: Tetsuya J. Kobayashi (The Univ. of Tokyo), Kyogo Kawaguchi (RIKEN), Akihiko Ishijima (Osaka Univ.)

Physical understanding of multi-cellular systems is the unexplored frontier in biophysics. Sparked by the rapid advancements in bioimaging, bioinformatics, symthetic biology and so on, multi-cellular systems are becoming a promising target of biophysics. In this symposium, we showcase the attempts to investigate the design principles of multi-cellular systems by using or integrating the methods of physics, informatics, and other disciplines.

2SAP-1 **多細胞系の情報物理学**
Information Physics of multi-cellular systems
○小林 徹也（生産研・東大）
Tetsuya J. Kobayashi (*IIS, UTokyo*)

2SAP-2 **内皮細胞集団動態と血管新生**
Collective endothelial cell migration and angiogenesis
○田久保 直子（東京大学アイソトープ総合センター）
Naoko Takubo (*Isotope Science Center, The University of Tokyo*)

2SAP-3 **細胞間コミュニケーションの操作による多細胞パターンのデザイン**
Programming multicellular pattern formation with synthetic cell-cell signaling
○戸田 聡（金沢大学・ナノ生命）
Satoshi Toda (*NanoLSI, Kanazawa Univ.*)

2SAP-4 **(3Pos118) グラフニューラルネットワークによる細胞間の時空間相互作用の推定**
(3Pos118) Graph-based machine learning reveals rules of spatiotemporal cell interactions in tissues
Takaki Yamamoto[1], Katie Cockburn[2], Valentina Greco[2,3], Kyogo Kawaguchi[1,4,5] ([1]*Nonequilibrium Physics of Living Matter RIKEN Hakubi Research Team, RIKEN BDR*, [2]*Department of Genetics, Yale School of Medicine*, [3]*Departments of Cell Biology and Dermatology, Yale Stem Cell Center, Yale Cancer Center, Yale School of Medicine*, [4]*RIKEN CPR*, [5]*Universal Biology Institute, The University of Tokyo*)

2SAP-5 **線虫の神経回路における多重情報コードの情報物理学的解析**
Analyisis of multiplexed information coding in the nervous system of C.elegans
○豊島 有, 松本 朱加, 飯野 雄一（東大・院理・生科）
Yu Toyoshima, Ayaka Matsumoto, Yuichi Iino (*Grad. Sch. Sci., Univ. of Tokyo*)

2SAP-6 **器官形態形成プロセスの種間スケーリング**
Scaling of organ morphogenetic process between species
○森下 喜弘（理化学研究所　生命機能科学研究センター）
Yoshihiro Morishita (*RIKEN Center for Biosystems Dynamics Research*)

おわりに
Closing Remarks

13:50〜16:20　B 会場（函館アリーナ 武道館 B）／Room B（Hakodate Arena Budokan B）
2SBP　【共催：「富岳」成果創出加速プログラム
「全原子・粗視化分子動力学による細胞内分子動態の解明」】

富岳を用いた高性能計算による生物物理
High-performance computational biophysics with supercomputer Fugaku

オーガナイザー：松永 康佑（埼玉大学），信夫 愛（理化学研究所）
Organizers: Yasuhiro Matsunaga (Saitama Univ), Ai Shinobu (RIKEN)

Computational approaches are becoming increasingly important in biophysics, not only for simulations but also for the detailed interpretation of various measurement data. In particular, with the recent launch of modern supercomputers such as Fugaku, enormous computational resources have become available, and new computational methods and applications that were not computationally feasible in the past are becoming possible. In this symposium, we invite researchers who conduct cutting-edge high-performance computations. We discuss current computational research using supercomputers as well as future directions of computational biophysics.

はじめに
Opening Remarks

2SBP-1　富岳と超並列分子動力学を用いたタンパク質の構造変化、会合と解離
Protein conformational change, association and dissociation observed using Fugaku and massively parallel molecular dynamics simulations
○北尾 彰朗（東工大・生命理工）
Akio Kitao (*Scl. Life Sci. Tech., Tokyo Tech*)

2SBP-2　Molecular dynamics study of multidrug efflux transporter complex embedded in lipid bilayer: Role of membrane lipids in the transporter
Keiko Shinoda, Hisashi Kawasaki (*AgTECH, GSALS, UTokyo*)

2SBP-3　(3Pos186) エンベロープ型ウイルス粒子の粗視化シミュレーション：B 型肝炎ウイルス
(3Pos186) Coarse-grained Molecular Dynamics Study of Enveloped Virus Particle: Hepatitis B Virus
○浦野 諒, 篠田 渉（岡山大学・異分野基礎研）
Ryo Urano, Wataru Shinoda (*Res. Inst. Interdiscip. Sci., Okayama Univ.*)

2SBP-4　Binding free energy landscapes of Src Kinase to its inhibitors sampled by two-dimensional replica exchange molecular dynamics simulations
Ai Shinobu[1], Suyong Re[1,2], Yuji Sugita[1] ([1]*RIKEN*, [2]*National Institutes of Biomedical Innovation, Health, and Nutrition*)

2SBP-5　REST シミュレーションによるタンパク質やペプチドリガンドの活性制御機構の解析
Applications of REST simulation to understanding regulation mechanism of protein activation and peptide ligands
○浴本 亨 [1], 山根 努 [2], 池口 満徳 [1,2]（[1] 横浜市大・生命医, [2] 理研・R-CCS）
Toru Ekimoto[1], Tsutomu Yamane[2], Mitsunori Ikeguchi[1,2] ([1]*Grad. Med. Life Sci., Yokohama City Univ.*, [2]*R-CCS, Riken*)

2SBP-6 (1Pos027) Automated Density Extraction of Isomorphous Difference map and Occupancy-estimation for Conformer Fitting
Sriram Srinivasa Raghavan[1], Florence Tama[1,2,3], Osamu Miyashita[1] ([1]*RIKEN Center for Computational Science, Kobe, Japan.*, [2]*Institute of Transformative Biomolecules (WPI-ITbM), Nagoya University, Aichi, Japan.*, [3]*Department of Physics, Graduate School of Science, Nagoya University, Aichi, Japan.*)

2SBP-7 スーパーコンピュータ「富岳」を用いたテンプレートマッチング法による生体分子のマルチコンフォメーション解析
Multi-conformational analysis of biomolecule by the template-matching method using the supercomputer Fugaku
○徳久 淳師（理研・R-CCS）
Atsushi Tokuhisa (*R-CCS, Riken*)

おわりに
Closing Remarks

13:50〜16:20　C 会場（函館アリーナ 武道館 C）／Room C（Hakodate Arena Budokan C）
2SCP　生体分子の人工設計：タンパク質、RNA、DNA
Design of biomolecules, protein, RNA, and DNA

オーガナイザー：古賀 信康（分子科学研究所），神谷 由紀子（名古屋大学）
Organizers: Nobuyasu Koga (IMS), Yukiko Kamiya (Nagoya Univ.)

The biomolecules, protein, RNA, and DNA, control cell functions. The design technologies for the biomolecules and their interactions have been greatly advanced, which made it possible to create a wide range of biomolecules not existing in nature. In this symposium, each of the biomolecular design geeks will present the basics of the design technology and latest results. We then discuss about future perspectives to create novel biomolecules.

2SCP-1 タンパク質構造の人工設計
De novo design of novel protein structures
○古賀 信康（自然・ 生命創成）
Nobuyasu Koga (*NINS, ExCELLS*)

2SCP-2 Towards the de novo design of binding proteins through beta-sheet folds
Enrique Marcos (*Molecular Biology Institute of Barcelona (IBMB-CSIC), Protein Design and Modeling Lab*)

2SCP-3 Protein engineering for biogeeks; practical examples of structural redesigns of a model protein and therapeutic antibody designs
Koki Makabe (*Grad. Sch. Sci. and Eng., Yamagata univ.*)

2SCP-4 非環状型人工核酸による天然核酸認識の設計
Understanding the design of acyclic artificial nucleic acids that recognize natural nucleic acids
○神谷 由紀子（名大・院工）
Yukiko Kamiya (*Grad. Sch. Eng., Nagoya Univ.*)

2SCP-5 Engineering RNA-protein interactions by directed evolution
Keisuke Fukunaga, Yohei Yokobayashi (*Nucleic Acid Chemistry and Engineering Unit, OIST*)

2SCP-6 DNA ナノ構造によるデザインされた人工細胞と人工オルガネラの実現へ向けて
Toward DNA nanostructure-based designed artificial cells and artificial organelles
○瀧ノ上 正浩（東工大・情報理工）
Masahiro Takinoue (*Sch. Computing, Tokyo Tech*)

13:50〜16:20　D 会場（函館アリーナ 多目的室 A）／Room D（Hakodate Arena Multipurpose Room A）
2SDP　金属イオン制御による酵素の動態
Metal-ion regulation of enzyme dynamics

オーガナイザー：織田 昌幸（京都府立大学），森川 耿右（京都大学）
Organizers: Masayuki Oda (Kyoto Prefectural Univ.), Kosuke Morikawa (Kyoto Univ.)

Enzyme function closely correlates with its structural dynamics, and is often regulated by metal-ion binding. In many cases, metal-ions bind to enzymes rather weakly, and induce protein conformations or conformational ensembles. This essential structure-function relationship is an attractive but difficult target to be analyzed. The invited speakers present challenging efforts on enzymes, such as cutinase, RNaseH, and DNAzyme, which are regulated by Ca2+ or Mg2+. We hope that discussions based on presented biophysical data could facilitate us to understand real dynamic views of metal-enzyme interactions.

はじめに
Opening Remarks

2SDP-1 酵素反応における弱い金属イオン結合の意義
Significance of weak metal-ion binding in enzymatic reactions
○織田 昌幸（京府大・院生環科）
Oda Masayuki (*Grad. Sch. Life Environ. Sci., Kyoto Pref. Univ.*)

2SDP-2 PET 分解酵素 Cut190 における弱く結合した Ca^{2+} イオンを介したアロステリック制御
Allosteric regulation of PET-degrading enzyme Cut190 through the weakly bound Ca^{2+} ion
○沼本 修孝（医科歯科大・難研）
Nobutaka Numoto (*Med. Res. Inst., Tokyo Med. Dent. Univ.*)

2SDP-3 RNaseHI の触媒反応機構：必須金属は 1 個か 2 個か？
Catalytic mechanism of RNaseHI: one metal or two metals?
○森川 耿右（京大・生命科学）
Kosuke Morikawa (*Kyoto Univ.*)

2SDP-4 エレクトロスプレーイオン化質量分析法による活性型リボヌクレアーゼ HI：RNA/DNA:金属イオン複合体の検出
Active ternary complex of ribonuclease HI: RNA/DNA hybrid: metal ions probed by ESI mass spectrometry
○高尾 敏文 [1], 安東 友繁 [1], 林 潤美 [1], Jongruja Nujarin[2], 奥村 宜明 [1], 森川 耿右 [3], 金谷 茂則 [2] ([1] 大阪大・蛋白研, [2] 大阪大・院工学, [3] 京都大・院生命科学)
Toshifumi Takao[1], Tomoshige Ando[1], Hiromi Hayashi[1], Nujarin Jongruja[2], Nobuaki Okumura[1], Kosuke Morikawa[3], Shigenori Kanaya[2] ([1]*Inst. Protein Res., Osaka Univ.*, [2]*Grad. Sch. Eng., Osaka Univ.*, [3]*Grad. Sch. Biostudies, Kyoto Univ.*)

2SDP-5 (2Pos026) Structural basis of the significant metal-histidine coordination in *E. coli* RNase HI
Zengwei Liao[1], Takuji Oyama[2], Yumi Kitagawa[3], Katsuo Katayanagi[4], Kosuke Morikawa[5], Masayuki Oda[3] ([1]*Grad. Sch. Agri. and Life Sci., the Univ. of Tokyo*, [2]*Faculty of Life and Environ. Sci., Univ. of Yamanashi*, [3]*Grad. Sch. Life Environ. Sci., Kyoto Pref. Univ.*, [4]*Grad. Sch. Integrated Sci. for Life, Hiroshima Univ.*, [5]*Grad. Sch. Biostudies, Kyoto Univ.*)

2SDP-6 Metal interaction and Conformational Changes in HIV-1 Reverse Transcriptase
Rieko Ishima (*University of Pittsburgh School of Medicine*)

2SDP-7 High-resolution and time-resolved insights into an RNA-cleaving DNA catalyst
Manuel Etzkorn[1,2] ([1]*Heinrich Heine University Düsseldorf*, [2]*Research Center Jülich*)

おわりに
Closing Remarks

13:50〜16:20　E 会場（函館アリーナ 多目的室 B）／Room E（Hakodate Arena Multipurpose Room B）
2SEP　ダイナミックな翻訳 その開始から終わりまで
Dynamic translation: from initiation to the end

オーガナイザー：丹澤 豪人（大阪大学），楊 倬皓（東京大学）
Organizers: Takehito Tanzawa (Osaka Unv.), Zhuohao Yang (The Univ. of Tokyo)

Translation on ribosomes is a fundamental biological phenomenon that requires strict spatiotemporal regulation and quality control. Since translation is a multi-step reaction, it is necessary to clarify the details of each step in order to understand its whole glance. Recently, with advancing and developing analytical methods such as structural analysis, single molecular imaging, and NGS, it has been uncovered that the translation cycle on ribosomes is regulated in various ways. In this symposium, we would like to have young researchers from different fields shed light on and discuss the dynamics of cis/trans-acting translational control on ribosomes from theoretical and experimental perspectives.

はじめに
Opening Remarks

2SEP-1 Novel repressive role of eIF4A1 during mTORC1 inhibition
Yuichi Shichino (*RIKEN CPR*)

2SEP-2 (1Pos121) 自由エネルギー地形から探る開始コドン認識機構
(1Pos121) Computational Analysis of the Start Codon Recognition Mechanism Based on Free Energy Landscape
○亀田 健 [1], 浅野 桂 [2,3,4], 冨樫 祐一 [1,5]（[1] 立命大 生命, [2] カンザス州立大 生物, [3] 広島大 HiHA, [4] 広島大 統合生命, [5] 理研 BDR）
Takeru Kameda[1], Katsura Asano[2,3,4], Yuichi Togashi[1,5] ([1]*Coll. Life Sci., Ritsumeikan Univ.*, [2]*Div. Biol., Kansas State Univ.*, [3]*HiHA, Hiroshima Univ.*, [4]*Grad. Sch. Integ. Sci. Life, Hiroshima Univ.*, [5]*RIKEN BDR*)

2SEP-3 (2Pos109) RNase T2 のリボソームへの結合を介した翻訳阻害機構
(2Pos109) Regulation mechanism of translation through the interaction of RNase T2 with ribosome
○南 篤 [1], 丹澤 豪人 [2], 楊 倬皓 [3], 船津 高志 [3], 加藤 貴之 [2], 葛山 智久 [1,4], 吉田 秀司 [5], 小川 哲弘 [1,4]
([1] 東大・院農生科, [2] 阪大・蛋白研, [3] 東大・院薬, [4] 東大・CRIIM, [5] 大阪医薬大・医)
Atsushi Minami[1], Takehito Tanzawa[2], Zhuohao Yang[3], Takashi Funatsu[3], Takayuki Kato[2], Tomohisa Kuzuyama[1,4], Hideji Yoshida[5], Tetsuhiro Ogawa[1,4] ([1]*Grad. Sch. Agri. and Life Sci., Univ. Tokyo*, [2]*IPR, Osaka Univ.*, [3]*Grad. Sch. Pharm. Sci., Univ. Tokyo*, [4]*CRIIM, Univ. Tokyo*, [5]*Fac. Med., Osaka Med. Pharm. Univ.*)

2SEP-4 High-speed AFM visualizes translational GTPase factor pool formed around the ribosomal P-stalk
Hirotatsu Imai[1,2], Toshio Uchiumi[3], Noriyuki Kodera[2] ([1]*Fac. Med., Univ. Ryukyus*, [2]*Nano-LSI, Kanazawa Univ.*, [3]*Fac. Sci., Niigata Univ.*)

2SEP-5 The mechanical stability of SecM translation arrest
Zhuohao Yang[1], Ryo Iizuka[2], Takashi Funatsu[1] ([1]*Grad. Sch. Pharm. Sci., The Univ. Tokyo*, [2]*Dept. Biol. Sci., Grad. Sch. Sci., The Univ. Tokyo*)

2SEP-6 Attempt to visualize the synthetic polypeptide during translational arrest
Takehito Tanzawa (*IPR., Osaka Univ.*)

2SEP-7 The final step of protein synthesis; the capture of an unfolded polypeptide by chaperonin GroEL
Kevin Mac Alister Stapleton (*Grad. Sch. Frontier BioSci., Osaka Univ.*)

2SEP-8 ER Redox shift through the ribosome translation
Ryo Ushioda[1,2] ([1]*Fac. of Life Sci., Kyoto Sangyo Univ.*, [2]*Inst. for Protein Dynamics, Kyoto Sangyo Univ.*)

おわりに
Closing Remarks

13:50〜16:20　F 会場（函館市民会館 1F 大ホール）／Room F（Hakodate Citizen Hall 1F Main Hall）
2SFP　【共催：学術変革領域研究（B）「遅延制御超分子化学」】

生物物理学による脳の理解と化学的再生
Biophysical elucidation of neural network and chemical regeneration of neural tissue

オーガナイザー：村岡 貴博（東京農工大学），齋尾 智英（徳島大学）
Organizers: Takahiro Muraoka (Tokyo Univ. of Agriculture and Tech.), Tomohide Saio (Tokushima Univ.)

In recent years, brain science has made remarkable progress. Understanding neural circuits and elucidation of signal transduction processes at the molecular level are being carried out. Not only neuroscience but also mechanistic biochemical studies on neural diseases are progressing. Neurodegenerative diseases are one representative example, and the structure and dynamics of the causative protein are being elucidated at the single-molecule level. Integrating discussions between biophysical neuroscience and chemical research of the brain should address important unexplored issues such as the precise elucidation of brain function and the development of neuronal tissue regeneration technology.

はじめに
Opening Remarks

2SFP-1 Phase separation provides a reaction chamber for autophagy progression
Yuko Fujioka (*Institute for Genetic Medicine, Hokkaido Univ.*)

2SFP-2 蛋白質ミスフォールディング病における蛋白質凝集の分子機構
The molecular mechanism of protein aggregation in protein misfolding disease
Young-Ho Lee[1,2,3] ([1]*Research Center for Bioconvergence Analysis, Korea Basic Sci. Inst., Korea*, [2]*Bio-Analytical Sci., Uni. of Sci. and Tech., Korea*, [3]*Grad. Sch. of Analytical Sci. and Tech., Chungnam National Uni., Korea*)

2SFP-3 脳神経疾患研究における 1 分子イメージング研究の現状・課題・可能性
Current status, problems, and potential of single molecule imaging studies in neurological disease research
○坂内 博子（早大・理工学術院）
Hiroko Bannai (*Fac. Sci. Eng., Waseda Univ.*)

2SFP-4 超分子ペプチドゲルを用いた損傷脳再生
Injured brain regeneration using supramolecular peptide hydrogels
○味岡 逸樹 [1,2]（[1] 東京医科歯科大学・脳統合機能研究センター, [2] 神奈川県立産業技術総合研究所）
Itsuki Ajioka[1,2] ([1]*Center for Brain Integration Research (CBIR), Tokyo Medical Dental Univ (TMDU)*, [2]*KISTEC*)

2SFP-5 相反する匂い価値の脳内表現と神経回路基盤
Representations and circuits for opposing odor values in the brain
○風間 北斗（理化学研究所脳神経科学研究センター）
Hokto Kazama (*RIKEN Center for Brain Science*)

おわりに
Closing Remarks

13:50～16:20　G 会場（函館市民会館 3F 小ホール）／Room G（Hakodate Citizen Hall 3F Small Hall）
2SGP　物理化学的解析から探るアミロイド・ゲルの構造ダイナミクス
Physicochemical analyses of structural dynamics for amyloid and gel

オーガナイザー：田中 元雅（理化学研究所），真板 宣夫（量子科学技術研究開発機構）
Organizers: Motomasa Tanaka (RIKEN), Nobuo Maita (QST)

Disease-associated proteins often form apparently rigid aggregates such as amyloids and gels. Interestingly, however, recent studies have found that amyloids and gels are not the final dead-end products of proteins, but rather undergo dynamic structural changes by cellular proteins and environmental factors, which potentially provide great impacts on cellular phenotypes. However, compared to static structures of amyloids and gels, the details of their dynamic structural changes remain poorly understood. In this symposium, we would like to share and discuss the latest findings that clarify the structural dynamics of amyloids and gels by physicochemical analyses through the development of new technologies, and contribute to further advances of the research field.

はじめに
Opening Remarks

2SGP-1 Putting prions in context: towards in vivo structural biology using DNP NMR
Kendra King Frederick (*UT Southwestern*)

2SGP-2 The single-particle cryo-electron microscopic analysis of amyloid disaggregation reaction
Takashi Nomura[1], Yoshiko Nakagawa[1], Yusuke Komi[1], Shingo Tamai[1,2], Masako Yamazaki[1], Motomasa Tanaka[1] ([1]*CBS, RIKEN*, [2]*Biomed. Sci. & Eng., Grad. Sch. of Med. &Dent. Sci., TMDU*)

2SGP-3 Critical Jamming and gel rheology of droplet suspensions in living cells
Daisuke Mizuno (*Kyushu University*)

2SGP-4 レオロジー NMR 法による SOD1 アミロイド形成の多状態その場観察
Multiple-state *in situ* observation of SOD1 amyloid formation by Rheo-NMR spectroscopy
○森本 大智 [1], ヴァリンダ エリック [2], 白川 昌宏 [1], シェラー ウルリッヒ [3], 菅瀬 謙治 [4] ([1] 京大・院工学, [2] 京大・院医学, [3]IPF, [4] 京大・院農学)
Daichi Morimoto[1], Erik Walinda[2], Masahiro Shirakawa[1], Ulrich Scheler[3], Kenji Sugase[4] ([1]*Grad. Sch. Eng., Kyoto Univ.*, [2]*Grad. Sch. Med., Kyoto Univ.*, [3]*IPF*, [4]*Grad. Sch. Agr., Kyoto Univ.*)

2SGP-5 TDP43-LC ドメインの病原性変異と線維形成能の網羅的解析
Comprehensive studies of disease-related mutations on cross-β polymerization of TDP43-LC domain
Nobuo Maita[1], Yuko Kajino[1], Masato Kato[1,2] ([1]*National Institutes for Quantum Science and Technology*, [2]*UT Southwestern Medical Center*)

13:50〜16:20　H 会場（函館市民会館 3F 大会議室）／Room H（Hakodate Citizen Hall 3F Conference Room）

2SHP　【共催：学術変革領域研究（A）「マルチファセットプロテインズ」】

マルチファセット・プロテインズへの生物物理アプローチ
Biophysical approach for multifaced protein world

オーガナイザー：渡邉 力也（理化学研究所），太田 元規（名古屋大学）
Organizers: Rikiya Watanabe (RIKEN), Motonori Ota (Nagoya Univ.)

In recent years, our perception of the "protein world" has been expanding and transforming with the discovery of many aspects that were previously unseen. In this symposium, we would like to discuss the biophysical approaches to clarify the molecular mechanism and physiological significance of the expanding and changing protein world from a "multifaceted" perspective.

2SHP-1 mRNA の翻訳制御を 1 分子解像度で in situ イメージングする
Translational regulation visualized at single-molecule resolution in cells
○小林 穂高 [1,2]（[1]JST さきがけ, [2] 東京大学 定量生命科学研究所）
Hotaka Kobayashi[1,2] ([1]*JST PRESTO*, [2]*IQB, The University of Tokyo*)

2SHP-2 SARS-CoV-2 nsp1 はホスト翻訳系をどう乗っ取るのか？
SARS-CoV-2 nsp1: how do they hijack the host translation?
○桜庭 俊 [1], 謝 祺琳 [2], 笠原 浩太 [3], 岩切 淳一 [4], 河野 秀俊 [1]（[1] 量研機構, [2] 立命館大・院生命科学, [3] 立命館大・生命, [4] 東京大・院新領域）
Shun Sakuraba[1], Qilin Xie[2], Kota Kasahara[3], Junichi Iwakiri[4], Hidetoshi Kono[1] ([1]*Natl. Inst. Quantum Sci. & Tech.*, [2]*Grad. Sch. Life Sci., Ritsumeikan Univ.*, [3]*Col. Life Sci., Ritsumeikan Univ.*, [4]*Grad. Sch. Frontier Sci., Univ. Tokyo*)

2SHP-3 神経変性疾患を引き起こすアミロイド線維のクライオ電顕解析
Cryo-EM analyses of the amyloid fibrils causing neurodegenerative diseases
○山形 敦史（理化学研究所・生命機能科学研究センター）
Atsushi Yamagata (*RIKEN Center for Biosystems Dynamics Research*)

2SHP-4 (2Pos260) 新規遺伝子の誕生と機能獲得の進化メカニズムに迫るゲノム計算科学：バイオインフォマティクスのその先に遺伝子の本質を探求する
(2Pos260) How do *de novo* genes evolve and acquire function?: Computational genomics to revisit the nature of genes beyond bioinformatics
○山内 駿 [1], 岩崎 渉 [1,2]（[1] 東大・院理学系, [2] 東大・院新領域）
Shun Yamanouchi[1], Wataru Iwasaki[1,2] ([1]*Grad. Sch. Sci., Univ. Tokyo*, [2]*Grad. Sch. Front. Sci., Univ. Tokyo*)

2SHP-5 Multifaceted view of protein diffusion
Eiji Yamamoto (*Dept. Syst. Des. Eng., Keio Univ.*)

2SHP-6 生体分子の 1 分子解析とその応用
Single-molecule analysis of bio-molecules and its applications
○渡邉 力也（理研・CPR）
Rikiya Watanabe (*CPR, RIKEN*)

3 日目（9 月 30 日（金））／Day 3（Sep. 30 Fri.）

09:00〜11:30　A 会場（函館アリーナ 武道館 A）／Room A（Hakodate Arena Budokan A）
3SAA　発光・蛍光計測と光学顕微鏡の標準化を目指して
Toward a standardization of luminescence, fluorescence measurements and light microscopy

オーガナイザー：佐々木 章（産業技術総合研究所），近江谷 克裕（産業技術総合研究所）
Organizers: Akira Sasaki (AIST), Yoshihiro Ohmiya (AIST)

The quantitative aspect of luminescence, fluorescence measurement and light microscopy is becoming significant. The challenge now lies in improving the accuracy and precision of the data obtained from such measurements. Standardization is the way to achieve precise, reproducible and inter-comparable measurement. Improving these will facilitate the comparison of results between different instruments/institutions and therefore ensure the reproducibility of results. In this symposium, recent standardization effort in the world (e.g. ISO) will be introduced in addition of leading edge researches of the related field.

はじめに
Opening Remarks

3SAA-1 定量的な蛍光顕微鏡計測に向けて - FCS を用いた顕微鏡ベンチマーク -
Toward traceable quantitative fluorescence microscopy - Benchmarking microscope using FCS technique -
○佐々木 章（産総研・バイオメディカル）
Akira Sasaki (*BMRI, AIST*)

3SAA-2 Supporting cellular analysis by quantitative imaging with standards and reference materials
Michael Halter, Ed Kwee, Alexander Peterson, John T Elliott (*National Institute of Standards and Technology (NIST), USA*)

3SAA-3 細胞を用いた分析・製造分野における細胞形態計測の信頼性向上を目指して～ISO 標準化活動の紹介
Towards improvement of the reliability of cell morphometry for analysis and manufacturing of cells - Role of ISO standardization
○能見 淑子（千代田化工建設株式会社）
Yoshiko Nomi (*Chiyoda Corporation*)

3SAA-4 (1Pos289) Morphological Analysis of Hydrogel Induced Cancer Stem Cells in Synovial Sarcoma Model Cells
Zannatul Ferdous[1], Masumi Tsuda[1,3,4], Jean-Emmanuel Clément[3], Jian Ping Gong[1,3,6], Shinya Tanaka[3,4,6], Tamiki Komatsuzaki[2,3,5], Koji Tabata[2] ([1]*Graduate School of Life Science, Hokkaido University*, [2]*Research Center of Mathematics for Social Creativity, Research Institute for Electronic Science, Hokkaido University, Sapporo, Japan*, [3]*Institute for Chemical Reaction Design and Discovery (WPI-ICReDD), Hokkaido University, Sapporo, Japan*, [4]*Department of Cancer Pathology, Hokkaido University Faculty of Medicine, Sapporo*, [5]*Graduate School of Chemical Sciences and Engineering, Hokkaido University, Sapporo, Japan*, [6]*Global Station for Soft Matter, Global Institution for Collaborative Research and Education (GI-CoRE), Hokkaido University, Sapporo, Japan*)

3SAA-5 Quantification of receptor clustering and activation at the cell surface using correlation and lifetime-based methods
Andrew Harry Albert Clayton (*Cell Biophysics, Optical Sciences Centre, Swinburne University of Technology, Hawthorn, Australia*)

3SAA-6 (1Pos288) Size determination of cytoplasmic condensates of optineurin using spatial image correlation spectroscopy (SICS)
Yuta Hamada[1], Masataka Kinjo[2], Akira Kitamura[2] ([1]*Grad. Sch. Sci. of Life Sci., Hokkaido Univ.*, [2]*Fac. of Adv. Life Sci., Hokkaido Univ*)

3SAA-7 絶対発光量計測技術に基づく生物発光反応の量子収率解析とバイオ分析機器標準化
Absolute light measurement for the investigation of bioluminescence quantum yield and standardization of bioanalysis instruments
○丹羽 一樹（産業技術総合研究所物理計測標準研究部門）
Kazuki Niwa (*National Metrology Institute of Japan (NMIJ), National Institute of Advanced Industrial Science and technology (AIST)*)

3SAA-8 定量的 in vivo, ex vivo 生物発光イメージング
Quantitative bioluminescence imaging in vitro and ex vivo
○近江谷 克裕 [1,2]（[1] 産業技術総合研究所, [2] 大阪工業大学）
Yoshihiro Ohmiya[1,2] ([1]*AIST*, [2]*Osaka Institute of technology*)

おわりに
Closing Remarks

09:00〜11:30　B 会場（函館アリーナ 武道館 B）／Room B（Hakodate Arena Budokan B）
3SBA　【共催：新学術研究領域「高速分子動画」】

様々な先端的手法で挑む生体分子の構造ダイナミクスの可視化
Visualization of structural dynamics of biomolecules using a variety of advanced techniques

オーガナイザー：梅名 泰史（名古屋大学），清水 伸隆（高エネルギー加速器研究機構）
Organizers: Yasufumi Umena (Nagoya Univ.), Nobutaka Shimizu (KEK)

Time-resolved serial femtosecond crystallography (TR-SFX) using X-ray free-electron laser (XFEL) has recently been established as one of the approaches to obtain structural dynamics of biological molecules. Furthermore, various biophysical analyses are necessary to understand complicated biological dynamic events properly, and novel methods have been proposed to obtain more detailed interpretations. The integrated collaborations between these methods and TR-SFX will take us to visualize biological processes as "molecular movies" in the future. In this session, we will introduce not only the latest SFX studies but also the various novel approaches to capture dynamic biological events and advance to understand the biomolecular functions through integrative research.

はじめに
Opening Remarks

3SBA-1　ポールシェーラー研究所でのいろいろな実験手法を組み合わせた時分割シリアル結晶学への取り組み
Time resolved serial crystallography with various methods at the Paul Scherrer Institut
Takashi Tomizaki, Tsujino Soichiro (*Paul Scherrer Institut*)

3SBA-2　分子動力学シミュレーションによるタンパク質の構造ダイナミクス研究
Structural dynamics of proteins studied using molecular dynamics simulations
○池口 満徳 [1,2]（[1] 横浜市大・生命医, [2] 理研・計算科学研究セ）
Mitsunori Ikeguchi[1,2] ([1]*Grad. Sch. Med Life Sci., Yokohama City Univ.*, [2]*R-CCS, RIKEN*)

3SBA-3　生体分子の動的構造解析のためのマイクロ流体デバイスの開発
Development of microfluidic devices for structural dynamics measurement of biomolecules
○真栄城 正寿 [1,2,3]（[1] 北海道大学大学院工学研究院, [2]JST・さきがけ, [3] 高エネルギー加速器研究機構 物質構造科学研究所）
Masatoshi Maeki[1,2,3] ([1]*Faculty of Engineering, Hokkaido University*, [2]*JST PRESTO*, [3]*Institute of Materials Structure Science, High Energy Accelerator Research Organization (KEK)*)

3SBA-4　Serial Femtosecond Crystallography reveals structural intermediates during CO-dissociation process in ba3-type Cytochrome c Oxidase
Swagatha Ghosh[1,2], Cecilia Safari[1], Rebecka Andersson[1], Jonatan Johannesson[1], Peter Dahl[1], Eriko Nango[3], Rie Tanaka[3], So Iwata[3], Richard Neutze[1], Gisela Brändén[1] ([1]*Dept. Chem. and Mol. Bio, Gothenburg University, Sweden*, [2]*Dept. Appl.Physics, Nagoya University, Japan*, [3]*RIKEN Spring-8 Center, Hyogo, Japan*)

3SBA-5　光化学系 II 酸素発生中心における V185 の役割についての QM/MM-MD 解析
QM/MM-MD study of the role of valine 185 in the oxygen-evolving center of photosystem II
○庄司 光男 [1,2], 宮川 晃一 [1], 三嶋 謙二 [1], 山口 兆 [3], 重田 育照 [1]（[1] 筑波大 CCS, [2] さきがけ, [3] 大阪大学）
Mitsuo Shoji[1,2], Koichi Miyagawa[1], Kenji Mishima[1], Kizashi Yamaguchi[3], Yasuteru Shigeta[1] ([1]*CCS, U.Tsukuba*, [2]*JST-PRESTO*, [3]*Osaka Univ.*)

3SBA-6 光活性化アデニル酸シクラーゼ OaPAC の動的構造解析による反応機構の解明
Reaction mechanisms of photoactivated adenylate cyclase OaPAC using dynamic structural analysis
○石本 直偉士 [1], 梅名 泰史 [3], Trampari Sofia[2], 辻野 壮一郎 [2], 富崎 孝司 [2], 朴 三用 [1] ([1] 横浜市大・院生命医科学, [2] ポールシェラー研究所, [3] 名大・シンクロトロン光研究センター）
Naito Ishimoto[1], Yasufumi Umena[3], Sofia Trampari[2], Soichiro Tsujino[2], Takashi Tomizaki[2], Sam-Yong Park[1] ([1]*Grad. Sch. MLS, Yokohama City Univ. / Japanese*, [2]*Paul Scherrer Institute / Switzerland*, [3]*Synchrotron Radiation Research Center, Nagoya University / Japanese*)

おわりに
Closing Remarks

09:00〜11:30　C 会場（函館アリーナ 武道館 C）／Room C（Hakodate Arena Budokan C）
3SCA　自主・自発の階層と適応：冗長性を行動力(健康)につなげる分子-細胞-筋-身体-脳連携
Hierarchies of autonomy and spontaneity and adaptation: Molecular-cell-muscle-bodybrain linkage of redundancy to action (health)

オーガナイザー：跡見 順子（東京農工大学），岩城 光宏（理化学研究所）
Organizers: Yoriko Atomi (Tokyo Univ. of Agriculture & Technology), Mitsuhiro Iwaki (RIKEN)

Fumio Osawa, the founder of the Biophysical Society of Japan, saw the essence of life as "independence and spontaneity. Humans, who are at the mercy of fragmented science, technology, and concepts, have lost sight of the larger framework for creating independence and spontaneity. This symposium will explore the path to extend the hierarchy of life's autonomy and spontaneity, in which protein interactions lead to emergence and molecular chaperones lead to adaptation, from the cell to the human body and mind. This will provide the basis for the creation of new health, industry, and medical science and education.

はじめに
Opening Remarks

3SCA-1 Myosin molecular motors convert information into motion
Toshio Yanagida[1,2,3,4] ([1]*NICT*, [2]*Grad. Sch. Info. Sci. Tech., Osaka Univ.*, [3]*Grad. Sch. Front. Biosci., Osaka Univ.*, [4]*iFReC*)

3SCA-2 The network of microtubule integrates the spatial information provided by the actin network along the cell periphery
Manuel Thery (*CEA (French Atomic Energy Reserch Center)*)

3SCA-3 Molecular mechanisms of the chaperones that assist in the folding of actin and tubulin
Masafumi Yohda (*Grad. Sch. Eng., Tokyo Univ. Agr. Tech.*)

3SCA-4 多細胞動物ヒトの筋適応の素過程：ストレス因子カルシウム、微小管及び分子シャペロン αB-クリスタリン
Elementary processes of slow muscle adaptation in multicellular human: calcium, microtubules and the molecular chaperone αB-crystallin
○跡見 順子（東京農工大）
Yoriko Atomi (*Tokyo University of Agriculture and Technology*)

3SCA-5 骨格筋幹細胞の活性化・分化と筋再生のサーカディアン制御
Circadian regulation of skeletal muscle stem cell activation differentiation, and muscle regeneration
○朝倉 淳（ミネソタ大学医学部・幹細胞研究所）
Atsushi Asakura (*Stem Cell Institute, University of Minnesota Medical School*)

3SCA-6 ヒトの不安定な立位姿勢における頭部-体幹部の構造的冗長性の制御
Control of structural redundancy from head to trunk during unstable upright standing in humans
○跡見 友章（杏林大学保健学部）
Tomoaki Atomi (*Health Sci., Univ. Kyorin*)

おわりに
Closing Remarks

09:00〜11:30　D 会場（函館アリーナ 多目的室 A）／Room D（Hakodate Arena Multipurpose Room A）
3SDA　【共催：学術変革領域研究（A）「新興硫黄生物学が拓く生命原理変革」】

硫黄のタンパク質科学の最前線
New implications of sulfur in protein science

オーガナイザー：増田 真二（東京工業大学），中林 孝和（東北大学）
Organizers: Shinji Masuda (Tokyo Tech), Takakazu Nakabayashi (Tohoku Univ.)

In recent years, attention has been focused on physiological phenomena involving sulfur, such as finding supersulfide molecules consisting of multiple sulfur atoms in mammals, including humans. In this symposium, six presenters introduce their recent results of structure-function relationships of sulfur-related proteins. We would like to discuss how biophysics can be applied to physiological phenomena involving sulfur.

はじめに
Opening Remarks

3SDA-1 Mechanism of sulfide/supersulfide sensing in bacteria
Shinji Masuda (*Grad. Sch. Life Sci. & Technol., Tokyo Inst. Tech.*)

3SDA-2 Intramolecular disulfide bond switches enzymatic activity of SOD1
Shinya Tahara[1], Kousuke Yamazaki[1], Takumi Ohyama[1], Kunisato Kuroi[2], Takakazu Nakabayashi[1]
([1]*Grad. Sch. Pharm. Sci., Tohoku Univ.*, [2]*Dept. Pharm. Sci., Kobe Gakuin Univ.*)

3SDA-3 Reaction mechanism of tRNA sulfur modifying enzyme using a cofactor iron-sulfur cluster
Min Yao (*Fac. Adv. Life Sci., Hokkaido Univ.*)

3SDA-4 2 つの異なるタイプの PLP 依存型システイン脱硫酵素と基質 L-システインおよび阻害剤との反応
Actions of two distinct types of PLP-dependent cysteine desulfurase enzymes with substrate L-cysteine and inhibitors
○藤城 貴史（埼玉大学大学院理工学研究科）
Takashi Fujishiro (*Grad. Sch. Sci. Engeneer., Saitama Univ.*)

3SDA-5 Structural and functional analyses of *E. coli* SufBCD complex involved in iron-sulfur clusters biogenesis

Kei Wada[1,2], Yoshikazu Tanaka[3], Yasuhiro Takahashi[4] ([1]*Department of Medical Sciences, University of Miyazaki*, [2]*Frontier Science Research Center, University of Miyazaki.*, [3]*Graduate School of Life Sciences, Tohoku University*, [4]*Graduate School of Science and Engineering, Saitama University*)

3SDA-6 アミノ酸とナノカーボンの相互作用：物理吸着およびシステインの化学反応
Interactions of carbon nanomaterials with amino acids: physical adsorption and chemical reaction with cysteine

○平野 篤（産総研・ナノ材料）
Atsushi Hirano (*NMRI, AIST*)

おわりに
Closing Remarks

09:00〜11:30　E 会場（函館アリーナ 多目的室 B）／Room E（Hakodate Arena Multipurpose Room B）

3SEA　【共催：NEDO ムーンショット型研究開発事業】

生物を利用したゼロエミッション・CO_2 資源化技術の可能性
Potential of zero-emission and CO_2-utilizing biotechnologies

オーガナイザー：加藤 創一郎（産業技術総合研究所），近藤 英昌（産業技術総合研究所）
Organizers: Souichiro Kato (AIST), Hidemasa Kondo (AIST)

"Zero-emission", which will reduce the emission of greenhouse-gases such as CO_2, CH_4, and N_2O to mitigate climate changes, are being tackled internationally. The technologies attracting attention in recent years are physicochemical methods such as Direct Air Capture (DAC) and CO_2 Capture and Storage (CCS). Considering the mitigation of greenhouse gases generated from agriculture and the utilization of CO_2, it is necessary to develop new technologies that utilize specific abilities of living organisms. In this symposium, research projects for innovative zero-emission and CO_2-utilizing biotechnologies conducted by Moonshot Research & Development Program are introduced.

はじめに
Opening Remarks

3SEA-1 微生物電気化学を活用した二酸化炭素資源化技術
CO_2 utilization technologies based on microbial electrochemistry

○加藤 創一郎（産総研・生物プロセス）
Souichiro Kato (*BPRI, AIST*)

3SEA-2 気相微生物反応
Microbial gas-phase reaction

○堀 克敏（名古屋大学大学院工学研究科）
Katsutoshi Hori (*Grad. Sch. Eng., Nagoya Univ.*)

3SEA-3 資源循環の最適化による農地由来の温室効果ガスの排出削減
Mitigation of greenhouse gas emissions from agricultural lands by optimizing nitrogen and carbon cycles

○南澤 究（東北大・院生命）
Kiwamu Minamisawa (*Graduate School of Life Sciences, Tohoku University*)

3SEA-4 土壌団粒構造と微生物
Soil aggregate structure and microorganisms
○和穎 朗太（農研機構・農業環境部門）
Rota Wagai (*NARO/NIAES*)

3SEA-5 ウシルーメンマイクロバイオーム制御による消化管メタンの削減をはかる新しい家畜生産システム開発に向けて
Toward a new livestock production system to reduce enteric methane through controlling bovine rumen microbiome
○小林 泰男（北海道大学大学院農学研究院）
Yasuo Kobayashi (*Research Faculty of Agriculture, Hokkaido University*)

3SEA-6 牛ルーメンからのメタン低減に向けた微生物利用の可能性
Potential microbial target for mitigating enteric methane production in the rumen of cows
○真貝 拓三（国立研究開発法人　農業・食品産業技術総合研究機構　畜産研究部門）
Takumi Shinkai (*Institute of Livestock and Grassland Science, National Agricultural and Food Research Organization*)

おわりに
Closing Remarks

09:00～11:30　F 会場（函館市民会館 1F 大ホール）／Room F（Hakodate Citizen Hall 1F Main Hall）
3SFA　クライオ電子顕微鏡が魅せる生命の未知なる動的なメカニズム
Unexpected dynamic mechanisms of life uncovered by Cryo-EM

オーガナイザー：濡木 理（東京大学），西増 弘志（東京大学）
Organizers: Osamu Nureki (The Univ. of Tokyo), Hiroshi Nishimasu (The Univ. of Tokyo)

Recent outstanding development of single particle analysis of cryo-EM allows high-resolution structure determinations of huge and flexible supramolecular complexes, which have been never available. In this symposium, we will present and discuss on current topics of unexpected dynamic molecular and cellular mechanisms of protein and nucleic acid supramolecular complexes involved in various life phenomena.

3SFA-1 Structure-function relationship of pump-like cation channelrhodopsins
Koichiro Kishi[1], Yoon Seok Kim[2], Masahiro Fukuda[1], Masatoshi Inoue[2], Tsukasa Kusakizako[3], Peter Wang[2], Toshiki Matsui[1], Keitaro Yamashita[4], Takashi Nagata[5], Masae Konno[5], Tomoko Uemura[6], Kehong Liu[6], Mikihiko Shibata[7], Norimichi Nomura[6], So Iwata[6], Osamu Nureki[3], Keiichi Inoue[4], Karl Deisseroth[2], **Hideaki Kato[1]** ([1]*Komaba Inst. Sci., Grad. Sch. Arts. Sci., Univ. Tokyo*, [2]*Stanford Univ.*, [3]*Grad. Sch. Sci., Univ. Tokyo*, [4]*MRC*, [5]*ISSP, Univ. Tokyo*, [6]*Grad. Sch. Med., Kyoto Univ.*, [7]*Kanazawa Univ.*)

3SFA-2 III-E 型 CRISPR-Cas7-11 エフェクター複合体の立体構造と分子改変
Structure and engineering of the type III-E CRISPR-Cas7-11 effector complex
○西増 弘志（東京大学）
Hiroshi Nishimasu (*The University of Tokyo*)

3SFA-3 (2Pos003) クライオ電子顕微鏡による高分解能解析によって明らかになってきた二成分毒素の膜透過機構
(2Pos003) High-resolution Cryo-EM analysis reveals the mechanism of binary toxin translocation
○山田 等仁 [1], 杉田 征彦 [2,3], 野田 岳志 [2], 津下 英明 [1]（[1] 京都産業大学 大学院生命科学研究科, [2] 京都大学 微細構造ウイルス学分野, [3] 京都大学 白眉センター）
Tomohito Yamada[1], Yukihiko Sugita[2,3], Takeshi Noda[2], Hideaki Tsuge[1] ([1]*Graduate School of Life Science, Kyoto Sangyo University*, [2]*Laboratory of Ultrastructural Virology, Institute for Life and Medical Sciences, Kyoto University*, [3]*Hakubi Center for Advanced Research, Kyoto University*)

3SFA-4 IscB–ωRNA 複合体による RNA 依存性 DNA 切断の構造基盤と Cas9 への進化的洞察
Structure of the IscB–ωRNA ribonucleoprotein complex, the likely ancestor of CRISPR-Cas9
○加藤 一希 [1], 岡崎 早恵 [1], Kannan Soumya[2], Zhang Feng[2], 西増 弘志 [1]（[1] 東大・先端研, [2]MIBR, MIT）
Kazuki Kato[1], Sae Okazaki[1], Soumya Kannan[2], Feng Zhang[2], Hiroshi Nishimasu[1] ([1]*RCAST, Univ. Tokyo*, [2]*MIBR, MIT*)

3SFA-5 ミトコンドリアのリボソームの成熟過程から翻訳開始過程に至る構造解析
Structural analysis of the late assembly states of mitochondorial ribosome to the translation initiation
Yuzuru Itoh[1,2], Anas Khawaja[3], Joanna Rorbach[3], Alexey Amunts[2] ([1]*Dept. BioSci., Grad. Sch. Sci., Univ. Tokyo*, [2]*SciLifeLab, DBB, Stockholm University*, [3]*Karolinska Institutet*)

3SFA-6 膜タンパク質と非翻訳 RNA の分子機構の構造基盤
Structural basis for molecular mechanisms of membrane proteins and non-coding RNA
○濡木 理（東京大学・院理）
Osamu Nureki (*Grad. Sch. Sci., Univ. Tokyo*)

09:00〜11:30　G 会場（函館市民会館 3F 小ホール）／Room G（Hakodate Citizen Hall 3F Small Hall）

3SGA　自己組織化で超分子生体膜を創る: 材料科学と生物物理学の接点
Creation of supramolecular biomembrane by the bottom-up self-assembly:Where material science meets biophysics

オーガナイザー：安原 主馬（奈良先端科学技術大学院大学），森垣 憲一（神戸大学）
Organizers: Kazuma Yasuhara (NAIST), Kenichi Morigaki (Kobe Univ.)

In biological systems, unique material properties of the membrane play central roles. The two-dimensional fluid and compartmentalization are essentially important in a variety of biological functions such as signal transduction and energy conversion. Bottom-up approaches based on the self-assembly of materials are promising to reproduce the unique membrane structures and functions, providing insights into the machinery of the biological membrane and enabling to exploit applications in real-life. This symposium will introduce unique studies to create novel artificial biomembranes using not only conventional phospholipids but also synthetic polymers, nanoparticles, and their hybrids to explore the interface between biophysics and material science.

はじめに
Opening Remarks

3SGA-1 ポリマー化脂質膜と天然脂質膜からなるパターン化人工膜
Micropatterned model membrane composed of polymerized and natural lipid bilayers
○森垣 憲一 [1,2]（[1] 神戸大・バイオシグナル, [2] 神戸大・院農学）
Kenichi Morigaki[1,2] ([1]*Biosignal Res. Cen., Kobe Univ.*, [2]*Grad. Sch. Agrobio., Kobe Univ.*)

3SGA-2 **メカノクロミック生体膜を用いたペプチドー脂質相互作用の検出**
Mechanochromic biomembranes for studying peptide-lipid interactions
○杉原 加織（東大・生研）
Kaori Sugihara (*IIS, Univ. Tokyo*)

3SGA-3 **多価不飽和脂質によって形成される脂質ドメイン**
Lipid domains generated by polyunsaturated lipids
ゴー メルヴィン ウェイ シェン, ○手老 龍吾（応化生命系・豊橋技科大）
Melvin Wei Shern Goh, **Ryugo Tero** (*Dept. Appl. Chem. Life Sci., Toyohashi Univ. Tech.*)

3SGA-4 **リキッドマーブル：粒子膜で安定化された液滴**
Liquid marble: Droplet covered by particulate membrane
○藤井 秀司（大阪工業大学）
Syuji Fujii (*Osaka Institute of Technology*)

3SGA-5 **(2Pos188) DNA ゲル骨格が決定する人工細胞の力学特性**
(2Pos188) Cytoskeletons of self-assembled DNA regulate the mechanical properties of artificial cells
○増田 和俊 [1], 大野 風優 [2], 柳澤 実穂 [1,2]（[1] 東京大学教養学部, [2] 東京大学大学院総合文化研究科）
Kazutoshi Masuda[1], Fuyu Ohno[2], Miho Yanagisawa[1,2] ([1]*College of Arts and Sciences, The University of Tokyo*, [2]*Graduate school of Arts and Sciences, The University of Tokyo*)

3SGA-6 **生体膜表面を模倣した高分子自己集合体**
Self-assembled polymer aggregates with mimetic cell membrane surface
○遊佐 真一（兵庫県立大学大学院工学研究科応用化学専攻）
Shin-ichi Yusa (*Department of Applied Chemistry, Graduate School of Engineering, University of Hyogo*)

3SGA-7 **合成高分子によって形成される最小モデル膜としての脂質ナノディスク**
Lipid nanodisc as a minimal model membrane formed with synthetic polymers
○安原 主馬 [1,2]（[1] 奈良先端大院・物質, [2] 奈良先端大・デジタルグリーンイノベーションセンター）
Kazuma Yasuhara[1,2] ([1]*Div. Mat. Sci, Nara Inst. Sci. Tech.*, [2]*Ctr. for Digital Green-innovation, Nara Inst. Sci. Tech.*)

おわりに
Closing Remarks

09:00～11:30　H 会場（函館市民会館 3F 大会議室）／Room H（Hakodate Citizen Hall 3F Conference Room）

3SHA　【共催：学術変革領域研究（A）「超越分子システム」 / 学術変革領域研究（B）「SPEED」】

高次機能性分子システム～創る方法の解明に向けて～
Construction of Higher-ordered Molecular Systems - How to Create Them?

オーガナイザー：松浦 友亮（東京工業大学），川野 竜司（東京農工大学），鈴木 雄太（京都大学）
Organizers: Tomoaki Matsuura (Tokyo Tech), Ryuji Kawano (Tokyo Univ. of Agriculture and Tech.), Yuta Suzuki (Kyoto Univ.)

We would like to take place a joint symposium collaborated with the “Cell-free molecular system” (Grant-in-Aid for Transformative Research Areas (A)) and the “SPEED” (Grant-in-Aid for Transformative Research Areas (B)). This symposium aims to shed light on the bottom-up construction of the cell-free system and the superior protein engineering by evolution and design.

はじめに
Opening Remarks

3SHA-1　Constructing an in vitro gene screening system for membrane proteins and its application
Tomoaki Matsuura (*ELSI, Tokyo Tech*)

3SHA-2　人工金属酵素を用いた触媒システムの構築
Artificial enzymes towards systems catalysis
○岡本 泰典（東北大・学際研）
Yasunori Okamoto (*FRIS, Tohoku Univ.*)

3SHA-3　2 次元ナノ材料界面を利用した高感度バイオセンサの開発
Development of Highly Sensitive Biosensor Using Two-Dimensional Nanomaterial Interface
○早水 裕平（東工大・物質理工）
Yuhei Hayamizu (*Sch.Mater, Tokyo Tech*)

3SHA-4　分子進化によるタンパク質集合体の構築
Directed evolution of protein assembly
○寺坂 尚紘 [1], 菅 裕明 [1], Hilvert Donald[2]（[1] 東京大・院理学, [2]Laboratory of Organic Chemistry, ETH Zurich）
Naohiro Terasaka[1], Hiroaki Suga[1], Donald Hilvert[2] ([1]*Grad. Sch. Sci., The Univ. of Tokyo*, [2]*Laboratory of Organic Chemistry, ETH Zurich*)

3SHA-5　人工細胞膜システム：デノボ設計ナノポアの構築
Artificial Cell-membrane system: the construction of *de novo* nanopores
○川野 竜司（東京農工大学 工学研究院 生命工学専攻）
Ryuji Kawano (*Dept. Biotech&Life Sci., Tokyo University of Agriculture and Technology*)

3SHA-6　合理設計による機能性タンパク質集合体の構築
Rational design of protein assembly
○鈴木 雄太（京大・白眉）
Yuta Suzuki (*Hakubi Center, Kyoto University*)

ポスター　Poster

＊ 学生発表賞候補演題
＊ Student Presentation Award Candidate Poster

1 日目（9 月 28 日（水））／Day 1（Sep. 28 Wed.）

蛋白質：構造／Protein: Structure

1Pos001 珪藻 *Thalassiosira pseudonana* 由来ルビスコの構造解析及び新規ピレノイドタンパク質との相互作用解析
Structural study of RubisCO from diatom *Thalassiosira pseudonana* and its interaction with novel pyrenoid proteins
Taiki Fukuzawa[1], Rei Tohda[1], Nawely Hermanus[2], Natumi Morishima[2], Ryosuke Okubo[2], Yoshinori Tsuji[2], Akihiro Kawamoto[1], Hideaki Tanaka[1], Gerle Christogh[1], Yusuke Matsuda[2], Genji Kurisu[1] ([1]*Institute for Protein Research, Osaka University*, [2]*School of Biological and Environmental Sciences, Kwansei Gakuin University*)

1Pos002 ヒト B 細胞抑制性共受容体 CD72 の構造解析
Structure analysis of human B cell inhibitory co-receptor CD72
Xibin Quan[1], Nobutaka Numoto[1], Takeshi Tsubata[2,3], Nobutoshi Ito[1] ([1]*Dept. Struct. Biol., Med. Res. Inst., Tokyo Med. Dent. Univ.*, [2]*Dept. Immunol., Med. Res. Inst., Tokyo Med. Dent. Univ.*, [3]*Sch. Dent., Nihon Univ.*)

1Pos003 Generation of protein distance matrices and novel structures utilizing Generative Adversarial Networks(GAN)
Taihei Yamaguchi (*Grad. Sch. Agr. Life Sci., Univ. Tokyo*)

1Pos004 ヒト由来電位依存性カリウムイオンチャネルのクライオ電子顕微鏡単粒子解析
Cryo-EM single particle analysis of a human voltage-gated potassium channel
Natsuko Sekido[1], Tomona Iizuka[2], Tomoyasu Aizawa[2], Makoto Sasaki[1], Haruhiko Fuwa[3], Mari Yotsu-Yamashita[4], Keiichi Konoki[4], Takeshi Yokoyama[1], Yoshikazu Tanaka[1] ([1]*Grad. Sch. Life Sci., Tohoku Univ.*, [2]*Grad. Sch. Life Sci., Hokkaido Univ.*, [3]*Fac. Sci. & Eng., Chuo Univ.*, [4]*Grad. Sch. Agri Sci., Tohoku Univ.*)

1Pos005 電子線クライオトモグラフィーで可視化したスピロプラズマの細胞骨格リボン
Cytoskeletal ribbon of *Spiroplasma* revealed by cryo electron tomography
Yuya Sasajima[1], Takayuki Kato[2], Tomoko Miyata[3], Akihiro Kawamoto[2], Fumiaki Makino[3,4], Keiichi Namba[3,5,6], Makoto Miyata[1,7] ([1]*Grad. Sch. Sci., Osaka Metropolitan Univ.*, [2]*IPR., Osaka Univ.*, [3]*Grad. Sch. Front. Biosci., Osaka Univ.*, [4]*JEOL Ltd.*, [5]*BDR & SPring-8 Center, Riken*, [6]*JEOL YOKOGUSHI Res. Alliance. Lab. Osaka Univ.*, [7]*OCARINA, Osaka Metropolitan Univ.*)

1Pos006 左巻き *βαβ* モチーフをもつタンパク質のデノボデザインに向けて
Toward *de novo* design of left-handed *βαβ*-motif-containing proteins
Hiroto Murata, George Chikenji (*Dept of Appl. Phys., Grad. Sch of Eng., Nagoya Univ.*)

1Pos007 CRISPR-Cas7-11 の構造とエンジニアリングによる RNA ノックダウンツールへの応用
Structure and engineering of the type III-E CRISPR-Cas7-11 effector complex
Kazuki Kato[1], Wenyuan Zhou[2], Sae Okazaki[1], Yukari Isayama[1], Tomohiro Nishizawa[3], Jonathan S. Gootenberg[2], Omar O. Abudayyeh[2], Hiroshi Nishimasu[1] ([1]*RCAST, Univ. Tokyo*, [2]*MIBR, MIT*, [3]*Grad. Sch. Med. Life Sci., Univ. Yokohama City*)

1Pos008 疑似電子顕微鏡画像を機械学習することにより生体分子の同定手法を開発する
Deep learning of computer-generated electron microsopy images to identify biomolecules
Atsushi Matsumoto (*Institute for Quantum Life Science, National Institutes for Quantum Science and Technology*)

1Pos009 Time-resolved X-ray crystallography of *E. coli* MutT, a Nudix hydrolase
Teruya Nakamura[1,2], Yuriko Yamagata[1,3] ([1]*Grad. Sch. of Pharmaceut. Sci., Kumamoto Univ.*, [2]*Priority Organization for Innovation and Excellence, Kumamoto Univ.*, [3]*Shokei University and Shokei University Junior College*)

1Pos010 X 線自由電子レーザーを用いた単粒子解析における分子サイズ効果
Molecular size effect on the single-particle analysis using X-ray free electron laser
Miki Nakano[1], Osamu Miyashita[1], Florence Tama[1,2,3] ([1]*RIKEN Center for Computational Science*, [2]*Grad. Sch. Sci., Nagoya Univ.*, [3]*ITbM, Nagoya Univ.*)

1Pos011 クライオ電子顕微鏡を用いた繊毛軸糸ダイニンコンポーネント Calaxin の機能解析
Cryo-electron tomography revealed that Calaxin stabilizes the docking of outer arm dyneins onto ciliary doublet microtubule in vertebrate
Hiroshi Yamaguchi, Masahide Kikkawa (*Grad. Sch. Med., Univ. Tokyo*)

1Pos012 スーパーフォールドを区別する構造ルールの探索:フェレドキシン構造とリバースフェレドキシン構造の解析
The structural rule distinguishing a superfold: A case study of ferredoxin fold and the reverse ferredoxin fold
Takumi Nishina, George Chikenji (*Dept of Appl. Phys., Grad. Sch. of Eng., Nagoya Univ.*)

1Pos013 ネフローゼ症候群原因タンパク質 podocin の調製と結晶化
Preparation and crystallization of podocin, associated with nephrotic syndrome
Koki Ando[1], Hideshi Yokoyama[2] ([1]*Grad. Sch. Pharm. Sci., Tokyo Univ. Sci.*, [2]*Fac. Pharm. Sci., Tokyo Uni. Sci.*)

1Pos014 TMD シミュレーションを用いたギャップ結合ファミリータンパク質のクローズ機構及び周囲の脂質分子の流動性の解析
Analysis on the closing mechanism of gap junction family proteins and fluidity of surrounding lipid molecules by TMD simulation
Ikuma Kaneshiro[1], Florence Tama[1,2], Osamu Miyashita[2] ([1]*Grad. Sch. Sci., Univ. Nagoya*, [2]*Kobe Inst., Riken*)

1Pos015 レジリン蛋白質における自己組織化能の評価
Evaluation of Self-Assembling Ability in Resilin Proteins
Risa Tani[1], Yoichi Yamazaki[1], Kento Yonezawa[1,2], Sachiko Toma[1], Hironari Kamikubo[1,2] ([1]*NAIST, MS*, [2]*NAIST, CDG*)

1Pos016 代謝安定型作動薬と LysoPS 受容体 LPS1 の構造解析
Cryo-EM structure of LysoPS Receptor LPS1 in complex with Metabolically Stable Agonist
Ryo Kawahara[1], Fumiya Sano[1], Akiharu Uwamizu[2], Luying Chen[2], Tomohiko Ohwada[2], Junken Aoki[2], Wataru Shihoya[1], Osamu Nureki[1] ([1]*Grad. Sch. Sci., Univ. Tokyo*, [2]*Grad. Sch. Pharm., Univ. Tokyo*)

1Pos017 免疫受容体 LILRA2 の ANGPTL6 認識機構
Molecular mechanism of ANGPTL6 recognition by immune activation receptor LILRA2
Jiaqi Wang[1], Atsushi Furukawa[1,2], Rika Yamazaki[1], Kouyuki Hirayasu[3,4], Tsuyoshi Kadomatsu[5], Yuichi Oike[5], Hisashi Arase[3], Katsumi Maenaka[1] ([1]*Pharm. Sci. Hokkaido Univ.*, [2]*Pharm. Kanazawa Univ.*, [3]*Res. Inst. Microbial Diseases, Osaka Univ.*, [4]*Adv. Preventive. Med. Sci. Res. Center., Kanazawa Univ.*, [5]*Med., Kumamoto Univ.*)

1Pos018 gREST 法による VHH 構造の効率的サンプリング
Enhanced Conformational Sampling of VHH by Generalized Replica-Exchange with Solute Tempering
Ren Higashida, Kouhei Yamaguchi, Yasuhiro Matsunaga (*Grad. Sch. Sci. Eng., Saitama Univ.*)

1Pos019 毛髪ダメージに伴う毛髪繊維の変形とその分光学的解析
Deformation of hair fibers due to hair damage and its spectroscopic analysis
Kazuki Kobayashi, Atsushi Baba, Kazuyuki Suzuta, Len Ito (*MILBON Co.,Ltd.*)

1Pos020 ミトコンドリア蛋白質搬入ゲート TOM 複合体の高速原子間力顕微鏡解析
High-speed atomic force microscopy analysis of the mitochondrial protein import gate TOM complex
Yuhei Araiso[1], Nanako Kobayashi[1], Kana Kuzasa[1], Hirotatsu Imai[2], Aimi Makino[2], Akihiro Inazu[1], Noriyuki Kodera[2], Toshiya Endo[3,4] ([1]*Dept. of Clin. Lab. Sci., Div. of Health Sci., Kanazawa Univ.*, [2]*WPI-NanoLSI, Kanazawa Univ.*, [3]*Fac. of Life Sci., Kyoto Sangyo Univ.*, [4]*Inst. of Protein Dynamics, Kyoto Sangyo Univ.*)

1Pos021 カイコ storage protein の単粒子解析
Single particle analysis of silkworm storage proteins
Shunsuke Kita, Yuki Anraku, Cong Tian, Katsumi Maenaka (*Faculty of Pharmaceutical Sciences, Hokkaido University*)

1Pos022 狂犬病ウイルスの P 蛋白質が宿主の JAK-STAT 経路を阻害する分子機構の解明
Molecular dissection on how rabies virus P-protein inhibits JAK-STAT pathway of host
Aoi Sugiyama[1], Miku Minami[1], Yukihiko Sugita[2], Mika Hirose[3], Shunsuke Kita[1,4], Katsumi Maenaka[1,4], Min Yao[1,5], Toyoyuki Ose[1,5] ([1]*Grad. Sch. Life Sci., Hokkaido Univ.*, [2]*Inst. Front. Life and Med. Sci., Kyoto Univ.*, [3]*Inst. Protein, Osaka Univ.*, [4]*Fac. Pharm. Sci., Hokkaido Univ.*, [5]*Fac. Adv. Life Sci., Hokkaido Univ.*)

1Pos023 一分子蛍光測定を目指した SARS-CoV2 の N 蛋白質の精製及びラベル化
Purification and fluorophore labeling of SARS-CoV2 N protein aiming at single molecule fluorescence measurements
Shun Endo[1,2], Leo Suzuki[1,2], Yuji Itoh[1,2], Hiroyuki Oikawa[1,2], Satoshi Takahashi[1,2] ([1]*Tohoku Univ.Inst.,Tagenken*, [2]*Grad.Sch.Sci.,Univ.Tohoku*)

1Pos024 高分解能中性子構造解析によるペプチド結合の平面性の再検討
Revisiting the peptide bond planarity by high-resolution neutron structure
Yuya Hanazono[1,2,3], Yu Hirano[2,4], Kazuki Takeda[1], Katsuhiro Kusaka[5], Taro Tamada[2], Kunio Miki[1] ([1]*Grad. Sch. Sci., Kyoto Univ.*, [2]*Inst. Quant. Lif. Sci., QST*, [3]*Med. Res. Inst., Tokyo Med. Dent. Univ.*, [4]*PRESTO, JST*, [5]*Front. Res. Cent. for Appl. Atom. Sci., Ibaraki Univ.*)

蛋白質：構造機能相関／Protein: Structure & Function

1Pos025 大腸菌由来 ribonuclease HI の金属イオン結合熱力学解析と活性との相関
Metal-ion binding and folding thermodynamics of *Escherichia coli* ribonuclease HI in correlation with its activity
Yumi Kitagawa[1], Zengwei Liao[1], Kosuke Morikawa[2], Masayuki Oda[1] ([1]*Grad. Sch. Life Environ. Sci., Kyoto Pref. Univ.*, [2]*Grad. Sch. Biostudies, Kyoto Univ.*)

1Pos026 大規模な薬剤データセットにおける心筋イオンチャネル-薬剤間の結合自由エネルギー計算
Calculation of the binding free energies between cardiac ion channels and drugs on a large data set
Tatsuki Negami, Tohru Terada (*Grad. Sch. Agr. Life Sci., Univ. Tokyo*)

1Pos027 (2SBP-6) Automated Density Extraction of Isomorphous Difference map and Occupancy-estimation for Conformer Fitting
Sriram Srinivasa Raghavan[1], Florence Tama[1,2,3], Osamu Miyashita[1] ([1]*RIKEN Center for Computational Science, Kobe, Japan.*, [2]*Institute of Transformative Biomolecules (WPI-ITbM), Nagoya University, Aichi, Japan.*, [3]*Department of Physics, Graduate School of Science, Nagoya University, Aichi, Japan.*)

1Pos028 HIV-1 の Nelfinavir 耐性プロテアーゼ D30N/N88D 変異体に対する動的残基間相互作用ネットワーク解析
Dynamic Residue Interaction Network Analysis of the Protease D30N/N88D Mutant Conferring Nelfinavir Resistance in HIV-1
Ayaka Ojima, Norifumi Yamamoto (*Chiba Tech*)

1Pos029 Elucidating the Mechanisms of the Bacterial Flagella ATPase Subcomplex
Thomas Stefan Davies[1,2], Peter John Bond[1], Alexander Krah[1], Chrystala Constantinidou[2] ([1]*A*STAR Singapore*, [2]*University of Warwick*)

1Pos030 Molecular dynamics study of phase behaviors of heat-resistant obscure proteins and their anti-aggregation functions
Cheng Tan[1], Ai Niitsu[2], Yuji Sugita[1,2,3] ([1]*Computational Biophysics Research Team, RIKEN Center for Computational Science*, [2]*Theoretical Molecular Science Laboratory, RIKEN Cluster for Pioneering Research*, [3]*Laboratory for Biomolecular Function Simulation, RIKEN Center for Biosystems Dynamics Research*)

1Pos031 インバース共溶媒分子動力学法による分子プローブ周辺アミノ酸残基環境の可視化
Inverse Mixed-Solvent Molecular Dynamics for Visualization of Amino Acid Residue Interaction Profile of Molecular Probes
Keisuke Yanagisawa[1], Ryunosuke Yoshino[2,3], Genki Kudo[4], Takatsugu Hirokawa[2,3] ([1]*Comput. Sci., Sch. Comput., Tokyo Tech*, [2]*Faculty Med., Univ. Tsukuba*, [3]*TMRC, Univ. Tsukuba*, [4]*Appl. Sci., Grad. Sch. Sci. Tech., Univ. Tsukuba*)

1Pos032 タイプ I インターフェロン経路を阻害する麻疹ウイルス V タンパク質の機能解析
Mechanistic analysis of type I interferon pathway inhibition by Measles virus V protein
Daiki Ito[1], Madoka Kimoto[1], Nanaka Goda[1], Kiichi Hirohata[2], Takahiro Maruno[2], Susumu Uchiyama[2], Min Yao[3], Toyoyuki Ose[3] ([1]*Grad. Sch. Life Sci., Univ. Hokkaido*, [2]*Grad. Sch. Eng., Univ. Osaka*, [3]*Grad. Sch. Adv. Life Sci., Univ. Hokkaido*)

1Pos033 SMN タンパク質のプロリン残基異性化による機能変化
Functional changes in SMN proteins by isomerization of proline residues
Saki Ohazama[1], Shinichi Nakagawa[2], Hiroshi Maita[2] ([1]*Graduate School of Life Science, Hokkaido Univ.*, [2]*Faculty of Pharmaceutical Sciences, Hokkaido Univ.*)

1Pos034 MD シミュレーションとクライオ電顕を用いた p97 の構造変化の研究
Conformational change of p97 by MD simulations and experimental data
Teppei Deguchi[1], Florence Tama[1,2,3], Osamu Miyashita[1,3] ([1]*Grad. Sch. Sci., Univ. Nagoya*, [2]*ITbM,. Univ. Nagoya*, [3]*R-CCS., RIKEN*)

1Pos035 ホソイトスギ由来パンアレルゲン、ポルカルシンの組換え発現と NMR 構造
Recombinant expression and NMR structural analysis of a pan-allergen, polcalcin from European cypress
Peiwen Fan, Shaokai Zhao, Tomona Iizuka, Jingkang Zheng, Mitsuki Shibagaki, Tomoyasu Aizawa (*Grad. Sch. Life Sci., Hokkaido Univ.*)

1Pos036 STAT2 との相互作用に必要な麻疹ウイルス V 蛋白質最小領域の同定と相互作用特性
Characterization of the minimum region of measles virus V protein to interact with STAT2
Nanaka Goda[1], Madoka Kimoto[1], Daiki Ito[1], Kaho Morita[1], Hiroyuki Kumeta[2], Min Yao[2], Toyoyuki Ose[2] ([1]*Grad. Sch. Life Sci., Univ. Hokkaido*, [2]*Grad. Sch. Adv. Life Sci., Univ. Hokkaido*)

1Pos037 ストレスファイバーにおけるアクチンサブユニットの張力依存的な構造状態
Tension-dependent structural state of actin subunits in stress fibers
Yuki Karan, Taro Q.P. Noguchi (*National Institute of Technology, Miyakonojo College*)

1Pos038 Structural dynamics and *in silico* design of pyrazolopyran-based inhibitors against *Plasmodium* serine hydroxymethyltransferases
Pitchayathida Mee-udorn[1], Bodee Nutho[2], Romchalee Chootrakool[3], Somchart Maenpuen[4], Ubolsree Leartsakulpanich[5], Penchit Chitnumsub[5], Thanyada Rungrotmongkol[1,3] ([1]*Program in Bioinformatics and Computational Biology, Grad. Sch., Chulalongkorn Univ., Bangkok, Thailand*, [2]*Department of Pharmacology, Science, Mahidol Univ., Bangkok, Thailand*, [3]*Biocatalyst and Environmental Biotechnology Research Unit, Biochemistry, Science, Chulalongkorn Univ., Bangkok, Thailand*, [4]*Department of Biochemistry, Science, Burapha Univ., Chonburi, Thailand*, [5]*National Center for Genetic Engineering and Biotechnology, Thailand Science Park, Bangkok, Thailand*)

1Pos039 SARS-CoV-2 スパイク蛋白質と NTD 結合抗体との糖鎖を介した相互作用の解析
Investigation of interactions between SARS-CoV-2 spike and NTD-binding antibody through glycans
Mao Oide[1], Yuji Sugita[1,2,3] ([1]*RIKEN CPR*, [2]*RIKEN BDR*, [3]*RIKEN R-CCS*)

1Pos040 Recombinant production, functional and structural analysis of antimicrobial peptides in mouse cryptdin family
Shaonan Yan, Yuchi Song, Yi Wang, Weiming Geng, Shinya Yoshino, Tomoyasu Aizawa (*Graduate School of Life Science, Hokkaido University*)

1Pos041 *Dictyostelium discoideum* の filopodia の cryo-EM 観察
Observation of filopodia in *Dictyostelium discoideum* by cryo-EM
Yuki Gomibuchi, Yukihisa Hayashida, Yusuke V. Morimoto, Takuo Yasunaga (*Grad. Sch Comp. Sci and Sys. Eng., KIT*)

1Pos042 Unraveling the coupling between conformational changes and ligand binding in ribose binding protein using MD simulations
Weitong Ren[1], Hisham Dokainish[1], Ai Shinobu[2], Hiraku Oshima[2], Yuji Sugita[1,2,3] ([1]*RIKEN Cluster for Pioneering Research*, [2]*RIKEN Center for Biosystems Dynamics Research*, [3]*RIKEN Center for Computational Science*)

1Pos043 コーヒーポリフェノールと乳タンパク質の相互作用に関する分光学的研究
Spectroscopic study of the interaction between coffee polyphenols and milk proteins
Kazuki Horita[1,2], Hiroshi Suga[1], Atsushi Hirano[1,2] ([1]*Grad. Sch. Eng., Chiba Tec.*, [2]*NMRI, AIST*)

1Pos044 CD28 ペプチドとの相互作用に伴う PI3K nSH2 ドメインの構造動態変化
Changes in structural dynamics of PI3K nSH2 upon interaction with CD28 peptide
Yohei Miyanoiri[2], Suyong Re[3], Yuhi Hosoe[1], Yuya Asahina[2], Toru Kawakami[2], Masataka Kuroda[3,4], Kenji Mizuguchi[2,3], Masayuki Oda[1] ([1]*Grad. Sch. Life Environ. Sci., Kyoto Pref. Univ.*, [2]*Inst. Prot. Res., Osaka Univ.*, [3]*ArCHER, Natl. Inst. Biomed. Innov. Health Nutrition*, [4]*Discov. Tech. Lab., Mitsubishi Tanabe Pharma Corp.*)

1Pos045 Acceleration of residue-level coarse-grained molecular dynamics by new development of parallelization
Jaewoon Jung[1,2], Cheng Tan[1], Chigusa Kobayashi[1], Diego Ugarte[1], Yuji Sugita[1,2,3] ([1]*RIKEN R-CCS*, [2]*RIKEN CPR*, [3]*RIKEN BDR*)

1Pos046 新型コロナウイルスのスパイクタンパク質の動的残基相互作用ネットワーク分析
Dynamic Residue Interaction Network Analysis of the Spike Protein of SARS-CoV-2
Hirokazu Murata, Norifumi Yamamoto (*Chiba Tech*)

1Pos047 詳細反応モデリングとベイズパラメタ推定による KaiC の多量体構造の機能的役割の解明
Functional roles of the multimeric structure of KaiC revealed by detailed kinetic modeling and Bayesian parameter inference
Shin-ichi Koda[1,2], Shinji Saito[1,2] ([1]*Institute for Molecular Science*, [2]*SOKENDAI*)

蛋白質：物性（安定性 折れたたみなど）／Protein: Property

1Pos048 抗体の親和性成熟と安定性の変化；成熟した C6 とそのジャームライン型抗体
Antibody evolution for antigen binding and stability; maturated C6 and its germline-type antibodies
Saaya Yabuno[1], Takahiro Hayashi[2], Masayuki Oda[1,2] ([1]*Faculty Life. Environ. Sci., Kyoto Pref. Univ.*, [2]*Grad. Sch. Life. Environ. Sci., Kyoto Pref. Univ.*)

1Pos049 抗体の親和性成熟と安定性の変化；抗ニトロフェニル抗体の重鎖 58 番と 102 番残基の役割
Antibody evolution for antigen binding and stability; Role of residues at 58 and 102 of heavy chain of anti-nitrophenyl antibody
Mutsumi Yoshida[1], Yumi Kitagawa[2], Masayuki Oda[1,2] ([1]*Faculty Life. Environ. Sci., Kyoto Pref. Univ.*, [2]*Grad. Sch. Life. Environ. Sci., Kyoto Pref. Univ.*)

1Pos050 Amyloid β aggregation and accumulation process under physiological conditions
Masahiro Kuragano, Shinya Yamanaka, Kiyotaka Tokuraku (*Grad. Sch. Eng., Muroran Inst. of Tech.*)

1Pos051 PSD95-PDZ3 の高温での可逆的なオリゴマー形成における速度論的効果の定量的な評価
The quantitative evaluation of kinetic effect on PSD95-PDZ3's reversible oligomerization at high temperature
Tomonori Saotome[1], Sawaros Onchaiya[2], Jose C Martinez[3], Yutaka Kuroda[2], Shun-ichi Kidokoro[1] ([1]*Dept. of Mate. Sci. and Bio., Nagaoka Univ. of Tech., Japan*, [2]*Dept. of Biotech. and Life Sci., Tokyo Univ. of Agric. and Tech., Japan*, [3]*Dept. of Phys. Chem., Univ. of Granada, Spain*)

1Pos052 変性して小さくなる蛋白質
Antibody proteins can be smaller by denaturation
Hiroshi Imamura[1,2,3], Ayako Ooishi[3], Shinya Honda[3] ([1]*Dept. Bio-sci., Nagahama Inst. Bio-Sci. Tech.*, [2]*Coll. Life Sci., Ritsumeikan Univ.*, [3]*Biomed. Res. Inst., AIST*)

1Pos053 タンパク質表面電荷が溶解性に及ぼす影響の格子モデル解析
Lattice-model analysis of protein surface charge distribution on amorphous aggregation and condensation
Yutaka Kuroda, Yuki Matsuzawa, Shin Kohara (*Tokyo University of Agriculture and Technology (TUAT)*)

1Pos054 (1SAA-8) GGGGCC-RNA は、TDP43 およびそのカルボキシ断片の凝集を抑制する
(1SAA-8) GGGGCC-RNA prevents aggregation of TDP43 and its carboxy terminal fragments
Ai Fujimoto[1], Masataka Kinjo[2], Akira Kitamura[2] ([1]*Grad. Sch. of Life Sci., Hokkaido. Univ*, [2]*Fac. Adv. Life Sci., Hokkaido. Univ*)

1Pos055 Difference between the Aβ40 and Aβ42 aggregation processes at the atomic level
Satoru G. Itoh[1,2,3], Maho Yagi-Utsumi[1,2,3,4], Koichi Kato[1,2,3,4], Hisashi Okumura[1,2,3] ([1]*IMS*, [2]*ExCELLS*, [3]*SOKENDAI*, [4]*Nagoya City Univ.*)

1Pos056 翻訳アレスト時のポリペプチド鎖を可視化する試み
Attempt to visualize the synthetic polypeptide during translational arrest
Takehito Tanzawa, Takayuki Kato (*IPR., Osaka Univ.*)

1Pos057 Kinetic mechanisms of amyloid-β-(16–22) fibrillation
Keisuke Ikeda[1], Moe Yamazaki[1], Tomoshi Kameda[2], Hiroyuki Nakao[1], Minoru Nakano[1] ([1]*Fac. Pharm. Sci., Univ. Toyama*, [2]*AIST*)

1Pos058 アミロイド β ペプチドの凝集に対する NaCl 結晶の過渡的形成の影響
Effect of temporary NaCl crystal on the aggregation of amyloid β peptides
Masafumi Gushiken, Ikuo Kurisaki, Shigenori Tanaka (*Grad. Sch. system infomatics., Univ. Kobe*)

1Pos059 リン酸基で修飾したジルコニア粒子を用いた His タグタンパク質の精製
Purification of histidine-tagged proteins using phosphate-modified zirconia particles
Shogo Kanoh[1,2], Kentaro Shiraki[3], Momoyo Wada[2], Takeshi Tanaka[2], Msahiro Kitamura[4], Katsuya Kato[5], Atsushi Hirano[2] ([1]*Pure & Appl. Sci., Univ. Tsukuba*, [2]*NMRI, AIST*, [3]*Pure & Appl. Sci., Univ. Tsukuba*, [4]*NGK SPARK PLUG CO., LTD*, [5]*MMRI, AIST*)

1Pos060 ヘモグロビンの S 字型酸素結合曲線によるカメレオンモデルの協同性の研究
Testing cooperativity of chameleon model by sigmoidal oxygen binding curve of hemoglobin
Itsuki Yoshida, Tomoki P. Terada (*Dept. Appl. Phys., Grad. Sch. Eng., Nagoya Univ.*)

1Pos061 SARS-CoV-2 3CL プロテアーゼと基質ペプチドの結合解離過程の解析
Binding and unbinding kinetics of peptide substrate on SARS-CoV-2 3CL protease
Kei Moritsugu[1,2], Akinori Kidera[1] ([1]*Grad. Sch. Med. Life Sci., Yokohama City Univ.*, [2]*Grad. Sch. Sci., OMU*)

1Pos062 クモ糸タンパク質フィブロインのナノファイバーの単位構造の解明
A Unit Structure of Nanofiber composed of Spider Silk Protein Fibroin
Rakuri Aiba[1], Kento Yonezawa[2], Yusuke Okamoto[1], Haruya Kajimoto[1], Takehiro Sato[3], Yoichi Yamazaki[1], Sachiko Toma-Fukai[1], Hironari Kamikubo[1,2] ([1]*MS.,NAIST*, [2]*CDG., NAIST*, [3]*Spiber Inc.*)

1Pos063 フィブロインナノファイバーの違いによる延伸乾燥ハイドロゲルの特性の比較
Comparison of Properties of Stretch-Dried Hydrogels with Different Fibroin Nanofibers
Kenta Kimura[1], Kento Yonezawa[1,2], Yuki Nakatani[1], Satoru Onishi[1], Haruya Kajimoto[1], Takehiro Sato[3], Yoichi Yamazaki[1], Sachiko Toma-Fukai[1], Hironari Kamikubo[1,2] ([1]*NAIST ,MS*, [2]*NAIST, CDG*, [3]*Supiber inc*)

蛋白質：機能（反応機構 生物活性など）／Protein: Function

1Pos064 Role of the si-face Tyr of *Bacillus subtilis* ferredoxin-NADPH oxidoreductase in the enzyme-substrate interactions
Daisuke Seo (*Grad. Sch. Nat. Sci. Tec., Kanazawa Univ.*)

1Pos065 SOD1 への基質接近に対する静電ループと Arg143 の役割
Role of electrostatic loop and Arg143 on substrate approach to SOD1
Miu Nakamura[1], Yoshifumi Fukunishi[2], Juha Lintuluoto[3], Masami Lintuluoto[1] ([1]*Grad. Sch. Life and Environ. Sci., Kyoto Pref. Univ.*, [2]*AIST, CMB*, [3]*Grad. Sch. Eng., Kyoto univ.*)

1Pos066 Truncated mutant of the hemolytic lectin CEL-III revealed the interaction between protomer in hemolytic oligomer
Shuichiro Goda[1,2], Keisuke Fukumoto[1], Yuta Yamawaki[1], Hideaki Unno[1], Tomomitsu Hatakeyama[1] ([1]*Grad. Sch. Of Eng., Nagasaki Univ.*, [2]*GaLSIC, Soka Univ.*)

1Pos067 Effect of microtubule-binding proteins on microtubule flexural rigidity
Takuto Nakamichi, Kosuke Matsumura, Keiya Shimamori, Kohei Nishida, Kiyotaka Tokuraku, Masahiro Kuragano (*Grad. Sch. Eng., Muroran Inst. of Tech*)

1Pos068 Characterization of fibrous condensations of CAHS proteins from an anhydrobiotic tardigrade
Seiji Nishimura[1], Maho Yagi-Utumi[1,2,3], Kazuhiro Aoki[2,4], Kazuharu Arakawa[2,5], Koichi Kato[1,2,3] ([1]*Graduate School of Pharmaceutical Sciences, Nagoya City University*, [2]*Exploratory Research Center on Life and Living Systems (ExCELLS), National Institutes of Natural Sciences*, [3]*Institute for Molecular Science (IMS), National Institutes of Natural Sciences*, [4]*National Institute for Basic Biology (NIBB), National Institutes of Natural Sciences*, [5]*Institute for Advanced Biosciences, Keio University*)

1Pos069 微小管切断酵素カタニンの活性評価と高速 AFM による可視化
Biochemical characterization and high-speed AFM visualization of AAA ATPase Katanin
Hayato Shibuya[1], Noriyuki Kodera[2], Ikuko Hayashi[1] ([1]*Grad. Sch. of Med. Lif. Sci., Yokohama City Univ.*, [2]*NanoLS., Kanazawa Univ.*)

1Pos070 Target DNA binding dynamics of *Staphylococcus aureus* Cas9 as revealed by high-speed atomic force microscopy
Leonardo Puppulin[1,2], Junichiro Ishikawa[3], Hiroshi Nishimasu[3], Mikihiro Shibata[1,4] ([1]*Nano Life Science Institute (WPI-NanoLSI), Kanazawa University*, [2]*Kyoto Prefectural University of Medicine, Department of Pathology and Cell Regulation*, [3]*Structural Biology Division, Research Center for Advanced Science and Technology, The University of Tokyo*, [4]*Infinity for Frontier Science Initiative, Kanazawa University*)

1Pos071 Analysis of amyloid β aggregation inhibitory activities and cytotoxicity suppressing activities of mushroom extracts from Hokkaido
Tuya Gegen[1], Rina Sasaki[1], Enkhmaa Enkhbat[2], Masahiro Kuragano[1], Keiya Shimamori[1], Yoshiko Suga[2], Yuta Murai[2], Masaki Anetai[2], Kenji Monde[2], Kiyokata Tokuraku[1] ([1]*Division of Sustainable and Environmental Engineering, Muroran Institute of Technology*, [2]*Frontier Research Center for Advanced Material and Life Science, Faculty of Advanced Life Science, Hokkaido University*)

1Pos072 Escherichia coli inhibited amyloid β aggregation in a concentration-dependent manner
Sohta Katagiri, Na Zhu, Masahiro Kuragano, Kiyotaka Tokuraku (*Grad. Sch. Eng., Muroran Inst. of Tech.*)

1Pos073 機械学習を用いたペプチドの血圧降下活性の予測
Prediction of antihypertensive activity of peptides using machine learning
Kazushi Tamura, Yoshitaka Moriwaki, Tohru Terada, Kentaro Shimizu (*Grad. Sch. Agri. & Life Sci., Univ. Tokyo*)

蛋白質：計測・解析の方法論／Protein: Measurement & Analysis

1Pos074 回転拡散と並進拡散の解析による凝集性タンパク質の検出
Detection of protein aggregates using rotational and translational diffusion analysis
Riku Ando[1], Johtaro Yamamoto[2,3], Akira Kitamura[3], Nori Nakai[4], Sumio Terada[4], Masataka Kinjo[3] ([1]*Grad. Sch. Life Sci., Hokkaido Univ.*, [2]*Nat. Inst. Adv. Ind. Sci. & Tech.*, [3]*Fac. Adv. Life Sci., Hokkaido Univ.*, [4]*Grad. Sch. Med. & Dent. Sci., Tokyo Med. & Dent. Univ.*)

1Pos075 非発光タンパク質の発光酵素反応
Enzymatic luminous reaction of non-bioluminescent proteins
Ryo Nishihara[1,2], Kazuki Niwa[1], Tatsunosuke Tomita[1], Ryoji Kurita[1] ([1]*National Institute of Advanced Industrial Science and Technology (AIST)*, [2]*Japan Science and Technology Agency (JST), PRESTO*)

1Pos076 (1SBA-4) 3D structural determination of proteins from fluctuation X-ray scattering data
Wenyang Zhao[1], Osamu Miyashita[1], Florence Tama[1,2] ([1]*Center for Computational Science, RIKEN*, [2]*Grad. Sch. Sci., Univ. Nagoya*)

1Pos077 残基特異的な熱力学・速度論解析が明らかにするスペクトリン SH3 ドメインの共同性の低いフォールディング
Reduced cooperativity of spectrin SH3 domain folding revealed by combined per-residue thermodynamic and kinetic analysis
Seiichiro Hayashi[1], Daisuke Fujinami[2], Daisuke Kohda[1] ([1]*Med. Inst. Bioreg., Kyushu Univ*, [2]*Grad. Sch. Integr. Pharm. Nutr. Sci., Univ. Shizuoka*)

1Pos078 残基特異的 QFER（自由エネルギー 2 次関係）はスムーズな蛋白質折れ畳みを実現するコンシステンシー原理の数学的表現である
Residue-based Quadratic Free Energy Relationship is a Mathematical Formulation of the Consistency Principle of Protein Folding
Daisuke Kohda[1], Seiichiro Hayashi[1], Daisuke Fujinami[2] ([1]*Med. Inst. Bioreg., Kyushu Univ.*, [2]*Grad. Sch. Integr. Pharm. Nutr. Sci., Univ. Shizuoka*)

1Pos079 自由エネルギー摂動法を用いた VHH フレームワーク部位のアミノ酸配列最適化
In silico optimization of VHH framework sequence using free energy perturbation method
Kazuma Okada, Yasuhiro Matsunaga (*Grad. Sch. Sci. Eng., Saitama Univ.*)

1Pos080 新型コロナウイルス並びにインフルエンザウイルス A 型を検出するチオ NAD サイクリング ELISA 法の開発
Development of Thio-NAD Cycling ELISA for Detection of SARS-CoV-2 and Influenza Virus Type A
Yuta Kyosei[1], Sou Yamura[1], Mayuri Namba[1], Etsuro Ito[1,2] ([1]*Department of Biology, Waseda University*, [2]*Waseda Research Institute for Science and Engineering, Waseda University*)

1Pos081 gr Predictor：深層学習を活用したタンパク質水和分布の高速計算法
gr Predictor : An Efficient Method for Computing the Hydration Structure around Proteins using Deep Learning
Kosuke Kawama[1], Yusaku Fukushima[1], Mitsunori Ikeguchi[2,3], Masateru Ohta[3], **Takashi Yoshidome**[1] ([1]*Dep. of Appl. Phys., Tohoku Univ.*, [2]*Grad. Sch. of Med. Life Sci., Yokohama City Univ.*, [3]*RIKEN*)

1Pos082 タンパク質の局所構造の形状操作性に関するロボット工学的解析手法
Robotics-Based Method for Analyzing Shape Manipulability of Localized Protein Structures
Keisuke Arikawa (*Fcl. Eng., Kanagawa Inst. of Tech.*)

1Pos083 マルチチェイン/マルチドメインタンパク質の構造変化の解析法について
A method for analyzing structural changes of protein with multi-chains/multi-domains
Chigusa Kobayashi[1], Hisham Dokainish[2], Suyong Re[3], Takaharu Mori[2], Jaewoon Jung[1,2], Yuji Sugita[1,2,4] ([1]*RIKEN R-CCS*, [2]*RIKEN CPR*, [3]*NIBIOHN*, [4]*RIKEN BDR*)

1Pos084 Cryo-CLEM 法および Cryo-ET 法による糸状仮足先端の三次元構造観察
Observation of three dimensional structure of filopodial tips by Cryo-CLEM and Cryo-ET methods
Miho Nakafukasako[1], Tomoya Higo[1], Yuki Gomibuchi[2], Hiroko Takazaki[3], Yusuke V. Morimoto[2], Takayuki Kato[3], Takuo Yasunaga[2] ([1]*Grad. Sch. Comp. Sci. Syst. Eng., Kyushu Inst. Tech.*, [2]*Dept. of Phys. Info. Tech., Kyushu Inst. Tech.*, [3]*IPR, Univ. Osaka*)

1Pos085 タイムタグ光子測定方式によるナノ秒蛍光相関分光測定システムの開発
Development of the time-tag photon detection method of nanosecond fluorescence correlation spectroscopy
Yutaka Sano[1,2], Hiroyuki Oikawa[1,2], Satoshi Takahashi[1,2] ([1]*Institute of Multidisciplinary Research for Advanced Materials, Tohoku University*, [2]*Department of Chemistry, Graduate School of Science, Tohoku University*)

1Pos086 生細胞中の細胞質タンパク質 CRAF の二量体化状態および構造状態遷移に関する詳細解析
Detailed analyses of dimerization state and conformational state transitions of cytoplasmic protein CRAF in live cells
Kenji Okamoto, Yasushi Sako (*RIKEN CPR*)

1Pos087 ラマン分光法を用いたタンパク質相分離液滴の濃度と熱力学的性質の検討
Investigation of concentration changes and thermodynamic properties of a single phase-separated protein droplet using Raman microscopy
Kohei Yokosawa[1], Shinji Kajimoto[1,2], Takakazu Nakabayashi[1] ([1]*Grad. Sch. Pharm. Sci., Tohoku Univ.*, [2]*JST PRESTO*)

蛋白質：蛋白質工学／進化工学／Protein: Engineering

1Pos088 Algorithm and Neural Network-Based Design, and Experimental Evaluations of Antimicrobial Peptides
Je-Wen Liou[1,2,3], Te-Man Liu[2], Yu-Ren Chen[2], Chin-Hao Yang[1], Hemalatha Mani[3] ([1]*Department of Biochemistry, School of Medicine, Tzu Chi University, Hualien, Taiwan*, [2]*Department of Laboratory Medicine and Biotechnology, Tzu Chi University, Hualien, Taiwan*, [3]*Institute of Medical Sciences, Tzu Chi University, Hualien, Taiwan*)

1Pos089 Generation of microtubule superstructures by mimicking ciliary microtubule structures
Muneyoshi Ichikawa[1], Hiroshi Inaba[2], Yurina Sueki[2], Arif Md. Rashedul Kabir[3], Takashi Iwasaki[4], Hideki Shigematsu[5], Akira Kakugo[3], Kazuki Sada[3], Tomoya Tsukazaki[1], Kazunori Matsuura[2] ([1]*Div. of Biol. Sci., NAIST*, [2]*Grad. Sch. of Eng., Tottori Univ.*, [3]*Grad. Sch. of Chem. Sci. and Eng., Hokkaido Univ.*, [4]*Grad. Sch. of Agric. Sci., Tottori Univ.*, [5]*Struct. Biol. Div., Jap. Synchrot. Radiat. Res. Instit.*)

1Pos090 ウシ由来抗菌ペプチド BMAPs の大量発現系構築および機能・構造解析
Construction of an overexpression system and functional and structural analysis of bovine antimicrobial peptides BMAPs
Fumi Hirai[1], Mitsuki Shibagaki[2], Kotaro Tsukioka[1], Hao Gu[2], Tomoyasu Aizawa[1,2] ([1]*Sch. Sci., Hokkaido Univ.*, [2]*Grad. Sch. Life Sci., Hokkaido Univ.*)

1Pos091 ヘリックス–ループ–ヘリックスモチーフのヘリックス–ヘリックス角に着目したタンパク質複合体構造の計算機デザイン
Computational design of protein complexes focusing on the helix–helix angle of the helix-loop-helix motif
Marino Yamamoto, Naoya Kobayashi, Shun Hirota (*NAIST, Mat. Sci.*)

1Pos092 機械学習を組み合わせたファージ提示法による抗体断片の指向性進化
Machine-learning application for in vitro selection of antibody fragments from a phage display library
Sakiya Kawada[1], Yoichi Kurumida[2], Tomoyuki Ito[1], Thuy Duong Nguyen[2], Hikaru Nakazawa[1], Hafumi Nishi[3,4,5], Yutaka Saito[2,6,7,8], Tomoshi Kameda[2,8], Koji Tsuda[7,8,9], Mitsuo Umetsu[1,8] ([1]*Grad. Sch. Eng., Tohoku Univ.*, [2]*AIRC, AIST*, [3]*Grad. Sch. Information Sci., Tohoku Univ.*, [4]*ToMMo, Tohoku Univ.*, [5]*Fac. Core Res., Ochanomizu Univ.*, [6]*CBBD-OIL, AIST-Waseda Univ.*, [7]*Grad. Sch. Frontier Sci., The Univ. of Tokyo*, [8]*Adv. Intell. Pro., RIKEN*, [9]*MaDIS, NIMS*)

1Pos093 ファージ提示ライブラリーを用いた進化分子工学操作への機械学習利用による抗体様分子開発
Machine-learning-assisted molecular evolution with a phage display library of antibody mimetics
Tomoyuki Ito[1], Thuy Duong Nguyen[2], Yutaka Saito[2,3,4,5], Yoichi Kurumida[2], Hikaru Nakazawa[1], Sakiya Kawada[1], Hafumi Nishi[6,7,8], Koji Tsuda[4,5,9], Tomoshi Kameda[2,5], Mitsuo Umetsu[1,5] ([1]*Grad. Sch. Eng., Tohoku Univ.*, [2]*AIRC, AIST*, [3]*CBBD-OIL, AIST-Waseda Univ.*, [4]*Grad. Sch. Frontier Sci., The Univ. of Tokyo*, [5]*Adv. Intell. Pro., RIKEN*, [6]*Grad. Sch. Information Sci., Tohoku Univ.*, [7]*ToMMo, Tohoku Univ.*, [8]*Fac. Core Res., Ochanomizu Univ.*, [9]*MaDIS, NIMS*)

1Pos094 抗菌ペプチド α ディフェンシンの高濃度変性剤存在下における野生型ジスルフィド結合形成機構の解析
Mechanism of correct disulfide bonds formation of α-defensins in the presence of high concentrations of denaturing agents
Shinya Yoshino, Hiromichi Taguchi, Yi Wang, Yuchi Song, Weiming Geng, Shaonan Yan, Tomoyasu Aizawa (*Grad. Sch. Life Sci., Hokkaido Univ.*)

1Pos095 PD-1 アゴニスト開発に向けた PD-1 結合タンパク質の合理的設計
Rational design of PD-1 binding proteins to develop PD-1 agonists
Hirotaro Shimamura[1], Shunji Suetaka[2], Nao Sato[2], Yuuki Hayashi[2,3], Munehito Arai[1,2] ([1]*Dept. Phys., Univ. Tokyo*, [2]*Dept. Life Sci., Univ Tokyo*, [3]*Environmental Science Center, Univ. Tokyo*)

1Pos096 Analysis of receptor signaling using growth factor mutants designed by an in silico approach
Yuga Okada[1], Akihiro Eguchi[2], Daisuke Kuroda[3], Kohei Tsumoto[1], Ryosuke Ueki[1], Shinsuke Sando[1] ([1]*Grad. Sch. Eng., Univ. Tokyo*, [2]*Faculty of Health and Medical Sciences, University of Copenhagen.*, [3]*National Institute of Infectious Diseases, Ministry of Health, Labour, and Welfare.*)

1Pos097 NMR 解析に向けたマウス由来抗菌ペプチド cathelicidin, CRAMP(cathelicidin related anti-microbial peptide)の大腸菌を用いた大量発現系構築
Construction of an overexpression system of mouse-derived antimicrobial peptide cathelicidin, CRAMP in *E. coli* for NMR analysis
Kotaro Tsukioka[1], Waka Ueda[1], Humi Hirai[1], Mitsuki Shibagaki[2], Hao Gu[2], Tomoyasu Aizawa[3] ([1]*Sch.Sci.,Hokkaido Univ.*, [2]*Grad. Sch. Life Sci., Hokkaido Univ.*, [3]*Fac. Adv. Life Sci., Hokkaido Univ.*)

ヘム蛋白質／Heme proteins

1Pos098 ナノディスクに再構成した鉄還元膜タンパク質 CYB561D2 によって誘起される脂質過酸化の解析
Analysis of lipid peroxidation induced by iron-reducing membrane heme protein; CYB561D2 in nanodiscs
Aoi Yamaguchi, Motonari Tsubaki, Tetsunari Kimura (*Dept. of Chem., Grad Sch. of Sci., Kobe Univ.*)

1Pos099 プロテオリポソーム中における Higd1A によるシトクロム *c* 酸化酵素の活性増強機構
The positive regulation mechanism of cytochrome *c* oxidase by Higd1A in proteoliposome
Wataru Sato[1], Sachiko Yanagisawa[1], Kyoko Shinzawa-Itoh[1], Yuya Nishida[2], Takemasa Nagao[2], Yasunori Shintani[2], Minoru Kubo[1] ([1]*Grad. Sch. Sci., Univ. Hyogo*, [2]*Mol. Pharmacol., NCVC*)

1Pos100 酸素バリア性フィルムを利用した嫌気下での構造解析の試み
Attempt to structural analysis under anaerobic condition using oxygen barrier film
Takehiko Tosha[1], Kanji Shimba[2], Hiroaki Matsuura[1], Kunio Hirata[1], Masaki Yamamoto[1], Yoshitsugu Shiro[2] ([1]*RIKEN SPring-8*, [2]*University of Hyogo*)

膜蛋白質／Membrane proteins

1Pos101 LoCoMock: Log*P* によって補正されたスコアによるタンパク質-リガンド-膜複合体のドッキングシミュレーション
LoCoMock: Log*P*-corrected Membrane Docking Score Screens Protein-Ligand-Membrane Complexes
Rikuri Morita, Yasuteru Shigeta, Ryuhei Harada (*CCS, Univ. Tsukuba*)

1Pos102 γ 切断酵素と APP/Notch のドッキング過程の粗視可モデルシミュレーション研究
Coarse-grained model Simulation study of the docking process of γ-secretase and APP/Notch
Chika Minami, Lisa Matsukura, Naoyuki Miyashita (*Grad. Sch. BOST, KINDAI Univ.*)

1Pos103 遺伝子変異が引き起こす EGFR 動態変化の 1 分子解析
Single-molecule analysis of mutation induced changes in EGF receptor behavior
Michio Hiroshima[1,2], Masahiro Ueda[1,3] ([1]*RIKEN BDR*, [2]*RIKEN CPR*, [3]*FBS, Osaka Univ.*)

1Pos104 1 分子イメージングを用いた薬剤スクリーニング
Drug screening platform using single molecule imaging
Daisuke Watanabe[1,2], Michio Hiroshima[2], Masahiro Ueda[1,2] ([1]*FBS Osaka Univ*, [2]*RIKEN BDR*)

核酸結合蛋白質／Nucleic acid binding proteins

1Pos105 計算科学的に明らかにするホモ二量体チロシル tRNA 合成酵素（TyrRS）のハーフサイト活性
A Computational Study on the Half-Site Activity Mechanism of Homodimeric Tyrosyl tRNA Synthetase（TyrRS）
Yoshino Okamoto[1], Takunori Yasuda[2], Rikuri Morita[3], Yasuteru Shigeta[3], Ryuhei Harada[3] ([1]*College of biological sciences, University of Tsukuba*, [2]*Doctoral program in biology, University of Tsukuba*, [3]*Center for computational Sciences*)

1Pos106 Elucidation of nucleosome sliding mechanism in all-atom detail via MD simulations
Syed Hashim Shah, Giovanni Bruno Brandani, Shoji Takada (*Department of Biophysics, Graduate school of science, Kyoto University, Kyoto*)

1Pos107 PPRP の RNA からの解離機構のシミュレーション研究
Simulation study of the dissociation mechanism of the PPRP with RNA
Sumile Tanaka[1], Lisa Matsukura[1], Masaki Ottawa[2], Naoyuki Miyashita[1] ([1]*Grad. Sch. BOST., KINDAI Univ.*, [2]*Sch. Phys. Sci., GUAS*)

1Pos108 部分的にアンラップされたヌクレオソームからの、Nap1 による H2A/H2B 解離メカニズム
Nap1 dismantles a H2A/H2B dimer from a partially unwrapped nucleosome
Fritz Nagae, Shoji Takada, Tsuyoshi Terakawa (*Grad. Sch. Sci., Kyoto Univ.*)

核酸：構造・物性／Nucleic acid: Structure & Property

1Pos109 Simulation for the phase separation of DNA droplet with chemical reactions
Ryohei Furuichi[1], Tomoya Maruyama[2], Akihiro Yamamoto[1], Masahiro Takinoue[1,2] ([1]*School of Computing, Tokyo Institute of Technology*, [2]*School of Life Science and Technology, Tokyo Institute of Technology*)

1Pos110 ヌクレオソーム上を動く酵母 RNApolymerase Ⅱ の粗子化 MD シミュレーション
Coarse-grained MD simulations of an elongation process of yeast RNA Pol2 moving toward a nucleosome
Takafumi Yamauchi, Genki Shino, Shoji Takada (*Kyoto University*)

1Pos111 Mg イオンによるリボザイムのフォールディングとミスフォールディング機構
Mg-induced folding and misfolding of ribozymes
Naoto Hori[1], D Thirumalai[2] ([1]*School of Pharmacy, University of Nottingham*, [2]*Department of Chemistry, University of Texas at Austin*)

1Pos112 線形および環状 DNA の交流電場応答の直接観測
Dynamics of circular and linear DNA under AC electric fields
Yunosuke Fuji, Shin Takano, Seiwa Yamagishi, Yuuta Moriyama, Toshiyuki Mitsui (*Dept. Phys. Sch. Sci. Aogaku Univ.*)

1Pos113 染色体レオロジー特性を介した核内ストレス顆粒のポジショニング機構
Mechanisms of nuclear stress granule positioning in the nucleus via rheological properties of chromatin
Takuya Nara, Haruko Takahashi, Yutaka Kikuchi (*Graduate School of Integrated Sciences for Life, Hiroshima University*)

1Pos114 高分子の表面吸着問題から理解する分裂酵母の構成的ヘテロクロマチン形成
Essence of assembly of constitutive heterochromatin in fission yeast lies in surface adhesion of polymers?
Tetsuya Yamamoto[1], Takahiro Asanuma[2], Yota Murakami[3] ([1]*ICReDD, Hokkaido Univ.*, [2]*Grad. Sch. Chem. Sci. Eng., Hokkaido Univ.*, [3]*Dep. Chem, Fac. Sci., Hokkaido Univ.*)

1Pos115 クロマチンのもつ液滴の性質
Intrinsic liquid droplet property of chromatin
Kazuhiro Maeshima[1], Sachiko Tamura[1], Tatsuya Fukuyama[2], Yusuke Maeda[2] ([1]*National Institute of Genetics & SOKENDAI*, [2]*Department of Physics, Kyushu University*)

1Pos116 修飾核酸特有の低質量プロダクトイオンによる定量を行うソフトウェア
Software for Quantification with Low-mass Product Ions peculiar to Modified Nucleic Acids
Yuki Matsubara[1], Masami Koike[2], Yuko Nobe[3], Hiroko Tsuchida[2], Yasuto Yokoi[1], Masato Taoka[3], Hiroshi Nakayama[2] ([1]*Mitsui Knowledge Industry*, [2]*RIKEN CSRS*, [3]*Tokyo Metropolitan University*)

1Pos117 単分散 GUV を用いた濃度制御による DNA 凝集体の生成
GENERATION OF DNA CONDENSATES BY CONCENTRATION CONTROL IN MONODISPERSE GIANT UNILAMELLAR VESICLES
Ryotaro Yoneyama[1], Ryota Ushiyama[1], Tomoya Maruyama[2], Masahiro Takinoue[2,3], Hiroaki Suzuki[1] ([1]*Graduate School of Science and Engineering, Chuo University*, [2]*Life Science and Technology, Tokyo Institute of Technology*, [3]*Department of Computer Science, Tokyo Institute of Technology*)

核酸：相互作用・複合体／Nucleic acid: Interaction & Complex formation

1Pos118 microRNA の機能発現を 1 細胞 1 分子レベルで可視化する新規技術の開発
In situ single-molecule imaging of microRNA function
Hotaka Kobayashi[1,2] ([1]*JST PRESTO*, [2]*IQB, The University of Tokyo*)

1Pos119 *In silico* アプローチによるアプタマー-IgG 結合の熱力学的プロファイルの解析
In silico approach for identification of the thermodynamic profiles of aptamer-IgG binding
Ryoji Yamazaki[1], Azumi Ito[2], Tomoki Sakamoto[3,4], Masaki Komine[2], Takeshi Ishikawa[5], Masato Katahira[3,4], Takashi Nagata[3,4], Taiichi Sakamoto[2], Kenji Yamagishi[1] ([1]*Graduate School of Engineering Nihon University*, [2]*Faculty of Advanced Engineering Chiba Institute of Technology*, [3]*Graduate School of Energy Science Kyoto University*, [4]*Institute of Advanced Energy, Kyoto University*, [5]*Graduate School of Science and Engineering Kagoshima University*)

1Pos120 IgG に結合するアプタマーへの化学修飾の影響
Effect of chemical modification on the aptamer that binds to IgG
Azumi Ito[1], Yuuki Yatabe[1], Hisae Yoshida[2], Masahiro Sekiguchi[2], Kazumasa Akita[3], Yoshikazu Nakamura[3], Yusuke Nomura[4], Takeshi Ishikawa[5], Kenji Yamagishi[2], Taiichi Sakamoto[1] ([1]*Chiba Institute of Technology*, [2]*Nihon University*, [3]*Ribomic Inc.* , [4]*National Institute of Health Science*, [5]*Kagoshima University*)

1Pos121 (2SEP-2) 自由エネルギー地形から探る開始コドン認識機構
(2SEP-2) Computational Analysis of the Start Codon Recognition Mechanism Based on Free Energy Landscape
Takeru Kameda[1], Katsura Asano[2,3,4], Yuichi Togashi[1,5] ([1]*Coll. Life Sci., Ritsumeikan Univ.*, [2]*Div. Biol., Kansas State Univ.*, [3]*HiHA, Hiroshima Univ.*, [4]*Grad. Sch. Integ. Sci. Life, Hiroshima Univ.*, [5]*RIKEN BDR*)

1Pos122 ヌクレオソームから H2A-H2B2 量体が脱離する際の自由エネルギー曲線解析
Analysis of free energy curve of H2A-H2B dimer displacement from the nucleosome
Hisashi Ishida, Hidetoshi Kono (*Institute for Quantum Life Science, National Institutes for Quantum Science and Technology*)

1Pos123 細菌の翻訳開始前複合体における tRNA とリボソームタンパク質の相互作用に関する理論的考察
Theoretical investigation of the interactions between a tRNA and ribosomal proteins in bacterial translation pre-initiation complex
Yoshiharu Mori, Shigenori Tanaka (*Grad. Sch. Sys. Inf., Kobe Univ.*)

1Pos124 遠隔操作が可能な DNA 流体のマイクロ流制御
Microflow manipulation of DNA fluid with remote controllability
Hirotake Udono[1], Shin-ichiro Nomura M.[2], Masahiro Takinoue[1] ([1]*Sch. Comp., TiTech*, [2]*Grad. Sch. Eng., Tohoku Univ.*)

1Pos125 光ピンセットを用いたソレ効果による相分離ドロップレットの生成と DNA 濃縮 II
Generation of Phase Separated Droplet Induced by Soret Effect and DNA Enrichment by Optical Tweezers II
Mika Kobayashi, Yoshihiro Minagawa, Hiroyuki Noji (*Grad. Sch. of Eng., Univ. Tokyo*)

電子状態／Electronic state

1Pos126 一定終状態光電子収量分光法を用いたタンパク質薄膜の電子構造観察
Application of Constant Final State Photoelectron Yield Spectroscopy to Protein Films to Elucidate Their Occupied Electronic Structure
Masaki Tomita[1], Bera Sudipta[4], Ryotaro Nakazawa[1], Rio Ushiroda[1], Ichiro Ide[1], Cahen David[4], Hisao Ishii[1,2,3] ([1]*GSSE Chiba Univ*, [2]*CFS Chiba Univ*, [3]*MCRC Chiba Univ*, [4]*Weizmann Inst*)

1Pos127 電子線回折を利用した構造解析における電子状態を考慮した構造精密化
Structural refinement considering the electron orbitals in structural analysis using electron diffraction
Yasuhisa Honda, Keigo Takahira, Takuo Yasunaga (*Dept of Computer Science and Engineering, Kyushu Institute of Technology*)

1Pos128 酸化型[NiFe]ヒドロゲナーゼの生成経路と活性中心の電子・幾何構造についての理論的研究
Theoretical characterization of the active site and its formation pathway in oxidized [NiFe]-hydrogenase
Yuta Hori, Yasuteru Shigeta (*Center for Computational Sciences, Univ. Tsukuba*)

1Pos129 Scala 言語を用いた生体高分子計算科学ツール STCSB への量子化学計算機能の追加
Further development of STCSB, Scala Tool for the Computational Science of Biomolecules, to add a quantum- chemistry calculation module
Ryoutarou Matsuda, Mika Mitsumatsu, Itaru Onishi, Masayuki Irisa (*Kyushu Inst. of tech*)

発生・分化／Development & Differentiation

1Pos130 Continuum model for analyzing mechanical properties of *Dictyostelium* fruiting-body development
Seiya Nishikawa, Satoshi Kuwana, Hidenori Hashimura, Satoshi Sawai, Shuji Ishihara (*Grad. Sch. Arts & Sci., Univ. Tokyo*)

1Pos131 ゼブラフィッシュ自己組織化細胞塊における細胞挙動の解析
Characterization of cell dynamics in the process of self-organization in zebrafish explants
Momoka Tochizawa (*Dept. Phys. Sch. Sci. Aogaku Univ.*)

1Pos132 線虫の初期胚発生における力学モデル
Mechanical Model in Early Embryogenesis of C. elegans
Takehiro Kurihara[1], Toshikaze Chiba[1], Naohito Urakami[2], Kazunori Yamamoto[3], Akatsuki Kimura[4] ([1]*Soft Matter and Biophysics Lab., Department of Physics, Faculty of Science, Tohoku University*, [2]*Graduate School of Sciences and Technology for Innovation, Yamaguchi University*, [3]*Department of Applied Bioscience, Faculty of Applied Bioscience, Kanagawa Institute of Technology*, [4]*Cell Architecture Laboratory, Department of Chromosome Science, National Institute of Genetics*)

1Pos133 多細胞系の形態形成の近似モデルとしての細胞間相互作用の実効ポテンシャル
Effective mechanical potential of cell-cell interactions: approximated model for multicellular morphogenesis
Hiroshi Koyama, Toshihiko Fujimori (*Div. Embryology., Nat. Inst. Basic Biology*)

分子モーター／Molecular motor

1Pos134 好熱菌 F_oF_1-ATPase のユニサイト触媒作用の構造的基盤
Structural basis of unisite catalysis of thermophilic F_oF_1-ATPase
Momoko Aoyama[1], Atsuki Nakano[1], Jun-ichi Kishikawa[2], Ken Yokoyama[1] ([1]*Department of Molecular Biosciences, Kyoto Sangyo Univ.*, [2]*IPR, Osaka Univ.*)

1Pos135 祖先型 ATPase の作製と機能解析
Resurrection of the Ancestral ATPase
Aya Suzuki[1], Ryutaro Furukawa[1], Hiroshi Ueno[1], Satoshi Akanuma[2], Hiroyuki Noji[1] ([1]*Grad. Sch. Eng., Univ.Tokyo*, [2]*Fac. Human Sci., Waseda Univ*)

1Pos136 Rotation dynamics and structure of F1-ATPase with all α-subunit-type P-loops
Hiroshi Ueno[1], Meghna Sobti[4,5], Rie Koga[2], Tomoko Masaike[3], Alastair Stewart[4,5], Nobuyasu Koga[2], Hiroyuki Noji[1] ([1]*Grad. Sch. Eng., Univ. Tokyo*, [2]*ExCELLs, NINS*, [3]*Dept. Appl. Biol. Sci., Tokyo Univ. Sci.*, [4]*Mol. Struct. Comp. Biol. Div., The Victor Chang Cardiac Research Institute*, [5]*Facul. Med., UNSW Sydney*)

1Pos137 (2SFA-5) Plus and minus ends of microtubules respond asymmetrically to kinesin binding by a long-range directionally driven allosteric mechanism
Huong T Vu[1], Zhechun Zhang[2], Riina Tehver[3], Dave Thirumalai[4] ([1]*University of Warwick*, [2]*Harvard University*, [3]*Denison University*, [4]*University of Texas*)

1Pos138 Kinesin-1 および Kinesin-14 の In vitro 合成とデザイン
In vitro synthesis and design of kinesin-1 and kinesin-14
Daisuke Inoue[1], Ohashi Keisuke[2,3], Takasuka Taichi[2,3], Kakugo Akira[4] ([1]*Fac. Des., Kyushu Univ.*, [2]*Grad. Sch. Glo. Food Res., Hokkaido Univ.*, [3]*Res. Fac. Agr. , Hokkaido Univ.*, [4]*Fac. Sci., Hokkaido Univ.*)

1Pos139 A novel photochromic regulator inhibits kinesin Eg5 at the ADP sate in the ATPase cycle
Md Alrazi Islam[1], Kozue Satoh[2], Shinsaku Maruta[1,2] ([1]*Grad. Sch. Sci & Eng., Soka Univ.*, [2]*Grad. Sch. Sci & Eng., Soka Univ.*)

1Pos140 野生型と疾患関連変異型で構成されるヘテロダイマー KIF1A(キネシン-3)の二足歩行運動モデル
A bipedal walking model for heterodimeric motors composed of wild-type KIF1A and disease-associated KIF1A
Tomoki Kita[1], Kazuo Sasaki[1], Shinsuke Niwa[2,3] ([1]*Grad. Eng., Tohoku Univ.*, [2]*Grad. Life. Sci., Tohoku Univ.*, [3]*FRIS., Tohoku Univ.*)

1Pos141 How does giraffe kinesin cope with the long distance axonal transport?
Taketoshi Kambara[1], Daisuke Taniguchi[2], Tomoya Mukai[3], Yasushi Okada[1,2,3,4,5] ([1]*BDR, RIKEN*, [2]*IRCN, Univ. Tokyo*, [3]*Grad. Sch. Sci., Univ. Tokyo*, [4]*Grad. Sch. Med., Univ. Tokyo*, [5]*UBI, Univ. Tokyo*)

1Pos142 QCM 測定による周波数変化から測定したアクトミオシン滑り運動の機構
Sliding mechanism of actomyosin motility assay measured from frequency change by QCM
Honoka Kobayashi, Naoki Matsumoto, Taiki Nishimura, Yuki Sakurai, Kaho Yokomuro, Kazuya Soda, Ikuko Fujiwara, Hajime Honda (*Dept. of Matl. Sci. and Bioeng., Nagaoka Univ. of Tech*)

1Pos143 QCM 上でのアクトミオシンの滑走速度と周波数変化の関係
The relation between sliding velocities and frequency changes of actomyosin on the QCM
Taiki Nisimura[1], Naoki Matumoto[1], Honoka Kobayasi[2], Yuuki Sakurai[1], Kaito Kobayasi[1], Kaho Yokomuro[1], Ikuko Hujiwara[2], Hajime Honda[2] ([1]*Dept. of Bioeng., Nagaoka Univ. of Tech.*, [2]*Dept. of Matl. Sci. and Bioeng., Nagaoka Univ. of Tech.*)

1Pos144 鞭毛内輸送を行うダイニンがどのように歩行する微小管を選択するのかに関する粗視化 MD 研究
Coarse-grained MD study on the function of dynein in selecting walking microtubules
Shintaroh Kubo[1,2], Huy Bui Khanh[2] ([1]*Grad. Sch. Med., The Univ. of Tokyo*, [2]*Dept. Anatomy and Cell Biol., McGill Univ.*)

1Pos145 Discovery of the fastest myosin, its amino acid sequence, and structural features
Takeshi Haraguchi[1], Masanori Tamanaha[1], Kano Suzuki[2], Kohei Yoshimura[1], Takuma Imi[1], Motoki Tominaga[3,4], Hidetoshi Sakayama[5], Tomoaki Nishiyama[6], Takeshi Murata[2], Kohji Ito[1] ([1]*Dept. of Bio. Sci., Grad. Sch. of Sci and Eng., Univ. of Chiba*, [2]*Dept. of Che. Sci., Grad. Sch. of Sci and Eng., Univ. of Chiba*, [3]*Grad. Sch. Adv. Sci. and Eng., Univ. Waseda*, [4]*Fac. Educ. Integrated Arts. Sci., Bio., Univ. Waseda*, [5]*Dept. of Bio. Sci., Grad. Sch. of Sci., Univ. of Kobe*, [6]*Adv. Sci. Res. Ctr., Univ. of Kanazawa*)

1Pos146 バクテリアのべん毛モーターは減速機を持つか？
Does bacterial flagellar motor have a reduction drive?
Ryota Iino[1,2] ([1]*IMS, NINS*, [2]*SOKENDAI*)

1Pos147 高度好塩菌アーキアの回転モーターのステップ状回転の検出
Detection of stepwise rotation of the archaellar motor in *Haloferax volcanii*
Yoshiaki Kinosita, Jun Ando, Tastuya Iida, Rikiya Watanabe (*Molecular Physiology Lab, RIKEN*)

1Pos148 Cryo-EM structure analysis of the PomAB complex, a bacterial flagellar stator of sodium-driven motor in *Vibrio alginolyticus*
Tatsuro Nishikino[1], Norihiro Takekawa[2], Jun-ichi Kishikawa[1], Mika Hirose[1], Seiji Kojima[3], Michio Homma[3], Takayuki Kato[1], Katsumi Imada[2] ([1]*IPR., Osaka Univ.*, [2]*Dept. of Macromol. Sci., Grad. Sch. of Sci., Osaka Univ.*, [3]*Div. Biol. Sci. Grad. Sch. Sci., Nagoya Univ.*)

1Pos149 バクテリアの膜電位揺らぎの解析手法の開発
Development of a method for analyzing membrane potential fluctuations in bacterial cells
Kenta Takemori, Yusuke V. Morimoto (*Fac, Comp. Sci. and Sys. Eng., Kyushu Inst. Tech*)

1Pos150 分子動力学シミュレーションによる SMC 蛋白質の DNA によって刺激される ATPase 活性の分子機構解明
Molecular Dynamics Simulations to Reveal Molecular Mechanism of DNA-Stimulated ATPase Activity of SMC Proteins
Masataka Yamauchi, Tsuyoshi Terakawa, Giovanni B. Brandani, Shoji Takada (*Dept. of Biophysics, Grad. of Sci., Kyoto Univ.*)

1Pos151 除膜クラミドモナス細胞の巨大リポソームへの封入
Encapsulation of demembranated *Chlamydomonas* cell into giant liposomes
Koichiro Akiyama, Syunsuke Shiomi, Masahito Hayashi, Tomoyuki Kaneko (*Frontier Bioscience, Hosei Univ.*)

細胞生物学的課題（接着，運動，骨格，伝達，膜）／Cell biology

1Pos152 リゾチームアミロイド線維との接触に対する運動するアクチン線維の応答
Response of a moving actin filament to a contact with a lysozyme amyloid fibril
Kuniyuki Hatori, Ryusei Murata, Kazuto Mima (*Dep. Mech. Eng., Yamagata Univ.*)

1Pos153 細胞配置換えの分子基盤の解明
Elucidating molecular basis of cell rearrangement
Keisuke Ikawa[1], Kaoru Sugimura[2] ([1]*Grad. Sch. Sci., Nagoya Univ.*, [2]*Grad. Sch. Sci., Univ. Tokyo*)

1Pos154 ウニ胚の細胞骨格分布極性に起因する外腸胚形成
Exogastrulation due to cytoskeletal polarity distribution in sea urchin embryo
Kaichi Watanabe[1], Yuhei Yasui[1], Yuta Kurose[2], Naoaki Sakamoto[1], Akinori Awazu[1] ([1]*Grad. Sch. Int., Univ. Hiroshima*, [2]*Grad. Sch. Sci., Univ. Hiroshima*)

1Pos155 アクチンとミオシン細胞骨格の組織化によって細胞質のカイラルな回転流が生まれる
Chiral cytoplasmic flow emerging from the spatial organization of actin and myosin cytoskeleton
Takaki Yamamoto, Tomoki Ishibashi, Sylvain Hiver, Mitsusuke Tarama, Yuko Mimori-Kiyosue, Masatoshi Takeichi, **Tatsuo Shibata** (*RIKEN BDR*)

1Pos156 サルモネラ菌の感染時におけるアクチン細胞骨格動態の顕微力学解析
Micromechanical analysis of actin cytoskeleton dynamics during the *Salmonella* infection
Hiroaki Kubota[1], Togo Shimozawa[2], Kai Kobayashi[1], Morika Mitobe[1], Jun Suzuki[1], Kenji Sadamasu[1] ([1]*Dept. Microbiol., Tokyo Metropolitan Institute of Public Health*, [2]*Sch. Sci., Univ. Tokyo*)

1Pos157 K^+-induced decrease in the matrix pH of mitochondria
Jannatul Naima[1,2], Yoshihiro Ohta[1] ([1]*Department of Biotechnology and Life Science, Tokyo University of Agriculture and Technology*, [2]*Department of Pharmacy, University of Chittagong, Bangladesh*)

1Pos158 RacGAP 因子 FilGAP は腎ポドサイトの細胞-基質接着と突起形成を制御する
FilGAP, a GAP for Rac1, controls cell-extracellular matrix adhesion and process formation of kidney podocytes
Koji Saito[1], Seiji Yokawa[1], Sari Mizuta[1], Kanae Tada[1], Moemi Oda[1], Hiroyasu Hatakeyama[2], Noriko Takahashi[2], Hidetake Kurihara[3], Yasutaka Ohta[1] ([1]*Division of Cell Biology, Department of Biosciences, School of Science, Kitasato University*, [2]*Department of Physiology, School of Medicine, Kitasato University*, [3]*Department of Physical Therapy, Faculty of Health Sciences, Aino University*)

1Pos159 パターン化モデル生体膜上でのアクチンのネットワーク形成
Actin network assembly on a patterned model membrane
Yosuke Yamazaki[1], Yuri Miyata[2], Kenichi Morigaki[2,3], Makito Miyazaki[1,4,5,6] ([1]*Dept. Phys., Kyoto Univ.*, [2]*Grad. Sch. Agr., Kobe Univ.*, [3]*Biosignal, Kobe Univ.*, [4]*Hakubi Ctr., Kyoto Univ.*, [5]*PRESTO, JST*, [6]*Inst. Curie*)

1Pos160 細胞中のジュール熱産生
Joule heat production in cells
Tetsuichi Wazawa, Kai Lu, Takeharu Nagai (*SANKEN, Osaka Univ*)

1Pos161 Highly conserved GYXLI motif of FlhA is directly involved in hierarchical flagellar protein export in *Salmonella*
Tohru Minamino[1], Miki Kinoshita[1], Keiichi Namba[1,2] ([1]*Grad. Sch. Frontier Biosci., Osaka Univ.*, [2]*RIKEN SPring-8*)

1Pos162 Aberrant shape formation of fission yeast spheroplasts under microfluidic conditions
Hironori Sugiyama[1], Yuhei Goto[1,2,3], Kazuhiro Aoki[1,2,3] ([1]*ExCELLS, NINS*, [2]*NIBB, NINS*, [3]*Sch. Life Sci., SOKENDAI*)

1Pos163 赤外線レーザー照射中の心筋細胞シートの伝導変化
Changes in conduction of cardiomyocyte sheet during infrared laser irradiation
Kentaro Kito, Masahito Hayashi, Tomoyuki Kaneko (*Frontier Bioscience, Grad. Sch. Sci. & Eng., Hosei Univ.*)

1Pos164 好中球様細胞に分化させた HL-60 細胞のケモタキシスにおけるミトコンドリア関連タンパク質の役割
Roles of mitochondria associated protein in chemotaxis of neutrophil-like differentiated HL-60 cells
Yuichi Mazaki[1], Tsunehito Higashi[1], Yasuhito Onodera[2] ([1]*Dept. Cell. Pharm., Grad. Sch. Med., Hokkaido Univ*, [2]*Glb. Ctr. Biomed. Sci. Eng., Fac. Med., Hokkaido Univ*)

1Pos165 Trans-dimer conformations of full-length ectodomains of Celsr cadherin in solution visualized using high-speed atomic force microscopy
Shigetaka Nishiguchi[1], Rinshi Kasai[2], Takayuki Uchihashi[1,3,4] ([1]*ExCELLS*, [2]*iGCORE, Gifu Univ.*, [3]*Nagoya Univ.*, [4]*iGCORE, Nagoya Univ.*)

1Pos166 アミロイドβ凝集体はヒト脳微小血管内皮細胞の異常なアクチンの組織化と細胞死を誘発する
Amyloid-β aggregates induce abnormal actin organization and death of human brain microvascular endothelial cell
Keiya Shimamori[1], Yushiro Take[2], Yusaku Chikai[1], Yukina Kuroraki[1], Masahiro Kuragano[1], Kiyotaka Tokuraku[1] ([1]*Grad. Sch. of Eng., Muroran Inst. of Tech.*, [2]*Ohkawara Neurosurgical Hospital*)

1Pos167 酸素消費を伴わないミトコンドリア電子伝達機構
Mitochondrial electron transfer mechanism without oxygen consumption
Marino Neda[1], Hinako Tanaka[1], Emika Shida[1], Yoshihiro Ohta[2] ([1]*Department of Biotechnology and Life Sciences, Graduate school of Engineering, Tokyo University of Agriculture and Technology*, [2]*Department of Biotechnology and Life Sciences, Associate Professor, Tokyo University of Agriculture and Technology*)

1Pos168 局所加熱法を用いた表皮細胞内変異型ケラチンフィラメント熱ストレス応答の経時変化解析
Time-course analysis of mutant keratin filament dynamics in cultured epidermal cells under thermal stress using a local heating method
Masato Kaya[1,2], Hideki Itoh[4], Yoshie Harada[2,3], E. Birgitte Lane[4], Madoka Suzuki[2] ([1]*Department of Biological Sciences, Graduate School of Science, Osaka University*, [2]*Institute for Protein Research, Osaka University*, [3]*Center for Quantum Information and Quantum Biology, Osaka University*, [4]*Skin Research Institute of Singapore*)

1Pos169 シグナル伝達機構解明のための巨大細胞利用
Use of giant cells to study cell-cell signaling mechanisms
Yukihisa Hayashida, Yusuke Morimoto (*Kyushu Institute of Technology (Grad. Sch. Comp. Sci. and Sys. Eng., Kyushu Inst. Tech)*)

1Pos170 べん毛のロッド-フック型タンパク質の輸送順序
Transport order of the flagellar rod-hook type proteins
Reika Igarashi, Norihiro Takekawa, Katsumi Imada (*Dept. Macromol. Sci., Grad. Sch. Sci., Osaka Univ.*)

1Pos171 無傷のミトコンドリアの単離・保存法の検討
Methods for isolating and preserving intact mitochondria
Asaka Ogihara, Arima Okutani, Wataru Uchiumi, Miki Kanatani, Yoshihiro Ohta (*Department of Biotechnology and Life Sciences, Graduate school of Engineering, Tokyo University of Agriculture and Technology*)

1Pos172 アミロイド β の凝集が細胞の集合に与える影響の解析
Analysis of the effect of amyloid β aggregation on cell assembly
Ayaka Ota, Masahiro Kuragano, Kiyotaka Tokuraku (*Grad. Sch. Eng., Muroran Inst. of Tech.*)

1Pos173 Theoretical studies on macrophase separation in systems composed of two solutes and one solvent using a solvent-free coarse-grained model
Yuki Norizoe, Naoki Iso, Takahiro Sakaue (*Department of Physical Sciences, Aoyama Gakuin University*)

1Pos174 自発運動する細胞の興奮系 Ras を抑制する GAP の同定
Identification of GAP that suppresses the excitatory Ras in spontaneous cell motility
Guangyu Cheng[1], Satomi Matsuoka[1,2,3], Masahiro Ueda[1,2,3] ([1]*Grad. Sch. Sci., Osaka University*, [2]*Grad. Sch. of Front. Biosci., Osaka University*, [3]*BDR, RIKEN*)

1Pos175 マイコプラズマ・モービレの滑走方向は細胞体の非対称な形状と相関がある
Gliding direction of *Mycoplasma mobile* correlates with asymmetric configuration of the cell body
Kana Suzuki[1], Daisuke Nakane[2], Azusa Kage[1], Takayuki Nishizaka[1] ([1]*Dept. Physics, Gakushuin Univ.*, [2]*Univ. of Electro-Communications*)

1Pos176 Direct observation of the functional dynamics by which CAP1 interacts with F-actin and cofilin by high-speed AFM
Phuong Doan N. Nguyen[1], Hiroshi Abe[2], Shoichiro Ono[3], Noriyuki Kodera[4] ([1]*Grad. Sch. NanoLS., Kanazawa Univ.*, [2]*Dept. Biol., Chiba Univ.*, [3]*Dept. Pathol. & Cell Biol., Emory Univ.*, [4]*WPI-NanoLSI, Kanazawa Univ.*)

1Pos177 細胞の自発運動において Ras 興奮系のノイズ強度の最適化にスフィンゴミエリン代謝系が関与する
Noise generation by sphingomyelin metabolism optimizes Ras excitability for cell migration
Dayoung Shin[1,2], Hiroaki Takagi[2,3], Michio Hiroshima[2], **Satomi Matsuoka**[1,2,4], Masahiro Ueda[1,2,4] ([1]*Grad. Sch. Sci., Osaka Univ.*, [2]*BDR, RIKEN*, [3]*Sch. Med., Nara Med. Univ.*, [4]*Grad. Sch. Frontier Biosci., Osaka Univ.*)

1Pos178 TIRF 観察によるアクチン線維に対するサイトカラシン D の作用理解
Inhibitory mechanism of cytochalasin D on actin by TIRF observations
Takahiro Mitani[1], Hikaru Empuku[2], Shuichi Takeda[3], Ikuko Fujiwara[2], Hajime Honda[2] ([1]*Dept. of Bioeng., Nagaoka Univ. of Tech.*, [2]*Dept. of Matl. Sci. and Bioeng., Nagaoka Univ. Tech.*, [3]*Okayama Univ., RIIS*)

1Pos179 極性形成に関わる膜タンパク質 Frizzled の細胞間隙での蛍光 1 分子観察
Single molecule observation of polarity-related membrane proteins at the cell-cell interface; immobilization and accumulation of Frizzled
Rinshi Kasai[1], Yuri Nemoto[2] ([1]*iGCORE, Gifu Univ.*, [2]*OIST*)

1Pos180 Bottom-up strategy による軸糸の屈曲波の再構築
Reconstitution of the axonemal beating by bottom-up strategy
Isabella Guido[1], Kenta Ishibashi[2], Hitoshi Sakakibara[2], Andrej Vilfan[3], Eberhard Bodenschatz[1], Ramin Golestanian[1], **Kazuhiro Oiwa**[2,4] ([1]*MPI. Dynamics Self-Organization*, [2]*Adv. ICT Res. Inst., NICT*, [3]*Jozef Stefan Inst.*, [4]*Grad. Sch. Sci., Univ. Hyogo*)

1Pos181 Anomalous dynamics of cardiomyocytes and fibroblasts on PDMS substrate
Arata Nagai, Kaito Kojima, Ryu Kidokoro, Shota Nozaki, Ayu Sasaki, Yuuta Moriyama, Toshiyuki Mitsui (*Dept. Phys. Sch. Sci. Aogaku Univ.*)

1Pos182 ミトコンドリア電子伝達系複合体の時間依存的酸化ダメージの検出
Detection of time-dependent oxidative damages of mitochondrial electron transfer complexes
Shizuku Saito, Yoshihiro Ohta (*Department of Biotechnology and Life Science, Graduate school of Engineering, Tokyo University of Agriculture and Technology*)

1Pos183 回転方向に依存した大腸菌べん毛モーターの回転揺らぎの原因
Investigation for the cause of rotational fluctuations depending on the rotational direction of flagellar motor
Kazumi Akahoshi, Yumiko Uchida, Yong-Suk Che, Akihiko Ishijima, Hajime Fukuoka (*Grad. Sch. Frontier Biosci. Osaka Univ*)

1Pos184 酵母ミトコンドリアの膜電位変動観察の試み
Observation of membrane potential fluctuations of yeast mitochondria
Sora Maekawa, Yoshihiro Ohta (*Department of Biotechnology and Life Sciences, Graduate school of Engineering, Tokyo University of Agriculture and Technology*)

1Pos185 デスミンフィラメントとアクチンフィラメントとの相互作用の観察
Observation of the interaction between single desmin filaments and single actin filaments in a reconstituted motility system
Takumi Ishizaka, Kuniyuki Hatori (*Grad. Sch. Sci. Eng., Yamagata Univ.*)

1Pos186 1 粒子観察による細胞外小胞の細胞選択的結合の分子機構解明
Molecular mechanisms of selective binding of small extracellular vesicles to recipient cells as revealed by single-particle imaging
Tatsuki Isogai[1], Koichiro M. Hirosawa[2], Miki Kanno[3], Ayano Syo[4], Yasuhiko Kizuka[2,5], Yasunari Yokota[6], Kenichi G. N. Suzuki[2,5] ([1]*UGSAS, Gifu Univ.*, [2]*iGCORE, Gifu Univ.*, [3]*Grad. Sch. Nat. Sci. Tech., Gifu Univ.*, [4]*Dept. App. Bio. Sci., Gifu Univ.*, [5]*CREST, JST*, [6]*Dept. Eng., Gifu Univ.*)

生体膜・人工膜：構造・物性／Biological & Artificial membrane: Structure & Property

1Pos187 Morphology of Adhering Vesicles
Toshikaze Chiba[1], Hironori Sugiyama[2], Taro Toyota[3], Yuka Sakuma[1], Masayuki Imai[1], Primož Ziherl[4,5] ([1]*Department of Physics, Tohoku University*, [2]*ExCELLS, National Institutes of Natural Sciences*, [3]*Department of Basic Science, Graduate School of Arts and Sciences, The University of Tokyo*, [4]*Faculty of Mathematics and Physics, University of Ljubljana*, [5]*Jožef Stefan Institute*)

1Pos188 基板支持リン脂質積層膜の軟 X 線直線偏光による相状態解析
Soft X-ray polarization analysis of lipid order for phospholipid multilayers supported on hydrophilic surfaces
Shin-ichi Wada[1,2], Masataka Tabuse[1] ([1]*Grad. Sch. Adv. Sci. Eng., Hiroshima Univ.*, [2]*HiSOR, Hiroshima Univ.*)

1Pos189 薬剤代謝におけるコレステロールの役割を探るためのモデル生体膜と薬剤の相互作用研究：リン脂質 POPE/コレステロール/クロルゾキサゾン系
A model biomembrane study on the role of cholesterol in cytochrome P450 drug metabolism: POPE/cholesterol/ chlorzoxazone systems
Shosei Kano, **Hiroshi Takahashi** (*Grad. Sch. Sci. Tech., Gunma Univ.*)

1Pos190 薬物添加による血液脳関門モデル膜の膜厚変化に関する X 線回折研究：スフィンゴミエリンの役割
An X-ray diffraction study of changes in the blood-brain barrier model membrane thickness induced by adding drugs : role of sphingomyelin
Anna Ajima, Hiroshi Takahashi (*Grad. Sch. Sci. Tech., Gunma Univ.*)

1Pos191 パターン化人工膜へのエクソソーム導入技術の開発
Reconstitution of exosomes into a patterned model membrane
Yu Yoshimura[1], Ayane Sugimachi[1], Fumio Hayashi[2], Koichiro M. Hirosawa[3], Rinshi S. Kasai[3], Kenichi G. N. Suzuki[3], Kenichi Morigaki[1,4] ([1]*Grad. Sch. Agri., Kobe Univ.*, [2]*Grad. Sch. Sci., Kobe Univ.*, [3]*iGCORE, Gifu Univ.*, [4]*Biosignal Research Center, Kobe Univ.*)

1Pos192 Laurdan の時間分解蛍光解析法からみる脂質膜水和状態
Lipid-Surrounding Hydration States Probed by Time-Resolved Emission Spectra of Laurdan
Nozomi Watanabe[1], Keishi Suga[2], J. Peter Slotte[3], Thomas K. M. Nyholm[3], Hiroshi Umakoshi[1]
([1]*Graduate School of Engineering Science, Osaka University*, [2]*Graduate School of Engineering, Tohoku University*, [3]*Faculty of Science and Engineering, Åbo Akademi University*)

生体膜・人工膜：ダイナミクス／Biological & Artificial membrane: Dynamics

1Pos193 エクソソーム評価系としてのブラウン運動解析
Brownian motion analysis as an exosome evaluation system
Kei Takahashi, Yui Miyabayashi, Takuo Yamaki (*CellSource Co., Ltd.*)

1Pos194 細胞質型ホスホリパーゼ A_2 活性化とセラミド 1-リン酸の膜動態の関連性
Relationship between the membrane dynamics of ceramide 1-phosphate domains and the activation of cytosolic phospholipase A_2
Tomokazu Yasuda[1,2], Daiki Ueura[1], Madoka Nakagomi[2], Shinya Hanashima[1], J Peter Slotte[3], Michio Murata[1] ([1]*Graduate School of Science, Osaka University,*, [2]*Research Foundation Itsuu Laboratory*, [3]*Åbo Akademi University*)

1Pos195 浸透圧下の巨大リポソームでの抗菌ペプチド・マガイニン 2 のポア形成とその進化
Antimicrobial peptide magainin 2 (Mag)-induced pore formation and its evolution in single GUVs under osmotic pressure (Π)
Md. Masum Billah[1], Samiron Kumar Saha[1], Masahito Yamazaki[1,2,3] ([1]*Grad. Sch. Sci. Tech., Shizuoka Univ.*, [2]*Res. Inst. Ele., Shizuoka Univ.*, [3]*Grad. Sch. Sci., Shizuoka Univ.*)

1Pos196 酸性アミノ酸の側鎖長を調整することによる環状ペプチドの pH 依存性膜透過性の制御
Control of pH-dependent membrane permeation of cyclic peptides by adjusting side chain length of acidic amino acids
Motomi Matsuda, Keisuke Ikeda, Minoru Nakano, Hiroyuki Nakao (*Grad. Sch. Med. Phar. Sci., Univ. Toyama / Japanese*)

1Pos197 粗視化陰溶媒脂質力場、iSoLF、を用いて GENESIS による多成分脂質システムの分子動力学シミュレーション
Extension of the Implicit Solvent Lipid Force Field, iSoLF, for the simulation of large multi-component lipidic systems using GENESIS
Diego Ugarte[1], Shoji Takada[2], Yuji Sugita[1,3,4] ([1]*Computational Biophysics Research Team, RIKEN R-CCS*, [2]*Dept. Biol., Sch. Sci., Kyoto Univ.*, [3]*Laboratory for Biomolecular Function Simulation, RIKEN BDR*, [4]*Theoretical Molecular Science Laboratory, RIKEN CPR*)

1Pos198 一定張力による GUV 中のポア形成に対する脂質成分や分布の効果
Effect of lipid composition and distribution on constant tension-induced pore formation in GUVs
Kanta Tazawa[1], Junichi Higuchi[1], Masahito Yamazaki[1,2,3] ([1]*Grad. Sch. Sci., Shizuoka Univ*, [2]*Res. Inst. Ele., Shizuoka Univ.*, [3]*Grad. Sch. Sci. Tech., Shizuoka Univ.*)

生体膜・人工膜：興奮・チャネル／Biological & Artificial membrane: Excitation & Channels

1Pos199 Design and characterization of enzyme-responsive synthetic ion channels
Iiro Kiiski[1], Nanami Takeuchi[1], Alexandre Legrand[2], Reiko Sakaguchi[3], Kenji Usui[4], Shuhei Furukawa[2], Ryuji Kawano[1] ([1]*Tokyo University of Agriculture and Technology*, [2]*Kyoto University*, [3]*University of Occupational and Environmental Health*, [4]*Konan University*)

1Pos200 膜水系における環状人工イオンチャネルの QM/MM シミュレーション
QM/MM simulations of cyclic artificial ion channel in membrane-water system
Mayuko Nakagawa[1], Toru Ekimoto[1], Tsutomu Yamane[2], Kohei Sato[3], Kazushi Kinbara[3], Mitsunori Ikeguchi[1,2] ([1]*Dept. of Med. Life Sci., Yokohama City Univ.*, [2]*R-CCS, Riken*, [3]*Sch. of Life Sci. and Tech., Tokyo Inst. of Tech.*)

1Pos201 CBB 法を用いた再構成膜でのアクアポリン 6 のイオン透過特性の解析
Ion conducting properties of Aquaporin 6 reconstituted in the contact bubble bilayer
Takahisa Maki[1], Shigetoshi Oiki[2], Masayuki Iwamoto[1] ([1]*Dept. Mol. Neurosci., Facul. Med. Sci., Univ. Fukui*, [2]*Biomed. Imaging Res. Center, Univ. Fukui*)

1Pos202 アガロースゲルビーズを用いた人工膜チャネル電流測定
An artificial lipid bilayer ion-channel recording method using agarose gel beads
Mami Asakura[1], Atsuya Mukuno[1], Minako Hirano[2], Toru Ide[2] ([1]*Fac. Eng., Okayama Univ.*, [2]*Grad. Sch. Health Sys., Okayama Univ.*)

生体膜・人工膜：輸送・情報伝達／Biological & Artificial membrane: Transport & Signal transduction

1Pos203 リポソーム内タンパク質機能発現制御のための膜透過性ペプチドの利用
Use of Cell penetrating peptide for the regulation of protein functional expression in giant unilamellar vesicles
Akari Miwa, Koki Kamiya (*Grad. Sch. Sci. Tech., Gunma Univ.*)

1Pos204 Development of DNA nanostructures that function as artificial channel/transducer on a giant vesicle membrane
Shoji Iwabuchi[1], Yusuke Sato[2], Ibuki Kawamata[1,3], Satoshi Murata[1], Shin-ichiro Nomura[1] ([1]*Tohoku University*, [2]*Kyushu Institute of Technology*, [3]*Ochanomizu University*)

1Pos205 Membrane Permeability of Mono-Amino Acids Estimated by Planar Lipid Bilayer System
Kaiyi Zheng, Kayano Izumi, Ryuji Kawano (*Department of Biotechnology and Life Science, Tokyo University of Agriculture and Technology, Japan*)

1Pos206 分子動力学計算による CLC^F における F^-輸送機構の解析
F^- export mechanism in CLC^F using molecular dynamics simulations
Akihrio Nakamura[1,2], Takashi Tokumasu[2], Takuya Mabuchi[2,3] ([1]*Graduate School of Engineering, Tohoku University*, [2]*Institute of Fluid Science, Tohoku University*, [3]*Frontier Research Institute for Interdisciplinary Sciences, Tohoku University*)

1Pos207 筋小胞体 Ca ポンプのヘリックス M2 と M6 の Ca 輸送における役割
Role of M2 and M6 helices of sarcoplasmic reticulum Ca pump in Ca transport
Takashi Daiho (*Asahikawa Med. Univ. Biochemistry*)

1Pos208 PI3K シグナル伝達は S-G2 期の ERK の時間的調節において重要な役割を果たす
PI3K signaling plays a critical role in the temporal regulation of ERK in the S-G2 phase
Ryo Yoshizawa, Nobuhisa Umeki, Yasushi Sako (*Wako Inst., Riken*)

1Pos209 ペプチドナノディスクを用いた光受容体ロドプシンのパターン化モデル生体膜への再構成
Reconstitution of photoreceptor rhodopsin into a patterned model membrane using peptide nanodisc
Masato Koezuka[1], Fuko Kueda[2], Fumio Hayashi[3], Kenichi Morigaki[2,4] ([1]*Fac. Agri., Kobe Univ.*, [2]*Grad. Sch. Agri., Kobe Univ.*, [3]*Grad. Sch. Sci., Kobe Univ.*, [4]*Biosignal Research Center, Kobe Univ.*)

1Pos210 色素再構成系を用いたシアノバクテリオクロム型光受容体の光変換機構の解析
Analysis of the photoconversion mechanism of cyanobacteriochrome-class photosensors using in vitro reconstitution approach
Takaaki Matsushita, Toshihiko Eki, Yuu Hirose (*Toyohashi Univ. of Tech*)

1Pos211 Thermodynamic and kinetic factors affecting the redox chemistry of a flavin cofactor in photolyases
Yuhei Hosokawa, Hiroyoshi Morita, Mai Nakamura, Shigenori Iwai, Junpei Yamamoto (*Grad. Sch. Eng. Sci., Osaka Univ.*)

1Pos212 ロドプシンクラスター上における G 蛋白質トランスデューシンの高速 AFM による 1 分子動態観察
Single molecule observation of G protein transducin on rhodopsin cluster by high-speed AFM
Hayato Yamashita[1], Akihiro Tsuji[1], Fumio Hayashi[2], Kenichi Morigaki[3,4], Masashi Fujii[5,6], Akinori Awazu[5,6], Kazuhiko Hoshikaya[1], Masayuki Abe[1] ([1]*Grad. Sch. Eng. Sci., Osaka Univ.*, [2]*Grad. Sch. Sci., Kobe Univ.*, [3]*Grad. Sch. Agr. Sci., Kobe Univ.*, [4]*Biosignal Research Center, Kobe Univ.*, [5]*Grad. Sch. Sci., Hiroshima Univ.*, [6]*Grad. Sch. Int., Hiroshima Univ.*)

1Pos213 繊毛型光受容細胞で機能するオプシンにおける収斂的な対イオン変位
Convergent evolutionary counterion displacement of ciliary opsins
Kazumi Sakai, Hiroki Ikeuchi, Chihiro Fujiyabu, Yasushi Imamoto, **Takahiro Yamashita** (*Grad. Sch. of Sci., Kyoto Univ.*)

1Pos214 光サイクル型視覚ロドプシンを用いた細胞内 cAMP 濃度の一過的変化誘導
Transient induction of intracellular cAMP level changes using photocyclic visual rhodopsin
Kazumi Sakai, Shion Aoki, Takahiro Yamashita (*Grad. Sch. Sci., Kyoto Univ.*)

1Pos215 新奇微生物ロドプシン・ベストロドプシンのユニークな発色団レチナール異性化特性
Unique chromophore isomerization properties of a novel microbial rhodopsin bestrhodopsin
Takashi Nagata[1], Yuma Kawasaki[1], Masae Konno[1,2], Yujiro Nagasaka[1], Mako Aoyama[3], Kota Katayama[2,3], Andrey Rozenberg[4], Igor Kaczmarczyk[5], Donna Matzov[5], Moran Shalev-Benami[5], Oded Béjà[4], Hideki Kandori[3], Keiichi Inoue[1] ([1]*ISSP, Univ. Tokyo*, [2]*PRESTO, JST*, [3]*Nagoya Inst. Tech.*, [4]*Technion–Israel Inst. Tech.*, [5]*Weizmann Inst. Sci.*)

1Pos216 新規微生物ロドプシン *Sm*ChR のイオン透過性
Ion permeability of the novel microbial rhodopsin *Sm*ChR
Yo Yamashita[1], Shoko Hososhima[1], Suneel Kateriya[2], Hideki Kandori[1], Satoshi Tsunoda[1] ([1]*Nagoya Institute of Technology*, [2]*Laboratory of Optobiology, Jawaharlal Nehru University, India*)

1Pos217 (2SCA-2) Conversion of light-driven outward proton pump rhodopsin into inward proton pump
Maria Del Carmen Marin Perez[1], Masae Konno[1,2], Himoru Yawo[1], Keiichi Inoue[1] ([1]*ISSP, Univ. Tokyo*, [2]*PRESTO, Japan Science and Technology Agency*)

1Pos218 宿主由来のレチナールを利用する共生細菌 Saccharibacteria 由来 Type-1 ロドプシンの分子特性
Molecular properties of Type-1 rhodopsin from Saccharibacteria that may use host-derived all-*trans* retinal
Masae Konno[1,2], Alexander L. Jaffe[3], Yuma Kawasaki[1], Chihiro Kataoka[4], Oded Béjà[5], Hideki Kandori[4,6], Jillian F. Banfield[7,8,9], Keiichi Inoue[1] ([1]*The Institute for Solid State Physics, The University of Tokyo*, [2]*PRESTO, Japan Science and Technology Agency*, [3]*Department of Plant and Microbial Biology, University of California*, [4]*Department of Life Science and Applied Chemistry, Nagoya Institute of Technology*, [5]*Faculty of Biology, Technion-Israel Institute of Technology*, [6]*OptoBioTechnology Research Center, Nagoya Institute of Technology*, [7]*Innovative Genomics Institute, University of California*, [8]*Department of Earth and Planetary Science, University of California*, [9]*Department of Environmental Science, Policy, and Management, University of California*)

1Pos219 高熱安定性光駆動型内向き H^+ポンプロドプシンにおける熱安定性要因の研究
Study on the factors contributing to the high thermal stability of thermostable light-driven inward H^+ pump rhodopsins
Yuma Kawasaki[1], Masae Konno[1,2], Keiichi Inoue[1] ([1]*ISSP, Univ. Tokyo*, [2]*JST・さきがけ*)

1Pos220 多様な温度環境に分布するプロトンポンプ型ロドプシンの熱力学的性質の網羅的解析
Comprehensive thermodynamic analysis for microbial proton pump rhodopsins identified in various temperature environments
Ryouhei Ohtake[1], Kaori Kondo[1], Makoto Demura[2], Takashi Kikukawa[2], Takashi Tsukamoto[2] ([1]*Graduate School of Life Science, Hokkaido University*, [2]*Faculty of Advanced Life Science, Hokkaido University*)

1Pos221 光駆動 Na^+/H^+ハイブリッドポンプ型ロドプシン KR2 における N112 変異体のプロトン選択的ポンプ機構の研究
Study of proton-selective pumping mechanism of N112 mutants in light-driven Na^+/H^+ hybrid pump-type rhodopsin KR2
Yuki Ichikawa[1], Yuji Furutani[1,2] ([1]*Graduate School of Engineering, Nagoya Institute of Technology*, [2]*OptoBio, Nagoya Institute of Technology*)

1Pos222 Time-resolved cryo-Raman study of Na^+ uptake and release by a sodium pumping rhodopsin from *Indibacter alkaliphilus*
Tomotsumi Fujisawa[1], Kouta Kinoue[1], Ryouhei Seike[1], Takashi Kikukawa[2], Masashi Unno[1] ([1]*Fac. Sci. Eng., Saga Univ.*, [2]*Fac. Adv. Life Sci., Hokkaido Univ.*)

光生物：光合成／Photobiology: Photosynthesis

1Pos223 励起子電荷分離混成が酸素発生型光合成を駆動する
Exciton-charge transfer mixing drives oxygenic photosynthesis
Yusuke Yoneda[1,2,3], Eric A. Arsenault[1,2], Shiun-Jr Yang[1,2], Kaydren Orcutt[1,2], Masakazu Iwai[1,2], Graham R. Fleming[1,2] ([1]*University of California, Berkeley*, [2]*Lawrence Berkeley National Laboratory*, [3]*Institute for Molecular Science*)

1Pos224 遠赤色光に適応した光化学系 I の光捕集における Chlorophyll-*f* と Red-Chlorophyll の役割に関する理論的研究
Theoretical study on the role of Chlorophyll-*f* and Red-Chlorophyll in light-harvesting mechanism in far-red light adapted photosystem I
Yuka Nakamura, Mikihito Okochi, Shigeru Itoh, Akihiro Kimura (*Grad. Sch. Sci., Nagoya Univ.*)

1Pos225 Electrostatic charge controls spectral properties and thermal stabilities of LH1-RCs from triply extremophilic *Halorhodospira halochloris*
Yukihiro Kimura[1], Kazuna Nakata[1], Shingo Nojima[1], Shinji Takenaka[1], Michael T. Madigan[2], Zheng-Yu Wang-Otomo[3] ([1]*Department of Agrobioscience, Graduate School of Agriculture, Kobe University*, [2]*Department of Microbiology, Southern Illinois University*, [3]*Faculty of Science, Ibaraki University*)

1Pos226 フェムト秒ポンプ・プローブ分光法によるヘリオバクテリア反応中心におけるカロテノイドの励起エネルギー移動解析
Analysis of excitation energy transfer of carotenoids in the reaction center of heliobacteria with femto-second pump-probe spectroscopy
Risa Kojima[1], Masatoshi Kida[2], Daisuke Kosumi[3], Hirozo Oh-oka[1,4] ([1]*CELAS, Osaka Univ.*, [2]*Grad. Sch. Sci. & Tech., Kumamoto Univ.*, [3]*IINa, Kumamoto Univ.*, [4]*Grad. Sch. Sci., Osaka Univ.*)

1Pos227 FTIR monitoring of photosynthetic quinone transport in the light-harvesting 1 reaction center complexes from purple bacteria
Yosuke Nakamoto[1], Rikako Kishi[1], Shinji Takenaka[1], Michael T. Madigan[2], Kenji V. P. Nagashima[3], Zheng-Yu Wang-Otomo[4], Yukihiro Kimura[1] ([1]*Department of Agrobioscience, Graduate School of Agriculture, Kobe University*, [2]*Department of Microbiology, Southern Illinois University*, [3]*Research Institute for Integrated Science, Kanagawa University*, [4]*Faculty of Science, Ibaraki University*)

1Pos228 Wavelength-Dependent Optical Response of Single Photosynthetic Antenna Complexes from Siphonous Macrogreen Alga *Codium fragile*
Tatas H. P. Brotosudarmo[1,2], Bernd Wittmann[1], Soichiro Seki[3], **Ritsuko Fujii**[3,4], Jürgen Köhler[1] ([1]*Spectrosc. Soft Matter, Univ. Bayreuth, Germany*, [2]*Dept. Food Tech., Univ. Ciputra, Surabaya, Indonesia*, [3]*Grad. Sch. Sci., Osaka City Univ., Japan*, [4]*ReCAP., Osaka Metropolitan Univ., Japan*)

1Pos229 クロロフィル *f* を含む光化学系 I の近赤外光による反応メカニズム解明を目指した蛍光バンドの帰属
Assignment of fluorescence bands of chlorophyll-f containing photosystem I to elucidate its reaction mechanism by near-infrared light
Rin Taniguchi[1], Toshiyuki Shinoda[2], Tatsuya Tomo[2], Shen Ye[1], Yutaka Shibata[1] ([1]*Department of Chemistry, Graduate School of Science, Tohoku University*, [2]*Department of Biology, Faculty of Science, Tokyo University of Science*)

1Pos230 緑色硫黄細菌の光合成反応中心複合体の表在性タンパク質の結合は PscB が足場となる
PscB is the scaffold for binding of other water-soluble subunits to the photosynthetic reaction center complex of green sulfur bacteria
Tomomi Inagaki, Kazuki Terauchi, Chihiro Azai (*Grad. Sch. Life Sci., Ritsumeikan Univ.*)

1Pos231 極性カロテノイドの結合性向上を目指したシフォナス緑藻の光合成アンテナの in-vitro 再構成
Enhancement of polar-carotenoid binding in in-vitro reconstitution of a photosynthetic light-harvesting complex from siphonous green alga
Hikari Takakura[1], Naoko Norioka[2], Naohiro Oka[3], Soichiro Seki[1], Hideaki Tanaka[2,4], Genji Kurisu[2,4], Ritsuko Fujii[1,5] ([1]*Grad. Sch. Sci., Osaka City Univ.*, [2]*Inst. Protein Res., Osaka Univ.*, [3]*BRIC., Tokushima Univ.*, [4]*Grad. Sch. Sci., Osaka Univ.*, [5]*ReCAP., Osaka Metropolitan Univ.*)

光生物：光遺伝学・光制御／Photobiology: Optogenetics & Optical Control

1Pos232 Ras photocontrol by regulatory factor GAP modified with azobenzene derivative.
Rajib Ahmed, Nobuyuki Nishibe, Natsuki Yamamura, Kazunori Kondo, Shinsaku Maruta (*Department of Biosciences, Graduate School of Science and Engineering Soka University, Hachioji, Tokyo.*)

1Pos233 藍色光を吸収するチャネルロドプシン KnChR のイオン選択性と光遺伝学
Ion selectivity and optogenetics application of a deep blue absorbing channelrhodopsin
Satoshi Tsunoda[1,2], Rintaro Tashiro[1], Shoko Hososhima[1,2], Hideki Kandori[1,2] ([1]*Nagoya Institute of Technology, Department of Life Science and Applied Chemistry*, [2]*Nagoya Institute of Technology, OptoBioTechnology Research Center*)

1Pos234 G タンパク質 βγ サブユニット依存的イオンチャネル応答を選択的に駆動する無脊椎動物オプシン
An invertebrate opsin functionally biased for Gβγ-dependent ion channel responses
Hisao Tsukamoto[1], Yoshihiro Kubo[2] ([1]*Department of Biology, Kobe University*, [2]*Department of Molecular Physiology, National Institute for Physiological Sciences*)

1Pos235 微生物型ロドプシンの吸収波長とプロトン移動の制御機構
Regulation of absorption wavelength and proton transfer in microbial rhodopsins
Masaki Tsujimura[1], Hiroshi Ishikita[1,2] ([1]*Grad. Sch. Eng., Univ. Tokyo*, [2]*RCAST., Univ. Tokyo*)

1Pos236 Photocontrol of chromatin remodelers Snf2 and BRG1 as an ATP driven molecular motor by photoresponsive protein Dronpa
Choi Eunji[1], Ziyun Zhang[1], Shinya Watanabe[2], Kazunori Kondo[1], Shinsaku Maruta[1] ([1]*Grad. Sch. Sci., Univ. Soka*, [2]*Med. Sch., Univ. Massachusetts*)

1Pos237 QM/MM 分子シミュレーションによる光活性化酵素 OaPAC の研究
Study on photoactivated enzyme OaPAC by QM/MM molecular simulation
Masahiko Taguchi, Shun Sakuraba, Justin Chan, Hidetoshi Kono (*Inst. Quant. Life Sci., QST*)

生命の起源・進化／Origin of life & Evolution

1Pos238 Cationic Polyester Microdroplets as RNA-containing Protocells
Tony Z Jia[1,2], Niraja V. Bapat[1,3], Ajay Verma[3], Irena Mamajanov[1], H. James Cleaves II[1,2], Kuhan Chandru[4] ([1]*Earth-Life Science Institute, Tokyo Institute of Technology*, [2]*Blue Marble Space Institute of Science*, [3]*Department of Biology, Indian Institute of Science Education and Research*, [4]*Space Science Centre (ANGKASA), Institute of Climate Change, National University of Malaysia*)

1Pos239 DNA 相互作用を用いたコアセルベート間でのタンパク質輸送
DNA-Mediated Protein Shuttling between Coacervate-Based Artificial Cells
Tsuyoshi Mashima[1], Jan van Hest[2], Luc Brunsveld[2] ([1]*NAIST*, [2]*Eindhoven Univ. Tech.*)

1Pos240 ベシクルの自己生産: 人工ミニマルセルのボトムアップなデザイン
Reproduction of Vesicles: The Bottom-up Design for Synthetic Minimal Cell
Minoru Kurisu[1], Peter Walde[2], Yuka Sakuma[1], Masayuki Imai[1] ([1]*Dept. Physics, Grad. Sch. Sci., Tohoku Univ.*, [2]*ETH Zurich*)

1Pos241 配列情報と連携したベシクル膜の成長：進化可能なミニマルセルを目指して
Vesicle membrane growth coupled with sequence information: toward evolvable minimal cell
Ryosuke Katayama, Minoru Kurisu, Yuka Sakuma, Masayuki Imai (*Grad. Sch. Sci., Tohoku Univ.*)

1Pos242 Formation of self-growing artificial cell droplets in aqueous two-phase separation system by internal amplification of nucleic acids
Yoshihiro Minagawa, Moe Yabuta, Hiroyuki Noji (*Department of Applied Chemistry, Graduate School of Engineering, The University of Tokyo.*)

1Pos243 細胞モデル進化における表現型拘束に起因した交差耐性
Cross-resistance induced by phenotypic constraint in a cell model evolution
Takuya Sato[1], Kunihiko Kaneko[2] ([1]*RIKEN, BDR*, [2]*Niels Bohr Institute*)

ゲノム生物学：ゲノム機能／Genome biology: Genome function

1Pos244 Coarse-grained modeling of Nanog gene locus: Towards understanding enhancer-promoter communication
Soundhara Rajan Gopi[1], Giovanni Brandani[1], Cheng Tan[2], Jaewoon Jung[2,3], Chenyang Gu[1], Azuki Mizutani[1], Chigusa Kobayashi[2], Hiroshi Ochiai[4,5], Yuji Sugita[2,3,6], Shoji Takada[1] ([1]*Department of Biophysics, Graduate School of Science, Kyoto University, Kyoto 606-8502, Japan*, [2]*Computational Biophysics Research Team, Riken Center for Computational Science, Kobe 650-0047, Japan*, [3]*Theoretical Molecular Science Laboratory, RIKEN cluster for Pioneering Research, Saitama 351-0198, Japan*, [4]*Program of Mathematical and Life Sciences, Graduate School of Integrated Sciences for Life, Hiroshima University, Higashi-Hiroshima, Hiroshima 739-8511, Japan*, [5]*Genome Editing Innovation Center, Hiroshima University, Higashi-Hiroshima, Hiroshima 739-8511, Japan*, [6]*Laboratory for Biomolecular Function Simulation, RIKEN center for Biosystems Dynamics Research, Kobe 650-0047, Japan*)

1Pos245 Biochemical fractionation separating open and compact chromatin based on local assembly of adjacent nucleosomes
Satoru Ishihara (*Fujita Health Univ. Sch. Med.*)

1Pos246 **1 分子イメージングで迫るヒト染色体の凝縮機構**
Single molecule imaging unveils human chromosome condensation
Kayo Hibino[1,2,3], Yuji Sakai[4], Masato Kanemaki[1,2], Kazuhiro Maeshima[1,2] ([1]*NIG*, [2]*SOKENDAI*, [3]*JST, PRESTO*, [4]*Inst. LiMe, Kyoto Univ.*)

生命情報科学：分子進化／Bioinformatics: Molecular evolution

1Pos247 HDV ゲノムの分子進化における二次構造の制約の解析
Constraint of Base Pairing on HDV Genome Evolution
Saki Nagata, Ryoji Kiyohara, Hiroyuki Toh (*Grad. Sch. of Sci. Tech., KGU*)

1Pos248 GPCR 間相互作用ペア予測手法の改善
Improvement of a method to predict interacting GPCR-GPCR pairs
Aoi Fukushima[1], Hiroaki Teruse[2], Sakie Shimamura[1], Hiroyuki Toh[2], Wataru Nemoto[1] ([1]*Dept. Sch. & Tech., Tokyo Denki Univ.*, [2]*Dept. of Sci. & Tech., Kwanseigakuin Univ.*)

1Pos249 Chiral selectivity mechanism on aminoacylation of an RNA minihelix studied by quantum mechanics/molecular mechanics simulations
Tadashi Ando (*Dep. of Appl. Elec., Tokyo Univ. of Sci.*)

1Pos250 **光ピンセットを用いた fL リアクタ回収技術の開発**
Development of new DNA recovery technology from fL droplet array using optical tweezers
Tetsuya Ohashi, Hiroshi Ueno, Yoshihiro Minagawa, Hiroyuki Noji (*Department of Applied Chemistry, Univ. Tokyo*)

1Pos251 **深層生成モデル CM-VAE を用いた RNA ファミリー人工配列生成**
CM-VAE: a generative model for designing artificial members of RNA family
Shunsuke Sumi[1,2], Michiaki Hamada[2], Hirohide Saito[2] ([1]*Center for iPS Cell Research and Application, Kyoto University*, [2]*Graduate School of Advanced Science and Engineering, Waseda University*)

生態／環境／Ecology & Environment

1Pos252 **人工的微生物複合系において観察された機能的安定性と不安定性**
Functional stability and instability observed in engineered microbial complex systems
Rei Ikeda[1], Koki Amano[1], Masahiro Honjo[2], Nobuhiro Takahashi[1], Kenshi Suzuki[3], Futoshi Kurisu[4], Motohiko Kimura[1], Yosuke Tashiro[1], Hiroyuki Futamata[5] ([1]*Department of Applied Chemistry and Biochemical Engineering, Graduate School of Engineering, Shizuoka University*, [2]*Graduate School of Science and Technology, Shizuoka University*, [3]*Microbial Ecotechnology, Department of Biotechnology, Graduate School of Agricultural and Life Sciences, The University of Tokyo*, [4]*Research Center for Water Environment Technology, School of Engineering, The University of Tokyo*, [5]*Research Institution of Green Science and Technology, Shizuoka University*)

1Pos253 Diversity of swimming endurance and foraging strategy in marine bacteria
Kyosuke Takabe[1], Yiyun Zhang[2], Katsuki Hara[2], Tomohiro Hirayama[2], Yutaka Yawata[1,3] ([1]*Faculty of Life and Environmental Sciences, University of Tsukuba*, [2]*Master's Program in Agro-Bioresources Science and Technology, University of Tsukuba*, [3]*Microbiology Research Center for Sustainability, University of Tsukuba*)

1Pos254 北海道南部産ダルス内の PE 量に光が与える影響
Effect of light on the amount of PE in dulse from southern Hokkaido
Yukiko Sawayama, Yuzuka Takahashi, Rio Fukuda, Hibiki Nakamura (*HAKURYO High School attached to Hakodate University*)

数理生物学／Mathematical biology

1Pos255 3 次元形態形成を表す隣接細胞間ネットワークモデル
Simulating Three-Dimensional Epithelial Morphogenesis: A Network Model Based on the Interactions Between Adjacent Cells
Tomohiro Mimura, Yasuhiro Inoue (*Grad. Sch. Eng.,Univ. Kyoto*)

1Pos256 空間的局所相互作用を伴う動的可塑的ネットワーク系の自発的構造形成
Spontaneous Network Organizations of Dynamic-Plastic Network System with Spatial Local Interactions
Taito Nakanishi (*Grad. Sch. Int., Univ. Hiroshima*)

1Pos257 乳がんの転移に関連するオントロジーグループに基づいた遺伝子相関ネットワーク解析による予後予測
Prognosis prediction of breast cancer by gene correlation network analysis based on Gene Ontology terms involved in metastasis
Ayaka Yakushi[1], Masahiro Sugimoto[2], Takanori Sasaki[1] ([1]*Fac. Adv. Math. Sci., Meiji Univ.*, [2]*Tokyo Med. Univ*)

1Pos258 種内多型から テントウムシの模様形成メカニズムを予測する
Prediction of the pattern formation mechanism in ladybirds from polymorphism
Ryo Takeda (*Grad.sch.Sci.,Univ.Osaka*)

1Pos259 大腸菌走化性応答における細胞内シグナル伝達のデータ駆動によるモデル構築
Data-driven model construction of intracellular signal transduction in E. coli chemotaxis response
Hiroto Tanaka, Yasuaki Kazuta, Hiroaki Kojima (*Frontier Research Lab, Adv ICT Res Inst, NICT*)

1Pos260 混雑下での分子の構造変化を考慮した反応拡散モデル
A reaction-diffusion model considering the conformational change of molecules and crowded states
Masaki Okada[1], Yuichi Togashi[2,3] ([1]*Grad. Sch. of Integr. Sci. for Life, Hiroshima Univ.*, [2]*Coll. Life Sci., Ritsumeikan Univ.*, [3]*Riken BDR*)

1Pos261 細胞の遺伝子発現制御における学習過程
Learning processes in gene-expression regulation
Tomoyuki Yamaguchi (*Research Institute, Nozaki Tokushukai Hospital*)

1Pos262 細胞集団運動における界面張力の効果
Interface Tension Effect on Collective Cell Migration
Katsuyoshi Matsushita, Taiko Arakaki, Naoya Kamamoto, Maki Sudo, Koichi Fujimoto (*Dep. Bio. Sci., Osaka Univ.*)

非平衡・生体リズム／Nonequilibrium state & Biological rhythm

1Pos263 筋芽細胞集団が示す位相欠陥と収縮性流れの幾何的制御
Geometric control of topological defects and contractile flow in confined myoblast cell populations
Ryo Ienaga[1], Yusuke Maeda[1], Kazusa Beppu[2] ([1]*Grad. Sch. Sci.Phys., Univ. Kyushu*, [2]*Applied Phys., Univ. Aalto*)

1Pos264 ヒト iPS 細胞由来ニューロンの神経突起伸長過程における形態変化の数理解析とタンパク質凝集体発現の観察
Analysis of morphological change and observation of protein aggregations in the developmental process of neurites of iPSC-derived neurons
Narumi Maeda[1], Rio Hine[1], Yudai Kitayama[2], Yusuke Shibasaki[1], Yuka Shirakawa[3], Minoru Saito[1,2,3] ([1]*Grad. Sch. of Integ. Bas. Sci., Nihon Univ.*, [2]*Coll. Hum. Sci., Nihon Univ.*, [3]*Nat. Inst., Coll. Hum. Sci., Nihon Univ.*)

1Pos265 解糖系の振動現象に及ぼす飢餓処理の影響
Effect of starvation on the glycolytic oscillation in yeast cells
Keiya Goto[1], Seiji Hatano[1], Noboru Nagata[1], Yutetsu Kuruma[2], Masayuki Imai[1] ([1]*Grad. Sch. Sci., Tohoku Univ.*, [2]*Japan Agency for Marine-Earth Science & Technology*)

1Pos266 Neuro2a 細胞の神経突起伸長過程における形態変化のリアルタイム数理解析
Real-time mathematical analysis of morphological change in the developmental process of neurites of Neuro2a cells
Rio Hine[1], Narumi Maeda[1], Yudai Kitayama[2], Yusuke Shibasaki[3], Yuka Shirakawa[3], Minoru Saito[1,2,3] ([1]*Grad. Sch. of Integ. Bas. Sci., Nihon Univ.*, [2]*Coll. Hum. Sci., Nihon Univ.*, [3]*Nat. Inst., Coll. Hum. Sci., Nihon Univ.*)

1Pos267 結合 BZ 反応の系の光応答性とその同期現象
Photoresponsivity and synchronization of coupled BZ reaction systems
Ryota Yamazaki[1], Sigeru Sakurazawa[2] ([1]*Grad. Sch., Future Univ. Hakodate, Systems Information Science*, [2]*Future Univ. Hakodate, School of systems information science, Department of complex and intelligent systems*)

1Pos268 上皮細胞の集団運動とペアリング秩序転移
Collective motion and pairing order transition of confined epithelial cells
Kazuyuki Shigeta[1], Kazusa Beppu[1], Aya Tanaka[2], Yusuke Maeda[1] ([1]*Dept. Phys. Kyushu Univ.*, [2]*NTT BRL, BMC*)

計測／Measurements

1Pos269 補償光学系と機械学習を用いて 1 分子輝点の 3 次元座標を精度良く計測する方法のシミュレーション研究
A simulation study to measure precisely three-dimensional coordinates of single molecule images using adaptive optics and machine learning
Xiang Zhou, Yuma Ito, **Makio Tokunaga** (*Sch. Life Sci. Tech., Tokyo Tech*)

1Pos270 細胞内ナノドメインにおける分子ダイナミクスの精密な測定を可能にする一粒子追跡手法の開発
A novel single-particle tracking system for precise measurement of molecular dynamics in intracellular nanodomains
Shinkuro Kobayashi, Shigeyuki Namiki, Daisuke Asanuma, Kenzo Hirose (*Grad. Sch. Med., Univ. Tokyo*)

1Pos271 Live prediction with image-based deep learning accesses temporal variability of single-cell transcriptomic states
Tobias Frick[1,2], Katsuyuki Shiroguchi[2] ([1]*Osaka University, Graduate School of Frontier Biosciences (FBS)*, [2]*RIKEN Center for Biosystems Dynamics Research (BDR)*)

1Pos272 聴覚の末梢器官である内耳蝸牛の感覚上皮振動に含まれる直流動作の検出と分析
Analyses of the sound-evoked nanoscale offset motion in the cochlea of the inner ear
Takeru Ota[1], Hiroshi Hibino[1,2] ([1]*Grad. Sch. Med., Univ. Osaka*, [2]*AMED-CREST, AMED*)

1Pos273 気液界面を用いた細胞メカニクス解析技術の開発
Development of gas-liquid interface-based cell mechanics analysis technology
Masaki Moriyama[1], Naoya Ishizawa[1], Ryo Kobayashi[1], Seri Hayashi[1], Makiko Takubo[1], Kaede Yokoyama[1], Masataka Murakami[1], Tetsuro Hoshino[1], Akio Iwasa[1], Masafumi Mimura[1], Hirohide Murai[2], Taichi Nakamura[2], Kiyoshi Nozaki[1], Shuhei Tanaka[1] ([1]*Nikon Corporation*, [2]*Nikon Systems Inc.*)

1Pos274 ラマンイメージングによる老化細胞のラベルフリー検出
Label-free detection of senescent cells by Raman imaging
Hiroko Kodama[1], Ren Shibuya[2], Shinji Kajimoto[1,2,3], Takakazu Nakabayashi[1,2] ([1]*Faculty of Pharmaceutical Sciences, Tohoku Univ.*, [2]*Graduate School of Pharmaceutical Sciences, Tohoku Univ.*, [3]*JST PRESTO*)

1Pos275 多様体学習と機械学習の外力下での細胞運動ダイナミクスへの適用
Manifold and machine learning techniques applied to cell movement dynamics under external forces
Hiroshi Fujisaki[1], Kenta Odagiri[2], Hiromichi Suetani[3], Hiroya Takada[1], Rei Ogawa[1] ([1]*Nippon Medical School*, [2]*Senshu Univ.*, [3]*Oita Univ.*)

1Pos276 ソリッドステートナノポアによる H2A.B ヌクレオソームの構造安定性に関する研究
A study on the structural dynamics of the nucleosome containing H2A.B using solid-state nanopores
Hikaru Nozawa[1], Hirohito Yamazaki[1], Ryo Iizuka[1], Rina Hirano[1,2], Tomoya Kujirai[2,3], Hitoshi Kurumizaka[1,2], Sotaro Uemura[1] ([1]*Department of Biological Sciences, Graduate School of Science, The University of Tokyo*, [2]*Institute for Quantitative Biosciences, The University of Tokyo*, [3]*RIKEN Center for Biosystems Dynamics Research.*)

1Pos277 ナノポア計測による CALHM2 チャネルダイナミクスの解明
Investigation of CALHM2 Channel Dynamics using Nanopore measurement
Sotaro Nakamura, Hirohito Yamazaki, Wataru Shihoya, Osamu Nureki, Sotaro Uemura (*Department of Biological Sciences, The University of Tokyo*)

1Pos278 赤外超解像顕微鏡による爪ケラチンタンパク質の分布・配向観察
IR super-resolution imaging of keratin proteins in human nails based on non-linear optical process
Hirona Takahashi, Tetsuya Ida, Kohei Katayama, Makoto Sakai (*Faculty of Sci., Okayama Univ. of Sci.*)

1Pos279 近赤外光検出が可能な微弱光検出器の現状
Current status of low-light photodetectors capable of detecting near-infrared light
Atsuhito Fukasawa[1], Minako Hirano[2], Toru Ide[2], Hiroaki Yokota[3] ([1]*Hamamatsu Photonics K.K.*, [2]*Grad. Sch. Interdiscip. Sci. Eng. Health Sci., Okayama Univ.*, [3]*Grad. Sch. Creation Photon Indust.*)

1Pos280 表面増強ラマン分光を用いたジペプチド繰り返し配列を有するペプチドの液-液相分離液滴の計測
Surface Enhanced Raman Spectroscopy of liquid-liquid phase separation droplets consisting of dipeptide repeats
Yui Yamazaki[1], Masayuki Fujiwara[2], Ryo Kato[2], Kohsuke Kanekura[3], Taka-aki Yano[2], Yuhei Hayamizu[1] ([1]*Dept. of Mat. Sci. and Eng., Tokyo Tech*, [2]*pLED, Tokushima Univ.*, [3]*Dept. of Molecular pathology, Tokyo Medical Univ.*)

1Pos281 CRISPR-Cas13 を用いたデュアルプローブシステムおよび液液相分離濃縮による RNA の高感度 1 分子計測
Sensitive CRISPR-Cas13 mediated digital bioassay of RNA with dual probe system and enrichment by liquid-liquid phase separation
Yutaro Ii, Yoshihiro Minagawa, Hiroyuki Noji (*Dept. Appl. Chem., Grad. Sch. Eng., Univ.Tokyo*)

1Pos282 高速原子間力顕微鏡で観察されたミオシン V の歩行運動の隠れマルコフモデル解析
Hidden Markov model analysis of myosin V walking observed by high-speed atomic force microscopy
Sotaro Fuchigami[1], Yasuhiro Matsunaga[2], Shoji Takada[1] ([1]*Grad. Sch. of Science, Kyoto Univ.*, [2]*Grad. Sch. Sci. Eng., Saitama Univ.*)

1Pos283 (1SEP-6) Centromere-kinetochore structures revealed by 12x modified expansion microscopy
Yasuhiro Hirano[1], Aussie Suzuki[2], Yasushi Hiraoka[1], Tatsuo Fukagawa[1] ([1]*Graduate School of Frontier Biosciences, Osaka University*, [2]*McArdle Laboratory for Cancer Research, University of Wisconsin-Madison*)

1Pos284 Fluorescence polarization light-sheet microscopy for studying 3D molecular architectures *in vivo*
Tomomi Tani (*Biomedical Research Institute, National Institute of Adavnced Industrial Science and Technology*)

1Pos285 細胞分化に伴うクロマチン構造における状態特異的なヒストン動態の 1 分子イメージング
Single-molecule analysis of state-specific histone mobility in chromatin subcompartments during cellular differentiation
Masanori Hirose, Yuma Ito, Makio Tokunaga (*Sch. Life Sci. Tech., Tokyo Tech*)

1Pos286 Alphafold2 による遺伝子にコードされた FRET 型カルシウム指示薬の設計
Alphafold2-assisted design of a genetically-encoded FRET-based calcium indicator
Shinya Sakai[1], Kei-ichi Okazaki[2], Tomoki Matsuda[3], Takeharu Nagai[3] ([1]*Graduate School of Frontier Biosciences, Osaka University, Japan,*, [2]*Research Center for Computational Science, Institute for Molecular Science, Japan*, [3]*SANKEN, Osaka University, Japan*)

1Pos287 細胞性粘菌における **c-di-GMP** シグナルの解析
Fluorescence imaging of cyclic di-GMP signal in *Dictyostelium discoideum*
Hayato Ide, Yusuke Morimoto (*Grad. Sch. Comp. Sci. and Sys. Eng., Kyushu Inst. Tech.*)

1Pos288 (3SAA-6) Size determination of cytoplasmic condensates of optineurin using spatial image correlation spectroscopy (SICS)
Yuta Hamada[1], Masataka Kinjo[2], Akira Kitamura[2] ([1]*Grad. Sch. Sci. of Life Sci., Hokkaido Univ.*, [2]*Fac. of Adv. Life Sci., Hokkaido Univ*)

1Pos289 (3SAA-4) Morphological Analysis of Hydrogel Induced Cancer Stem Cells in Synovial Sarcoma Model Cells
Zannatul Ferdous[1], Masumi Tsuda[1,3,4], Jean-Emmanuel Clément[3], Jian Ping Gong[1,3,6], Shinya Tanaka[3,4,6], Tamiki Komatsuzaki[2,3,5], Koji Tabata[2] ([1]*Graduate School of Life Science, Hokkaido University*, [2]*Research Center of Mathematics for Social Creativity, Research Institute for Electronic Science, Hokkaido University, Sapporo, Japan*, [3]*Institute for Chemical Reaction Design and Discovery (WPI-ICReDD), Hokkaido University, Sapporo, Japan*, [4]*Department of Cancer Pathology, Hokkaido University Faculty of Medicine, Sapporo*, [5]*Graduate School of Chemical Sciences and Engineering, Hokkaido University, Sapporo, Japan*, [6]*Global Station for Soft Matter, Global Institution for Collaborative Research and Education (GI-CoRE), Hokkaido University, Sapporo, Japan*)

1Pos290 細胞内ストレス顆粒の近赤外蛍光・ラマンイメージング：細胞固定化の相分離液滴への影響
Near-infrared fluorescence and Raman imaging of intracellular stress granules: Effects of cell fixation on droplets formed by LLPS
Ren Shibuya[1], Shinji Kajimoto[1,2], Tetsuro Ariyoshi[3,4], Yasushi Okada[3,4], Takakazu Nakabayashi[1] ([1]*Grad. Sch. Pharm. Sci., Tohoku Univ.*, [2]*JST PRESTO*, [3]*RIKEN BDR*, [4]*Grad. Sch. Med., Univ. Tokyo*)

1Pos291 情報理論を使ったラマン画像に含まれる化学情報と形態情報の関係性の定量
Quantification of the relationship between chemical and spatial information in Raman images using information theory
Ryoya Kondo[1], James Nicholas Taylor[2], Yuta Mizuno[1,2,3], Jean-Emmanuel Clement[2,3], Katsumasa Fujita[4], Yoshinori Harada[5], Tamiki Komatsuzaki[1,2,3] ([1]*Grad. Chem. Sci. Eng., Hokkaido Univ.*, [2]*Res. Inst. Electr. Sci., Hokkaido Univ.*, [3]*WPI-ICReDD, Hokkaido Univ.*, [4]*Grad. Eng., Osaka Univ.*, [5]*Kyoto Pref. Univ. Med.*)

1Pos292 シグナル伝達反応進行過程における細胞膜上受容体動態の変化
Oligomerization and dynamics of receptor molecules during the signaling process
Hideaki Yoshimura, Takeaki Ozawa (*Sch. Sci., Univ. Tokyo*)

1Pos293 デュアルコム干渉計を用いた細胞膜電位のラベルフリー検出
Label-free detection of membrane potential using dual-comb interferometry
Satoshi Araoka[1,3], Yusuke Takashima[2], Yoshiki Naoi[2,3], Akira Emoto[3], Kazumichi Yoshii[3], Masatake Akutagawa[2], Hiroki Takanari[3] ([1]*Graduate School of Sciences and Technology for Innovation, Tokushima University*, [2]*Graduate School of Technology, Industrial and Social Science, University of Tokushima*, [3]*Institute of Post-LED Photonics, University of Tokushima*)

1Pos294 脂質、ヌクレオチド依存的 Prx 高分子量複合体形成メカニズムの解明
Study on the formation mechanism of peroxiredoxin high molecular weight complex with lipid and nucleotide
Ryusei Yamada[1], Hiroki Konno[2] ([1]*Grad. Sch. of Nat. Sci. & Technol., Kanazawa University*, [2]*WPI Nano Life Sci. Inst. (WPI-NanoLSI), Kanazawa Univ*)

1Pos295 イメージプロセッシングによる細胞内小胞輸送の 3 次元トラッキングデータ解析の自動化に関する研究
An automatic detection and tracking method for the 3D reconstruction of vesicle movement in a living cell
Seohyun Lee[1], Hyuno Kim[2], Hideo Higuchi[3] ([1]*Institute for quantitative biosciences, The University of Tokyo*, [2]*Institute of Industrial Science, The University of Tokyo*, [3]*Graduate School of Science, The University of Tokyo*)

1Pos296 機械学習を駆使して高速 AFM 画像から細胞骨格ネットワーク構造の再構成
Machine learning-guided reconstruction of cytoskeleton network from Live-cell AFM Images
Kanaki Kiku[1], Shigehiro Yoshimura[1], Skibbe Henrik[2], Naoki Honda[3] ([1]*Graduate School of Biostudies, Kyoto University, Japan*, [2]*Brain Image Analysis Unit, RIKEN Center for Brain Science, Wako, Japan*, [3]*Graduate School of Integrated Sciences for Life, Hiroshima University, Japan*)

1Pos297 ランダムドメイン挿入法を用いた FRET 型植物ホルモンセンサーのスクリーニング
Screening of FRET-type plant hormone sensor using Random domain insertion method
Ami Nakano (*Grad. Sch. Sci. Eng., Saitama Univ.*)

1Pos298 寒天培地上での海洋微生物の構造色の出現と発達のタイムラプス観察
Timelapse observation of the emergence and development of structural color of a marine bacterium on agar plates
Mikiko Tsudome, Shigeru Deguchi (*JAMSTEC*)

1Pos299 生体内高感度シングルショット 3D 温度イメージング技術の開発
Sensitive single-shot 3D temperature imaging *in vivo*
Haruka Maeoka[1], Ryuji Igarashi[2], Shin Usuki[3], Takuma Sugi[1] ([1]*Program of Biomedical Science, Graduate School of Integrated Sciences for Life, Hiroshima University*, [2]*Quantum Science and Technology Organization*, [3]*Research Institute of Electronics, Shizuoka University*)

1Pos300 Kilohertz imaging of intracellular heat diffusion with a genetically encoded temperature indicator
Kai Lu[1], Tetsuichi Wazawa[1], Joe Sakamoto[3], Cong Quang Vu[1,2], Masahiro Nakano[1], Yasuhiro Kamei[3], Takeharu Nagai[1,2] ([1]*SANKEN, Osaka Univ.*, [2]*Graduate School of Frontier Biosciences, Osaka Univ.*, [3]*NIBB*)

1Pos301 従来の超解像用、生理機能用蛍光指示薬による生理機能超解像イメージング法
Functional super-resolution (fSR) imaging with conventional SR and functional fluorescent indicators
Ryohei Noma[1], Satoshi Hara[1], Tomoki Matsuda[1], Tetsuichi Wazawa[1], Takashi Washio[1,2], Takeharu Nagai[1,2] ([1]*SANKEN (The Institute of Scientific and Industrial Research), Osaka University, Japan*, [2]*Transdimensional Life Imaging Division, Institute for Open and Transdisciplinary Research Initiatives, Osaka University, Japan*)

1Pos302 長期間ライブイメージングを可能にする光損傷を軽減する撮影条件の最適化
Optimization of image acquisition methods to reduce photodamage for long-term live-imaging
Go Shioi[1], Tomonobu M Watanabe[1], Junichi Kaneshiro[1], Yusuke Azuma[2], Shuichi Onami[2] ([1]*Laboratory for Comprehensive Bioimaging, RIKEN Center for Biosystems Dynamics Research*, [2]*Laboratory for Developmental Dynamics, RIKEN Center for Biosystems Dynamics Research*)

1Pos303 1 分子動態と局在による機能的クロマチン-RNA polymerase II 相互作用の統合解析
An integrated analysis of functional chromatin-RNA polymerase II interaction using single-molecule dynamics and localization
Yuma Ito, Makio Tokunaga (*Sch. Life Sci. Tech., Tokyo Tech*)

1Pos304 クライオ電子線トモグラフィー法による糸状仮足中のアクチン繊維上ファシンのサブトモグラム平均化
Subtomogram Averaging of Fascin on Actin Filaments in Filopodia by Cryo-Electron Tomography
Kaoru Mitsuoka[1], Naoko Kajimura[1], Takuo Yasunaga[2] ([1]*Research Center for Ultra-High Voltage EM, Osaka Univ.*, [2]*Grad. Sch. Comp. Sci. Syst. Eng., KIT*)

1Pos305 *Gloeobacter violaceus* の顕微分光イメージング
Microimaging of *Gloeobacter violaceus*
Kento Hashimoto[1], Reo Minami[1], Akio Murakami[2], Mamoru Nango[3], Mitsuru Sugisaki[3,4] ([1]*Grad. Sch. Sci., Osaka City University*, [2]*Grad. Sch. Sci., Kobe University*, [3]*Grad. Sch. Sci., Osaka Metropolitan University*, [4]*NITEP, Osaka Metropolitan University*)

1Pos306 骨格アニメーション法を活用したタンパク質構造変化の検証法
Utilizing skeletal animation for understanding structural change of proteins
Yutaka Ueno (*Artificial Intelligence Research Center, AIST*)

バイオエンジニアリング／Bioengineering

1Pos307 CRISPR 関連タンパク質によるプログラム可能な哺乳類細胞翻訳調節器
Programmable mammalian translational modulators by CRISPR-associated proteins
Shunsuke Kawasaki, Takeru Kuwabara, Hirohide Saito (*Center for iPS Cell Research and Application, Kyoto University*)

1Pos308 カップ型微小電極を用いた非接着細胞表面分子計測技術の開発
Development of a technology to detect surface molecules on non-adherent cells by using Cup-shaped microelectrodes
Taro Sasaki[1,2], Kohki Uchiyama[1,2], Tomoyuki Kamata[3], Dai Kato[3], Naoshi Kojima[3], Shohei Yamamura[3], Hyonchol Kim[1,2] ([1]*Cell. Mol. Biotechnol. Res. Inst., AIST*, [2]*Grad. Sch. Eng., Tokyo Univ. Agric. Technol*, [3]*Health Med. Res. Inst., AIST*)

1Pos309 3D DNA nanostructure-based assembled structures toward a construction of chromatin-like heterogeneous system
Hong Xuan Chai[1], Masahiro Takinoue[2] ([1]*Department of Life Science and Technology, School of Life Science and Technology, Tokyo Institute of Technology*, [2]*Department of Computer Science, School of Computing, Tokyo Institute of Technology*)

1Pos310 DNA 増幅を動力源とするナノモーターの設計と評価
Design and evaluation of nanomotors powered by DNA amplification
Riku Yoshino[1], Richard James Archer[1], Satoshi Murata[1], Shinichiro Nomura[1], Ibuki Kawamata[1,2] ([1]*Grad. Sch. Eng., Univ. Tohoku*, [2]*Fuc. Core Reserch, Univ Ochanomizu*)

1Pos311 DNA を用いたシグナル伝達のための核酸生成回路の検証
Characterization of Nucleic Acid Generation Circuits for DNA-based Signal Transduction
Ken Komiya, Chizuru Noda (*X-star, JAMSTEC*)

1Pos312 リン脂質-タンパク質非対称膜小胞を用いた小胞分裂モデルの構築
Construction of vesicle fission model using asymmetric phospholipid-protein vesicles
Masato Suzuki (*Facut. Sci. Tech., Gunma. Univ*)

1Pos313 原子間力顕微鏡液中測定によるパパイン分子と DNA で被覆された単層カーボンナノチューブ との相互作用の pH の影響の研究
Effects of pH on interaction of papain and DNA wrapped single walled carbon nanotubes studied by atomic force microscopy in fluid
Masaki Kitamura, Kazuo Umemura (*Physics. Science. Tokyo university of science/ Japanese*)

1Pos314 フェリチンに内包されたマグネタイトナノ粒子の高周波磁場による加熱
Heat production by magnetite nanoparticles encapsulated in ferritin under alternating magnetic field
Kanamaru Tomoko[1], Yuta Hayashi[1], Hiroto Goshima[1], Toshiki Higuchi[1], Arun Kasimchetty[1], Shuji Kanamaru[2], **Hideyuki Yoshimura**[1] ([1]*Meiji Univ.*, [2]*Tokyo Institute of Techinology*)

1Pos315 Inhibitory effect of nucleotides on acetylcholinesterase activity and its microflow based actuation in human plasma
Deshwal Akshi[1], Gill Arshdeep Kaur[2], Nain Surajmal[1], Patra Dr.Debabrata[2], Maiti Subhabrata[1] ([1]*Indian Institute of Science Education and Research Mohali, Punjab 140306 , India*, [2]*Institute of Nano Science and Technology , Mohali, Punjab 140306*)

結晶成長・結晶化技術／Crystal growth & Crystallization technique

1Pos316 無細胞合成を用いたタンパク質結晶化と構造解析
Protein crystallization and structure analaysis using cell-free protein synthesis
Satoshi Abe, Junko Tanaka, Mariko Kojima, Takafumi Ueno (*Sch. Life Sci. Tech., Tokyo Tech.*)

1Pos317 細胞内タンパク質結晶を用いた天然変性タンパク質の網羅的構造解析
Comprehensive structure analysis of intrinsically disordered protein using in-cell protein crystal
Mariko Kojima, Satoshi Abe, Takafumi Ueno (*Sch. Life Sci. & Tech., Tokyo Tech*)

その他／Miscellaneous topics

1Pos318 大気圧温度制御プラズマによる植物細胞への直接タンパク質導入法の開発及び導入機構解明
Direct protein introduction into plant cells by a temperature controllable atmospheric-pressure plasma and elucidation of the mechanism
Yuki Yanagawa[1,2], Yusuke Iijima[3], Toshiki Aizawa[3], Yuma Suenaga[3], Akitoshi Okino[3], Ichiro Mitsuhara[4] ([1]*Grad. Sch. Hortic., Chiba Univ.*, [2]*CSRS, RIKEN*, [3]*FIRST, Tokyo Inst. Tech.*, [4]*NIAS, NARO*)

1Pos319 新規カロテノプロテインの分離と構造解析—青色にもピンク色にもなるアスタキサンチン
Isolation and structure analysis of a novel marine sponge carotenoprotein
Momoko Ishida, Momose Kuroda, Suzuho Iseya, Yui Fujita, Satoko Matsunaga (*N.I.T., Hakodate Col.*)

1Pos320 Construction of novel lipidomics platform combined of targeted and non-targeted analysis
Hideaki Kasahara, Yasuto Yokoi, Hideya Kuwabara, Tadahiro Hoshino (*MITSUI KNOWLEDGE INDUSTORY CO., LTD.*)

1Pos321 ヒト角栓内部における脂質の不均一分布
Heterogeneous spatial distribution of lipid components in a follicular cast
Hitomi Matsushita[1], Hiromitsu Nakazawa[1], Noboru Ohta[2], Taro Moriwaki[2], Satoru Kato[1] ([1]*Grad. Sch. SciTech., Kwansei Gakuin Univ.*, [2]*JASRI/SPring-8*)

1Pos322 変分オートエンコーダを用いた下顎骨形態の定量化
A method for morphological feature extraction based on variational auto-encoder: an application to mandible shape
Masato Tsutsumi[1], Nen Saito[2,3,4], Daisuke Koyabu[5,6], Chikara Furusawa[4,7] ([1]*Dept. of Physics, Grad. Sch. Sci., The Univ. of Tokyo*, [2]*Grad. Sch. Integr. Sci. for Life, Hiroshima Univ.*, [3]*ExCELLS, NIBB*, [4]*UBI, The Univ. of Tokyo*, [5]*Res. and Dev. Center for Precision Med., Tsukuba Univ.*, [6]*Jockey Club College of Veterinary Medicine and Life Sciences, City University of Hong Kong*, [7]*BDR, RIKEN*)

1Pos323 Evaluation of the Potent SARS-CoV-2 Main Protease Inhibitors using LB-PaCS-MD/FMO Technique
Kowit Hengphasatporn, Ryuhei Harada, Yasuteru Shigeta (*Center for Computational Sciences, Univ. Tsukuba*)

1Pos324 Flory-Huggins 理論を用いた 3 成分系における相分離挙動の解析
Analysis of phase separation behavior in three-component systems based on the Flory-Huggins theory
Naoki Iso, Takahiro Sakaue, Yuki Norizoe (*Aoyama Gakuin University*)

1Pos325 多孔質ハイドロゲル固体試料中における紫膜積層に適した孔サイズ分布
Pore size distributions related to spontaneous purple membrane stacking in porous hydrogels
Yasunori Yokoyama[1,2], Morise Karasawa[1], Kingo Takiguchi[3], Hiroshi Takahashi[4], Takashi Kikukawa[5], Masashi Sonoyama[4,6,7], Koshi Takenaka[1] ([1]*Grad. Sch. Eng., Nagoya Univ.*, [2]*Natl. Inst. Tech., Hakodate Coll.*, [3]*Grad. Sch. Sci., Nagoya Univ.*, [4]*Grad. Sch. Sci. Tech., Gunma Univ.*, [5]*Fac. Adv. Life Sci., Hokkaido Univ.*, [6]*GIAR, Gunma Univ.*, [7]*GUCFW, Gunma Univ.*)

2 日目（9 月 29 日（木））／Day 2（Sep. 29 Thu.）

蛋白質：構造／Protein: Structure

2Pos001* クライオ電子顕微鏡によるヒト LPA1 受容体の構造解析
Cryo-EM structure of Human Lysophosphatidic Acid Receptor 1
Hiroaki Akasaka, Tatsuki Tanaka, Fumiya Sano, Wataru Shihoya, Osamu Nureki (*Grad. Sch. Sci., The Univ. of Tokyo*)

2Pos002* クライオ電子顕微鏡を用いたコレラ菌 Na^+輸送性 NADH-ユビキノン酸化還元酵素の構造解明
Cryo-EM structures of Na^+-pumping NADH-ubiquinone oxidoreductase from *Vibrio cholerae*
Moe Ishikawa[1], Jun-ichi Kishikawa[2], Takahiro Masuya[1], Masatoshi Murai[1], Yuki Kitazumi[1], L. Nicole Butler[3], Takayuki Kato[2], Blanca Barquera[3,4], Hideto Miyoshi[1] ([1]*Grad. Sch. Agri., Kyoto Univ./ Japanese*, [2]*Inst. Prot. Res., Osaka Univ./ Japanese*, [3]*Bio. Sci., RPI/ USA*, [4]*CBIS, RIP/ USA*)

2Pos003* (3SFA-3) クライオ電子顕微鏡による高分解能解析によって明らかになってきた二成分毒素の膜透過機構
(3SFA-3) High-resolution Cryo-EM analysis reveals the mechanism of binary toxin translocation
Tomohito Yamada[1], Yukihiko Sugita[2,3], Takeshi Noda[2], Hideaki Tsuge[1] ([1]*Graduate School of Life Science, Kyoto Sangyo University*, [2]*Laboratory of Ultrastructural Virology, Institute for Life and Medical Sciences, Kyoto University*, [3]*Hakubi Center for Advanced Research, Kyoto University*)

2Pos004 タンパク質間相互作用阻害を機序とする抗新型コロナウイルス薬の創出
Screening for new types of coronavirus inhibitors that block protein-protein interaction
Ryusei Hamajima[1], Haruka Takagi[1], Takeshi Tenno[1], Youichi Suzuki[2], Hong Wu[2], Hidekazu Hiroaki[1] ([1]*Grad. Sch. Pharm. Sci., Nagoya Univ.*, [2]*School of Medicine, Osaka Medical and Pharmaceutical University*)

2Pos005* クライオ電子顕微鏡によるヒト由来メラトニン受容体シグナル伝達複合体の立体構造解析
Cryo-EM structure of the human MT_1–G_i signaling complex
Hiroyuki Okamoto[1], Hirotake Miyauchi[1], Asuka Inoue[2], Francesco Raimondi[3], Hirokazu Tsujimoto[4], Tsukasa Kusakizako[1], Wataru Shihoya[1], Keitaro Yamashita[1,5], Ryoji Suno[6], Norimichi Nomura[4], Takuya Kobayashi[6], So Iwata[4,7], Tomohiro Nishizawa[8], Osamu Nureki[1] ([1]*Graduate School of Science, The University of Tokyo.*, [2]*Graduate School of Pharmaceutical Sciences, Tohoku University.*, [3]*Laboratorio di Biologia Bio@SNS, Scuola Normale Superiore.*, [4]*Graduate School of Medicine, Kyoto University.*, [5]*MRC Laboratory of Molecular Biology.*, [6]*Department of Medical Chemistry, Kansai Medical University.*, [7]*RIKEN SPring-8 Center.*, [8]*Graduate School of Medical Life Science, Yokohama City University.*)

2Pos006* FlhAc の高速原子間力顕微鏡画像の解析
Analysis of High Speed Atomic Force Microscopy Image of FlhAc
Riku Osawa[1], Naoya Terahara[2], Noriyuki Kodera[3], Katsumi Imada[4], Tohru Minamino[5], Akio Kitao[1] ([1]*Sch. Life Science and Technology, Tokyo Tech*, [2]*Dep. Physics Faculty of Science and Engineering, Chuo Univ*, [3]*Bio-AFM Frontier Research Center, Kanazawa Univ*, [4]*Dep. Macromolecular Science, Grad. Sch. Science, Osaka Univ*, [5]*Grad. Sch. Frontier Biosciences, Osaka Univ*)

2Pos007 デングウイルス由来 RNA 依存性 RNA ポリメラーゼと天然物ライブラリーから得られたその阻害剤との複合体の立体構造解析
Structure analysis of the dengue viral RNA-dependent RNA polymerase in complex with its inhibitor obtained from marine natural products
Nami Hosoi[1], Haruka Nakatani[2], Lakkana Thaveepornkul[3], Arisa Suto[4], Naoki Sakai[5,6], Hiroaki Matsuura[6], Masaki Yamamoto[6], Takashi Matsui[7,8], Yoshio Kodera[7,8], Sarin Chimnaronk[3], Ryuichi Sakai[2], Takeshi Yokoyama[1], Yoshikazu Tanaka[1] ([1]*Grad. Sch. Life Sci., Tohoku Univ.*, [2]*Grad. Sch. Fisheries Sci., Hokkaido Univ.*, [3]*The Laboratory of RNA Biology, Institute of Molecular Biosciences, Mahidol University*, [4]*Grad. Sch. Sci., Kitasato Univ.*, [5]*Strut. Biol. Div. JASRI*, [6]*Life Sci. Res. Infra. Gr., RIKEN RSC*, [7]*Sch. Sci., Kitasato Univ.*, [8]*Cent. Disease Proteomics, Kitasato Univ.*)

2Pos008* フェレドキシン-$NADP^+$還元酵素の中性子結晶構造解析
Neutron crystallographic analysis of ferredoxin-$NADP^+$ reductase
Midori Uenaka[1,2], Yusuke Ohnishi[1], Hideaki Tanaka[1,2], Genji Kurisu[1,2] ([1]*IPR., Osaka Univ.*, [2]*Grad. Sch. Sci., Osaka Univ.*)

2Pos009* クライオ電子顕微鏡を用いたビタミン C トランスポーター SVCT1 の構造解析
Cryo-EM structures of vitamin C transporter SVCT1
Takaaki Kobayashi, Hiroto Shimada, Fumiya Sano, Tsukasa Kusakizako, Osamu Nureki (*Dept. Biol. Sci., Grad. Sch. Sci., Univ. Tokyo*)

2Pos010 赤色蛍光タンパク質の単一復帰変異による赤色蛍光消失の構造基盤
Structural basis of the loss of red fluorescence by single back mutation of an artificial red fluorescent protein
Shiho Otsubo[1], Hiromi Imamura[2], Norihiro Takekawa[1], Katsumi Imada[1] ([1]*Grad. Sch. Sci., Osaka Univ.*, [2]*Grad. Sch. Biost., Kyoto Univ.*)

2Pos011 MD シミュレーションによる LIM2 ドメインの構造解析
Structural analysis of Lim2 domain by MD simulation
Motokuni Nakajima[1], Yoh Noguchi[1,3], Hironao Yamada[2,3], Ryota Morikawa[1], Masako Takasu[1], Yukiko K. Hayashi[4] ([1]*Sch. of Life Sci., Tokyo Univ. of Pharm. and Life Sci.*, [2]*Sch. of Pharm., Tokyo Univ. of Pharm. and Life Sci.*, [3]*The Inst.of Statist. Math.*, [4]*Tokyo Med. Univ.*)

2Pos012 尿素とトリエチルアミン N-オキシドが KaiC の ATPase 活性に及ぼす影響
Effects of urea and trimethylamine N-oxide on the ATPase activity of KaiC
Nanaka Hara[1], Keita Mitsuhashi[2], Haruka Horiuchi[3], Masahiro Miyamoto[1], Ayumi Masuda[1], Soichiro Kitazawa[3], Ryo Kitahara[3] ([1]*Graduate School of Pharmaceutical Sciences, Ritsumeikan University*, [2]*Graduate School of Life Sciences, Ritsumeikan University*, [3]*College of Pharmaceutical Sciences, Ritsumeikan University*)

2Pos013 原子分解能でみた概日時計の朝夕昼夜
Visualizing a Day of Circadian Clock at Atomic Resolution
Yoshihiko Furuike[1,2], Atsushi Mukaiyama[1,2], Eiki Yamashita[3], Takao Kondo[4], Shuji Akiyama[1,2] ([1]*Research Center of Integrative Molecular Systems (CIMoS), Institute for Molecular Science (IMS)*, [2]*The Graduate University for Advanced Studies (SOKENDAI)*, [3]*Institute for Protein Research (IPR), Osaka University*, [4]*Graduate School of Science, Nagoya University*)

2Pos014 分子動力学シミュレーションを活用した VHH-抗原複合体のアンサンブルドッキング
Ensemble Docking of VHH-Antigen Complexes using Molecular Dynamics Simulations
Kohei Yamaguchi, Ren Higashida, Yasuhiro Matsunaga (*Grad. Sch. Sci. Eng., Saitama Univ.*)

2Pos015 Structure and stability analysis of Cry j 7, an antimicrobial peptide from Japanese cedar that causes the pollen-food allergic syndrome
Jingkang Zheng, Tomona Iizuka, Hiroyuki Kumeta, Yasuhiro Kumaki, Ami Hanaoka, Ichiho Yoshikawa, Yurie Nakajima, Soma Ishihara, Tomoyasu Aizawa (*Grad. Sch. Life Sci., Hokkaido Univ.*)

2Pos016 細菌由来グルカンスクラーゼのアクセプター特異性に関連するループ構造
The loop structure responsible to the acceptor specificity of bacterial glucansucrase
Takafumi Inoue, Hideyuki Komatsu (*Dept. of Bioscience and Bioinfomatics, Kyushu Inst. Tech.*)

2Pos017 構造解析に向けたヒト免疫不全ウイルス 2（HIV-2）エンベロープ糖タンパク質の調製
Preparation of human immunodeficiency virus type-2 (HIV-2) envelope glycoprotein for structure analysis
Yuki Anraku[1], Shunsuke Kita[1], Hideo Fukuhara[1], Haruka Kawabata[1], Takaki Akiyama[1], Simon Davis[2], Atsushi Furukawa[1], Thushan I. de Silva[2], James E. Robinson[3], Yuguang Zhao[2], E. Yvonne Jones[2], David Stuart[2], Juha T Huiskonen[2], Sarah Rowland-Jones[2], Katsumi Maenaka[1] ([1]*Fac. Pharm. Sci., Univ. Hokkaido*, [2]*Univ. Oxford*, [3]*Univ. Tulane*)

2Pos018 粗視化モデルによる微小管の安定性の理論的研究
Theoretical study of stability of microtubules by a coarse-grained model
Ayasa Kurahashi, Hiro Takeda, Kazutomo Kawaguchi, Hidemi Nagao (*Grad. Sch. Nat. Sci. Tech., Kanazawa Univ.*)

2Pos019 X 線小角散乱測定を用いたクラミドモナス由来クリプトクロムの溶液構造解析
Structural analyses of the animal-like cryptochrome from *Chlamydomonas reinhardtii* by small angle X-ray scattering
Soma Matsuda, Satoshi Nagao, Daichi Yamada, Minoru Kubo (*Grad. Sch. Sci., Univ. Hyogo*)

2Pos020 蛋白質天然変性領域を模倣する生理活性化合物の探索
Search of bioactive compounds that imitate intrinsically disordered regions of proteins
Haruki Fukuyama[1], Takuya Takahashi[2], Kota Kasahara[2] ([1]*Grad. Sci. Life Sci., Ritsumeikan Univ.*, [2]*Coll. Life Sci., Ritsumeikan Univ.*)

2Pos021 Effect of a narrowest clamp of binary toxin on cell toxicity
Yuto Uchida[1], Toru Yoshida[2], Tomohito Yamada[1], Hideaki Tsuge[1] ([1]*Graduate of Life Scienc, kyoto Sangyo University*, [2]*Fac. Sci., Japan Women's Univ.*)

2Pos022 β シートにおける隣接ストランド間でのペア特異的 Cα 距離の解析
Pair-specific analysis of Cα distances between adjacent strands in β-sheets
Hiromi Suzuki (*Sch. Agri., Meiji Univ.*)

2Pos023 分子動力学シミュレーションによる凝集性を有するペプチドの密度依存性に着目した構造分布解析
Distribution and structure analysis of fibril-forming peptides focusing on concentration dependency by molecular dynamics simulation
Yoshitake Sakae[1,2], Takeshi Kawasaki[2], Yuko Okamoto[3] ([1]*RIST*, [2]*Dep. Phys., Nagoya Univ.*, [3]*Info. and Comm., Naogya Univ.*)

2Pos024 An extended bound-water network and hydrophobic hydration determine the activity of microbial antifreeze protein
Hidemasa Kondo[1,2], N. M.-Mofiz Uddin Khan[2,3], Tatsuya Arai[4], Sakae Tsuda[4,5,6], Yasushi Ohyama[1] ([1]*Bioproduction Research Institute, National Institute of Advanced Industrial Science and Technology (AIST)*, [2]*Graduate School of Life Science, Hokkaido University*, [3]*Department of Chemistry, Dhaka University of Engineering and Technology, Gazipur*, [4]*Graduate School of Frontier Sciences, The University of Tokyo*, [5]*OPERANDO Open Innovation Laboratory, National Institute of Advanced Industrial Science and Technology (AIST)*, [6]*Faculty of Advanced Life Science, Hokkaido University*)

蛋白質：構造機能相関／Protein: Structure & Function

2Pos025 Gly-kink 導入 β バレルナノポアを用いた単一分子検出
Single-molecule detection using β-barrel nanopore with Gly-kink
Ikuro Mizoguchi[1], Masataka Usami[1], Keisuke Shimizu[1], Shuhei Yoshida[2], Yoshio Hamada[2], Yuto Suzuki[3], Yuzuha Araki[3], Kenji Usui[2], Izuru Kawamura[3], Ryuji Kawano[1] ([1]*Department of Biotechnology and Life Science, Tokyo University of Agriculture and Technology*, [2]*Faculty of Frontiers of Innovative Research in Science and Technology, Konan University*, [3]*Graduate School of Engineering Science, Yokohama National University*)

2Pos026* (2SDP-5) Structural basis of the significant metal-histidine coordination in *E. coli* RNase HI
Zengwei Liao[1], Takuji Oyama[2], Yumi Kitagawa[3], Katsuo Katayanagi[4], Kosuke Morikawa[5], Masayuki Oda[3] ([1]*Grad. Sch. Agri. and Life Sci., the Univ. of Tokyo*, [2]*Faculty of Life and Environ. Sci., Univ. of Yamanashi*, [3]*Grad. Sch. Life Environ. Sci., Kyoto Pref. Univ.*, [4]*Grad. Sch. Integrated Sci. for Life, Hiroshima Univ.*, [5]*Grad. Sch. Biostudies, Kyoto Univ.*)

2Pos027* *De novo* ペプチドナノポアの無細胞合成へのアプローチ
Approaches to cell-free synthesis of *de novo* peptide nanopores
Shoko Fujita, Miyu Fukuda, Ikuro Mizoguchi, Ryuji Kawano (*Department of Biotechnology and Life Science, Tokyo University of Agriculture and Technology*)

2Pos028* K48 結合型環状ユビキチン鎖の物性解析
Physical property analysis of cyclic K48-linked ubiquitin chains
Tomoki Sorada[1], Daichi Morimoto[1], Erik Walinda[2], Kenji Sugase[3] ([1]*Grad. Sch. Eng., Univ. Kyoto*, [2]*Grad. Sch. Med., Univ. Kyoto*, [3]*Grad. Sch. Agr., Univ. Kyoto*)

2Pos029 アミノ酸生産菌の呼吸鎖の拡張型超複合体の電子顕微鏡による観察と解析
Electron microscopic observation and analysis of extended supercomplexes of the respiratory chain of amino acid-producing bacteria
Ayumi Moriyasu[1], Tomoichirou Kusumoto[1], Hiroko Takazaki[2], Takuo Yasunaga[1], Takayuki Kato[2] ([1]*Grad. Sch. Comp. Sci. Syst. Eng., KIT*, [2]*IPR, Univ. Osaka*)

2Pos030 グルタミン酸脱水素酵素における補酵素結合経路のクライオ電子顕微鏡観察
Cofactor binding pathway in glutamate dehydrogenase studied using cryoTEM
Taiki Wakabayashi[1,2], Mao Oide[1,2], Takayuki Kato[3], Masayoshi Nakasako[1,2] ([1]*Dept. Phys., Keio Univ.*, [2]*RSC, RIKEN*, [3]*Protein Inst., Osaka Univ.*)

2Pos031* *In silico* design of cross-reactive antibodies binding to SARS-CoV and SARS-CoV-2 spike RBDs
Yoshiki Yasuda[1], Daisuke Kuroda[2], Jiei Sasaki[3], Makoto Nakakido[1], Ryo Matsunaga[1], Hashiguchi Takao[3], Kouhei Tsumoto[1] ([1]*Grad. Sch. Eng., The University of Tokyo*, [2]*Research Center for Drug and Vaccine development, National Institute of Infectious Diseases*, [3]*Laboratory of Medical Virology, Institute for Life and Medical Sciences, Kyoto University*)

2Pos032 動的・静的構造解析による南極産好冷細菌由来グルコキナーゼの低温適応・高熱安定性機構の解明
X-ray crystallography and spin-labeling ESR reveal cold adaptation and high thermal stability mechanism of cold-adapted glucokinase
Akane Yato[1], Rio Asaka[2], Hiroshi Sugimoto[3], Keiichi Watanabe[2], Masaki Horitani[2] ([1]*United Grad. Sch. Agri. Sci., Kagoshima Univ.*, [2]*Agri., Saga Univ.*, [3]*SPring-8, RIKEN*)

2Pos033 EPR 法による中温菌、好冷細菌由来複核 Mn 酵素の活性中心における微細構造変化の検出
EPR Spectroscopy Reveals the Differences of Active Site Structures for Di-Mn Enzymes from Mesophilic and Psychrophilic Bacteria
Masaki Horitani[1,2], Yuri Kasu[1] ([1]*Fac. Agric., Saga Univ.*, [2]*Unit. Grad. Sch. Agric. Sci., Kagoshima Univ.*)

2Pos034* FixL 二量体感覚領域のリガンド認識機構
Computational Study on the Ligand Discrimination of Dimeric Sensory Domain of FixL Protein
Tingting Wang, Takahisa Yamato (*Graduate School of Science, Nagoya University*)

2Pos035 QM/MM 法による *C*-メチル基転移酵素 Fur6 の反応機構解析
QM/MM study on the catalytic mechanism of the *C*-methyltransferase Fur6
Fan Zhao[1], Tomohiro Noguchi[1], Yoshitaka Moriwaki[1], Tohru Terada[1], Tomohisa Kuzuyama[1,2], Kentaro Shimizu[1] ([1]*Grad. Sch. of Agri. and Life Sci., Univ. of Tokyo*, [2]*CRIIM, Univ. of Tokyo*)

2Pos036 CD28 結合と構造安定性に寄与する Grb2 のドメイン間相互作用
Interdomain interactions in Grb2 contribute to the conformational stability and CD28 binding
Saki Ochi, Momoka Iiyama, Masayuki Oda (*Grad. Sch. Life Environ. Sci., Kyoto Pref. Univ.*)

2Pos037* リョビュウイルスの核蛋白質 **-RNA** 複合体のクライオ電子顕微鏡構造
Cryo-EM structure of the nucleoprotein-RNA complex of a novel filovirus, Lloviu virus
Shang fan Hu[1,2,3], Yoko Fujita-Fujiharu[1,2,3], Yukihiko Sugita[1,2,4], Lisa Wendt[5], Yukiko Muramoto[1,2,3], Masahiro Nakano[1,2,3], Thomas Hoenen[5], Takeshi Noda[1,2,3] ([1]*Laboratory of Ultrastructural Virology, Institute for Life and Medical Sciences, Kyoto University*, [2]*Laboratory of Ultrastructural Virology, Graduate School of Biostudies, Kyoto University*, [3]*CREST, Japan Science and Technology Agency*, [4]*Hakubi Center for Advanced Research, Kyoto University*, [5]*Laboratory for Integrative Cell and Infection Biology, Institute of Molecular Virology and Cell Biology, Friedrich-Loeffler-Institut*)

2Pos038 シトクロム P450 によるメチレンジオキシブリッジ形成の反応機構
Reaction mechanism of methylenedioxybridge formation by cytochrome P450
Kenshin Kondoh, Ryo Yonezawa, Eiichi Mizohata (*Grad.Sch.Eng., Osaka Univ.*)

2Pos039* ヒト stomatin SPFH ドメインのリン酸イオンに依存した線維状構造
The SPFH domain of human stomatin forms fibril-like assembly at high concentrations, whose formation is promoted by phosphate ions
Koki Kataoka[1], Shota Suzuki[1], Takeshi Tenno[1], Natsuko Goda[1], Emi Hibino[1], Atsunori Oshima[1,2,3], Hidekazu Hiroaki[1,2] ([1]*Grad. Sch. Pharm. Sci., Nagoya Univ.*, [2]*Cellular and Structural Physiology Institute (CeSPI)*, [3]*iGCORE, Toaki National Higher Education and Research System*)

2Pos040* 天然変性タンパク質が引き起こす滑膜肉腫発生の新規メカニズム
A Novel Mechanism of Synovial Sarcoma Induced by Intrinsic Disordered Proteins
Kanami Takahashi[1], Naoki Horikoshi[2], Kazutoshi Tani[3], Yohei Miyanoiri[4], Noriyuki Kodera[5], Masahiro Nishimura[2], Kohsuke Kato[6], Satoshi Takenaka[7], Hitoshi Kurumizaka[2], Kenji Iwasaki[8] ([1]*Grad. Sch. Sci. and Tech., Univ. of Tsukuba*, [2]*IQB, Univ. of Tokyo*, [3]*Grad. Sch. of Med., Mie Univ.*, [4]*IPR, Osaka Univ.*, [5]*NanoLSI, Kanazawa Univ.*, [6]*Grad. Sch. of Comprehensive Human Sciences, Univ. of Tsukuba*, [7]*Osaka International Cancer Inst. Hosp.*, [8]*TARA, Univ. of Tsukuba*)

2Pos041 HSP40 結合による HSP70 の安定性への影響
HSP40 binding affects the stability of HSP70
Lisa Matsukura, Naoyuki Miyashita (*Grad. Sch. BOST, KINDAI Univ.*)

2Pos042* 緑藻クラミドモナス由来シトクロム b_6f 複合体のクライオ電子顕微鏡構造が示す Rieske 鉄硫黄蛋白質の機能的構造変化
Cryo-EM structure of cytochrome b_6f complex from *Chlamydomonas reinhardtii* reveals the functional domain movement of Rieske ISP
Hatsuki Tanabe[1,2], Shinichiro Ozawa[3], Akihiro Kawamoto[1,2], Hideaki Tanaka[1,2], Yuichiro Takahashi[4], Genji Kurisu[1,2] ([1]*IPR., Osaka Univ.*, [2]*Grad. Sch. Eng., Osaka Univ.*, [3]*IPSR., Okayama Univ.*, [4]*RIIS., Okayama Univ.*)

2Pos043 疾患関連変異のタンパク質構造上の三次元分布に基づく新規機能部位の探索
Search for undiscovered protein functional sites based on the spatial distribution of disease-associated missense variants
Chie Motono[1,2], Atsushi Hijikata[3], Takatsugu Hirokawa[4,5], Kenichiro Imai[1] ([1]*Cell. Mol. Biotechnology RI, AIST*, [2]*CBBD-OIL, AIST*, [3]*Sch.Life Sci., Tokyo Univ. Pharm. Life Sci.*, [4]*Faculty Med., Univ. of Tsukuba*, [5]*Transborder Med. Res. Center, Univ. of Tsukuba*)

2Pos044 拡張アンサンブル法を用いた 3 次元ドメインスワッピング(3D-DS)の研究
3 Dimensional Domain Swapping (3D-DS) Studied by Advanced Molecular Dynamics Simulation
Hiromitsu Shimoyama, Yasuteru Shigeta (*CCS, Tsukuba Univ.*)

2Pos045 構造に基づくキラターゼ CfbA のポルフィリン型基質選択性の理解
Structural insights into porphyrinoid substrate selectivity of chelatase CfbA
Shoko Ogawa[1], Yuma Oyamada[1], Masahide Hikita[2], Takashi Fujishiro[1] ([1]*Dept. of Biochem. Mol. Biol., Grad. Sch. Sci. Engineer., Saitama Univ. / Japanese*, [2]*IMSS, KEK / Japanese*)

2Pos046 Structure-function relationship of Zn finger domain in Heliorhodopsin
Manish Singh[1], Kota Katayama[1], Yuji Furutani[1], Oded Béjà[2], Rohit Ghai[3], Hideki Kandori[1] ([1]*Nagoya Institute of Technology (Japan)*, [2]*Technion –Israel Institute of Technology (Israel)*, [3]*Department of Aquatic Microbial Ecology (Czech Republic)*)

2Pos047 Torque transmission of the F_1-ATPase with an inelastic driveshaft
Shou Furuike, Yasushi Maki, Hideji Yoshida (*Dept. of Phys. Osaka Med. Pharm. Univ.*)

蛋白質：物性（安定性 折れたたみなど）／Protein: Property

2Pos048 環境変化によるタンパク質の構造変化を取り込んだ粗視化タンパク質モデル
An improved coarse grained protein model to include an environment-driven conformational change
Teppei Yamada[1], Wataru Shinoda[2] ([1]*Graduate School of Natural Science, Okayama University*, [2]*Research Institute for Interdisciplinary Science, Okayama University*)

2Pos049* 表面電荷改変抗体のコロイド安定性・結合親和性とその溶媒依存性の解析
Analysis of buffer-dependent colloidal stability and binding affinity of supercharged antibodies
Keisuke Kasahara[1], Daisuke Kuroda[2], Satoru Nagatoishi[3], Kouhei Tsumoto[1,3] ([1]*Dept. Bioeng., Grad. Sch. Eng., Univ. Tokyo*, [2]*Res. Ctr. Drug Vaccine Dev., NIID*, [3]*Inst. Med. Sci., Univ. Tokyo*)

2Pos050* (1SBA-3) タンパク質ケージ内における芳香環相互作用ネットワークの熱力学・分子動力学的解析
(1SBA-3) Thermodynamic and Molecular Dynamic Analysis of Aromatic Interaction Networks in Protein Cages
Yuki Hishikawa[1], Noya Hiroki[1], Asuka Asanuma[1], Basudev Maity[1], Satoru Nagatoishi[2], Kouhei Tsumoto[2,3], Satoshi Abe[1], Takafumi Ueno[1] ([1]*Sch. Life Sci. Technol., Tokyo Inst. Technol.*, [2]*Inst. Med. Sci., Univ. Tokyo*, [3]*Sch. Eng., Univ. Tokyo*)

2Pos051 (1SAA-7) 蝶々型金ナノデバイスが可能にするタンパク質液液相分離過程の制御
(1SAA-7) Control of protein condensation by butterfly-shaped gold nanodevices
Tomohiro Nobeyama[1], Koji Takata[2], Tatsuya Murakami[2], Kentaro Shiraki[1,2] ([1]*Pure and Appli.Sci., Univ.Tsukuba*, [2]*Grad. Sch. Sci. Toyama Pref. Univ*)

2Pos052 6 M 塩化グアニジニウム中でアンフォールドした 3 ヘリックス・バンドル蛋白質の残存構造の H/D 交換 2 次元 NMR による研究
Residual structures in the unfolded state in a three-helix-bundle protein in 6 M guanidinium chloride studied by H/D-exchange 2D NMR
Kunihiro Kuwajima[1], Saeko Yanaka[2], Maho Yagi-Utsumi[2], Koichi Kato[2] ([1]*Grad. Sch. Sci., Univ. Tokyo*, [2]*ExCELLS & IMS, NINS*)

2Pos053 Isolation and characterization of a 200kDa fibroin precursor
Kok Sim Chan[1], Kento Yonezawa[2], Haruya Kajimoto[1], Takehiro Sato[3], Yoichi Yamazaki[1], Sachiko Toma-Fukai[1], Hironari Kamikubo[1,2] ([1]*1Division of Materials Science, Graduate School of Science and Technology, Nara Institute of Science and Technology*, [2]*Center for Digital Green-innovation, Nara Institute of Science and Technology*, [3]*Spiber Inc.*)

2Pos054 スタフィロコッカル・ヌクレアーゼにおける、自発的フォールディングからリガンド誘導フォールディングへの機構転移
How to shift the mechanisms from spontaneous folding to ligand-induced folding of staphylococcal nuclease?
Yujiro Mori[1], Issei Suzuki[2], Shingo Fukazawa[2], Kosuke Maki[1] ([1]*Grad. Sch. Sci., Nagoya Univ.*, [2]*Sch. Sci., Nagoya Univ.*)

2Pos055 液-液相分離により形成されるドロップレット内部でのタンパク質及び RNA の分子ダイナミクス
Molecular dynamics of proteins and RNA within droplets formed by liquid-liquid phase separation
Fuga Watanabe[1], Takuma Akimoto[2], Eiji Yamamoto[3] ([1]*Grad. Sch. Sci. Tech., Keio Univ.*, [2]*Dept. Phys., Tokyo Univ. Sci.*, [3]*Dept. Syst. Des. Eng., Keio Univ.*)

2Pos056 剪断応力がフィブロインナノファイバーに及ぼす影響
Effect of shear stress on fibroin nanofibers
Keita Iwasaki[1], Kento Yonezawa[1,2], Satoru Onishi[1], Muneya Daidai[1], Haruya Kajimoto[1], Takehiro Sato[3], Yoichi Yamazaki[1], Sachiko Toma-Fukai[1], Hironari Kamikubo[1,2] ([1]*NAIST, MS*, [2]*NAIST, CDG*, [3]*Spiber Inc*)

2Pos057* 神経変性疾患関連タンパク質 Ataxin-3 の液-液相分離と凝集ダイナミクスのポリ Q 鎖長依存性
PolyQ chain length dependence of liquid-liquid phase separation and aggregation dynamics of a neurodegeneration-related protein ataxin-3
Uchu Matsuura[1], Shinya Tahara[1], Shinji Kajimoto[1,2], Takakazu Nakabayashi[1] ([1]*Graduate School of Pharmaceutical Sciences, Tohoku University*, [2]*JST PRESTO, Japan.*)

2Pos058 疾病関連 α-シヌクレイン変異体の構造およびダイナミクス特性
Structural and dynamical properties of the disease-related mutants of α-synuclein
Satoru Fujiwara[1], Kai Nishikubo[1], Kensuke Ikenaka[2], César Aguirre[2], Hideki Mochizuki[2] ([1]*Inst. Quantum Life Science, QST*, [2]*Grad. Sch. Medicine, Osaka Univ.*)

2Pos059 統計力学モデルによるアポミオグロビンのフォールディング反応機構の予測
Folding mechanisms of apomyoglobin predicted by an extended statistical mechanical model
Koji Ooka[1], Munehito Arai[2,3] ([1]*Col. Arts & Sci., Univ. Tokyo*, [2]*Dept. Life Sci., Univ. Tokyo*, [3]*Dept. Phys., Univ. Tokyo*)

2Pos060 コンタクト計算を厳密化した改良型統計力学モデルによるタンパク質フォールディング経路の予測
Predicting protein folding pathways using the statistical mechanical model modified with accurate contact calculation
Runjing Liu[1], Koji Ooka[2], Munehito Arai[1,3] ([1]*Dept. Life Sci., Univ. Tokyo*, [2]*Col. Arts & Sci., Univ. Tokyo*, [3]*Dept. Phys., Univ. Tokyo*)

2Pos061 AlphaFold は条件付きでフォールドする天然変性タンパク質・天然変性領域（ProS）の構造をどのように予測したか
How AlphaFold predicts conditionally-foldable segments in intrinsically disordered proteins
Koya Sakuma[1], Hiroto Anbo[2], Satoshi Fukuchi[2], Motonori Ota[1] ([1]*Grad. Sch. Informatics, Nagoya Univ.*, [2]*Faculty of Engineering, Maebashi Inst. of Technology*)

2Pos062 Liquid-liquid phase separation and amyloid formation of Sup35 from four different yeast species
Yumiko Ohhashi[1], Suguru Nishinami[2], Kentaro Shiraki[2], Eri Chatani[1] ([1]*Grad. Sch of Sci., Kobe Univ.*, [2]*Inst. Appl. Phys., Univ. of Tsukuba*)

2Pos063 トランスサイレチン断片のアミロイド線維形成
Amyloid fibril formation of transthyretin fragments
Keisuke Yuzu[1], Misato Matsumura[1], Naoki Yamamoto[2], Masatomo So[3], Keiichi Yamaguchi[4], Yuji Goto[4], Eri Chatani[1] ([1]*Grad. Sch. Sci., Kobe Univ.*, [2]*Fac. Med., Jichi Med. Univ.*, [3]*Inst. Protein Res., Osaka Univ.*, [4]*Grad. Sch. Eng., Osaka Univ.*)

蛋白質：機能（反応機構 生物活性など）／Protein: Function

2Pos064* β アレスチンの新規 PIP2 結合サイトとその機能
Novel PIP2 binding site of βarrestin and its function
Ritsuki Kuramoto, Tatsuya Ikuta, Koki Kawakami, Asuka Inoue (*Graduate School of Pharmaceutical Sciences, Tohoku University*)

2Pos065 クチナーゼ様酵素 Cut190 による微粉化 PET 分解
Degradation of homogenized PET with cutinase-like enzyme Cut190 form *Saccharomonospora viridis* AHK190
Fumiya Kondo[1], Miho Emori[2], Masayuki Oda[1,2] ([1]*Faculty Life. Environ. Sci., Kyoto Pref. Univ.*, [2]*Grad. Sch. Life. Environ. Sci., Kyoto Pref. Univ.*)

2Pos066 不凍タンパク質と粘性物質を組み合わせた培養細胞の新規凍結保護剤
Novel cryoprotectants consist of antifreeze protein and viscous additive for cryopreservation of cultured cells
Luyan Zhang[1,2], Akari Yamauchi[6], Sakae Tsuda[3,4,5], Yasushi Ohyama[2], Hidemasa Kondo[1,2] ([1]*Graduate School of Life Science, Hokkaido University*, [2]*Bioproduction Research Institute, National Institute of Advanced Industrial Science and Technology (AIST)*, [3]*Graduate School of Frontier Sciences, The University of Tokyo*, [4]*OPERANDO Open Innovation Laboratory, National Institute of Advanced Industrial Science and Technology (AIST)*, [5]*Faculty of Advanced Life Science, Hokkaido University*, [6]*Hibernation Metabolism, Physiology and Development Group, Institute of Low Temperature Science, Hokkaido University*)

2Pos067 オオクワガタ由来不凍タンパク質の特性評価
Characteri zation of antifreeze protein from a stag beetle *Dorcus hopei binodulosus*
Yuki Iida[1,2], Tatsuya Arai[3], Akari Yamauchi[6], Sakae Tsuda[3,4,5], Yasushi Ohyama[2], Hidemasa Kondo[1,2] ([1]*Graduate School of Life Science, Hokkaido University*, [2]*Bioproduction Research Institute, National Institute of Advanced Industrial Science and Technology*, [3]*Graduate School of Frontier Sciences, The University of Tokyo*, [4]*OPERANDO Open Innovation Laboratory, National Institute of Advanced Industrial Science and Technology*, [5]*Faculty of Advanced Life Science, Hokkaido University*, [6]*Hibernation Metabolism, Physiology and Development Group, Institute of Low Temperature Science, Hokkaido University*)

2Pos068 氷結晶結合蛋白質の非凍結細胞保護機能の分子メカニズム解明
Elucidating the molecular mechanism of cell protective function of ice-binding proteins at non-freezing temperature
Tatsuya Arai[1,2], Yue Yang[1], Sakae Tsuda[1], Kazuhiro Mio[2], C. Yuji Sasaki[1,2] ([1]*Grad. Sch. Fontier Sci., Univ. Tokyo*, [2]*AIST-UTokyo OPERANDO-OIL*)

2Pos069* アミロイドβと細胞骨格蛋白質のアクチンおよびチューブリンの間の相互作用は、それらの重合状態に依存する
The interaction between amyloid β and cytoskeletal proteins, actin and tubulin, depends on their polymerization state
Yukina Kurotaki[1], Ragheed H. Yousif[2], Masahiro Kuragano[1], Kiyotaka Tokuraku[1] ([1]*Muroran Institute of Technology*, [2]*Al-Farahidi University*)

2Pos070 ヒト血清のアミロイドβ凝集阻害活性の評価
Evaluation of Amyloid β aggregation inhibitory activity of human serum
Yuku Yamada, Keiya Shimamori, Tomohiko Katakawa, Masahiro Kuragano, Kiyotaka Tokuraku (*Grad. Sch. Eng. , Muroran Inst. of Tech.*)

2Pos071 セリンプロテアーゼ Neuropsin の基質特異性の決定因子に関する MD 研究
MD simulation study on determinant factors for substrate specificity of serine protease neuropsin
Masami Lintuluoto[1], Yota Horioka[1], Mitsumasa Abe[1], Yoshifumi Fukunishi[2], Juha Mikael Lintuluoto[3], Hideki Tamura[4] ([1]*Grad. Sch. Life and Env. Sci., Kyoto Pref. Univ.*, [2]*AIST, CMB*, [3]*Grad. Sch. Eng. Kyoto Univ.*, [4]*Hoshi Univ. Sch. Pharm. and Pharm. Sci.*)

2Pos072* 改良型 Raichu を用いた静水圧印加時の Ras 活性測定
Ras activity measurement under hydrostatic pressure using improved Raichu
Teruhiko Matsuda[1], Minki Chang[2], Katsuko Furukawa[2], Takashi Ushida[3], Taro QP Uyeda[1] ([1]*Dept. Pure & Appl. Physics, Grad. Sch. Adv. Sci. & Eng., Waseda Univ./ Japanese*, [2]*Dept. Bio Eng., Fac. Eng., Univ. Tokyo/ Japanese*, [3]*Dept. Mech. Eng., Fac. Eng., Univ. Tokyo/ Japanese*)

2Pos073 *Eco*RV による DNA 加水分解におけるプロトン移動の量子化学計算による観察
Proton-transfer in hydrolysis of DNA by EcoRV calculated by quantum-chemical metadynamics
Mika Mitsumatsu[1], Itaru Onishi[1], Norio Yoshida[2], Fumio Hirata[3], Masayuki Irisa[1] ([1]*Kyushu Inst. of Tech.*, [2]*Nagoya Univ.*, [3]*IMS*)

蛋白質：計測・解析の方法論／Protein: Measurement & Analysis

2Pos074* Molecular structure dynamics identification method development based on High speed AFM imaging data
Yui Kanaoka[1], Yuto Nonaka[1], Norie Hamaguchi[2], Takeshi Murata[2], Florence Tama[1,3], Takayuki Uchihashi[1] ([1]*Grad. Sch. Sci., Univ. Nagoya*, [2]*Grad. Sch. Sci., Univ. Chiba*, [3]*R-CSS*)

2Pos075* ブリルアン・ラマン同時イメージングによる液-液相分離によるタンパク質液滴の変化の観測
Observation of the change in physical condition of a liquid droplet formed by liquid-liquid phase separation using Brillouin-Raman imaging
Daiki Shibata[1], Shinji Kajimoto[1,2], Takakazu Nakabayashi[1] ([1]*Grad. Sch. Sci., Tohoku Univ.*, [2]*JST PRESTO*)

2Pos076 タンパク質モーフィング手法と半自動簡略化経路探索法の膜タンパク質二量体のダイナミクスへの適用
Application of the Protein Morphing Method and the Semi-automatic Simplified Path Exploration to the Membrane Protein Dimers Dynamics
Ryota Kiyooka[1], Masaki Otawa[2], Lisa Matsukura[1], Naoyuki Miyashita[1] ([1]*Grad. Sch. BOST, KINDAI Univ.*, [2]*Grad. Sch. Phys. Sci., GUAS*)

2Pos077* 蛍光寿命を用いた LLPS によって生じた FUSLC 液滴の時間変化ダイナミクスの定量解析
Quantitative analysis of time-dependent dynamics of FUS LC droplets formed by LLPS using fluorescence lifetime
Kaichi Nagai[1], Shinya Tahara[2], Uchuu Matusura[2], Mizuki Sugimoto[3], Eita Sasaki[4], Shinji Kajimoto[2,5], Kenjiro Hanaoka[4], Takakazu Nakabayashi[2] ([1]*Faculty of Pharmaceutical Sciences, Tohoku University*, [2]*Graduate school of Pharmaceutical Sciences, Tohoku University*, [3]*Faculty of Pharmacy, Keio University*, [4]*Graduate School of Pharmaceutical Sciences, Keio University*, [5]*JST PRESTO*)

2Pos078 スプリット Akaluc を用いた個体深部における GPCR/β-アレスチン相互作用と細胞融合の検出法
Split Akaluc reconstitution methods for detecting GPCR/β-arrestin interaction and cell fusion event in deep tissues
Yiling Li, Genki Kawamura, Qiaojing Li, Takeaki Ozawa (*Department of Chemistry, School of Science, The University of Tokyo*)

2Pos079 X 線 1 分子追跡法によるイベルメクチン存在下での nAChR α7 の逆回転運動の測定
The Opposite Twisting Motions of Ivermectin-nAChR α7 Monitored by Diffracted X-ray Tracking
Yue Yang[1], Tatsuya Arai[1,2], Daisuke Sasaki[1], Masahiro Kuramochi[1,3], Hiroshi Sekiguchi[4], Kazuhiro Mio[2], Tai Kubo[5], Yuji C. Sasaki[1,2,4] ([1]*Grad Sch. of Fron. Sci., Univ. Tokyo*, [2]*AIST-UTokyo*, [3]*Grad Sch. of Sci. and Eng., Univ. Ibaraki*, [4]*JASRI/ SPring-8*, [5]*GlyTech Inc.*)

2Pos080* 凝集体形成機構解明に向けた電場存在下におけるタンパク質の動的構造解析基盤の確立
Development of a platform for dynamic structural analysis of proteins in electric fields to elucidate the mechanism of aggregate formation
Yusuke Shuto[1], Erik Walinda[3], Daichi Morimoto[2], Kenji Sugase[1] ([1]*Grad. Agr., Univ. Kyoto*, [2]*Grad. Eng., Univ. Kyoto*, [3]*Grad. Med., Univ. Kyoto*)

2Pos081 糊化デンプンを使用したマイクロプレートへの MBP 融合タンパク質固定化法の開発及びタンパク質間相互作用解析への応用
An immobilization method of MBP-fusion proteins using a gelatinized starch-agarose mixture and its application for PPI analysis
Ryoya Katayama[1], Yuri Emoto[2], Reiji Hijikata[3], Emi Hibino[2], Natsuko Goda[2], Takeshi Tenno[2], Hidekazu Hiroaki[2], Akihiro Narita[1] ([1]*Graduate School of Science, Nagoya University*, [2]*Graduated School of Pharmaceutical Sciences, Nagoya University*, [3]*School of Science, Nagoya University*)

2Pos082* インタクトなミトコンドリアにおける電子伝達複合体活性計測
Measurements of electron transfer complex activities in intact mitochondria
Saki Koyama, Momoka Kutami, Yoshiki Suganuma, Hiroko Kashiwagi, Yoshihiro Ohta (*Department of Biotechnology and Life Sciences, Graduate school of Engineering, Tokyo University of Agriculture and Technology*)

2Pos083 ペプチドの伸長に伴うエネルギー準位統計の分化と分子進化
Evolution of Energy Level Statistics and Molecular Evolution with Peptide Elongation
Masanori Yamanaka (*CST, Nihon Univ.*)

2Pos084 ポリアミノ酸検出のためのナノポア阻害電流解析法の開発
Developing Current Analyses for Nanopore Detection of Poly(amino acid)s
Misa Yamaji, Ryuji Kawano (*Department of Biotechnology and Life Science, Tokyo University of Agriculture and Technology*)

2Pos085* 生体用ナノポア用いた α-helix 及び β-hairpin ペプチドのアンフォールディング挙動観察
Observation of unfolding behavior of peptides with a-helix and b-hairpin through a biological nanopore
Miyu Fukuda, Ryuji Kawano (*Department of Biotechnology and Life Science, Tokyo University of Agriculture and Technology.*)

2Pos086* 合理的設計手法による SARS-CoV-2 変異体に対する中和抗体の開発
Development of neutralizing antibodies against SARS-CoV-2 variants by rational design
Rina Aoyama[1], Sairi Matsumoto[1], Nao Sato[1], Shunji Suetaka[1], Yuuki Hayashi[1,2], Munehito Arai[1,3] ([1]*Dept. Life Sci., Univ. Tokyo*, [2]*Environmental Sci. Ctr., Univ. Tokyo*, [3]*Dept. Phys., Univ. Tokyo*)

2Pos087* Reverse Engineering Analysis of the High-Temperature Reversible Oligomerization and Amyloidogenicity of PSD95-PDZ3
Sawaros Onchaiya[1], Tomonori Saotome[2], Kenji Mizutani[3], Jose C. Martinez[4], Jeremy R. H. Tame[3], Shun-ichi Kidokoro[2], Yutaka Kuroda[1] ([1]*Department of Biotechnology and Life Science, Tokyo University of Agriculture and Technology, 2-24-16, Naka-cho, Koganei-shi 184-8588, Tokyo, Japan*, [2]*Department of Bioengineering, Nagaoka University of Technology, 1603-1, Kamitomioka-cho, Nagaoka-shi 940-2188, Niigata, Japan*, [3]*Graduate School of Medical Life Science, Yokohama City University, 1-7-29 Suehiro, Yokohama 230-0045, Kanagawa, Japan*, [4]*Department of Physical Chemistry, Institute of Biotechnology, Faculty of Sciences, University of Granada, 18071 Granada, Spain*)

2Pos088 アレルギー疾患を阻害しうるタンパク質の合理的設計
Rational design of proteins that can inhibit allergic diseases
Mizuki Teranishi[1], Nao Sato[1], Shunji Suetaka[1], Mio Sano[1], Yuuki Hayashi[1,2], Munehito Arai[1,3] ([1]*Dept. Life Sci., Univ. Tokyo*, [2]*Environment Science Center, Univ. Tokyo*, [3]*Dept. Phys., Univ. Tokyo*)

2Pos089* タンパク質間相互作用を阻害するヘリックス模倣化合物の探索
Search for helix-mimetic compounds that inhibit protein-protein interactions
Nao Sato[1], Shunji Suetaka[1], Eiji Honda[2], Hajime Takashima[2], Dai Takehara[2], Atsushi Yoshimori[3], Yuuki Hayashi[1,4], Munehito Arai[1,5] ([1]*Department of Life Sciences, The University of Tokyo.*, [2]*PRISM BioLab Co., Ltd.*, [3]*Institute for Theoretical Medicine, Inc.*, [4]*Environmental Science Center, The University of Tokyo.*, [5]*Department of Physics, The University of Tokyo.*)

2Pos090* *Pichia pastoris* を用いた組換えタンパク質発現系におけるシステインに富んだタンパク質の折りたたみと収量に関わる因子の解明
Factors involved in the folding and yield of cysteine-rich proteins in recombinant expression system using *Pichia pastoris*.
Ami Hanaoka[1], Tomona Iizuka[1], Jingkang Zheng[1], Ichiho Yoshikawa[2], Wenqing Cai[1], Yurie Nakajima[1], Soma Ishihara[2], Tomoyasu Aizawa[1,2] ([1]*Grad. Sch. Life Sci., Hokkaido Univ.*, [2]*Sch. Sci., Hokkaido Univ.*)

2Pos091* 細胞内光遺伝学ツール Magnets 変異体の比較とさらなる改良
Comparison and further improvement of the intracellular optogenetic tool Magnets variants
Masataka Yoshimura[1], Yuki Aono[1], Yuuki Hayashi[1,2], Fuun Kawano[1], Moritoshi Sato[1], Munehito Arai[1,3] ([1]*Dept. Life Sci., Univ. Tokyo*, [2]*Env. Sci. Ctr., Univ. Tokyo*, [3]*Dept. Phys., Univ. Tokyo*)

2Pos092 ピキア酵母を用いたシステインリッチアレルゲン蛋白質の過剰発現系における非天然型ジスルフィド結合と修飾の検討
Investigation of non-native disulfide bonds and modification in the overexpression of cysteine-rich allergens by *Pichia pastoris*
Ichiho Yoshikawa[1], Ami Hanaoka[2], Tomona Iizuka[2], Jingkang Zheng[2], Wenqing Cai[2], Soma Ishihara[1], Yurie Nakajima[2], Tomoyasu Aizawa[1,2] ([1]*Sch. Sci., Hokkaido Univ.*, [2]*Grad. Sch. Life Sci., Hokkaido Univ.*)

2Pos093* LL-37 型 cathelicidin ファミリー抗菌ペプチドの組換え発現と NMR 解析による免疫進化研究
Immunological evolution studies combining NMR and recombinant overexpression of the LL-37-like cathelicidin family antimicrobial peptides
Mitsuki Shibagaki[1], Waka Ueda[1], Kohei Kano[1], Hao Gu[1], Tomoyasu Aizawa[1,2] ([1]*Grad. Sch. Life Sci., Hokkaido Univ.*, [2]*Fac. Adv. Life Sci., Hokkaido Univ.*)

2Pos094* 相分離タンパク質の天然変性領域の配列に基づく、相分離ペプチドの合理的設計
Rational design of phase-separating peptides based on natural phase-separating protein disordered sequence
Atsumi Hando[1,2], Maulana Ariefai[1,3], Nanako Iwaki[1,4], Saori Kanbayashi[1], Keisuke Ikeda[5], Kiyoto Kamagata[1,2,3,4] ([1]*IMRAM, Tohoku Univ.*, [2]*Grad. Sch. Life Sci., Tohoku Univ.*, [3]*Dep. Chem., Fac. Sci., Tohoku Univ.*, [4]*Dep. Chem., Grad. Sch. Sci., Tohoku Univ.*, [5]*Fac. Pharm. Sci., Univ. Toyama*)

ヘム蛋白質／Heme proteins

2Pos095* シトクロム P450BM3 の非天然反応を誘起するペプチド性小分子の開発およびその作用の解明
Evolution of Dipeptidic Molecules for the Induction of the Non-native Catalysis of Cytochrome P450BM3 and the Analysis of the Mechanisms
Kai Yonemura[1], Shinya Ariyasu[1], Hiroshi Sugimoto[2], Shigeru Matsuoka[3], Osami Shoji[1] ([1]*Graduate School of Science, Nagoya University*, [2]*RIKEN/SPring-8*, [3]*Faculty of Medicine, Oita University*)

2Pos096 Direct Visualization of Hydrogen Atoms in the Haem-Acquisition Protein HasA Capturing a Synthetic Metal Complex by Protein Crystallography
Yuma Shisaka[1], Hiroshi Sugimoto[2], Naomine Yano[3], Katsuhiro Kusaka[3], Masaki Unno[3,4], Osami Shoji[5] ([1]*RIKEN Center for Sustainable Resource Science*, [2]*RIKEN SPring-8 Center*, [3]*Frontier Research Center for Applied Atomic Sciences, Ibaraki University*, [4]*Graduate School of Science and Engineering, Ibaraki University*, [5]*Graduate School of Science, Nagoya University*)

2Pos097 インドールアミン 2,3-ジオキシゲナーゼの電気化学的なレドックス制御と迅速な阻害アッセイ
Redox control of human indoleamine 2,3-dioxygenase at nanostructured electrode surface and its inhibitor screening
Yasuhiro Mie[1], Chitose Mikami[1], Yoshiaki Yasutake[1,2], Yuki Shigemura[3], Hirofumi Tsujino[3,4], Taku Yamashita[5] ([1]*Bioproduction Res. Inst., AIST*, [2]*CBBD-OIL, AIST-Waseda Univ.*, [3]*Grad. Sch. Pharm. Sci., Osaka Univ.*, [4]*Museum, Osaka Univ.*, [5]*Sch. Pharm., Mukogawa Women's Univ.*)

2Pos098 ミオグロビンへの協同的な配位子結合性付与に向けた二量体の合理的設計
Rational design of myoglobin dimers for ligand binding cooperativity
Satoshi Nagao[1], Chihiro Maruo[2], Masashi Yamada[2], Daichi Yamada[1], Minoru Kubo[1] ([1]*Grad. Sch. Sci., Univ. Hyogo*, [2]*Sch. Sci., Univ. Hyogo*)

膜蛋白質／Membrane proteins

2Pos099 シュウ酸トランスポーター OxlT の未解明構造の分子動力学的探索
Molecular dynamics search for the unknown structural state of oxalate transporter OxlT
Jun Ohnuki, Kei-ichi Okazaki (*Institute for Molecular Science*)

2Pos100 ヒト L 型アミノ酸トランスポーター LAT1-CD98hc 複合体の基質輸送シミュレーション
Substrate transport simulations of human L-type amino acid transporter LAT1-CD98hc complex coupled with conformational changes
Natsumi Yoshida[1], Toru Ekimoto[1], Tsutomu Yamane[2], Mitsunori Ikeguchi[1,2] ([1]*Grad. Sch. Med. Life Sci., Yokohama City Univ.*, [2]*RIKEN R-CCS*)

2Pos101 病原菌ヘム ABC トランスポーターのクライオ電子顕微鏡解析
Cryo-EM analysis of bacterial heme ABC transporter
Machika Kataoka[1,2], Ayaho Abe[1,2], Gopalashingam Chai[2], Gerle Christoph[2], Yoshitsugu Shiro[1], Masaki Yamamoto[2], Hideki Shigematsu[3], Hiroshi Sugimoto[1,2] ([1]*Grad. Sch. Sci., Univ. Hyogo*, [2]*RIKEN SPring-8 Center*, [3]*JASRI*)

2Pos102 高速 AFM による ABC トランスポーター P-gp の動態観察
HS-AFM Observation of Conformational Dynamics of ABC transporter P-gp
Yuto Nonaka[1], Norie Hamaguchi[2], Fumi Nakagawa[2], Satoru Ogasawara[2], Takesi Murata[2], Takayuki Uchihashi[1] ([1]*Grad. Sch. Phys., Univ. Nagoya / Japanese*, [2]*Grad. Sch. sci., Univ. Chiba. / Japanese*)

2Pos103* 局所熱パルス法を用いた 1 型リアノジン受容体の中間領域変異体の高熱感受性解析
Malignant hyperthermia-implicated heat hypersensitive mutations in the central region of RyR1 channel studied by a local heat pulse method
Chujie Liu[1,2], Takashi Murayama[3], Toshiko Yamazawa[4], Kotaro Oyama[5], Yoshie Harada[2,6], Madoka Suzuki[2] ([1]*Department of Biological Sciences, Graduate School of Science, Osaka University*, [2]*Institute for Protein Research, Osaka University*, [3]*Department of Cellular and Molecular Pharmacology, Juntendo University Graduate School of Medicine*, [4]*The Jikei University School of Medicine*, [5]*National Institutes for Quantum Science and Technology*, [6]*Center for Quantum Information and Quantum Biology, Osaka University*)

2Pos104 ナノディスクに挿入したカリウムチャネル **KcsA** の構造
KcsA K+ Channel Structure Incorporated into Nanodisc
Hiroko Takazaki[1], Hirofumi Shimizu[2], Takuo Yasunaga[3] ([1]*IPR, Univ. Osaka*, [2]*Fac. Med. Sci., Univ. Fukui*, [3]*Grad. Sch. Comp. Sci. Syst. Eng., KIT*)

2Pos105 X 線 1 分子追跡法を用いた TRPV1 チャネルの細胞内ドメイン動態計測
Intramolecular dynamics of TRPV1 channel using Diffracted X-ray Tracking
Tatsunari Ohkubo[1,2], Shoko Fujimura[2,3], Kazuhiro Mio[1,2], Hiroshi Sekiguchi[4], Yuji C. Sasaki[2,3,4] ([1]*Grad. Sch. Med. Sci., Yokohama CU*, [2]*Operand OIL, AIST*, [3]*Grad. Sch. of Front. Sci., The Univ of Tokyo*, [4]*JASRI*)

2Pos106* EXP2 ナノポアとその変異体を用いたペプチドの 1 分子検出
Single-molecule detection of peptides using EXP2 nanopore and its variant
Mitsuki Miyagi, Sotaro Takiguchi, Kazuaki Hakamada, Masafumi Yohda, Ryuji Kawano (*Department of Biotechnology and Life Science, Tokyo University of Agriculture and Technology*)

核酸結合蛋白質／Nucleic acid binding proteins

2Pos107 DNA 液滴内での DNA 結合タンパク質の標的 DNA 探索の単分子観察
Single-molecule characterization of target search of DNA-binding proteins inside liquid DNA droplets
Ryo Kusano[1,2], Trishit Banerjee[1,2], Saori Kambayashi[1], Kiyoto Kamagata[1] ([1]*IMRAM, Tohoku Univ.*, [2]*Department of Chemistry, Tohoku Univ.*)

2Pos108 Molecular dynamics study of the three prime repair exonuclease 1 and its mutants
Hiroki Otaki (*Grad. Sch. of Biomedical Sci., Nagasaki Univ.*)

2Pos109* (2SEP-3) RNase T2 のリボソームへの結合を介した翻訳阻害機構
(2SEP-3) Regulation mechanism of translation through the interaction of RNase T2 with ribosome
Atsushi Minami[1], Takehito Tanzawa[2], Zhuohao Yang[3], Takashi Funatsu[3], Takayuki Kato[2], Tomohisa Kuzuyama[1,4], Hideji Yoshida[5], Tetsuhiro Ogawa[1,4] ([1]*Grad. Sch. Agri. and Life Sci., Univ. Tokyo*, [2]*IPR, Osaka Univ.*, [3]*Grad. Sch. Pharm. Sci., Univ. Tokyo*, [4]*CRIIM, Univ. Tokyo*, [5]*Fac. Med., Osaka Med. Pharm. Univ.*)

2Pos110 ヌクレオリン核酸結合ドメインと 4 重鎖 DNA との結合過程
The binding process of quadruplex DNA to RNA/DNA binding domains of nucleolin
Masato Morikawa[1], Kota Yamaguchi[1], Kazuki Kawada[2], Koji Umezawa[1,2,3] ([1]*Grad. Sch. of Sci. & Tech., Shinshu Univ.*, [2]*Dept. Agri., Shinshu Univ.*, [3]*IBS., Shinshu Univ.*)

核酸：構造・物性／Nucleic acid: Structure & Property

2Pos111 微小閉鎖空間がポリヌクレオソーム凝縮に与える影響の検討
Investigation of the effect of spherical (three-dimensional) confinement on the higher order structure of 12-mer nucleosome arrays
Masahiro Okabe (*Dept. Biol. Sci., Grad. Sch. Sci., The Univ. Tokyo*)

2Pos112 一本鎖 DNA は核小体周囲に凝集体を形成する
Single-stranded DNA forms condensates surrounding nucleoli
Koichiro Maki[1,2], Jumpei Fukute[1,3], Taiji Adachi[1,2,3] ([1]*Inst. Life Med. Sci., Kyoto University*, [2]*Grad. Sch. Eng., Kyoto University*, [3]*Grad. Sch. Biostudies, Kyoto University*)

2Pos113* ヒト生細胞内環境における三重鎖 DNA 分子の構造及びダイナミクスの解析
Analysis of the structure and dynamics of triplex forming oligodeoxynucleotide in living human cells
Tomoki Sakamoto[1,2], Yudai Yamaoki[1,2], Takashi Nagata[1,2], Masato Katahira[1,2] ([1]*Inst. Adv. Energy, Kyoto Univ.*, [2]*Grad. Sch. Energy Sci., Kyoto Univ.*)

2Pos114 動的ループによる染色体コンパートメントの形成と変化
Dynamic loops shape and reshape chromosome compartments
Shin Fujishiro[1,2], Masaki Sasai[1,2] ([1]*Fukui Inst. Fund. Chem., Kyoto Univ.*, [2]*Dept. Complex Sys. Sci., Nagoya Univ.*)

2Pos115 FRET study of the sequence dependence of nucleosomal DNA unwrapping
Tomoko Sunami, Hidetoshi Kono (*QST, iQLS*)

2Pos116* (2SBA-4) 細胞核内における underwound DNA の蛍光イメージング
(2SBA-4) Fluorescence imaging of underwound DNA in the cell nucleus
Jumpei Fukute[1,2], Koichiro Maki[1,3], Taiji Adachi[1,2,3] ([1]*Inst. Life & Med. Sci., Kyoto Univ.*, [2]*Grad. Sch. Biostudies, Kyoto Univ.*, [3]*Grad. Sch. Eng., Kyoto Univ.*)

2Pos117 ラマン顕微鏡を用いた生細胞内のクロモセンターのラベルフリー成分・構造解析
Label-free compositional and structural analysis of chromocenters in living cells using Raman microscopy
Masato Machida[1], Atsushi Shibata[2], Kentaro Hujii[3], Shinji Kajimoto[1,4], Takakazu Nakabayashi[1] ([1]*Grad. Sch. Pharm. Sci., Univ. Tohoku*, [2]*GIAR., Univ. Gunma*, [3]*QST.*, [4]*JST PRESTO.*)

核酸：相互作用・複合体／Nucleic acid: Interaction & Complex formation

2Pos118* 高速原子間力顕微鏡による H2A.Z.1 ヌクレオソームの DNA 上での自発的スライディングの直接観察
Direct imaging of spontaneous sliding along DNA of H2A.Z.1 nucleosome by high-speed atomic force microscopy
Shin Morioka[1], Shoko Sato[2], Naoki Horikoshi[2], Tomoya Kujirai[2], Hitoshi Kurumizaka[2], Mikihiro Shibata[3,4] ([1]*Grad. Sch. Math. & Phys., Kanazawa Univ.*, [2]*Institute of Quantitative Biosciences, Tokyo Univ.*, [3]*WPI-NanoLSI, Kanazawa Univ.*,, [4]*InFiniti, Kanazawa Univ.*)

2Pos119* DNA ハイブリダイゼーションのカイネティックなエラー抑制
Kinetic error suppression of DNA hybridization
Hiroyuki Aoyanagi[1], Simone Pigolotti[2], Shinji Ono[1], Shoichi Toyabe[1] ([1]*Grad. Sch. Eng., Tohoku Univ*, [2]*OIST*)

2Pos120* (1SGA-2) 人工核酸 PNA を用いた DNA の液ー液相分離制御
(1SGA-2) Regulation of liquid-liquid phase separation of DNA using peptide nucleic acid (PNA)
Rikuto Soma, Yuichiro Aiba, Masanari Shibata, Shinya Ariyasu, Osami Shoji (*Graduate School of Science, Nagoya University.*)

2Pos121* 非平衡ダイナミクスを示す酵素反応によって活性化された DNA 液滴
Enzymatically activated DNA-droplets exhibiting non-equilibrium dynamics
Tomoya Maruyama[1], Masahiro Takinoue[1,2] ([1]*School of Life science and Technology, Tokyo Institute of Technology*, [2]*School of Computer Science, Tokyo Institute of Technology*)

2Pos122* 再構成転写翻訳系におけるトランスファー RNA の合成と共役した翻訳および DNA 複製システム
Transfer RNA synthesis-coupled translation and DNA replication in a reconstituted transcription/translation system
Ryota Miyachi[1], Yoshihiro Shimizu[2], Norikazu Ichihashi[1,3,4] ([1]*Grad. Sch. Arts Sci., Univ. Tokyo*, [2]*Center for Biosystems Dynamics Research, Riken*, [3]*Komaba Institute for Science, Univ. Tokyo*, [4]*Research Center for Complex Systems Biology, Universal Biology Institute, Univ. Tokyo*)

水・水和／電解質／Water & Hydration & Electrolyte

2Pos123 MD シミュレーションによるタンパク質モデルペプチド周囲の水和ダイナミクスの解明
MD simulations reveals hydration dynamics around protein model peptides
Takuya Takahashi[1], Ryutaro Inou[2], Yui Nakamura[2] ([1]*Coll. Life Sci., Ritsumeikan Univ.*, [2]*Grad. Sch. Life Sci., Ritsumeikan Univ.*)

2Pos124* Effect of local electric field on the rotational dynamics of water dipole in protein solutions
Kang Hu[1,2], Ryo Shirakashi[1] ([1]*IIS, Univ. Tokyo*, [2]*Grad. Sch. Eng., Univ. Tokyo*)

2Pos125 ニューラルネットワークと経験分布の融合的手法による膜蛋白質の水和構造予測
Prediction of hydration structures of membrane proteins using neural networks in combination with the empirical hydration distribution
Kochi Sato[1,2], Mao Oide[1,2], Masayoshi Nakasako[1,2] ([1]*Dept. Phys., Keio Univ.*, [2]*RSC, RIKEN*)

2Pos126 Free energy analysis of the addition of small molecules with simple structures to elucidate co-solvent effects in insulin dissociation
Simon Hikiri, Nobuyuki Matubayasi (*Grad. Sch. Eng. Sci., Osaka Univ.*)

2Pos127* 酸性タンパク質凝集解明のための分子シミュレーションによる電解質溶液中のアニオン間実効引力の研究
Molecular simulation study of effective attraction between anions in an electrolyte solution for elucidation of acidic protein aggregation
Michika Takeda[1], Ryo Akiyama[2] ([1]*Grad. Sch. Sci. Kyushu Univ.*, [2]*Inst. Sci. Kyushu Univ.*)

2Pos128 水と生体分子のシミュレーションにおける静電相互作用計算：オンサーガモデルによる理論的検証
Theoretical study on the electrostatic calculation in biomolecular simulation
Yoshiteru Yonetani (*QST*)

発生・分化／Development & Differentiation

2Pos129* 幹細胞分化のモデル系を模した人工遺伝子回路の生じる空間パターン
Spatial patterns formed by a synthetic genetic circuit mimicking the model of stem cell differentiation
Kei Ikemori, Yuichi Wakamoto (*Grad. Sch. of Art. & Sci., Univ. Tokyo*)

2Pos130 Planar cell polarity–dependent asymmetric organization of microtubules for polarized positioning of the basal body in node cells
Xiao Rei Sai[1], Kastura Minegishi[2], Hiroshi Hamada[1] ([1]*Riken BDR*, [2]*National Center of Neurology and Psychiatry*)

2Pos131 マウスノード不動繊毛は変形の向きを感知して左右軸を決定する: 非対称性を生み出すメカニカルな機構
Mouse nodal immotile cilia sense bending direction for left-right determination: Mechanical regulation in initiation of symmetry breaking
Takanobu A Katoh[1], Toshihiro Omori[2], Katsutoshi Mizuno[3], Takeshi Itabashi[1], Atsuko H. Iwane[1], Takuji Ishikawa[2], Yasushi Okada[1,4], Takayuki Nishizaka[5], Hiroshi Hamada[1] ([1]*BDR, Riken*, [2]*Grad. Sch. Eng., Tohoku Univ.*, [3]*Fac. Med. Sci., Univ. of Fukui*, [4]*Grad. Sch. Med., Grad. Sch. Sci., UBI, WPI-IRCN, The Univ. of Tokyo*, [5]*Fac. Sci., Gakushuin Univ.*)

2Pos132* 物理的環境の非対称性が上皮折り畳みパターン選択に果たす役割
Role of asymmetry of physical environment in epithelial folding pattern selection
Kentaro Morikawa, Daich Kuroda, Yasuhiro Inoue (*Grad. Sch. Eng., Kyoto Univ.*)

筋肉（筋蛋白質・収縮）／Muscle

2Pos133 微小管脱重合薬により骨格筋の粘弾性は変化する
The viscoelasticity of skeletal muscle is altered by microtubule destabilized agent
Takuya Kobayashi, Takashi Murayama, Nagomi Kurebayashi (*Dept. of Cellular and Molecular Pharmacology, Juntendo University*)

2Pos134 細菌アクチン MreB の繊維構造多型
Filament structural polymorphism of bacterial actin MreB
Daichi Takahashi[1], Ikuko Fujiwara[1,2,3], Akihiro Narita[4], Makoto Miyata[1,2] ([1]*Grad. Sch. Sci., Osaka Metropolitan Univ.*, [2]*OCARINA, Osaka Metropolitan Univ.*, [3]*Dept. Mater. Sci. Bioeng., Nagaoka Univ. Tech.*, [4]*Grad. Sch. Sci., Nagoya Univ.*)

2Pos135 Absolute Reward in Large Feature Space: Tracking by Linear Bandit
Md Menhazul Abedin[1,2], Koji Tabata[3,4], Tamiki Komatsuzaki[1,3,4] ([1]*Graduate School of Chemical Sciences and Engineering, Hokkaido University, Japan*, [2]*Khulna University, Bangladesh*, [3]*Institute for Chemical Reaction Design and Discovery (ICReDD), Hokkaido University, Japan*, [4]*Research Institute for Electronic Science, Hokkaido University, Japan*)

2Pos136 アクトミオシンの弱結合ー強結合転移におけるクーロン駆動機構
Coulombic drive for the weak-to-strong binding transition in actomyosin
Kyohei Shoji, Mitsunori Takano (*Dept. of Pure & Appl. Phys., Grad. Scl. Adv. Sci. & Eng., Waseda Univ.*)

2Pos137 自由エネルギーランドスケープの切り替えとパワーストロークを考慮した筋収縮の 6 状態モデルの構築
Construction of six-state model of muscle contraction with switched free energy landscape and power stroke
Shunta Oda, Tomoki P. Terada (*Dept. Appl. Phys., Grad. Sch. Eng., Nagoya Univ.*)

分子モーター／Molecular motor

2Pos138 F_oF_1-ATPase の非触媒部位の機能解明
Functional elucidation of the non-catalytic site of F_oF_1-ATPase
Ren Kobayashi, Atsuki Nakano, Ken Yokoyama (*Department of Molecular Biosciences,Kyoto Sangyo*)

2Pos139* 無細胞タンパク質合成と 1 分子回転観察を組み合わせた F_1-ATPase の *in vitro* スクリーニング
In vitro screening of F_1-ATPase based on single molecule rotation assay coupled to cell-free protein synthesis
Mai Taguchi, Hiroshi Ueno, Hiroyuki Noji (*Grad. Sch. Eng., Univ. Tokyo*)

2Pos140 H⁺輸送律速における変異型 F_oF_1-ATPase の回転
ATP driven rotation of mutant F_oF_1 where H^+ translocation is rate-limiting
Kiyoto Yasuda[1], Daichi Ando[1], Ryohei Kobayashi[1,2], Hiroshi Ueno[1], Hiroyuki Noji[1] ([1]*Appl. Chem., Grad. Sch. Eng., Univ. Tokyo*, [2]*Inst. for Mol. Sci.*)

2Pos141* Vo 部分での回転によるプロトン輸送機構の分子基盤
Structural basis on the rotary mechanism of Vo domain by proton translocation
Yui Nishida[1], Junichi Kishikawa[2], Atsuko Nakanishi[3], Atsuki Nakano[4], Ken Yokoyama[1,4] ([1]*Dept. of Bioscience., Kyoto Sangyo Univ.*, [2]*IPR, Osaka Univ.*, [3]*Research Center for UHVEM.*, [4]*Grad. Sch. Bioscience., Kyoto Sangyo Univ.*)

2Pos142 分子動力学計算による F_1-ATPase のリン酸放出経路の探索
Exploration of phosphate release pathway of F1-ATPase with molecular dynamics calculation
Masahiro Motohashi[1], Mao Oide[2], Eiro Muneyuki[1], Yuji Sugita[2] ([1]*Grad. Sch. Sci. Eng., Univ. Chuo*, [2]*Wako Inst., Riken*)

2Pos143 Single molecule observation of kinesin-1 on collectively aligned microtubules
Tomoka Kashiwabara[1], Syeda Rubaiya Nasrin[2], Arif Md. Rashedul Kabir[2], Akira Kakugo[2], Yusuke T. Maeda[1] ([1]*Fac. Sci. Grad. Sch. Sci., Univ. Kyushu*, [2]*Fac. Science, Hokkaido University*)

2Pos144 Hybrid kinesin-1 dimer conjugated with synthetic PEG linker shows processive and fast motion with robust hand-over-hand mechanism
Jakia Jannat Keya[1], Akasit Visootsat[1], Kimitoshi Takeda[1], Akihiro Otomo[1], Wijak Yospanya[2], Sanghun Han[2], Kazushi Kinbara[2], Ryota Iino[1] ([1]*Institute for Molecular Science, National Institutes of Natural Sciences*, [2]*School of Life Science and Technology, Tokyo Institute of Technology*)

2Pos145* The movement of kinesin with the neck linker hanging free in solution
Rieko Sumiyoshi, Masahiko Yamagishi, Mitsuhiro Sugawa, Junichiro Yajima (*Grad. Arts & Sci., Univ. Tokyo*)

2Pos146 架橋微小管-キネシンの *in vitro* 運動系でマクロに出力する微小管群の観察
Observation of cross-linked microtubules transmitting integrated forces of multiple kinesin motors *in vitro*
Ryuzo Kawamura[1], Naruaki Tsuji[1], Naritaka Kobayashi[2], Takahisa Matsuzaki[1,3], Hiroshi Y. Yoshikawa[1,3] ([1]*Grad. Sch. Sci. Eng., Saitama Univ.*, [2]*Sch. Eng., Univ. of Shiga Pref.*, [3]*Grad. Sch. Eng., Osaka Univ.*)

2Pos147 タンパク質の 2D 投影像の深層学習によるミオシンの構造分類法の研究
Structure classification of myosin by deep learning of 2D projection images
Hitomi Wada[1], Hiroko Takazaki[2], Takuo Yasunaga[1] ([1]*Grad. Sch. Comp. Sci. Syst. Eng., KIT.*, [2]*IPR, Univ. Osaka*)

2Pos148* ミオシン 1c に駆動される F-アクチンのコークスクリュー運動
Corkscrew motion of F-actin driven by myosin-1c
Yusei Sato[1], Kohei Yoshimura[2], Kyohei Matsuda[1], Akisato Marumo[1], Takeshi Haraguchi[3], Masahiko Yamagishi[1], Mitsuhiro Sugawa[1], Kohji Ito[2,3], Junichiro Yajima[1] ([1]*Dep. of Life Sciences, Grad. School of Arts and Sciences, The University of Tokyo*, [2]*Dep. of Biology, Chiba Uni.*, [3]*Dep. of Biology, Chiba Uni.*)

2Pos149 軸糸ダイニンの協調性は外腕ダイニン中間鎖 2 によって制御される
Cooperative interactions between axonemal dyneins are regulated by the intermediate chain 2 of outer-arm dynein
Yusuke Kondo[1], Tomoka Ogawa[2], Emiri Kanno[3], Masafumi Hirono[4], Takako Minoura[3], Ritsu Kamiya[3], Toshiki Yagi[1,2] ([1]*Grad. Sch. comp. Sci., Pref. univ. Hiroshima*, [2]*Fac. Biores. Sci., Pref. univ. Hiroshima*, [3]*Fac. Sci., Chuo. Univ*, [4]*Dept. of Front . Life Sci., Hosei Univ.*)

2Pos150 細菌べん毛モーター回転子ー固定子間相互作用のアミノ酸レベルでの解析
Analysis of the interaction interface between the rotor and stator of the bacterial flagellar motor at the amino acid residue level
Jin Nakaya[1], Yumi Kumazaki[1], Tsubasa Ishida[2], Myu Yoshida[3], Rie Ito[3], Yoshiyuki Sowa[1,2,3] ([1]*Grad. Sch. Sci. & Eng., Hosei Univ.*, [2]*Res. Cent. Micro-nano Tech., Hosei Univ.*, [3]*Dept. Frontier Biosci., Hosei Univ.*)

2Pos151 真核生物鞭毛・繊毛軸糸構造の X 線回折トモグラフィー：クシクラゲ櫛板の利用
X-ray diffraction-based computed tomography of axonemal structure of eukaryotic flagella/cilia: Use of Ctenophore comb plates
Hiroyuki Iwamoto[1], Kei Jokura[2], Kazuhiro Oiwa[3], Kazuo Inaba[2] ([1]*SPring-8, JASRI*, [2]*Shimoda Marine Res. Ctr., Univ. Tsukuba*, [3]*Bio-ICT Lab., Nat. Inst. Inf. Com. Tech.*)

2Pos152 べん毛 III 型輸送 ATPase 複合体の構造変化と作動機構
Structural change of the ATPase ring complex of the flagellar Type III export apparatus
Asako Usui[1], Tatsunari Yano[1], Yuki Tajimi[2], Norihiro Takekawa[1], Miki Kinoshita[3], Tohru Minamino[3], Takayuki Uchihashi[2], Katsumi Imada[1] ([1]*Dept. of Macromol. Sci., Grad. Sch. of Sci., Osaka Univ.*, [2]*Dept. of phys. Sci., Grad. Sch. of Sci., Nagoya Univ.*, [3]*Grad. Sch. of Frontier Biosci., Osaka Univ.*)

2Pos153 Structural modeling of condensin by assimilating high-speed atomic force microscopy images
Hiroki Koide[1], Noriyuki Kodera[2], Mayu Terakawa[1], Shoji Takada[1], Tsuyoshi Terakawa[1] ([1]*Grad. Sch. Sci. Kyoto Univ.*, [2]*NanoLSI Kanazawa Univ.*)

2Pos154* べん毛 III 型分泌装置の ATPase FliI の HS-AFM 観察
Observation of flagellar type III secretion system ATPase FliI by HS-AFM
Yuki Tajimi[1], Asako Usui[2], Tatsunari Yano[2], Norihiro Takekawa[2], Katsumi Imada[2], Takayuki Uchihashi[1,3] ([1]*Dept. of phys. Sci., Grad. Sch. of Sci., Nagoya Univ.*, [2]*Dept. of Macromol. Sci., Grad. Sch. of Sci., Osaka Univ*, [3]*ExCELLS*)

細胞生物学的課題（接着，運動，骨格，伝達，膜）／Cell biology

2Pos155* 蛍光色や偏光方向を選択可能な汎用的分子配向プローブ Nanobody-based POLArIS の開発
Nanobody-based POLArIS: a versatile molecular orientation probe with options of colors and fluorescence polarization orientations
Nori Nakai-Kadowaki[1], Keisuke Sato[1], Tomomi Tani[2], Masahiko Kawagishi[1], Hiromasa Ka[1], Kenta Saito[1], Sumio Terada[1] ([1]*Dept. of Neuroanatomy and Cellular Neurobiology, Grad. Sch. Med. & Dent. Sci., Tokyo Med. & Dent. Univ.*, [2]*Biomedical Research Institute, Nat. Inst. Adv. Ind. Sci. & Tech.*)

2Pos156 Understanding of robustness in cancer morphology in cold temperature
Yuta Sekiguchi, Hideo Higuchi, Motoshi Kaya (*Grad. Sch. Sci., Univ. Tokyo*)

2Pos157* 酵母胞子の形成・復帰過程における分子混雑の可逆的な制御
Reversible regulation of molecular crowding in fission yeast during sporulation and germination
Keiichiro Sakai[1,2,3], Yuhei Goto[1,2,3], Yohei Kondo[1,2,3], Kazuhiro Aoki[1,2,3] ([1]*NIBB*, [2]*ExCELLS*, [3]*SOKENDAI*)

2Pos158 光照射による多細胞システムの運動制御
Regulation of cell motility in a multicellular system by photodamage
Shinji Yokoyama (*grad. Sch Comp. Sci and Sys .Eng.,Kyushyu Inst. Tech*)

2Pos159 深層学習を用いた *D. discoideum* の 2 細胞型混合集団運動における運動規則の推定
Deep learning-based estimation of motion rules for 2-cell type mixed collective motion of *D. discoideum*
Masahito Uwamichi, Hidenori Hashimura, Tomoko Adachi, Sumie Eto, Satoshi Sawai (*Grad. Sch. Arts and Sci., The Univ. of Tokyo*)

2Pos160* ATP 産生阻害した細胞における細胞内流動性低下の定量的評価
Quantitative evaluation of the decrease in intracellular mobility of cells in which ATP synthesis is inhibited
Hideaki Ota, Hideo Higuchi (*Grad. Sch. Sci., Univ. Tokyo*)

2Pos161 プライマリー神経堤細胞の定量的運動解析
Quantitative characterization of random and persistent locomotion in neural crest cell primary cultures
Takehiro Nakamura, Satoshi Sawai (*Grad. Sch. Arts & Sci., Univ. Tokyo*)

2Pos162* ケラトサイト細胞集団運動におけるアクトミオシンケーブルの切断と集団運動での役割
Breaking of actomyosin cables in keratocyte collectives and their role in the coordinated collective migration
Misaki Iwanaga[1], Chika Okimura[1], Tatsunari Sakurai[2], Tasuku Ueno[3], Yasuteru Urano[3,4], Yoshiaki Iwadate[1] ([1]*Grad. Sch. Sci. Tech., Yamaguchi Univ.*, [2]*Dept. Math. Eng., Musashino Univ.*, [3]*Grad. Sch. Pharm. Sci., Univ. Tokyo*, [4]*Grad. Sch. Med. Univ., Tokyo*)

2Pos163 真核生物の走化性に焦点を当てた、細胞膜上での Gα2 の PALM イメージングと空間的解析
PALM imaging and spatial analysis of Gα2 across the cell membrane: exploring the meaning in eukaryotic chemotaxis
Atsuhiro Mii[1], Satomi Matsuoka[1,2,3], Masahiro Ueda[1,2,3] ([1]*Grad. Sch. Front. Biosci., Osaka Univ.*, [2]*Dept. Biol. Sci., Grad. Sch. Sci., Osaka Univ.*, [3]*BDR, RIKEN*)

2Pos164* GEFB と GEFX は細胞運動に重要な興奮系 Ras の自発的対称性の破れを制御する
GEFB and GEFX regulate spontaneous symmetry breaking of the excitable system Ras for cell motility
Koji Iwamoto[1], Satomi Matsuoka[1,2,3], Masahiro Ueda[1,2,3] ([1]*Grad. Sch. Sci. Bio, Univ. Osaka*, [2]*Grad. Sch. of Front. Biosci., Univ. Osaka*, [3]*BDR., Riken*)

2Pos165 Loss of synchronous behavior in cardiomyocyte networks is independent of their spatial network patterns during hERG ion channel blocking
Kazufumi Sakamoto, Kenji Yasuda (*Dept. Pure & Appl. Phys., Grad. Sch. Adv. Sci. & Eng., Waseda Univ.*)

2Pos166* 電子線トモグラフィーによる *Mycoplasma mobile* 内部滑走装置の解析
Mycoplasma mobile internal gliding machinery analyzed by electron tomography
Minoru Fukushima[1], Takuma Toyonaga[1,2], Yuhei Oba Tahara[1], Daisuke Nakane[3], Makoto Miyata[1,2] ([1]*Grad. Sch. Sci., Osaka Metropolitan Univ. Osaka*, [2]*OCARINA, Osaka Metropolitan Univ.*, [3]*Grad. Sch. Info. Eng., Univ. Electro-Communication. Tokyo*)

2Pos167 ヒト原腸形成の自己組織化を模倣する：ヒト iPS 細胞のマイクロパターン培養
Mimicking the self-organization of human gastrulation: micro pattern culture of human iPS cells
Chihiro Takeuchi[1], Ryo Kobayashi[1], Kiyoshi Ohnuma[2] ([1]*Grad. Sch. Eng., Univ. Nagaoka Tech.*, [2]*Inn., Univ. Nagaoka Tech.*)

2Pos168 Real-Time Feedback 機構を用いた細胞集合体への機械刺激
Mechanical stimulus on cell aggregation with Real-Time Feedback control
Ayu Sasaki, Ryu Kidokoro, Shota Nozaki, Kaito Kojima, Arata Nagai, Yuuta Moriyama, Toshiyuki Mitsui (*Grad. Sch. Sci., Univ. Aogaku*)

2Pos169 ゆらぎの定理に基づく細胞張力ホメオスタシスに関する研究
Analyzing cellular tensional homeostasis from a physical point of view
Shinji Deguchi, Yuika Ueda (*Grad. Sch. Eng. Sci., Osaka Univ.*)

2Pos170 制御理論に基づくアクチン細胞骨格の力学・生化学応答に関する理論解析
Modeling mechanochemical reaction of the actin cytoskeleton based on control theory
Eiji Matsumoto, Daiki Matsunaga, Shinji Deguchi (*Grad. Sch. Eng. Sci., Osaka Univ.*)

2Pos171* 脱水ストレス依存に細胞骨格様の線維やゲルを形成するクマムシタンパク質 CAHS による細胞の機械的強度の向上
Stress-dependent cell stiffening by tardigrade tolerance proteins CAHS reversibly forming cytoskeleton-like filament networks and gels
Akihiro Tanaka[1], Tomomi Nakano[1], Kento Watanabe[1], Kazutoshi Masuda[2,3], Gen Honda[2,3], Shuichi Kamata[1], Reitaro Yasui[1], Satoshi Sawai[1,3], Miho Yanagisawa[2,3], Takekazu Kunieda[1] ([1]*Dept. of Bio. Sci., Grad. Sch. of Sci., Univ. of Tokyo.*, [2]*Komaba Inst. for Sci., Grad. Sch. of Arts and Sci., Univ. of Tokyo.*, [3]*Dept. of Basic Sci., Grad. Sch. of Arts and Sci., Univ. of Tokyo*)

2Pos172 Jasplakinolide または Phalloidin が結合したアクチンフィラメントのゆらぎの違いを FRET 解析により可視化した
Fluctuation difference in actin filaments bound Jasplakinolide or Phalloidin was visualized by using FRET
Ai Takahashi[1], Miku Nezasa[2], Kuruto Toda[2], Irfan Huzifah Ahmad[2], Ichiro Nishikata[4], Kenji Kamimura[3], Ikuko Fujiwara[1], Hajime Honda[1] ([1]*Dept. of Matl. Sci. and Bioeng., Nagaoka Univ. of Tech.*, [2]*Dept. Bioeng., Nagaoka Univ. of Tech.*, [3]*Dept. of Elect.Ctrl.Eng ., NIT. Nagaoka College*, [4]*ACEM., NIT. Nagaoka college*)

2Pos173* 2 種の細菌アクチン MreB が駆動する最小の細胞運動システム
Minimal cell motility system driven by two bacterial actin MreB
Hana Kiyama[1], Shigeyuki Kakizawa[2], Yuya Sasajima[1], O Yuhei Tahara[1,3], Daichi Takahashi[1], Makoto Miyata[1,3] ([1]*Graduate school of Science, Osaka Metropolitan University, Japan*, [2]*Bioproduction Research Institute, National Institute of Advanced Industrial Science and Technology (AIST), Japan*, [3]*OCARINA, Osaka Metropolitan University, Japan*)

2Pos174 腫瘍微小環境におけるエクソソーム中 GRP78 タンパク質の増加が腫瘍進行を促進する
Increased GRP78 protein in exosomes in the tumor microenvironment promotes tumor progression
Kanako Iha, Etsuro Ito (*Department of Biology, Waseda University*)

2Pos175* 細胞の生死の網羅的・定量的理解に向けた、機械学習による細胞の運命予測
Predicting cell fates by image-based machine learning for comprehensive and quantitative understanding of cell death and survival
Tomoaki Okaniwa[1,2], Katsuyuki Shiroguchi[1] ([1]*RIKEN BDR*, [2]*Grad. Sch. Frontier Biosciences, Osaka Univ.*)

2Pos176 Understanding the results of black box Convolution Neural Network to identify Follicular thyroid cancer
Abdul Halim Bhuiyan[1,2], Jean-Emmanuel Clément[3,4], Kentaro Mochizuki[5], James Nick Taylor[3], Koji Tabata[3,4], Yuta Mizuno[1,3,4], Atsuyoshi Nakamura[6], Yoshinori Harada[7], Katsumasa Fujita[5,8,9], Tamiki Komatsuzaki[1,3,4] ([1]*Graduate School of Chemical Sciences and Engineering, Hokkaido University, Sapporo, Japan.*, [2]*Bangladesh University of Engineering and Technology, Dhaka 1000, Bangladesh.*, [3]*Research Center of Mathematics for Social Creativity, Research Institute for Electronic Science, Hokkaido University, Sapporo, Japan*, [4]*Institute for Chemical Reaction Design and Discovery, Hokkaido University, Sapporo, Japan*, [5]*Department of Applied physics, Graduate School of Engineering, Osaka University, Japan*, [6]*Graduate school of Information Science and Technology, Hokkaido University, Japan*, [7]*Department of Pathology & Cell Regulation, Kyoto Prefectural University of Medicine, Japan*, [8]*Advanced Photonics and Biosensing Open Innovation Laboratory, AIST-Osaka University, Japan*, [9]*Transdimensional Life Imaging Division, Osaka University, Japan*)

2Pos177 Elucidation of macrophage's spatial discrimination limit between target antigen and non-target objects
Maiha Ando[1], Dan Horonushi[2], Sota Suzuki[2], Masato Yamazaki[1], Amane Yoshida[2], Kenji Yasuda[1,2] ([1]*Dept. Phys., Sch. Adv. Sci. & Eng., Waseda Univ.*, [2]*Dept. Pure & Appl. Phys., Grad. Sch. Adv. Sci. & Eng., Waseda Univ.*)

2Pos178 細胞内のタンパク質動態の 3 次元の流れとその定量化に関する研究
Research on three-dimensional flow of protein dynamics in cells and its quantification
Yuya Enokida (*Grad. Sch. Comp. Sci. and Sys. Eng., Kyushu Inst. Tech*)

2Pos179 海洋ビブリオ細胞分化におけるべん毛モーター回転制御因子 CheY の役割
Role of the flagellar motor-controlling factor CheY in cell differentiation of marine *Vibrio*
Karin Yamane[1], Mayu Ito[2], Masatoshi Nishikawa[1,2], Hirotaka Tajima[3], Ikuro Kawagishi[1,2,3] ([1]*Grad. Sch. Eng., Hosei Univ.*, [2]*Dept. Frontier Biosci., Hosei Univ.*, [3]*Res. Cen. Micro-Nano Tech., Hosei Univ.*)

2Pos180 海洋性ビブリオ菌において細胞極局在膜タンパク質 HubP はべん毛本数制御因子 FlhG の ATPase 活性を上昇させる
The polar landmark protein HubP enhances the ATPase activity of the flagellar number regulator FlhG in *Vibrio alginolyticus*
Yuxi Hao[1], Norihiro Takekawa[2], Michio Homma[1], Seiji Kojima[1] ([1]*Div. Biol. Sci., Grad. Sch. Sci., Nagoya Univ.*, [2]*Dept. Macromol. Sci., Grad. Sch. Sci., Osaka Univ.*)

2Pos181 クラスリン軽鎖の細胞膜上での構造変化は被覆構造、そしてエンドサイトーシスを制御する
A conformational switch in clathrin light chain regulates lattice structure and endocytosis at the plasma membrane of mammalian cells
Kazuki Obashi, Kem Sochacki, Marie-Paule Strub, Justin Taraska (*National Heart, Lung, and Blood Institute, National Institutes of Health*)

2Pos182 歯周病菌の Fim 線毛の先端タンパク質 FimC の構造
Structure of FimC, a tip protein of the Fim pilus in a gum disease bacterium *Porphyromonas gingivalis*
Norihiro Takekawa[1], Rei Kojima[1], Mikio Shoji[2], Katsumi Imada[1] ([1]*Grad. Sch. Sci., Osaka Univ.*, [2]*Grad. Sch. Biomed Sci., Nagasaki Univ.*)

2Pos183 細胞外小胞が引き起こす標的細胞でのシグナル伝達機構の解明：超解像顕微鏡法と 1 粒子追跡による研究
Intracellular signaling triggered by small extracellular vesicles as revealed by super-resolution microscopy and single-particle tracking
Koichiro M. Hirosawa[1], Yasunari Yokota[2], Kenichi G. N. Suzuki[1,3] ([1]*iGCORE, Gifu Univ.*, [2]*Dept. Eng., Gifu Univ.*, [3]*CREST・JST*)

2Pos184* アミノアシル tRNA 合成酵素 20 種の自己再生産と共役した DNA 複製系の構築
In vitro transcription/translation-coupled DNA replication through the regeneration of 20 aminoacyl-tRNA synthetases
Katsumi Hagino[1], Norikazu Ichihashi[1,2,3] ([1]*Department of Life Science, Graduate School of Arts and Science, The University of Tokyo.*, [2]*Komaba Institute for Science, The University of Tokyo.*, [3]*Research Center for Complex Systems Biology, Universal Biology Institute, The University of Tokyo.*)

2Pos185 1 細胞内での CheB 局在変化による忌避応答および適応
Repellent response and adaptation through the CheB-localization in single E. coli cell
Taiga Deguchi[1], Yumiko Uchida[1], Yong-Suk Che[1], Akihiko Ishijima[1], Tatsuki Hamamoto[2], Hajime Fukuoka[1] ([1]*Grad. Sch. Frontier Biosci. Osaka Univ.*, [2]*OIST. Grad. Univ.*)

生体膜・人工膜：構造・物性／Biological & Artificial membrane: Structure & Property

2Pos186* 膜融合性リポソーム膜のデザインのための系統的な膜特性解析
Systematic membrane characteristic analysis for the design of fusogenic liposome
Natsuumi Ito, Nozomi Watanabe, Yukihiro Okamoto, Hiroshi Umakoshi (*Bio-Inspired Chemical Engineering Laboratory / Division of Chemical Engineering / Graduate School of Engineering Science / Osaka University*)

2Pos187 A Liposome Prepared by Microfluidic Device Vomits the Inner Solution
Jiajue Ji, Kayano Izumi, Ryuji Kawano (*Department of Biotechnology and Life Science, University of Agriculture and Technology*)

2Pos188* (3SGA-5) DNA ゲル骨格が決定する人工細胞の力学特性
(3SGA-5) Cytoskeletons of self-assembled DNA regulate the mechanical properties of artificial cells
Kazutoshi Masuda[1], Fuyu Ohno[2], Miho Yanagisawa[1,2] ([1]*College of Arts and Sciences, The University of Tokyo*, [2]*Graduate school of Arts and Sciences, The University of Tokyo*)

2Pos189 両親媒性ブロックポリマーを用いたポリマー二分子膜の作製
Preparation of planar bilayer polymer membrane using amphiphilic di- and tri-block copolymers
Hiroaki Kihara, Harune Suzuki, Ryuji Kawano (*Department of Biotechnology and Life Science, Tokyo University of Agriculture and Technology*)

2Pos190 海水中で長期間安定に存在し得るリポソームの調製
Preparation for long-term stable liposomes in seawater
Kayano Izumi[1], Keiichiro Koiwai[2], Ryuji Kawano[1] ([1]*Tokyo University of Agriculture and Technology*, [2]*Tokyo University of Marine science and Technology*)

2Pos191* 脂質二重膜へのエタノール分子の浸透に対する塩添加の影響：分子動力学法による検討
Effect of salt addition on the penetration of ethanol molecules into lipid bilayers: a molecular dynamics study
Haru Kitaoka, Naoya Nishi, Yuko Yokoyama, Tetsuo Sakka (*Graduate School of Engineering, Kyoto University*)

2Pos192 高分子液滴を用いた細胞サイズ依存的な相分離
Cell-size dependent phase separation in polymer droplet
Chiho Watanabe[1,2], Tomohiro Furuki[2], Yuki Kanakubo[2], Fumiya Kanie[2], Keisuke Koyanagi[3], Jun Takeshita[2], Miho Yanagisawa[2] ([1]*Hiroshima Univ.*, [2]*Univ. Tokyo*, [3]*Tokyo Univ. Agri. Tech.*)

2Pos193 マガイニン 2 の膜相互作用に対する膜相転移の効果
Contributions of Membrane Phase Transitions to Interaction of Magainin 2 with Membrane
Ryoga Tsuji[1], Munehiro Kumashiro[2], Koichi Matsuo[3] ([1]*Grad. Sch. Adv. Sci. Eng., Hiroshima Univ.*, [2]*Inst. Adv. Med. Sci., Tokushima Univ.*, [3]*HiSOR., Hiroshima Univ.*)

生体膜・人工膜：ダイナミクス／Biological & Artificial membrane: Dynamics

2Pos194* 生体膜の不均一性が分子の拡散性に与える影響
Effect of biological membrane's heterogeneity on the diffusivity of molecules
Ken Sakamoto[1], Takuma Akimoto[2], Mayu Muramatsu[3], Mark S. P. Sansom[4], Ralf Metzler[5], Eiji Yamamoto[6] ([1]*Grad. Sch. Sci. Tech., Keio Univ.*, [2]*Dept. Phys., Tokyo Univ. Sci.*, [3]*Dept. Mech. Eng., Keio Univ.*, [4]*Dept. Biochem., Univ. Oxford*, [5]*Inst. Phys. Astron., Univ. Potsdam*, [6]*Dept. Syst. Des. Eng., Keio Univ.*)

2Pos195* 抗菌ペプチドによる膜細孔形成の分子シミュレーション研究
Molecular dynamics simulation study of membrane pore formation by antimicrobial peptides
Issei Kawabata[1], Yusuke Miyazaki[2], Wataru Shinoda[2] ([1]*Grad. Sch. Eng., Univ. Nagoya*, [2]*RIIS., Univ. Okayama*)

2Pos196 光重合性脂質を用いた単分子/二分子のハイブリッド膜
Patterned monolayer/bilayer hybrid membrane composed of polymerized and natural lipids
Yasushi Tanimoto[1], Fumio Hayashi[2], Kenichi Morigaki[3,4] ([1]*Grad. Sch. Sci., OMU / Japanese*, [2]*Grad. Sch. Sci., Unv. Kobe / Japanese*, [3]*Grad. Sch. Agr., Unv. Kobe / Japanese*, [4]*Bios. R. C., Unv. Kobe*)

2Pos197* 分子動力学シミュレーションによるエンドソーム脱出分子機構の解明
Exploring Molecular Mechanism of Endosomal Escape: A Molecular Dynamics Study
Kana Shibata[1], Akhil Pratap Singh[1], Wataru Shinoda[2] ([1]*Grad. Sch. Eng., Univ. Nagoya*, [2]*RIIS., Univ. Okayama*)

生体膜・人工膜：興奮・チャネル／Biological & Artificial membrane: Excitation & Channels

2Pos198* (1SFP-3) Mechanism study of antimicrobial peptide synergistic effects at the molecular level by combining spectroscopy and electrochemical methods
Yuge Hou, Kaori Sugihara (*Institute of Industrial Science, The University of Tokyo,*)

2Pos199 電位依存性プロトンチャネルは細胞内 ATP による活性制御を受ける
Intracellular ATP controls the voltage-gated proton channel
Akira Kawanabe, Maki Takata, Yuichiro Fujiwara (*Fac. Med., Kagawa Univ.*)

2Pos200 Smooth 型 LPS を用いたグラム陰性細菌外膜模倣膜への抗菌ペプチドの作用評価
Reconstitution of smooth-type LPS as an outer membrane of Gram-negative bacteria
Wakana Hashimoto, Mitsuki Miyagi, Ryuji Kawano (*Dep. of Biotech. and Life Sci., Tokyo Univ. of Agri. and Tech.*)

生体膜・人工膜：輸送・情報伝達／Biological & Artificial membrane: Transport & Signal transduction

2Pos201* 脂質膜水透過現象の解析: アクアポリン水透過モデルとの比較
Water Permeation through the Lipid Membrane: from the Comparison with Aquaporin Study
Natsuki Fukuda[1], Nozomi Watanabe[1], Mizuki Teraoka[2], Yukihiro Okamoto[1], Hiroshi Umakoshi[1] ([1]*Graduate School of Engineering Science, Osaka University.*, [2]*Doshisha Girl's Senior High School.*)

2Pos202 リポソーム型分子ロボットへの標的分子取込み
Transport of the target molecules into liposome-type molecular robots
Harune Suzuki, Kohei Hayashi, Ryuji Kawano (*Grad. Sch. Biotech & Life Sci., TUAT*)

2Pos203 レセプター機能を有する膜中 DNA システムの開発
Construction of a membrane-spanning receptor-like DNA system
Sotaro Takiguchi, Ryuji Kawano (*Dept. Biotech. Life Sci., Grad. Sch. Eng., Tokyo Univ. Agri. Tech.*)

化学受容／Chemoreception

2Pos204 細胞性粘菌の cAMP シグナルにおけるレチナールの効果
Effect of retinal on cAMP signaling in *Dictyostelium discoideum*
Kazuki Akiyama, Yusuke Morimoto (*Kyusyu Institute of Technology (Grad. Sch. Comp. Sci. and Sys. Eng., Kyushu Inst. Tech.)*)

2Pos205* ヒトアセチルコリン受容体のアロステリック機構の振動分光研究
Vibrational spectroscopic study of Allosteric Mechanism on human muscarinic acetylcholine receptor
Yuya Sugiura[1], Kota Katayama[1], Ryoji Suno[2], Hideki Kandori[1] ([1]*Grad. Sch. Eng., Nagoya Inst. Tech.*, [2]*Kansai Medical University. Medical.*)

2Pos206 センサーキナーゼ BaeS のインドール感知部位の同定
Identification of the indole-sensing region of the sensor kinase BaeS
Hirotaka Tajima[1,2], Kenichiro Kashihara[3], Kentaro Yamamoto[4], Yoshiyuki Sowa[1,2,3], Ikuro Kawagishi[1,2,3] ([1]*Fac. of Biosci. and Appl. Chem., Hosei Univ.*, [2]*Res. Cent. for Micro-Nano Tech., Hosei Univ.*, [3]*Grad. Sch. Sci. and Engin., Hosei Univ.*, [4]*Leprosy Res. Center, Nat. Ins. of Infectious Diseases*)

2Pos207 サルモネラクエン酸走性受容体 Tcp のリガンド認識における二価金属イオンの役割
Role of divalent metal cations in ligand recognition by the *Salmonella* citrate chemoreceptor Tcp
Fuga Omori[1], Mariko Matsuda[1], Katsumi Imada[4], Hirotaka Tajima[2,3], Yoshiyuki Sowa[1,2,3], Ikuro Kawagishi[1,2,3] ([1]*Grad. Sch. Sci. and Engin., Hosei Univ.*, [2]*Fac. of Biosci. and Appl. Chem., Hosei Univ.*, [3]*Res. Cent. for Micro-Nano Tech., Hosei Univ.*, [4]*Grad. Sch. Sci., Osaka Univ.*)

神経・感覚（細胞・膜蛋白質・分子）／Neuroscience & Sensory systems

2Pos208* シナプス後肥厚におけるグルタミン酸受容体と PSD-95 のメソスコピックシミュレーション
Mesoscopic simulation of glutamate receptor and PSD-95 in postsynaptic density
Risa Yamada, Shoji Takada (*Grad. Sch. Sci., Kyoto Univ.*)

2Pos209 海馬興奮性ニューロンにおける NMDA 型イオンチャネル受容体に依存した双方向シナプス可塑性の大規模数理モデルによる研究
Mechanism underlying hippocampal long-term potentiation and depression based on competition between endocytosis and exocytosis of AMPAR
Tomonari Sumi[1], Kouji Harada[2] ([1]*Research Inst. for Interdisciplinary Sci., Okayama Univ.*, [2]*Center for IT-Based Edu., Toyohashi Univ. of Tech.*)

2Pos210 高頻度で持続的なシナプス伝達をささえるシナプス小胞ナノスケール動態
Actin filaments restrict synaptic vesicle movement for high-frequency neurotransmission
Takafumi Miki (*Grad. Sch. Brain Sci., Doshisha Univ.*)

2Pos211* 細胞内輸送関連分子の新規解析手法の開発と病態モデルへの応用
A new approach to analysis of intracellular trafficking-related molecules using Cellprofiler and ImageJ in combination
Akito Hattori[1], Etsuro Ohta[2,3,4,5], Makiko Nagai[6], Kazuya Iwabuchi[1], Hideyuki Okano[5] ([1]*Program in Cellular Immunol, Gradu Sch Med Sci Kitasato Univ*, [2]*R&D center for Cell Design, Institute for Regenerative Medicine and Cell Design, Kitasato Univ*, [3]*Dept ImmunolII, Kitasato Univ of Allied Health Sci*, [4]*Div Clinical Immunol, Gradu Sch Med Sci Kitasato Univ*, [5]*Dept Physiol Keio Univ Sch Med*, [6]*Dept Neurol, Kitasato Univ Sch of Med*)

神経回路・脳の情報処理／Neuronal circuit & Information processing

2Pos212 ダブル Y 字型アガロース微細構造における神経突起同士の相互作用
Interactions of two elongating neurites in double Y-shaped agarose microstructure
Nanami Abe[1], Yuhei Tanaka[2], Ryohei Yamazaki[2], Yuri Kamiya[1], Haruki Watanabe[2], Kenji Yasuda[1,2] ([1]*Dept. Pure & Appl. Phys., Sch. Adv. Sci. & Eng., Univ. Waseda*, [2]*Dept. Pure & Appl. Phys., Grad. Sch. Adv. Sci. & Eng., Univ. Waseda*)

2Pos213 カルシウムイメージングによるアガロースマクロチャンバー内の神経回路活動の可視化
Visualization of neural circuit activity in agarose micro chamber by calcium imaging
Rika Fuchikami, Masahito Hayashi, Tomoyuki Kaneko (*FB, Grad. Sch. Sci. &Eng., Hosei Univ.*)

2Pos214 海馬が合成する男性・女性ホルモンやストレスホルモンは記憶シナプスを蛋白キナーゼ信号系で制御する
Kinase-dependent modulation of neuronal synapses by hippocampus-synthesized androgen, estrogen and stress hormone
Suguru Kawato[1,2], Mika Soma[1,2], Mari Ogiue-Ikeda[1,2], Saria Mabashi[2], Ayako Takasu[3], Minoru Saito[2] ([1]*Grad. Sch. Medicine, Juntendo Univ.*, [2]*Coll. Hum. Sci., Nihon Univ.*, [3]*Grad. Sch. Integ. Bas. Sci., Nihon Univ.*)

2Pos215 ミトコンドリア β 酸化に関与する HADH が線虫の介在ニューロンにおいて低温馴化を制御する
HADH involved in mitochondrial β-oxidation regulates temperature acclimation in interneurons of *C.elegans*
Akihisa Fukumoto[1], Misaki Okahata[1], Yohei Minakuchi[2], Atsushi Toyoda[2], Akane Ohta[1], Atsushi Kuhara[1,3] ([1]*Grad. Sch. Sci., Konan Univ*, [2]*Natl. Inst, of Genetics, Japan*, [3]*PRIME, AMED*)

2Pos216 全身を周回する神経回路が腸の脂質含量を調節する
Whole-body neural circuit regulates intestinal fat storage
Haruka Motomura[1,2], Makoto Ioroi[1,2], Kazutoshi Murakami[1,2], Atsushi Kuhara[1,2,3], Akane Ohta[1,2] ([1]*Grad. Sch of Nat. Sci., Konan Univ.*, [2]*Ins. integrative Neurobio., Konan Univ., Japan*, [3]*PRIME, AMED*)

2Pos217 環境の酸素情報が温度応答性に影響を与えることで低温馴化多様性が決定される
Cold acclimation diversity is determined by oxygen information, which affect neural activity of thermo sensory neuron in *C. elegans*
Misaki Okahata[1], Sawako Yoshina[2], Yohei Minakuchi[3], Atsushi Toyoda[3], Shohei Mitani[2], Toru Miura[1], Akane Ohta[1], Atsushi Kuhara[1,4] ([1]*Inst. for Integrative Neurobio., Konan Univ.*, [2]*Tokyo Women's Med. Univ.*, [3]*National Inst. of Genetics*, [4]*PRIME, AMED*)

2Pos218 ミミズ非連合学習におけるセロトニンシグナル
Serotonin signaling in non-associative learning in earthworm
Yoshiichiro Kitamura, Toshifumi Yakuwa, Daichi Morikawa (*Dept Math Sci Phys, Col Sci Eng, Kanto Gakuin Univ*)

2Pos219 異種混合培養神経回路網における神経情報伝達
Functional connections in a heterologous cultured chimera neuronal network
Ayumi Nishikawa, **Suguru N. Kudoh** (*Dep. of Engineering, Kwansei Gakuin University*)

2Pos220 網羅的定量的光計測によるマウス前頭葉前帯状皮質の興奮伝播の解析:膜電位感受性色素 VSD による
Analysis of neural activity propagation in the mouse prefrontal cortex using comprehensive quantitative optical recording: VSD study
Takashi Tominaga[1,2], Pooja Gusain[3], Makiko Taketoshi[1], Yoko Tominaga[1] ([1]*Inst. Neurosci., Tokushima Bunri Univ.*, [2]*Kagawa Sch Pharm., Tokushima Bunri Univ.*, [3]*Dept. Ophth, Sch Med, Keio Univ*)

行動／Behavior

2Pos221 咽頭筋のアミノ酸トランスポーター SLC46 は *C. elegans* の低温耐性を制御する
Amino acid transporter SLC46 in pharyngeal muscle regulates cold tolerance of *C. elegans*
Serina Yamashiro[1], Satomi Mizuno[1], Haruka Motomura[1], Akane Ohta[1], Atsushi Kuhara[1,2] ([1]*Laboratory of Molecular and Cellular Regulation Graduate school of Natural Science Konan University*, [2]*PRIME, AMED*)

2Pos222 蟻の探索行動における 3 次元的空間知覚
Three dimensional perception on ant foraging
Tomoko Sakiyama (*Faculty of Science and Engineering, Soka University*)

2Pos223 タイリクバラタナゴの赤色に対する特異な行動
Unusual behavior of rosy bitterlings in response to red coloration
Ririka Yamamoto[1], Rio Yoshizawa[1], Rikiya Ogawa[2] ([1]*Osaka Prefecture Tondabayashi High School*, [2]*Rikijuku Science School*)

2Pos224 ミクロ社会とマクロ社会におけるカラス属の社会行動が示すカラスの社会性
Crows (*corvus*) society based on crows' behaivor in micro-society and macro-society
Haruki Kon, Kosei Ando, Aoba Sasaki, Hina Nakamura (*Sapporo Kaisei secondary school*)

2Pos225 シアノバクテリオクロム RcaE におけるユニークな C15 - *E,syn* 型ビリン発色団のラマン分光法による研究
Raman Spectroscopy of an Atypical C15-*E,syn* Bilin Chromophore in Cyanobacteriochrome RcaE
Yuji Okuda[1], Risako Miyoshi[1], Takanari Kamo[2], Tomotsumi Fujisawa[1], Takayuki Nagae[3], Masaki Mishima[3], Toshihiko Eki[2], Yuu Hirose[2], Masashi Unno[1] ([1]*Fac.Sci.Eng.,Saga.Univ*, [2]*Toyohashi Univ. of Tech. Appl. Chem. & Life Sci.*, [3]*Tokyo Univ. of Pharmacy and Life Sciences Dep. Mol. Biophys.*)

2Pos226* 青色光センサータンパク質 SyPixD の C 末端領域による 10 量体構造の安定化
Stabilization of decamer structure by the C-terminal region of the blue light sensor protein SyPixD
Shunrou Tokonami, Yusuke Nakasone, Masahide Terazima (*Grad. Sch. Sci., Univ. Kyoto*)

2Pos227* 新奇塩化物イオンポンプロドプシンの輸送メカニズム研究
Study on the transport mechanism of the novel chloride-ion pump rhodopsin
Tomohiro Ishizuka[1], Kano Suzuki[2], Yuma Kawasaki[1], Masae Konno[1,3], Takeshi Murata[2,4], Keiichi Inoue[1] ([1]*ISSP, Univ. of Tokyo*, [2]*Grad. Sch. Sci., Chiba Univ.*, [3]*JST, PRESTO*, [4]*MPRC, Chiba Univ.*)

2Pos228* クリプトクロムが触媒する DNA 光修復反応の時間分解分光解析
Time-resolved spectroscopic analysis of DNA photorepair reaction catalyzed by cryptochrome
Tatsumi Maeno[1], Daichi Yamada[1], Ai Kadono[1], Junpei Yamamoto[2], Minoru Kubo[1] ([1]*Grad. Sch. Sci., Univ. Hyogo, Japan*, [2]*Grad. Sch. Eng. Sci., Osaka Univ., Japan*)

2Pos229 光と苦味のセンサーとしてはたらくキイロショウジョウバエ Rh7 の赤外分光研究
FTIR study of Drosophila Rh7, a light and bitter taste sensor
Kouhei Watanabe, Kota Katayama, Hideki Kandori (*Grad. Sch. Eng., Nagoya Inst.Tech.*)

2Pos230* 霊長類青感受性視物質の 200 K 以上での赤外分光解析
FTIR study of primate blue-sensitive cone pigment at >200 K
Yosuke Mizuno[1], Kota Katayama[1], Hiro Imai[2], Hideki Kandori[1] ([1]*Grad. Sch. Eng, Nagoya Inst. Tech.*, [2]*Center for the Evolutionary Origins of Human Behavior, Kyoto University*)

2Pos231 全トランス型から 11 シス型の光反応を示す新規微生物ロドプシンの分光解析
Spectroscopic analysis of novel microbial rhodopsin showing photoreaction from all-*trans*- to 11-*cis*-retinal
Mako Aoyama[1], Kota Katayama[1], Rei Abe-Yoshizumi[1], Masahiro Sugiura[1], Andrey Rozenberg[2], Igor Kaczmarczyk[3], Donna Matzov[3], Takashi Nagata[4], Moran Shalev-Benami[3], Oded Béjà[2], Keiichi Inoue[4], Yuji Furutani[1], Hideki Kandori[1] ([1]*Grad. Sch. Eng., Nagoya Inst. Tech.*, [2]*Technion – Israel Inst. Tech.*, [3]*Weizmann Inst. Sci.*, [4]*ISSP, Univ. Tokyo*)

2Pos232 異なる位置にカウンターイオンを持つクラゲオプシンの光異性化機構解析
Spectroscopic study of photoisomerization mechanism of Jellyfish Opsin having counterion at different position
Shino Inukai[1], Kota Katayama[1], Mitsumasa Koyanagi[2], Akihisa Tereakita[2], Hideki Kandori[1] ([1]*Grad. Sch. Eng., Nagoya Inst. Tech.*, [2]*Grad. Sch. Sci., Osaka Metro. Univ.*)

2Pos233* 固体 NMR を用いた Zn^{2+}結合型 TaHeR の脂質二重膜中の構造解析
Solid-state NMR study of membrane embedded TaHeR in the presence of Zn^{2+}
Sari Kumagai[1], Shibuki Suzuki[1], Kota Katayama[2], Hideki Kandori[2], Izuru Kawamura[1] ([1]*Grad. Sch. Eng. Sci., Yokohama Natl. Univ.*, [2]*Dep. Life Sci. Appl. Chem., Nagoya Inst. Technol.*)

2Pos234 霊長類の緑色感受性タンパク質の原子構造決定に向けて
Toward determining the atomic structure of primate green cone pigment
Sayaka Ohashi[1], Kota Katayama[1], Ryoji Suno[2], Nipawan Nuemket[3,4], So Iwata[3,4], Eriko Nango[4,5], Takuya Kobayashi[2], Hideki Kandori[1] ([1]*Grad. Sch. Eng., Nagoya Inst.Tech.*, [2]*Kansai Medical University*, [3]*Kyoto University*, [4]*Japan Synchrotron Radiation Research Institute*, [5]*Tohoku University*)

2Pos235 RcPYP と PBP 相互作用における表面電荷の効果
Effects of surface charge on RcPYP and PBP interactions
Yoichi Yamazaki[1], Yoko Narahara[1], Hironari Kamikubo[1,2] ([1]*NAIST, MS*, [2]*NAIST, CDG*)

2Pos236 固体 NMR による膜中 TAT ロドプシンの構造解析
Solid-state NMR study of membrane-embedded TAT rhodopsin
Sui Arikawa[1], Teppei Sugimoto[2], Kota Katayama[2], Hideki Kandori[2], Izuru Kawamura[1] ([1]*Grad. Sch. Eng. Sci., Univ. Yokohama Natl.*, [2]*Dep. Life Sci. Appl. Chem., Nagoya Inst. Technol.*)

2Pos237 低温ラマン分光法による photoactive yellow protein の L 中間体の構造解析
Structural analysis of the L intermediate in the photoactive yellow protein by low-temperature Raman spectroscopy
Shota Kawasaki[1], Tomotsumi Fujisawa[1], D. Hoff Wotuer[2], Masashi Unno[1] ([1]*Fac. Sci. Eng., Saga Univ.*, [2]*Oklahoma state Univ.*)

光生物：光合成／Photobiology: Photosynthesis

2Pos238 PELDOR 法により決定した光化学系Ⅱの 2 つの Mn^{2+}親和サイト
Location of the two high-affinity Mn^{2+} site in photosystem II detected by PELDOR
Hiroyuki Mino[1], Mizue Asada[1,2] ([1]*Grad. Sch. Sci., Nagoya Univ.*, [2]*Inst. Molecular Sci.*)

2Pos239 光化学系 II におけるストロマおよびルーメン側における摂動が第一キノン電子受容体 Q_A の酸化還元電位に及ぼす影響
Effects of stromal and lumenal side perturbations on the redox potential of the primary quinone Q_A in photosystem II
Yuki Kato, Takumi Noguchi (*Grad. Sch. Sci, Nagoya Univ.*)

2Pos240* 一分子過度吸収測定による光合成光捕集アンテナ複合体のダイナミクスとエネルギー移動の相関解析
Single-molecule transient absorption spectroscopy of energy transfer in photosynthetic antenna complex
Shun Arai[1], Tomomi Inagaki[2], Chihiro Azai[2], Toru Kondo[1] ([1]*Dept. of Life Sci. and Tech., Tokyo Tech.*, [2]*Grad. Sch. Life Sci., Ritsumeikan Univ.*)

2Pos241 光合成カロテノイドシフォナキサンチンにおける非共役官能基の共役系への影響
Effect of the non-conjugated functional group on the optical properties of a photosynthetic carotenoid, siphonaxanthin
Soichiro Seki[1], Kazuhiro Yoshida[1], Yumiko Yamano[2], Naohiro Oka[3], Mitsuru Sugisaki[1], Ritsuko Fujii[1,4] ([1]*Grad. Sch. Sci., Osaka Metropolitan Univ.*, [2]*Comp. Edu. Res. Cntr, Kobe Pharmaceutical Univ.*, [3]*Bio-Innovation Res. Cntr, Tokushima Univ.*, [4]*Res. Cntr. Artif. Photosynth., Osaka Metropolitan Univ.*)

2Pos242 光化学系Ⅱにおける水分解マンガンクラスターの光構築機構の時間分解赤外分光解析
Time-resolved infrared study on the mechanism of photoassembly of the water-oxidizing Mn_4CaO_5 cluster in photosystem II
Shunya Watanabe, Yuichiro Shimada, Takumi Noguchi (*Grad. Sch. Sci., Nagoya Univ.*)

2Pos243 光化学系 II の酸素発生中心における S_2 状態の中間体構造の DFT と CC 法による解析
DFT and DLPNO-CC calculation of relative stability and electronic states in the S_2 state of the $CaMn_4O_5$ cluster of the OEC of the PSII
Koichi Miyagawa[1], Takashi Kawakami[2,3], Mitsuo Shoji[1], Hiroshi Isobe[4], Kizashi Yamaguchi[3,5], Yasuteru Shigeta[1] ([1]*Center for Computational Sciences, University of Tsukuba*, [2]*Graduate School of Science, Osaka University*, [3]*RIKEN Center for Computational Science*, [4]*Research Institute for Interdisciplinary Science, Okayama University*, [5]*Center for Quantum Information and Quantum Biology, Osaka University*)

2Pos244 分子動力学シミュレーションによる紅色細菌の光捕集アンテナ LH2 の吸収スペクトルの解析
The analysis of absorption spectra of light-harvesting antenna LH2 in purple bacteria by molecular dynamics simulation
Shunsuke Yabu[1], Hirofumi Sato[1,2], Masahiro Higashi[1] ([1]*Graduate School of Engineering, Kyoto Univ.*, [2]*FIFC, Kyoto Univ.*)

2Pos245 X 線自由電子レーザーを用いた解析による光化学系 II の基質水分子の取り込みと水分子の酸化に関する構造的知見
Structural insights into the substrate water delivery and water oxidation in photosystem II by analysis with an X-ray free-electron laser
Michi Suga, Yoshiki Nakajima, Hongjie Li, Jian-Ren Shen (*Okayama Univ*)

光生物：光遺伝学・光制御／Photobiology: Optogenetics & Optical Control

2Pos246* 内向きおよび外向きプロトンポンプロドプシンの駆動力の解明
Driving force of inward and outward proton pump rhodopsins
Akari Okuyama, Shoko Hososhima, Satoshi Tsunoda, Hideki Kandori (*Grad. Sch. Eng., Nagoya Inst. Tech.*)

2Pos247* Ca^{2+}結合型 TAT ロドプシンの分光研究
Spectroscopic study of TAT rhodopsin bound with Calcium ion
Teppei Sugimoto, Kota Katayama, Hideki Kandori (*Graduate school of Engineering, Nagoya institute of technology*)

2Pos248* LED 光源を用いた微生物型ロドプシン AR3 による膜電位の長時間イメージング
Long-term membrane voltage imaging by microbial rhodopsin AR3 with LED light source
Shiho Kawanishi[1], Keiichi Kojima[2], Atsushi Shibukawa[1], Masayuki Sakamoto[3], Yuki Sudo[2] ([1]*Grad. Sch., Med. Dent. & Pharm. Sci., Okayama Univ.*, [2]*Grad. Sch., Med. Dent. & Pharm. Sci., Okayama Univ.*, [3]*Grad. Sch., Biostudies, Kyoto Univ.*)

2Pos249* ポンプ型チャネルロドプシン ChRmine のクライオ電子顕微鏡構造解析と次世代光遺伝学ツール開発
Cryo-EM structural analysis of pump-like channelrhodopsin ChRmine and structure guided engineering
Koichiro Kishi[1], Yoon Kim[2], Masahiro Fukuda[1], Masatoshi Inoue[2], Tsukasa Kusakizako[3], Peter Wang[2], Charu Ramakrishnan[2], Eamon Byrne[2], Elina Thadhani[4], Joseph Paggi[4], Toshiki Matsui[1], Keitaro Yamashita[5], Takashi Nagata[6], Masae Konno[6], Sean Quirin[2], Maisie Lo[2], Tyler Benster[2], Tomoko Uemura[7], Kehong Liu[7], Mikihiro Shibata[8], Norimichi Nomura[7], So Iwata[7], Osamu Nureki[3], Ron Dror[4], Keiichi Inoue[6], Karl Deisseroth[2], Hideaki Kato[1] ([1]*Komaba Inst. Sci., Univ. Tokyo*, [2]*Dept. Bioeng., Stanford Univ.*, [3]*Dept. Bio. Sci., Univ. Tokyo*, [4]*Dept. Comp. Sci., Stanford Univ.*, [5]*MRC Lab. Mol. Biol.*, [6]*ISSP Univ. Tokyo*, [7]*Dept. Cell Biol., Kyoto Univ.*, [8]*Inst. Front. Sci. Init., Kanazawa Univ.*)

2Pos250 光活性化アデニル酸シクラーゼの活性化に伴う構造変化の解明
Structural changes of adenylate cyclase from Oscillatoria acuminata in response to blue light stimulation
Yuki Kitamura, Toru Ide, Minako Hirano (*Grad. Sch. Health Sys,. Okayama Univ.*)

2Pos251 藻類シオミドロが持つ 4 種の Aureochrome の類似性と多様性
Similarity and Diversity of aureochromes, *Es*Au1-*Es*Au4, in a brown alga, *E. siliculosus.*
Yuta Nagano, Yumiko Adachi, Osamu Hisatomi (*Grad. Sch. Sci., Univ. Osaka*)

2Pos252 近赤外光で駆動可能なバイオアクチュエータの創製
Creation of Bioactuators Drivable by Near-Infrared Light
Daisuke Maemura, Son Le The, Mari Takahashi, Kazuaki Matsumura, Shinya Maenosono (*Sch. Mater. Sci., JAIST*)

2Pos253 *In vivo* optogenetic system to control deep tissue insulin signaling
Qi Dong, Mizuki Endo, Takeaki Ozawa (*Grad. Sch. Sci., Univ. Tokyo*)

生命の起源・進化／Origin of life & Evolution

2Pos254 プロトセルの適応度地形
Fitness Landscape of Protocell
Akiko Baba[1], Keidai Sato[1], Kazuki Yokoyama[1], Ulf Olsson[2], Masayuki Imai[1] ([1]*Grad. Sch. Sci., Univ. Tohoku*, [2]*Grad. Sch. Sci., Univ. Lund*)

2Pos255* Host-Parasite 分子複製体が織りなす複製反応ネットワークの複雑化過程とその性質
Complexification Process and Property of Replication Network by Host-Parasite Molucular Replicator
Rikuto Kamiura[1], Ryo Mizuuchi[2,3], Norikazu Ichihashi[1,2] ([1]*Grad. Sch. Arts and Sci., Univ. Tokyo*, [2]*Komaba inst., Univ. Tokyo*, [3]*JST, PRESTO*)

2Pos256 無細胞翻訳系を用いた DNA 自己複製により成長する相分離液滴の開発
Phase-separated Dex droplets grow coupled with internal DNA self-replication
Moe Yabuta, Yoshihiro Minagawa, Hiroyuki Noji (*Dept. App. Chem., Grad. Sch. Eng., Univ. Tokyo*)

2Pos257 試験管内の DNA 複製、転写、翻訳反応は最適条件が異なる
Different conditions are optimal for in vitro DNA replication, transcription, and translation
Kaito Seo[1], Norikazu Ichihashi[1,2,3] ([1]*Grad. Sch. Arts. Sci., Univ. Tokyo*, [2]*Komaba Inst. Sci., Univ. Tokyo*, [3]*Res. Cen. Complex Syst. Bio., Univ. Bio. Inst., Univ. Tokyo*)

2Pos258* RNA 自己複製系を用いた RNA ゲノム再編成を伴う RNA 集団の進化の観察
Observation of RNA population evolution with RNA genome reorganization using RNA self-replication system
Kensuke Ueda[1], Ryo Mizuuchi[2], Norikazu Ichihashi[1,2,3] ([1]*Graduate School of Arts and Science, The University of Tokyo*, [2]*Komaba Institute for Science, The University of Tokyo*, [3]*Universal Biology Institute, The University of Tokyo*)

2Pos259 Trp を含まない酵素群によって構成される解糖系に依存して生育する大腸菌の作成に向けた活性測定
Activity measurement for the creation of Escherichia coli dependent on glycolysis composed of a group of Trp-free enzymes
Naosato Takagi[1], Mana Hashimoto[1], Akifumi Nishida[1], Kenji Tsuge[2], Daisuke Kiga[1] ([1]*Faculty of Science and Engineering, Waseda University*, [2]*Graduate School of Science, Technology and Innovation, Kobe University*)

ゲノム生物学：ゲノム解析／Genome biology: Genome analysis

2Pos260* (2SHP-4) 新規遺伝子の誕生と機能獲得の進化メカニズムに迫るゲノム計算科学：バイオインフォマティクスのその先に遺伝子の本質を探求する
(2SHP-4) How do *de novo* genes evolve and acquire function?: Computational genomics to revisit the nature of genes beyond bioinformatics
Shun Yamanouchi[1], Wataru Iwasaki[1,2] ([1]*Grad. Sch. Sci., Univ. Tokyo*, [2]*Grad. Sch. Front. Sci., Univ. Tokyo*)

2Pos261 PLA2 産生に関与する遺伝子と経路の同定
Identification of the genes and pathways responsible for PLA2 production
Hiroki Oura[1], Eri Hayashi[1], Yuto Kimura[1], Yusuke Nomura[1], Satoko Nakamura[3], Norimasa Kashiwagi[3], Chiaki Ogino[3], Shuichi Hirose[2], Wataru Nemoto[1] ([1]*Dept. Sch. & Tech., Tokyo Denki Univ*, [2]*NAGASE R & D Center NAGASE & CO*, [3]*Org. of Adv Sci & Tec., Kobe Univ*)

2Pos262* Sequel II を用いた単一インフルエンザウイルス集団中のゲノム配列分布測定
Heterogeneity of Genetic Sequence within Population in Single Plaque of Influenza Virus Revealed by Sequel II analysis
Kenji Tamao[1], Masayuki Suetsugu[2], Hiroyuki Noji[1], Kazuhito Tabata[1] ([1]*Appl. Chem., Grad. Sch. Eng., Univ. Tokyo*, [2]*Dept. Life. Sci., Col. Sci., Univ. Rikkyo*)

ゲノム生物学：ゲノム構造／Genome biology: Genome structure

2Pos263* マウス胚性幹細胞の初期分化過程における X 染色体のエピゲノム構造変化は Xic 対合を促進する
Epigenetic-structural changes in X chromosomes promote Xic pairing during early differentiation process from embryonic stem cell of mouse
Tetsushi Komoto, Masashi Fujii, Akinori Awazu (*Grad. Sch. Integrated Sciences for Life, Univ. Hiroshima*)

2Pos264 Bayesian inference of chromatin folding from Hi-C data and application to enhancer-promoter communication in the Nanog locus
Giovanni Bruno Brandani, Chenyang Gu, Soundhara Rajan Gopi, Shoji Takada (*Grad. Sch. Sci., Univ. Kyoto*)

2Pos265* Polymer physics model of chromatin dynamics during early embryogenesis in *Caenorhabditis elegans*
Yesbolatova Aiya[1], Akatsuki Kimura[1], Takahiro Sakaue[2] ([1]*Grad. Univ. for Adv. Stud., SOKENDAI, National Institute of Genetics*, [2]*Aoyama Gakuin University, Department of Physics and Mathematics*)

2Pos266 Building a Coarse-grained Model of Chromatin
Justin Chan, Hidetoshi Kono (*Molecular Modelling and Simulation (MMS) Team, National Institutes for Quantum Science and Technology (QST)*)

生命情報科学：構造ゲノミクス／Bioinformatics: Structural genomics

2Pos267 PDB における ATP アーゼ複合体の構造変化
Structural changes of ATPase complexes in the PDB
Ryotaro Koike (*Grad. Sch. Info., Nagoya Univ.*)

2Pos268 Accurate modeling and mechanistic investigation of the complexes of the SRK/SP11 proteins of *Brassicaceae*
Hanting Jiang[1], Kentaro Shimizu[1], Tohru Terada[1], Yoshitaka Moriwaki[1], Kohji Murase[2], Seiji Takayama[2] ([1]*Dept. of Biotechnol., Grad. Sch. of Agri. and Life Sci., Univ. of Tokyo*, [2]*Dept. of Appl. Biol. Chem., Grad. Sch. of Agri. and Life Sci., Univ. of Tokyo*)

2Pos269 AlphaFoldDB の予測立体構造と既知の実験立体構造との構造比較
Structure comparison of predicted 3D models in AlphaFoldDB with known experimentally determined 3D structures
Takeshi Kawabata, Kengo Kinoshita (*Grad.Sch.Info.Sci.,Tohoku Univ.*)

生態／環境／Ecology & Environment

2Pos270 大和川水系石川におけるオオシマドジョウの生活史
Life History of *Cobitis* sp. BIWAE Type A in the Ishi River in the Yamato River System
Teppei Sakurai[1], Rikiya Ogawa[2] ([1]*Osaka Prefecture Tondabayashi High School*, [2]*Rikijuku Science School*)

2Pos271 石川の魚類相の変遷とその要因についての一考察
Transition of fish fauna in Ishi River and a consideration about that factors
Shohei Umegawa[1], Kyoka Matsuo[1], Rikiya Ogawa[2] ([1]*Osaka Prefecture Tondabayashi High School*, [2]*Rikijuku Science School*)

2Pos272 自然浄化に必要なものは
What is needed for natural purification?
Kyoka Matsuo[1], Cocona Okada[1], Rikiya Ogawa[2] ([1]*Osaka Prefecture Tondabayashi High School*, [2]*Rikijuku Science School*)

数理生物学／Mathematical biology

2Pos273* 皮膚疾患の環状紅斑を対象とした数理解析による炎症調節機構の解明
Mathematical analysis of erythema annulare to elucidate the pattern formation mechanism of skin inflammation
Maki Sudo, Koichi Fujimoto (*Grad. Sch. Sci., Osaka University*)

2Pos274 嗅覚系における匂い物質・受容体の多対多の相互作用による類似匂い混合物の識別に関する理論的解析
Mathematical analysis of the discrimination of odorant mixtures via collective interactions of multiple odorants and olfactory receptors
Karin Suwazono[1], Tetsuya J. Kobayashi[2] ([1]*Dept. Biophys. and Biochem., Fuc. Sci., Univ. Tokyo*, [2]*Inst. Ind. Sci., Univ. Tokyo*)

2Pos275* 免疫系における予測符号化に基づく適応的な抗原の有害/無害識別
Adaptive discrimination between harmful and harmless antigens based on predictive coding in immune system
Kana Yoshido[1], Naoki Honda[1,2,3] ([1]*Grad. Sch. of Biostudies, Kyoto Univ.*, [2]*Grad. Sch. of Integrated Sciences for Life, Hiroshima Univ.*, [3]*ExCELLS, NINS*)

2Pos276* 化学反応ネットワークの改変がダイナミクスに与える影響の解析
Analyzing the effect of modifications to the chemical reaction network on dynamics
Atsuki Hishida[1], Atsushi Mochizuki[2] ([1]*Grad. Sch. Sci., Univ. Kyoto*, [2]*Inst. Life Med. Sci, Kyoto Univ.*)

2Pos277 新しいパターン伝播機構: 曲率により駆動されるパターン伝播
New mechanism of pattern propagation: Pattern propagation driven by surface curvature
Ryosuke Nishide, Shuji Ishihara (*Grad. Sch. Arts and Sci., Univ. Tokyo*)

2Pos278* ゲノム縮小は内部共生の進化を加速するのだろうか？
Does Genome Reduction Accelerate Evolution of Endosymbiosis?
Yuki Kanai[1], Chikara Furusawa[1,2] ([1]*Grad. Sch. Sci., Univ. Tokyo*, [2]*BDR, Riken*)

2Pos279 A mathematical model for emergence of polar order induced by contact following locomotion in a multicellular system
Biplab Bhattacherjee, Masayuki Hayakawa, Tatsuo Shibata (*Laboratory for Physical Biology, BDR, RIKEN*)

非平衡・生体リズム／Nonequilibrium state & Biological rhythm

2Pos280 ミクロ経済学としての代謝制御の理解：ワールブルク効果とギッフェン財を例として
Microeconomics of Metabolism: The Warburg effect as Giffen behavior
Jumpei Yamagishi, Tetsuhiro Hatakeyama (*Grad. Sch. of Arts and Sci., Univ. Tokyo*)

2Pos281 Growing and competing cell colonies in a hybrid mechanochemical model
Jintao Li[1], **Simon Kaspar Schnyder[1,2]**, Matthew S. Turner[3], Ryoichi Yamamoto[1] ([1]*Department of Chemical Engineering, Kyoto University, Kyoto 615-8510, Japan*, [2]*Institute of Industrial Science, The University of Tokyo, 4-6-1 Komaba, Meguro-ku, Tokyo 153-8505, Japan*, [3]*Department of Physics, University of Warwick, Coventry CV4 7AL, United Kingdom*)

2Pos282 人工細胞内で再構成された細胞分裂面を決定する反応拡散波の動態と周期の制御
Tuning dynamics and period of a reaction-diffusion wave for cell division in artificial cells
Sakura Takada[1], Natsuhiko Yoshinaga[2,3], Nobuhide Doi[1], Kei Fujiwara[1] ([1]*Dept. Biosci. Info., Keio Univ.*, [2]*AIMR, Tohoku Univ.*, [3]*MathAM-OIL, AIST*)

2Pos283 無細胞発現系における液滴形成のダイナミクス
Dynamics of droplet formation in cell-free expression systems
Shuzo Kato[1], David Garenne[2], Vincent Noireaux[2], Yusuke Maeda[1] ([1]*Dept. Phys., Kyushu Univ.*, [2]*Sch. Phys. Astro., Univ. of Minnesota*)

2Pos284 接着力を取り入れたアクティブブラウン粒子モデルによる細胞集団運動のモデル化
Adhesive Active Brownian Particle Model for Collective Cell Motion
Sota Shimamura[1], Nen Saito[2], Shuji Ishihara[1] ([1]*Grad. Sch. Arts and Sci., U. Tokyo.*, [2]*Grad. Sch. of Integrated Sci. for Life, Hiroshima Univ.*)

計測／Measurements

2Pos285* ダイヤモンド量子センサによる単一細胞測定へ向けたピコリットル溶液 NMR 装置の開発
Development of pico-litter liquid NMR for single cell measurement by using diamond quantum sensor
Kohki Morita[1], Izuru Ohki[1,2], Masanori Fujiwara[1], Yuta Nakano[3], Norio Tokuda[3], Norikazu Mizuochi[1,4] ([1]*ICR, Kyoto Univ.*, [2]*QST*, [3]*NanoMaRi, Kanazawa Univ.*, [4]*CSRN, Kyoto Univ.*)

2Pos286* In vitro およびヒト生細胞中における超硫黄分子と S_8 のラマン解析
Raman analyses of supersulfides and S_8 in vitro and in human living cells
Lisa Kageyama[1], Shinji Kajimoto[1,2], Shinya Tahara[1], Takakazu Nakabayashi[1] ([1]*Graduate School of Pharmaceutical Sciences, University of Tohoku.*, [2]*JST PRESTO*)

2Pos287* Single Exosome 内包 miRNA 検出に向けた半導体ナノポアを用いた 1 粒子内包物検出法の開発
Development of a single-particle inclusions detection method by solid-state nanopore for miRNA in single exosome detection
Takumi Uchida, Hirohito Yamazaki, Ryo Iizuka, Sotaro Uemura (*Grad. Sch. Sci., The Univ. of Tokyo*)

2Pos288* Nanopore sensing of femtomolar DNAs using the excess complementary probes
Nanami Takeuchi, Ryuji Kawano (*Department of Biotechnology and Life Science, Tokyo University of Agriculture and Technology*)

2Pos289* ガラスピペットナノポアによるエクソソームの電気的検出
Electrical detection of exosomes by a glass capillary nanopore
Kohei Hayashi, Ryuji Kawano (*Department of Biotechnology and Life Science, Tokyo University of Agriculture and Technology*)

2Pos290* (2SDA-4) Nanopore direct determination of DNA methylation and demethylation intermediates
Ping Liu[1], Masayuki Honda[1], Ryuji Kawano[2] ([1]*Department of Food and Energy Systems Science, Tokyo University of Agriculture and Technology*, [2]*Institute of Engineering, Tokyo University of Agriculture and Technology*)

2Pos291* 原子間力顕微鏡による神経管閉鎖中のホヤ胚の 1 細胞力学特性の測定
Mechanical properties of single cells in ascidian embryo during neural tube closure measured by atomic force microscopy
Yosuke Tsuboyama, Yuki Miyata, Takaharu Okajima (*Graduate School / Faculty of Information Science and Technology, Hokkaido University*)

2Pos292 Optimization of protocols for metabolomics studies of human breast milk samples using benchtop NMR

Jiaxi Jiang[1], Zhiyan Hu[1], Li Gan[1], Zihao Song[1], Yuki Ohnishi[1], Seiji Osada[2], Hiroyuki Kumeta[1], Yasuhiro Kumaki[1], Kazuo Yamauchi[3], Tomoyasu Aizawa[1] ([1]*Grad. Sch. Life Sci., Hokkaido Univ.*, [2]*Nakayama Co.,Ltd.*, [3]*IAS, OIST*)

2Pos293 α-グルコシダーゼ阻害物質を含むクワ葉の投与によるマウス腸内環境への影響の NMR メタボロミクス解析

NMR metabolomics of administration of mulberry leaves containing α-glucosidase inhibitors on the intestinal environment of mice

Li Gan, Yuga Inamura, Zihao Song, Yuki Ohnishi, Yasuhiro Kumaki, Tomoyasu Aizawa (*Grad. Sch. Life Sci., Univ. Hokkaido*)

バイオイメージング／Bioimaging

2Pos294* Spatiotemporal Dynamics of Small Extracellular Vesicle Nanotopology in Response to Physicochemical Stresses Revealed by HS-AFM

Elma Sakinatus Sajidah[1], Lim Keesiang[2], Tomoyoshi Yamano[3], Takeshi Yoshida[2,3], Akiko Kobayashi[4], Masaharu Hazawa[2,4], Rikinari Hanayama[2,3], Toshio Ando[2], Richard W. Wong[1,2,4] ([1]*Division of Nano Life Science in the Graduate School of Frontier Science Initiative, Kanazawa University*, [2]*WPI-Nano Life Science Institute, Kanazawa University*, [3]*Department of Immunology, Kanazawa University Graduate School of Medical Sciences*, [4]*Cell-Bionomics Research Unit, Institute for Frontier Science Initiative, Kanazawa University*)

2Pos295* 高周波集束超音波スペクトロスコピーによる培養単一細胞への非侵襲局所力学刺激付与システムの開発とヒト iPS 細胞の核の共振による超音波吸収帯

Development of ultrasound spectroscopic imaging system for applying highly controlled local mechanical stimulation on cells

Natsumi Fujiwara, Takaki Matsumotio, Akira Nagakubo, Masahiro Kino-oka, Hirotsugu Ogi (*Graduate School of Engineering, University of Osaka*)

2Pos296 神経分化における細胞内温度の貢献

Contribution of Intracellular Thermogenesis to Neural Differentiation

Shunsuke Chuma[1,2], Hirotaka Okita[2], Shingo Sotoma[2], Kohki Okabe[3,4], Yoshie Harada[2,5] ([1]*Dept. Biol. Sci., Grad. Sch. Sci., Osaka Univ.*, [2]*IPR, Osaka Univ.*, [3]*Grad. Sch. Pharm. Sci., The Univ. Tokyo*, [4]*JST PRESTO*, [5]*QIQB Osaka Univ.*)

2Pos297* 高速 AFM の更なる高速化に向けた Z-スキャナの共振制御装置

Resonance-controller of the Z-scanner for faster high-speed AFM

Kazuma Tatsumi[1], Kenichi Umeda[2], Toshio Ando[2], Noriyuki Kodera[2] ([1]*Grad. Sch. Math. & Phys., Kanazawa Univ.*, [2]*WPI-NanoLSI, Kanazawa Univ.*)

2Pos298 細胞内高速マッピングが細胞内の非伝導性の熱散逸の存在を明らかにする

High-speed Intracellular Temperature Mapping Reveals the Existence of Non-Conductive Heat Dissipation within Cells

Masaharu Takarada[1], Kohki Okabe[1,2], Takashi Funatsu[1] ([1]*Grad. Sch. of Pharm. Sci., The Univ of Tokyo*, [2]*JST, PRESTO*)

2Pos299* がん免疫において細胞傷害性指標となる液性因子分泌のライブセルイメージング

Live Cell Imaging of Liquid Factor Secretion as an Indicator of Cytotoxicity in Cancer Immunity

Yuto Kurisu[1], Zhuohao Yang[1], Koji Nagaoka[2], Sotaro Kamimura[3], Kazuhiro Kakimi[2], Takashi Funatsu[1], Yoshitaka Shirasaki[1] ([1]*Grad. Sch. Pharmaceutical Sciences ., Univ.Tokyo*, [2]*The Department of Immunotherapeutics ., Univ. Tokyo. Hospital*, [3]*Grad. Sch. Sciences ., Univ.Tokyo*)

2Pos300* 高速原子間力顕微鏡のさらなる高速化を目指した超微小カンチレバーの開発
Development of ultra-small cantilever for faster high-speed atomic force microscopy
Noriki Katayama[1], Kenichi Umeda[2], Toshio Ando[2], Noriyuki Kodera[2] ([1]*Grad. Sch. Math. & Phys., Kanazawa Univ.*, [2]*WPI-NanoLSI, Kanazawa Univ.*)

2Pos301 ゴルジ体と小胞体の超解像顕微鏡による可視化解析
Observation and analysis of Golgi body and ER with super resolution microscopy
Kaoru Katoh[1,2], Totai Mitsuyama[2] ([1]*Biomed Res Inst, AIST*, [2]*AIRC, AIST*)

2Pos302* 高分解能ライトフィールド顕微鏡の開発によるシングルショット 3D イメージング
Development of high-resolution light-field microscopy for single-shot 3D volumetric imaging
Ryuki Imamura[1], Shin Usuki[2], Takuma Sugi[1] ([1]*Program of Biomedical Science, Graduate School of Integrated Sciences for Life, Hiroshima University*, [2]*Research Institute of Electronics, Shizuoka University*)

2Pos303* (2SBA-2) ヒト生細胞の局所クロマチン動態は細胞周期を通して一定である
(2SBA-2) Single-nucleosome imaging reveals steady-state motion of interphase chromatin in living human cells
Shiori Iida[1,2], Soya Shinkai[3], Yuji Itoh[1], Sachiko Tamura[1], Masato Kanemaki[2,4], Shuichi Onami[3], Kazuhiro Maeshima[1,2] ([1]*Genome Dynamics Lab., Natl. Inst. of Genet.*, [2]*Dept. of Genet., Sch. of Life Sci., SOKENDAI*, [3]*RIKEN BDR*, [4]*Mol. Cell Eng. Lab., Natl. Inst. of Genet.*)

2Pos304 High-speed atomic force microscopy mapping of *Bacillus subtilis'* mechanical properties
Christian Ganser[1], Shigetaka Nishiguchi[1], Takayuki Uchihashi[1,2] ([1]*ExCELLS, NINS*, [2]*Grad. Sch. Sci., Nagoya Univ.*)

2Pos305* 高速 AFM 観察を用いた E6AP/E6/p53 複合体の構造ダイナミクスの解明
Structural dynamics of E6AP/E6/p53 complex revealed by high-speed AFM (HS-AFM)
Kazusa Takeda[1], Ikumi Muro[1], Hiroki Konno[2] ([1]*Grad. Sch. of Nat. Sci. & Technol., Kanazawa University*, [2]*WPI Nano Life Sci. Inst. (WPI-NanoLSI), Kanazawa Univ*)

2Pos306 透過型電子顕微鏡の最大感度をもたらす新規ヒルベルト位相板
Novel Hilbert Phase Plates for Maximum Sensitivity in Transmision Electron Microscopy
Kuniaki Nagayama (*N-EM Laboratories Inc.*)

2Pos307* Dynamic unfolding of the laminin coiled-coil domain revealed by high-speed AFM
Lucky Akter[1], Holger Flechsig[1], Arin Marchesi[1,2], Clemens Martin Franz[1] ([1]*WPI Nano Life Science Institute, Graduate School of Frontier Science Initiative, Kanazawa University, Japan*, [2]*Faculty of Medicine and Surgery, Università Politechnica delle Marche, Italy*)

2Pos308 脂肪細胞内脂質分布の TOF-SIMS 解析
Subcellular lipid analysis in a 3T3-L1 adipocyte by TOF-SIMS
Noritaka Masaki (*National Institute of Genetics*)

2Pos309 Development of genetically encodable tool for live-imaging and manipulation of endogenous RNAs in living cells
Akira Takai[1,2], Yasushi Okada[1,2,3] ([1]*Dept. Cell Biol., Grad. Sch. Med., Univ. Tokyo*, [2]*BDR, RIKEN*, [3]*Dept. Phys., Grad. Sch. Sci., Univ. Tokyo*)

2Pos310* 表面形状計測システムに向けた生体ナノポアプローブの特性
Characteristics of Biological Nanopore Probes as a Topological Imaging System
Shuta Nomi, Kan Shoji (*Nagaoka University of Technology*)

2Pos311 Raman spectral analysis of induced pluripotent stem cell during spontaneous differentiation
Hideaki Fujita[1,2], Kensuke Sasaki[2], Kazuhiro Sudo[3], Yukio Nakamura[3], Kuniya Abe[3], Yasuhiko Yoshida[4], Takayuki Haruki[4], Keiichi Koizumi[5] ([1]*Dept. Stem Cell Biol., RIRBM, Hiroshima Univ.*, [2]*Lab. Comp. Biol., BDR, Riken*, [3]*BRC, Riken*, [4]*Faculty Sust. Design, Academic Assembly, Univ. Toyama*, [5]*RCPDS, Toyama Univ.*)

2Pos312* 真核細胞における翻訳活性変化の温度シグナリング機構の解明
Thermal Signaling Mechanisms of Translational Control in Eukaryotic Cells
Naoko Kamiya[1], Kohki Okabe[1,2], Takashi Funatsu[1] ([1]*Grad. Pharm. Sci., The Univ. of Tokyo*, [2]*PRESTO,JST*)

バイオエンジニアリング／Bioengineering

2Pos313 Structure mechanism for color tuning of red-colored chromoprotein, R-Velour
Le Zhai[1,2], Ryosuke Nakashima[2], Tomoki Matsuda[1,2], Takeharu Nagai[1,2] ([1]*Graduate School of Frontier Bioscience, Osaka University, Japan*, [2]*SANKEN (The Institute of Scientific and Industrial Research), Osaka University, Japan*)

2Pos314 統合情報理論に基づいたスイッチング DNA 論理回路の構築
Construction of Switching DNA Logic Circuit based on Integrated Information Theory
Fumika Kambara[1], Sotaro Takiguchi[1], Hiroki Watanabe[2], Masahiro Takinoue[2], Ryuji Kawano[1] ([1]*Department of Biotechnology and Life Science, Tokyo University of Agriculture and Technology / Japanese*, [2]*Department of Life Science and Technology, Tokyo Institute of Technology / Japanese*)

2Pos315 (2SDA-5) ATP を検出可能な DNA ナノポアセンサの開発
(2SDA-5) ATP-detectable DNA nanopore sensor
Hiromu Akai, Kan Shoji (*Nagaoka University of Technology*)

2Pos316* カスケード反応における酵素複合体形成の寄与
Contribution of three-enzyme complex via 3-way junction DNA to activity of the cascade reaction
Aoi Mameuda, Koki Kamiya (*Grad. Sch. Sci. Tech. , Gunma Univ.*)

2Pos317 様々な形状の DNA 検出のための β ストランド数変化した改変型 β バレルナノポアタンパク質の構築
Modified β-barrel nanopore-forming protein with changed the number of β-strands for detection of various-shaped of DNA
Toshiyuki Tosaka, Koki Kamiya (*Grad. Sch. Sci. Tech. Gunma Univ.*)

2Pos318 塩基配列の設計による DNA 液滴の安定化
Stabilization of DNA droplets by designing base sequences
Kazuki Kobayashi[1], Satoshi Takahashi[2], Masahiro Takinoue[1,2] ([1]*Dept. Life Sci. Tech., Tokyo Tech*, [2]*Dept. Computer Sci., Tokyo Tech*)

2Pos319* 液-液相分離に基づく分子検出ための DNA 液滴コンピュータ
Computational DNA droplets based on liquid-liquid phase separation for molecular detection
Jing Gong[1], Nozomi Tsumura[2], Yusuke Sato[3], Masahiro Takinoue[4] ([1]*School of Life Science and Technology, Univ. Tokyo Tech / Japanese*, [2]*School of Engineering, Univ. Tokyo Tech / Japanese*, [3]*Department of Intelligent and Control Systems, Univ. Kyushu Tech / Japanese*, [4]*Department of Computer Science, Univ. Tokyo Tech / Japanese*)

2Pos320* 油中水滴を活用した新規蛍光 RNA アプタマー創出法の開発
Feasibility study of the method for obtaining fluorogenic RNA aptamers using water-in-oil microdroplets
Keisuke Ito, Ryo Iizuka, Sotaro Uemura (*Dept. Biol. Sci., Grad. Sch. Sci., The Univ. Tokyo*)

その他／Miscellaneous topics

2Pos321 有殻アメーバの頑健な卵型被殻構築過程の 4D イメージングおよび模型作成
4D Imaging and 3D modeling of the robust egg-shaped shell construction process of testate amoeba
Mami Nomura[1], Yukinori Nishigami[2], Josephine Galipon[3], Masatoshi Ichikawa[4], Takuro Nakayama[5], Keisuke Ohta[6], Kei-ichiro Nakamura[6] ([1]*Fac. Sci., Yamagata Univ.*, [2]*RIES, Hokkaido Univ.*, [3]*IAB, Keio Univ.*, [4]*Dept. Phys., Kyoto Univ.*, [5]*CCS, Univ. Tsukuba*, [6]*Sch. of Med., Kurume Univ.*)

2Pos322* ナノダイヤモンドを用いたアミロイドβ蛋白への新規標的治療法の検証
Verification of a new targeted therapy against amyloid-β using nanodiamonds
Miwa Shintani[1,2], Shin-ichiro Yanagiya[2], Hiroki Takanari[2] ([1]*Grad. Sch. opt., Uni. Tokushima / Japanese*, [2]*Post-LED Photonics Inst., Uni Tokushima / Japanese*)

2Pos323 関西におけるアカハライモリの警戒色の斑紋パターンの多様性
Diversity of warning coloration pattern in Kansai red-bellied newts
Sora Kazumi[1], Rikiya Ogawa[2] ([1]*Osaka Prefecture Tondabayashi High School*, [2]*Rikijuku Science School*)

2Pos324 クサカゲロウの翅の反射防止性能
Anti-reflectivity in green lacewing wings
Yuro Katsurashima[1], Leona Takahashi[2], Kazunari Yoshida[1] ([1]*Grad. Sch. Sci. Eng., Univ. Yamagata*, [2]*Grad. Sch. Sci. Eng., Univ. Aoyama Gakuin*)

2Pos325 Enzymatically controlled micro-patterning of self-assembled nanoparticles by surface-bound ATP
Ekta Shandilya, Subhabrata Maiti (*Indian Institute of Science Education and Research (IISER) Mohali, Punjab, India - 140306*)

3 日目（9 月 30 日（金））／Day 3（Sep. 30 Fri.）

蛋白質：構造／Protein: Structure

3Pos001 全原子シミュレーションを用いた βαβ モチーフのレジスタシフトルールの解明
Explaining empirical rules of register shift of βαβ-motif by physical interactions
Senji Mishima, Hiroto Murata, George Chikenji (*Dept. of App. Phys., Grad. Sch of Eng., Nagoya Univ.*)

3Pos002 Structural Validation Properly Regulates Boost Potentials in the Biased Sampling of Proteins
Takunori Yasuda[1], Rikuri Morita[2], Yasuteru Shigeta[2], Ryuhei Harada[2] ([1]*University of Tsukuba, Doctral Program in Biology*, [2]*University of Tsukuba, Center for Computational Sciences*)

3Pos003 補酵素結合と二量体化による細菌の 3α - ヒドロキシステロイド脱水素酵素（3αHSDs）の構造揺らぎ変化に対する MD シミュレーション
MD simulation study of fluctuation changes of bacterial 3a-Hydroxysteroid Dehydrogenases (3aHSDs) by coenzyme binding and dimerization
Kahoru Amakawa[1], Hiroki Suzuki[2], Ayako Shiota[2], Masayuki Oda[2], Juha Lintuluoto[3], Masami Lintuluoto[2] ([1]*Fac. Life and Env., Univ. Kyoto Prefectural*, [2]*Grad. Sch. Life and Env. Sci., Univ. Kyoto Prefectural*, [3]*Grad. Sch. Eng., Univ. Kyoto*)

3Pos004 Structural determinants for distinguishing frequently and rarely occurring psi-loop motifs
Tomoki C. Terada, Takumi Nishina, George Chikenji (*Dept of Appl. Phy., Grad. Sch. of Eng., Nagoya Univ.*)

3Pos005 蛋白質の荷電性残基が液-液相分離に及ぼす影響に関する粗視化分子動力学法による検討
A Coarse-Grained Molecular Dynamics Study to elucidate the effect of charged residues of proteins on liquid-liquid phase separation
Yuji Kuriki[1], Kota Kasahara[2], Junichi Higo[3], Takuya Takahashi[2] ([1]*Grad. Sch. Life Sci., Univ. Ritsumeikan*, [2]*Coll. Life. Sci., Univ. Ritsumeiakn*, [3]*Grad. Sch. Simulation Studies. Univ. Hyogo*)

3Pos006 3D Convolutional Neural Network を用いたタンパク質-ペプチドドッキングモデルの評価
Structure evaluation for protein-peptide docking models using 3D convolutional neural networks
Hyeri Lim[1], Shigeyuki Matsumoto[1], Shuntaro Chiba[2], Yuta Isaka[2], Mayumi Kamada[1], Yasushi Okuno[1,2] ([1]*Grad. Sch. Med., Univ. Kyoto*, [2]*R-CCS, RIKEN*)

3Pos007 深層学習を用いたタンパク質ドメインの予測研究
A deep-learning model for the prediction of protein domains
Renta Sato[1], Toru Ekimoto[2], Takashi Yoshidome[1] ([1]*Dep. of Appl. Phys., Tohoku Univ.*, [2]*Grad. Sch. of Med. Life Sci., Yokohama City Univ.*)

3Pos008 Structure of the IscB–ωRNA ribonucleoprotein complex, the likely ancestor of CRISPR-Cas9
Kazuki Kato[1], **Sae Okazaki[1]**, Soumya Kannan[2], Han Altae-Tran[2], Yukari Isayama[1], Junichiro Ishikawa[1], Rhiannon K Macrae[2], Tomohiro Nishizawa[3], Kira S Makarova[4], Eugene V Koonin[4], Feng Zhang[2], Hiroshi Nishimasu[1] ([1]*RCAST.,Univ.Tokyo*, [2]*MIT*, [3]*Grad.Sch.Medical Life Science.,Univ.Yokohama City*, [4]*NCBI*)

3Pos009 Benchmark of force fields to characterize the short intrinsically disordered region of FUS-LC domain
Maud Chan-Yao-Chong, Justin Chan, Hidetoshi Kono (*Molecular Modelling and Simulation (MMS) Team, National Institutes for Quantum Science and Technology (QST)*)

3Pos010 Photon Factory における BioSAXS 測定システムの高度化
Upgrade of BioSAXS measurement system at the Photon Factory
Nobutaka Shimizu, Hideaki Takagi, Yasuko Nagatani, Takeharu Mori, Keiko Yatabe, Masatsuyo Takahashi, Noriyuki Igarashi (*PF, IMSS, KEK*)

3Pos011 Structure determination of Ferritin at room temperature in microfluidic chips
Yusuke Kono, Leonard Chavas (*Dept of Appl. Phys., Grod. Sch. of Eng., Nagoya Univ.*)

3Pos012 分子動力学計算による FtsZ の構造変化機構の解析
Molecular dynamics simulations on the conformational stability of FtsZ with the different bound nucleotides
Taichi Takasawa[1], Go Watanabe[2,3], Yoshio Kodera[2,4], Takashi Matsui[2,4] ([1]*Grad. Sch. Sci., Kitasato Univ.*, [2]*Sch. Sci., Kitasato Univ.*, [3]*KISTEC*, [4]*Cent. Disease Proteomics*)

3Pos013 (2SEA-7) Optineurin の E50K 緑内障変異はオリゴマー粒径を増大させる
(2SEA-7) The E50K mutation of optineurin increases the oligomer size
Rintaro Kawamura[1], Soya Uetsuki[1], Takehito Tanzawa[2], Takayuki Kato[2], Masataka Kinjo[3], Akira Kitamura[3] ([1]*Grad. Sci. Life Sci., Hokkaido Univ.*, [2]*Inst., for Proteins Res., Osaka Univ.*, [3]*Fac. Adv. Life sci., Hokkaido Univ.*)

3Pos014 鶏卵白リゾチームの D/H コントラスト法を利用した中性子結晶解析
Neutron crystallography of hen-egg white lysozyme using D/H contrast technique
Toshiyuki Chatake[1], Ichiro Tanaka[2], Katsuhiro Kusaka[3], Satoru Fujiwara[4] ([1]*Inst. Integ. Rad. Nucl. Sci., Kyoto Univ.*, [2]*Grad. Sci. Eng., Ibaraki Univ.*, [3]*Front. Res. Cent. App. Atom. Sci., Ibaraki Univ.*, [4]*Inst. Quantum Life Science, QST*)

3Pos015 多分散溶液中の生体高分子の構造解析のための超遠心分析と小角散乱による統合アプローチ
Integrated approach to biomacromolecular structure in polydisperse solution with analytical ultracentrifugation and small-angle scattering
Ken Morishima, Rintaro Inoue, Aya Okuda, Nobuhiro Sato, Masahiro Shimizu, Yasuhiro Yunoki, Reiko Urade, Masaaki Sugiyama (*Institute for Integrated Radiation and Nuclear Science, Kyoto University*)

3Pos016 クライオ電子顕微鏡による高精度構造解析
High-precision structural analysis by cryo-electron microscopy
Tasuku Hamaguchi[1], Keisuke Kawakami[2], Saori Maki-Yonekura[2], Koji Yonekura[1,2] ([1]*IMRAM, Tohoku Univ.*, [2]*RIKEN SPring-8 Center*)

3Pos017 Preparation of phosphorylated FROUNT protein, a regulator of chemokine receptors, for structural and functional analyses
Keisuke Uchida[1], Sosuke Yoshinaga[1], Takafumi Sato[1], Mitsuhiro Takeda[1], Yuya Terashima[2,3], Etsuko Toda[2,3,4], Kouji Matsushima[2,3], Hiroaki Terasawa[1] ([1]*Fac. Life Sci., Kumamoto Univ.*, [2]*Grad. Sch. Med., Univ. Tokyo*, [3]*RIBS, Tokyo Univ. Sci.*, [4]*Nippon Med. Sch.*)

3Pos018 Computational analysis on the effects of active-site reduction on structures and dynamics of plant-type ferredoxin
Tomoki Nakayoshi[1], Yusuke Ohnishi[2], Hideaki Tanaka[2], Genji Kurisu[2], Yu Takano[1] ([1]*Grad. Sch. Inf. Sci., Hiroshima City Univ.*, [2]*Inst. Protein Res., Osaka Univ.*)

3Pos019 Efficient Conformational Sampling with an Adaptive Coarse-Grained Elastic Network Model using Dynamic Cross-Correlation Coefficient
Ryo Kanada[1], Kei Terayama[2], Atsushi Tokuhisa[1], Shigeyuki Matsumoto[3], Yasushi Okuno[1,3] ([1]*RCCS, RIKEN*, [2]*Grad. Sch. Medical Life Sci., Yokohama City Univ.*, [3]*Grad. Sch. Medicine, Kyoto Univ.*)

3Pos020 Structural basis of actin-microtubule crosstalk mediated by GAS2
Jiancheng An, Tsukasa Makino, Masahide Kikkawa (*The University of Tokyo*)

3Pos021 Cryo-EM structure of an osmotically sensitive Ca^{2+} ion channel
Honoka Hosoki, Tatsuya Hagino, Kanae Demura, Wataru Shihoya, Tsukasa Kusakizako, Osamu Nureki (*Grad.Sch.Sci.,Univ.Tokyo*)

3Pos022 結晶構造から明らかになったシゾロドプシンの内向きプロトン輸送機構
Crystal structure of schizorhodopsin reveals mechanism of inward proton pumping
Wataru Shihoya[1], Akimitsu Higuchi[1], Masae Konno[2], Tatsuya Ikuta[1], Hideki Kandori[3], Keiichi Inoue[2], Osamu Nureki[1] ([1]*Grad. Sch. Sci., The Univ of TOkyo*, [2]*ISSP, The Univ of TOkyo*, [3]*Life Sci. Appl. Chem., Nagoya Inst. Tech.*)

3Pos023 タンパク質中性子回折実験における水素高感度検出のための技術開発
Technological development for high-sensitivity detection of hydrogen in protein neutron diffraction experiments
Ichiro Tanaka[1,2], Hideki Yamauchi[1], Yohei Noda[1,2], Tomoki Maeda[2], Satoshi Koizumi[1,2] ([1]*Grad. Sch. Sci. Eng., Ibaraki Univ.*, [2]*Frontier Res. Center Appl. Atomic Sci., Ibaraki Univ.*)

蛋白質：構造機能相関／Protein: Structure & Function

3Pos024 FAP47, HYDIN, and CPC1 in the central pair apparatus of *Chlamydomonas*
Yuma Tani[1], Haruaki Yanagisawa[1], Toshiki Yagi[2], Masahide Kikkawa[1] ([1]*Grad. Sch. Med., Univ. Tokyo*, [2]*Life Sci., Pref. Univ. Hiroshima*)

3Pos025 昆虫由来不凍タンパク質は哺乳動物細胞を－5℃でも生存可能にする
Insect-derived antifreeze protein allows mammalian cells to survive at －5°C
Akari Yamauchi[1], Hidemasa Kondo[2,3], Tatsuya Arai[4], Sakae Tsuda[2,4,5] ([1]*Inst. Low Temp. Sci., Univ. Hokkaido*, [2]*Grad. Sch. Life Sci., Univ. Hokkaido*, [3]*Hokkaido Inst., AIST*　, [4]*Grad. Sch. Frontier Sci., Univ. Tokyo*, [5]*Tokyo Inst., AIST*　)

3Pos026 Integration of *In Silico* Strategies for Drug Repositioning towards P38α Mitogen-Activated Protein Kinase (MAPK) at the Allosteric Site
Utid Suriya[1], Panupong Mahalapbutr[2], Thanyada Rungrotmongkol[3,4] ([1]*Program in Biotechnology, Faculty of Science, Chulalongkorn University, Bangkok, Thailand*, [2]*Department of Biochemistry, and Center for Translational Medicine, Faculty of Medicine, Khon Kaen University, Khan Kaen 40002, Thailand*, [3]*Structural and Computational Biology Research Unit, Department of Biochemistry, Chulalongkorn University, Bangkok, Thailand*, [4]*Ph.D. Program in Bioinformatics and Computational Biology, Graduate School, Chulalongkorn University, Bangkok 10330, Thailand*)

3Pos027 Designed darunavir derivatives against HIV-1 protease: A computational study
Hathaichanok Chuntakaruk[1], Tanatorn Khotavivattana[2], Chanat Aonbangkhen[2], Phornphimon Maitarad[3], Thanyada Rungrotmongkol[1,4], Supot Hannongbua[1,5] ([1]*Program in Bioinformatics and Computational Biology, Grad. Sch., Chulalongkorn Univ., Bangkok 10330, Thailand*, [2]*Center of Excellence in Natural Products Chemistry, Department of Chemistry, Faculty of Science, Chulalongkorn Univ., Bangkok 10330, Thailand*, [3]*Research Center of Nano Science and Technology, Shanghai Univ., NO 99, Shangda Road, PO Box 111, Baoshan district, Shanghai, 200444 People's Republic of China*, [4]*Biocatalyst and Environmental Biotechnology Research Unit, Department of Biochemistry, Faculty of Science, Chulalongkorn Univ., Bangkok 10330, Thailand*, [5]*Center of Excellence in Computational Chemistry (CECC), Department of Chemistry, Faculty of Science, Chulalongkorn Univ., Bangkok 10330, Thailand*)

3Pos028 Structural effects of spike variants that reshaped the pandemic
Hisham Dokainish[1,2], Yuji Sugita[1,3,4] ([1]*Theoretical Molecular Science Laboratory, RIKEN Cluster for Pioneering Research, Wako, Japan*, [2]*Faculty of Pharmaceutical Sciences, Hokkaido University*, [3]*Computational Biophysics Research Team, RIKEN Center for Computational Science, Kobe, Japan*, [4]*Laboratory for Biomolecular Function Simulation, RIKEN Center for Biosystems Dynamics Research, Kobe, Japan*)

3Pos029 コレラ菌走化性受容体 Mlp3 のリガンド認識機構
Ligand recognition mechanism of Mlp3, a chemoreceptor of *Vibrio cholerae*
Yuka Ueda[1], Yuzuki Yabunaka[1], Norihiro Takekawa[1], So-ichiro Nishiyama[2], Hirotaka Tajima[3], Ikuro Kawagishi[3], Katsumi Imada[1] ([1]*Dept. Macromol. Sci., Grad. Sch. Sci., Osaka Univ.*, [2]*Dept. Appl Life Sci, Niigata Univ of Pharm and Appl Life Sci.*, [3]*Dept. Front Biosci., Hosei Univ.*)

3Pos030 HIV 逆転写酵素の薬剤耐性変異に対する動的残基間相互作用ネットワーク解析
Dynamic Residue Interaction Network Analysis of HIV-1 Reverse Transcriptase for Drug Resistance Mutations
Ryuki Hashimoto, Norihumi Yamamoto (*Chiba Tech*)

3Pos031 HIV-1 の Nelfinavir 耐性プロテアーゼ D30N/L90M 変異体に対する動的残基間相互作用ネットワーク解析
Dynamic Residue Interaction Network Analysis of the Protease D30N/L90M Mutant Conferring Nelfinavir Resistance in HIV-1
Ryoga Miyawaki, Norihumi Yamamoto (*Chiba Tech*)

3Pos032 イオタ毒素 Ia-GFP キメラのタンパク質膜透過の確認と構造解析
Confirmation of protein membrane translocation and structural analysis of Iota toxin Ia-GFP chimera
Shun Tomoda, Tomohito Yamada, Hideaki Tsuge (*Graduate School of Life Science, Kyoto Sangyo University*)

3Pos033 酸化還元感受性の鉄硫黄クラスターを利用する tRNA 硫黄修飾酵素の反応機構
The reaction mechanism of tRNA sulfur modification enzymes using redox-sensitive iron-sulfur clusters
Masato Ishizaka[1], Minghao Chen[1,2], Shun Narai[1], Yoshikazu Tanaka[2,3], Masaki Horitani[4,5], Min Yao[2] ([1]*Grad. Sch. Life Sci., Hokkaido Univ.*, [2]*Fac. Adv. Life Sci., Hokkaido Univ.*, [3]*Grad. Sch. Life Sci., Tohoku Univ.*, [4]*Fac. Agri., Saga Univ.*, [5]*United Grad. Sch. Agri. Sci., Kagoshima Univ.*)

3Pos034 A new enzyme from tardigrades which consists of ferritin-like and IgG-like domains
Subaru Kato, Yota Fukuda, Tsuyoshi Inoue (*Graduate School of Pharmaceutical Sciences, Osaka University*)

3Pos035 生物発光タンパク質イクオリンのアロステリックな発光反応制御機構についての理論的研究
Theoretical study on allosteric control mechanism of a luminescent reaction of bioluminescent protein aequorin
Tomohiro Ando, Shigehiko Hayashi (*Grad. Sch. Sci., Kyoto Univ.*)

3Pos036 Structural dynamics and kinase inhibitory activity of tyrosine kinase inhibitors against wild-type and mutant forms of EGFR
Rungrotmongkol Thanyada[1,5], Todsaporn Duangjai[1], Mahalapbutr Panupong[2], P. Poo-arporn Rungtiva[3], Choowongkomon Kiattawee[4] ([1]*Center of Excellence in Biocatalyst and Sustainable Biotechnology, Department of Biochemistry, Faculty of Science, Chulalongkorn University, Bangkok 10330, Thailand*, [2]*Department of Biochemistry, and Center for Translational Medicine, Faculty of Medicine, Khon Kaen University, Khon Kaen 40002, Thailand*, [3]*Biological Engineering Program, Faculty of Engineering, King Mongkut's University of Technology Thonburi, Bangkok, Thailand*, [4]*Department of Biochemistry, Faculty of Science, Kasetsart University, Bangkok 10900, Thailand*, [5]*Program in Bioinformatics and Computational Biology, Graduate School, Chulalongkorn University, Bangkok 10330, Thailand*)

3Pos037 RNA-seq 解析によるセイヨウイトスギの新規アレルゲン候補の探索
Searching for new allergen candidates in European cypress by RNA-seq analysis
Tomona Iizuka[1], Hélène Sénéchal[2], Pascal Poncet[3], Tomoyasu Aizawa[1] ([1]*Grad. Sch. Life Sci., Hokkaido Univ.*, [2]*Allergy & Environment, Armand Trousseau Children Hospital, Paris, France*, [3]*Immunology Department, Institute Pasteur, Paris, France*)

3Pos038 分子動力学法による自己集合性ペプチドの配列最適化
Sequence optimization of self-assembly peptides by using MD simulations
Koya Sato[1], Kota Kasahara[2], Hiroshi Imamura[2], Takuya Takahashi[2] ([1]*Grad. Sch. Life Sci., Univ. Ritsumeikan*, [2]*Coll. Life. Sci., Univ. Ritsumeikan*)

3Pos039 緑色蛍光タンパク質のループ領域の静電ポテンシャルに影響を及ぼす部位特異的アミノ酸置換と分子構造および発光特性の相関
Correlation of amino acid substitutions affecting the electrostatic potential of loop region with structure and luminescence properties
Kaori Chiba, Kokomi Takanashi (*Indust. Eng. Natl. Inst. Tech, Ibaraki Coll. Japan*)

3Pos040 分子動力学計算によるダイナミンの誘電アロステリー解析
Dielectric allostery of dynamin studied by molecular dynamics simulation
Masataka Yaguchi[1], Jun Ohnuki[2], Mitsunori Takano[1] ([1]*Dept. of Pure & Appl. Phys., Grad. Scl. Adv. Sci. & Eng., Waseda Univ.*, [2]*Inst. for Mol. Sci.*)

3Pos041 HIV-1 Vif タンパク質によるヒト抗ウイルス因子 APOBEC3 タンパク質のマルチファセットな無力化: ユビキチン化と脱アミノ化阻害
HIV-1 Vif drived multifaceted neutralization against human APOBEC family proteins: ubiquitination/degradation and deamination inhibition
Keisuke Kamba[1], Li Wan[1,2], Kentaro Tozawa[1,2], Ryo Iwaoka[1,2], Satoru Unzai[3], Ryo Morishita[4], Akifumi Takaori-Kondo[5], Takashi Nagata[1,2], Masato Katahira[1,2] ([1]*Inst. of Adv. Energy, Kyoto Univ.*, [2]*Grad. Sch. Energy Sci., Kyoto Univ.*, [3]*Frontier Bioscience, Hosei Univ.*, [4]*CellFree Sciences Co.,Ltd.*, [5]*Grad. Sch. Med., Kyoto Univ.*)

3Pos042 タンパク質構造の熱揺らぎと進化しやすさは相関している
Dynamics-Evolution Correspondence in Protein Structures
Qianyuan Tang[1,2], Kunihiko Kaneko[1] ([1]*Center for Complex Systems Biology, Universal Biology Institute, University of Tokyo*, [2]*Lab for Neural Computation and Adaptation, RIKEN Center for Brain Science*)

3Pos043 シアン化物結合シトクロム酸化酵素の結晶構造から示唆される、金属中心の酸化状態変化による活性制御機構
Crystallographic cyanide-probing of cytochrome oxidase provides insights into its activity regulation by the redox change of metal sites
Atsuhiro Shimada[1], Kazumasa Muramoto[2], Kyoko Shinzawa-Itoh[2], Tomitake Tsukihara[3], Shinya Yoshikawa[2] ([1]*Dept. Appl. Life Sci., Fac. Appl. Biol. Sci., Gifu Univ.*, [2]*Grad. Sch. Sci., Univ. Hyogo*, [3]*Inst. Protein Res., Osaka Univ.*)

3Pos044 アクチンフィラメントの張力依存的な構造変化の解析
Analysis of the tension dependent structural changes of actin filament
Fumito Matsuzaki, Tao Q.P. Noguchi (*National Institute of Technology, Miyakonojo College*)

3Pos045 Kai 時計システムにおける分子の統合運動
Orchestration of proteins in a Kai clock system
Masaaki Sugiyama[1], Ken Morishima[1], Yasuhiro Yunoki[1], Rinatro Inoue[1], Nobuhiro Sato[1], Hirokazu Yagi[2], Koichi Kato[3] ([1]*KURNS*, [2]*Grad. Sch. Phar., Nagoya City Univ.*, [3]*ExCELLS*)

3Pos046 高分子クラウディング環境下での蛋白質溶解度の進化
Evolution of protein solubility in macromolecular crowding
Yasuhiro Isogai[1], Hiroshi Imamura[2], Tomonari Sumi[3], Tsuyoshi Shirai[4] ([1]*Dept. Pharmaceutical Engineering, Toyama Prefectural Univ.*, [2]*Dept. Bio-Science, Nagahama Inst. Bio-Science and Technology*, [3]*Research Inst. Interdisciplinary Science, Okayama University*, [4]*Dept. Computer Bioscience, Nagahama Inst. Bio-Science and Technology*)

3Pos047 Dispersion Effect of Molecular Crowding on Ligand-Protein Surface Binding Sites of *Escherichia coli* RNase HI
Chikashi Ota[2], Hikari Suzuki[1], Shun-ichi Tanaka[1], **Kazufumi Takano**[1] ([1]*Kyoto Prefectural University*, [2]*Ritsumeikan University*)

3Pos048 線維形成前駆状態 β2 ミクログロブリンの残余構造がアミロイド線維のモルフォロジーに与える影響
The residual structure of acid-denatured β_2-microglobulin is relevant to an ordered fibril morphology
Ryosuke Tomiyama[1], Masatomo So[2], Yohei Miyanoiri[3], **Kazumasa Sakurai**[1,4] ([1]*Graduate School of Biology-Oriented Science and Technology, Kindai University*, [2]*Astbury Centre for Structural Molecular Biology, University of Leeds*, [3]*Institute for Protein Research, Osaka Univeristy*, [4]*Institute of Advanced Technology, Kindai University*)

3Pos049 透析アミロイドーシスの発症機構における分子夾雑環境の役割
Role of macromolecular crowding in the onset mechanism of dialysis-related amyloidosis
Kichitaro Nakajima[1], Keiichi Yamaguchi[1], Suguru Yamamoto[2], Yuji Goto[1] ([1]*Global Center for Med. Eng. Info., Osaka Univ.*, [2]*Grad. Sch. Med. Dent. Sci., Niigata Univ.*)

3Pos050 異種フィブロイン混合系におけるナノファイバー/前駆体形成評価
Evaluation of nanofiber/precursor formation in heterogeneous fibroin mixtures
Haruya Kajimoto[1], Kento Yonezawa[2], Kok Sim Chan[1], Takehiro Sato[3], Yoichi Yamazaki[1], Sachiko Toma-Fukai[1], Hironari Kamikubo[1,2] ([1]*NAIST, MS*, [2]*NAIST, CDG*, [3]*Spiber Inc.*)

3Pos051 アラニンスキャン変異解析による c-Myb–KIX 間相互作用に重要なアミノ酸残基の同定
Identifying key residues of c-Myb–KIX interaction by alanine scanning mutagenesis
Shunji Suetaka[1], Yuuki Hayashi[1,2], Munehito Arai[1,3] ([1]*Dept. Life Sci., Univ. Tokyo*, [2]*Environmental Science Center, Univ. Tokyo*, [3]*Dept. Phys., Univ. Tokyo*)

3Pos052 高温条件下における耐熱化デンプンブランチングエンザイムの MD シミュレーションによる構造解析
Molecular Dynamics Simulation of Heat-Resistant Starch Branching Enzyme under High Temperature Conditions
Kosuke Nariyama[1], Yoh Noguchi[1,3], Motokuni Nakajima[1], Hironao Yamada[2,3], Ryota Morikawa[1], Masako Takasu[1], Shoko Fujiwara[1] ([1]*Sch. of Life Sci., Tokyo Univ. of Pharm. and Life Sci.*, [2]*Sch. of Pharm., Tokyo Univ. of Pharm. and Life Sci.*, [3]*The Institute of Statistical Mathematics*)

3Pos053 分子シミュレーションにおける高次項を用いた補間による自由エネルギー地形の推定
Estimation of Free-Energy Landscape for Molecular Simulations by Interpolation with Higher-Order Terms
Shohei Toyama[1,2], Yuji Higuchi[3], Hiroshi Noguchi[1] ([1]*ISSP., Univ. Tokyo*, [2]*Dept. Phys., Univ. Tokyo*, [3]*RIIT., Univ. Kyushu*)

3Pos054 アミロイド β タンパク質の分子構造動態に D-アスパラギン酸が与える影響
Effect of D-Aspartic Acid on the Conformational Dynamics of Amyloid-$\beta_{1\text{-}42}$ Protein
Yu Fukuda[1], Takeru Kameda[1], Shin-ichi Tate[3], Yuichi Togashi[1,2] ([1]*Coll. Life Sci., Ritsumeikan Univ.*, [2]*Riken BDR*, [3]*Grad. Sch. Integ. Sci. Life, Hiroshima Univ.*)

3Pos055 タンパク質複合体における複数残基間相互作用の解析
Analysis of multiple residue interactions in protein complexes
Masaki Koyama, George Chikenji (*Dept. of Appl. Phys., Grad. Sch. of Eng., Nagoya Univ.*)

3Pos056 蛍光タンパク質イクオリンとカルシウムの結合に関する熱力学的解析
Thermodynamic analysis of the calcium binding with photoluminescence protein; aequorin
Urara Kuroki[1], Toshiya Funahashi[2], Yusuke Onishi[3], Toru Nakatsu[3], Tetsunari Kimura[1] ([1]*Grad. Sch. of Sci., Kobe Univ.*, [2]*Grad. Sch. of Pharm. Sci., Kyoto Univ.*, [3]*Sch. of Pharm. Sci., Univ. Wakayama Med.*)

3Pos057 CHARMM C36m 力場のタンパク質-水相互作用の強化によるタンパク質の水溶液環境及び混雑環境における拡散性及び熱力学的特性の改善
Improved diffusive and thermodynamic properties of proteins with modified interactions between water and protein in CHARMM c36m
Daiki Matsubara[1], Kento Kasahara[2], Hisham Dokainish[3], Hiraku Oshima[1], Yuji Sugita[1,3,4] ([1]*Kobe Inst., RIKEN*, [2]*Grad. Sch. Eng., Univ. Osaka*, [3]*Wako Inst., RIKEN*, [4]*Kobe Inst., RIKEN*)

3Pos058 Structural Characteristics Investigation of Hero Peptides Using All-atom Molecular Dynamics Simulations
Haeri Im[1], Ai Niitsu[1], Cheng Tan[2], Yuji Sugita[1,2,3] ([1]*Theoretical Molecular Science Laboratory, RIKEN Cluster for Pioneering Research, Wako, Japan*, [2]*Computational Biophysics Research Team, RIKEN Center for Computational Science, Kobe, Japan*, [3]*Laboratory for Biomolecular Function Simulation, RIKEN Center for Biosystems Dynamics Research, Kobe, Japan*)

3Pos059 乾燥耐性生物クマムシのミトコンドリア局在性熱可溶性タンパク質 MAHS ・LEAM における乾燥誘導性 LLPS
Dehydration inducible LLPS of the mitochondria localized heat-soluble protein MAHS & LEAM of an anhydrobiotic tardigrade
Sae Tanaka[1,2], Kazuharu Arakawa[1,2] ([1]*National Institutes of Natural Sciences, Exploratory Research Center on Life and Living Systems, Section for Exploration of Life in Extreme Environments*, [2]*Institute for Advanced Biosciences, Keio University*)

3Pos060 ベイズ学習による格子タンパク質模型のデザイン
Lattice protein design using Bayesian learning
Tomoei Takahashi[1], George Chikenji[2], Kei Tokita[1] ([1]*Grad. Sch. Inf. Nagoya Univ.*, [2]*Grad. Sch. Eng. Nagoya Univ.*)

3Pos061 がん抑制タンパク質 p53 のアモルファス凝集体・アミロイド凝集体への新たなる知見
New insights into morphous & amyloid aggregates of the tumor suppressor p53
Emi Hibino[1], Reiji Hijikata[2], Takeshi Tenno[1,3], Hidekazu Hiroaki[1,3] ([1]*Grad. Sch. Pharm. Sci., Nagoya Univ.*, [2]*Sch. Sci., Nagoya Univ.*, [3]*BeCellBar*)

3Pos062 細胞質中のヌクレオチド三リン酸によって改変される生体高分子の相互作用と安定性
Stability and interaction of macromolecules altered by nucleoside triphosphates in cytoplasm
Isseki Yu[1], Ryuto Yamazaki[1], Michael Feig[2], Yuji Sugita[3] ([1]*Maebashi Institute of Technology Information Systems Program*, [2]*Michigan State University Department of Biochemistry and Molecular Biology*, [3]*Riken Theoretical Molecular Science Laboratory*)

蛋白質：機能（反応機構 生物活性など）／Protein: Function

3Pos063 自由エネルギー解析によるトリプトファン合成酵素におけるアロステリックなトリプトファン合成機構の解明
Allosteric regulation mechanism of tryptophan synthesis in tryptophan synthase by free energy analysis
Shingo Ito, Kiyoshi Yagi, Yuji Sugita (*Theor. Mol. Sci. Lab., CPR, RIKEN*)

3Pos064 Cryptdin-4, a mouse α-defensin, with multiple antibacterial mechanisms regulated by its redox structure and environmental conditions
Yi Wang, Yuchi Song, Rina Hiramine, Tomoyasu Aizawa (*Grad. Sch. Life Sci., Hokkaido Univ.*)

3Pos065 Insights into the allosteric modulation of catalysis via a single surface mutation on a flexible loop in dihydrofolate reductase
Sandhya Premnath Tiwari, Shinichi Tate (*Grad. Sch. of Integrated Sciences for Life, Hiroshima University*)

3Pos066 大腸菌フェリチンの鉄酸化とミネラル化に与えるリン酸の効果
Effect of phosphate on the iron oxidation and mineralization in *Escherichia coli* ferritin
Takumi Kuwata, Kazuo Fujiwara, Masamichi Ikeguchi (*Dept. of Biosci., Grad. Sch. of Sci and Eng., Soka Univ*)

3Pos067 テロメアブーケ形成における Mps3、Rpf2-Rrs1、Ebp2-Brx1 間の結合関係
Binding relationships among Mps3, Rpf2-Rrs1 and Ebp2-Brx1 in telomere bouquet formation
Hao Li[1], Takuma Eguchi[1], Isao Tanaka[1,2], Toyoyuki Ose[1,2], Min Yao[1,2] ([1]*Graduate School of Life Science, Hokkaido University*, [2]*Faculty of Advanced Life Science, Hokkaido University*)

3Pos068 IL-6 刺激下における非リン酸化型 STAT3 動態の解析
Analyses of the unphosphorylated STAT3 dynamics in the IL-6 activated pathway
Rin Tanaka[1,2], Michio Hiroshima[2], Masahiro Ueda[1,2] ([1]*Grad. Sch. Sci., Univ. Osaka*, [2]*Osaka Inst., Riken*)

3Pos069 A simple coarse-grained model for ADP binding to HSP90
Kazutomo Kawaguchi, Hidemi Nagao (*Inst. Sci. Eng., Kanazawa University*)

3Pos070 分子動力学に基づく混雑環境がタンパク質-リガンド結合に与える影響の速度論的解析
Kinetic analysis of the crowder effects on protein-ligand processes based on the molecular dynamics
Kento Kasahara (*Grad. Sch. Engr. Sci., Osaka Univ.*)

3Pos071 ジアゾ化酵素 Fur5 のジアゾ化反応機構の計算化学的解析
Computational analysis of the diazotization reaction mechanism of diazo-forming enzyme Fur5
Shota Kaneko, Yoshitaka Moriwaki, Tomohiro Noguchi, Tomohisa Kuzuyama, Tohru Terada, Kentaro Shimizu (*Grad. Sch. of Agri. and Life Sci., Univ. of Tokyo*)

3Pos072 二重スピンラベル-ESR 分光法による ABC トランスポーターの膜貫通ドメインのコンフォメーション変化
Conformational changes in transmembrane domain of ABC transporter revealed by double spin label-ESR spectroscopy
Ayaka Naka[1], Yasuhiro Kobori[1,2], Motonari Tsubaki[1], Yoshitsugu Shiro[3], Hiroshi Sugimoto[3,4], Tetsunari Kimura[1] ([1]*Grad. Sch. Sci., Kobe Univ.*, [2]*Mol. Photo. Res. Cent., Kobe Univ.*, [3]*Grad. Sch. Sci., Univ. Hyogo*, [4]*SPring-8, RIKEN*)

3Pos073 時間分解分光測定を用いた ABC トランスポーター BhuUV-T におけるヘム輸送機構の解析
Tire-resolved spectroscopic analysis of allocrite transport mechanism in heme ABC transporter; BhuUV-T
Akiho Hara[1], Yoshitsugu Shiro[2], Hiroshi Sugimoto[2,3], Tetsunari Kimura[1] ([1]*Grad. Sch. of Sci., Kobe Univ.*, [2]*Grad. Sch. Sci., Univ. of Hyogo*, [3]*SPring-8, RIKEN*)

蛋白質：計測・解析の方法論／Protein: Measurement & Analysis

3Pos074 Refinement of MD-derived conformational ensemble by referring to experimental SANXS data in framework of Bayesian statistics
Tomotaka Oroguchi[1,2] ([1]*Faclt. Sci. Tech., Keio Univ.*, [2]*RIKEN SPring-8 Center*)

3Pos075 蛍光相関分光法を用いたリボソーム-新生鎖複合体と相互作用する大腸菌 **Trigger Factor** シャペロンの動態観察

Application of fluorescence correlation spectroscopy to investigate dynamics of a ribosome-associated trigger factor chaperone in *E. coli.*

Tatsuya Niwa[1,2], Koki Nakazawa[1], Kensuke Hoshi[1], Hisashi Tadakuma[3], Koichi Ito[4], Hideki Taguchi[1,2] ([1]*Dept.of Life Science and Technology, Tokyo Tech.*, [2]*Cell Biology Center, IIR, Tokyo Tech.*, [3]*Sch. of Life Science and Technology & Gene Editing Center, ShanghaiTech University*, [4]*Dept. of Computational Biology & Medical Sciences, Grad. Sch. of Frontier Sciences, Tokyo University*)

3Pos076 BLI 法を用いた変性 LDL と LDL 関連受容体との結合特性

Binding properties of LDL to recombinant receptors were investigated by biolayer interfere layer method

Seiji Takeda[1], Nozomu Sato[1], Ao Hamamuki[1], Kanako Usirogata[2], Taichi Takasuka[2] ([1]*Dept. Pharm., Hokkaido Univ. of Sci.*, [2]*Grad. Sch. GFR., Hokkaido University*)

3Pos077 一定力下での非平衡分子動力学シミュレーションの再検討

Non-equilibrium molecular dynamics simulation under constant force revisited

Shinji Iida, Tomoshi Kameda (*National Institute of Advanced Industrial Science and Technology*)

3Pos078 量子ビームを利用した膜タンパク質分子内ダイナミクスの直接検出

Direct detection of intramolecular dynamics of membrane proteins using X-ray based analysis techniques

Kazuhiro Mio[1,2], Tatsunari Ohkubo[1,2], Shoko Fujimura[1,3], Tatsuya Arai[3], Hiroshi Sekiguchi[4], Yuji C. Sasaki[1,3,4] ([1]*Operand OIL, AIST*, [2]*Grad. Sch. Med. Sci., Yokohama CU*, [3]*Grad. Sch. of Front. Sci., The Univ of Tokyo*, [4]*JASRI*)

3Pos079 ノイズのある原子間力顕微鏡像からの探針形状推定法の開発

Development of blind tip reconstruction method for noisy atomic force microscopy images

Ryuhei Oshima (*Grad. Sch. Sci. Eng., Saitama Univ.*)

3Pos080 木探索分子動力学法による Interleukin-2-inducible T-cell kinase 活性化経路の探索

Activation Pathway of Interleukin-2-inducible T-cell kinase Explored by Tree-Search Molecular Dynamics

Yukina Nakai[1], Toru Ekimoto[1], Tsutomu Yamane[2], Naoki Ogawa[1], Masao Inoue[1], Kei Terayama[1], Mitsunori Ikeguchi[1,2] ([1]*Dept. of Med. Life Sci., Yokohama City Univ.*, [2]*R-CCS, Riken*)

3Pos081 微分可能な多状態ベネット受容比法を用いたシミュレーションモデルパラメータの効率的なチューニング

Efficient parameter tuning of simulation models by differentiable multistate Bennett's acceptance ratio method

Haruto Uchino, Yasuhiro Matsunaga (*Grad. Sch. Sci. Eng., Saitama Univ.*)

3Pos082 深層学習によるグリッドベースの水和自由エネルギー計算

A deep-learning model for Grid-based Solvation Free Energy

Yusaku Fukushima, Takashi Yoshidome (*Dep. of Appl. Phys., Tohoku Univ.*)

3Pos083 生体分子による液-液相分離とその環境要因を予測する機械学習モデルの開発

Development of machine learning models to predict liquid-liquid phase separation of biomolecules and its environmental factors

Kayin Chin, Shoichi Ishida, Kei Terayama (*Grad. Sch. Med. Life Sci., Yokohama City Univ.*)

3Pos084 自由エネルギー摂動法を用いた VHH 抗体の等電点の制御

In silico control of isoelectric point of VHH using free energy perturbation method

Soichiro Oda, Yasuhiro Matsunaga (*Grad. Sch. Sci. Eng., Saitama Univ.*)

3Pos085 X 線構造解析とラマン分光によるテトラペプチド結晶中の水素結合ネットワークの解析

Hydrogen network in a tetrapeptide crystal characterized by X-ray diffraction and Raman spectroscopy

Kazunori Motai[1], Masaki Kawano[2], Yuji Mochizuki[3,4], Takehiko Mori[1], Yuhei Hayamizu[1] ([1]*Department of Materials Science and Engineering, Tokyo Tech*, [2]*Department of Chemistry, School of Science, Tokyo Tech*, [3]*Department of Chemistry and Research Center for Smart Molecules, Faculty of Science, Rikkyo University*, [4]*Institute of Industrial Science,The University of Tokyo*)

蛋白質：蛋白質工学／進化工学／Protein: Engineering

3Pos086 気軽に試せる計算機タンパク質デザインに向けて
Towards easy-to-try computational protein design
Naoya Kobayashi, Shun Hirota (*NAIST, Mat. Sci.*)

3Pos087 phi29 ファージ DNA 複製を用いた人工 DNA ゲノム進化系の構築
Development of an artificial DNA genome evolution platform using the phi29 DNA replication
Taro Furubayashi[1,2], Yoshihiro Minagawa[1], Hiroyuki Noji[1] ([1]*Grad. Sch. Eng., Univ. Tokyo*, [2]*JSPS*)

3Pos088 RNA メチル基転移酵素の配列特異性および補酵素選択性を改変する進化分子工学的手法の開発
Development of a directed evolution method for changing sequence specificity and cofactor selectivity of RNA methyltransferases
Yoshiki Ochiai, Paola Laurino (*Protein Engineering and Evolution Unit, OIST*)

3Pos089 ヘリックス-ループ-ヘリックスペプチドを分子基盤とする細胞内タンパク質間相互作用阻害剤の分子設計
A Cyclized Helix-Loop-Helix Peptide as a Molecular Scaffold to Design Inhibitors against Iintracellular Protein-Protein Interactions
Daisuke Fujiwara, Masataka Michigami, Ikuhiko Nakase, Ikuo Fujii (*Grad. Sch. Sci., Osaka Metropolitan Univ.*)

3Pos090 cDNA display 法により取得されたペプチドアプタマーの迅速かつ最適なダイマー化への新しいコンビナトリアル手法の開発
High-throughput identification of bivalent peptide aptamers selected by cDNA display with a newly combinatorial approach
Taro Noguchi[1], Kanako Nakao[1], Shigefumi Kumachi[1], Masayuki Tsuchiya[1], **Naoto Nemoto**[1,2] ([1]*Epsilon Molecular Engineering, Inc.*, [2]*Grad. Sch. Sci. & Eng., Saitama Univ.*)

3Pos091 Model screening of a peptide by individual evaluation and separation using a combination of FACS and peptide ligase display (PL display)
Shingo Ueno, Fumi Toshioka, Takanori Ichiki (*iCONM, Kawasaki Inst. Industry. Promo.*)

3Pos092 CRISPR-Cas ファミリータンパク質のデザインと標的探索の解明
Engineering and elucidation of target search by CRISPR-Cas family proteins
Trishit Banerjee[1,2], Hiroto Takahashi[2], Kiyoto Kamagata[1,2] ([1]*Grad.Sch.Sci., Tohoku Uni.*, [2]*IMRAM, Tohoku Uni.*)

3Pos093 (1SEP-5) Control of small G-protein Ras using calmodulin-based ionochromic molecular device
Yassine Sabek, Nobuyuki Nishibe, Kazunori Kondo, Shinsaku Maruta (*Graduate school of science and engineering , department of biosciences , soka university, Hachioji TOKYO*)

3Pos094 ヒト・ノイラミニダーゼの構造解析に向けたハイブリッドモデル作成
The investigation of hybrid models for the structure determination of human Neuraminidases
Takeru Nakajima (*Dept. Appl. Phys., Nagoya Univ. / Japanese*)

膜蛋白質／Membrane proteins

3Pos095 Deciphering the signal transmission of activation mechanism for chemokine CXCL12-bound receptor CXCR4 in complex with G_i-protein
Ting-Yu Hu[1], Hao-Jen Hsu[1,2], Chun-Chun Chang[3,4] ([1]*Department of Life Sciences, College of Medicine, Tzu chi University*, [2]*Department of Biochemistry, School of Medicine, Tzu Chi University*, [3]*Department of Laboratory Medicine, Hualien Tzu Chi Hospital, Buddhist Tzu Chi Medical Foundation*, [4]*Department of Laboratory Medicine and Biotechnology, College of Medicine, Tzu Chi University*)

3Pos096 GPCR の相互作用ネットワーク解析
Interaction Network Analysis of GPCRs
Yusuke Higaki[1], Wataru Nemoto[2], Yoshihiro Yamanishi[3], Hiroyuki Toh[1] ([1]*Dept. of Bio. Med. Sci., Grad. Sch. of Sci., Univ. of Kangaku*, [2]*Dept. of Life. Sci. Eng., Grad. Sch. of Sci., Univ. of Touden*, [3]*Dept. of Biosci. Bioinfo., Grad. Sch. of Com. Sci., Univ. of Kyukou*)

3Pos097 全反射赤外分光法による GPCR のリガンド認識機構研究
ATR-FTIR study of ligand recognition on GPCRs
Seiya Iwata[1], Kota Katayama[1], Kohei Suzuki[1], Ryoji Suno[2], Chiyo Suno[2], Takuya Kobayashi[2], Hirokazu Tsujimoto[3], So Iwata[3], Hideki Kandori[1] ([1]*Grad. Sch. Eng., Nagoya Inst. Tech.*, [2]*Grad. Sch. Med., Kansai Med. Univ.*, [3]*Grad. Sch. Med., Kyoto Univ.*)

3Pos098 ソラベグロンおよびイソプレテレノールに結合した β3 アドレナリン受容体のクライオ電顕構造
Cryo-EM structures of the β3 adrenergic receptor bound to solabegron and isoproterenol
Ikko Nureki[1], Tatsuki Tanaka[1], Kazuhiro Kobayashi[1], Asuka Inoue[2], Wataru Shihoya[1], Osamu Nureki[1] ([1]*Grad. Sch. Sci., Univ. Tokyo*, [2]*Grad. Sch. Pharm. Sci. Univ. Tohoku*)

3Pos099 The Off-Axis Rotor of *Enterococcus hirae* V-type ATPase by Volta Phase Contrast and Conventional Phase Cryo-EM
Raymond N. Burton-Smith[1], Jun Tsunoda[1,2], Chihong Song[1,2], Hiroshi Ueno[3], Takeshi Murata[4], Ryota Iino[5], Kazuyoshi Murata[1,2] ([1]*ExCELLS, Okazaki, Japan*, [2]*SOKENDAI, Okazaki, Japan*, [3]*Univ. Tokyo, Tokyo, Japan*, [4]*Chiba Univ. Chiba, Japan*, [5]*IMS, Okazaki, Japan*)

3Pos100 PANX1 の K346E 変異型の発現系の確立と構造的基盤の検討
Establishment of the expression system and structural basis of the K346E mutation of PANX1
Kana Taniguchi, Taiichi Tsuyama, Ken Yokoyama (*Department of Molecular Biosciences, Kyoto Sangyo*)

3Pos101 Structural insights into the HBV receptor and bile acid transporter NTCP
Jae-Hyun Park[1], Masashi Iwamoto[2], Ji-Hye Yun[3], Tomomi Uchikubo-Kamo[4], Donghwan Son[3], Zeyu Jin[1,3], Hisashi Yoshida[1], Mio Ohki[1], Naito Ishimoto[1], Kenji Mizutani[1], Mizuki Oshima[2,5], Masamichi Muramatsu[2], Takaji Wakita[2], Mikako Shirouzu[4], Kehong Liu[6], Tomoko Uemura[6], Norimichi Nomura[6], So Iwata[6,7], Koichi Watashi[2,5,8], Jeremy R. H. Tame[1], Tomohiro Nishizawa[1], Weontae Lee[3], Sam-Yong Park[1] ([1]*Grad. Sch. MLS, Yokohama City University*, [2]*Department of Virology II, National Institute of Infectious Diseases*, [3]*Department of Biochemistry, College of Life Science and Biotechnology, Yonsei University*, [4]*Laboratory for Protein Functional and Structural Biology, RIKEN Center for Biosystems Dynamics Research*, [5]*Department of Biological Sciences, Tokyo University of Science*, [6]*Department of Cell Biology, Graduate School of Medicine, Kyoto University*, [7]*RIKEN SPring-8 Center*, [8]*Research Center for Drug and Vaccine Development*)

3Pos102 インフルエンザ菌アドヘシンの膜貫通ドメインのナノディスクへの挿入における BamA の役割
Role of BamA on the insertion of the transmembrane domain of *Haemophilus Influenzae* adhesin into nanodiscs
Eriko Aoki[1], Kazuo Fujiwara[2], Masamichi Ikeguchi[2] ([1]*GaLSIC, Soka Univ.*, [2]*Dept. Biosci., Soka Univ.*)

核酸結合蛋白質／Nucleic acid binding proteins

3Pos103 大腸菌 UvrD C 末端アミノ酸欠損変異体の DNA 結合・巻き戻しダイナミクス
Dynamics of DNA binding and unwinding by *Escherichia coli* UvrD lacking C-terminal amino acids
Hiroaki Yokota (*Grad. Sch. Creation New Photon. Indust.*)

3Pos104 転写因子 Nanog についての粗視化および全原子分子動力学シミュレーション
Coarse-grained and all-atom molecular simulations for transcription factor Nanog
Azuki Mizutani[1], Cheng Tan[2], Yuji Sugita[2], Shoji Takada[1] ([1]*Grad. Sch. Sci., Univ. Kyoto*, [2]*RIKEN, Comput. Sci.*)

3Pos105 スピンラベル ESR による HP1 天然変性ヒンジ領域と DNA 相互作用の動的構造解析
Dynamics of HP1 intrinsic disorderd hinge region with DNA measured by site-directed spin labeling-ESR spectroscopy
Isao Suetake[2,4], Kazunobu Sato[3], Tohru Kawakami[4], Tomoaki Sugishita[4], Risa Mutoh[5], Yuichi Mishima[4], Takeji Takui[3], Toshimichi Fujiwara[4], Hironobu Hojo[4], Makoto Miyata[1], **Toshiaki Arata[1,4]** ([1]*Dept.Biol. Grad. Sch. Sci. Osaka Met.Univ.*, [2]*Nakamura Gakuen Univ.*, [3]*Dept.Chem. Grad. Sch. Sci. Osaka Met.Univ.*, [4]*IPR. Osaka Univ.*, [5]*Fac. Sci. Toho Univ.*)

3Pos106 Through the Looking-Glass: Functional 'Ambidexterity' in an Ancient Nucleic Acid Binding Protein
Liam M Longo[1], Orit Ktorza[2], Yael Fridmann Sirkis[3], Dragana Despotović[3], Norman Metanis[2] ([1]*Earth-Life Science Institute, Tokyo Institute of Technology, Japan*, [2]*The Hebrew University of Jerusalem, Israel*, [3]*The Weizmann Institute of Science, Israel*)

水・水和／電解質／Water & Hydration & Electrolyte

3Pos107 分子動力学法を用いたシニョリン及び変異体周囲の水和ダイナミクスの解明
Elucidation of hydration dynamics around chignolin and mutants using molecular dynamics
Yui Nakamura[1], Ryutaro Inou[1], Shingo Nobunaga[1], Takuya Takahashi[2] ([1]*Grad. Sch. Life Sci., Ritsumeikan Univ.*, [2]*Affiliation 1 所属 1: Coll. Life Sci., Ritsumeikan Univ.*)

3Pos108 溶質周囲の水分子の配置・立体構造の歪みを解析するツール開発
Development of a program to analyze water's structure around solutes and the applications
Ryutaro Inou[1], Yui Nakamura[1], Takuya Takahashi[2] ([1]*Grad. Sch. Life Sci., Univ. Ritsumeikan*, [2]*Coll. Life. Sci., Univ. Ritsumeikan*)

3Pos109 データ駆動的に構築した記述子を用いた液相水分子の静的・動的構造の研究
Static and dynamic structure of liquid water investigated by means of data-driven atomic descriptor
Taku Mizukami[1], Viet Cuong Nguyen[2], Hieu Chi Dam[3] ([1]*JAIST Materials Science*, [2]*HPC systems*, [3]*JAIST Knowledge Science*)

3Pos110 サブテラヘルツ波照射によるタンパク質水和の非熱的促進：誘電緩和測定による解析
Nonthermal acceleration of protein hydration by sub-terahertz irradiation: Analysis of dielectric relaxation measurements
Masahiko Imashimizu, Jun-ichi Sugiyama, Masahito Tanaka (*National Institute of Advanced Industrial Science and Technology*)

3Pos111 濃厚な糖溶液の構造：単糖類と二糖類の特性の比較とトレハロースの特異性
Structures of concentrated sugar solutions: Comparison of characteristics of mono- and disaccharides and specificity of trehalose
Mitsuhiro Hirai (*Gunma Univ.*)

3Pos112 MD と 3D-RISM 理論による SARS-CoV-2 スパイクタンパク質と ACE2 タンパク質間相互作用の研究
MD and 3D-RISM study of the interaction between SARS-CoV-2 spike and ACE2 proteins
Yutaka Maruyama[1], Ayori Mitsutake[1], Norio Yoshida[2] ([1]*Dep. Phys., Meiji Univ.*, [2]*Grad. Sch. Info., Nagoya Univ.*)

3Pos113 ガン関連タンパク質 MDM2 のリガンド結合能に対する共溶媒効果の定量的評価
Quantitative evaluation of cosolvent effects on ligand binding abilities of cancer-associated protein MDM2
Naoki Komiya, Kento Kasahara, Nobuyuki Matubayasi (*Division of Chemical Engineering, Graduate School of Engineering Science, Osaka University*)

3Pos114 タンパク質およびその多量体の共溶媒添加に伴う安定性変化のエネルギー解析
Free-energy Analysis of Stability Change of Proteins and Their Oligomers upon Addition of Cosolvent
Yuka Hamada, Kento Kasahara, Nobuyuki Matubayasi (*Division of Chemical Engineering, Graduate School of Engineering Science, Osaka University*)

3Pos115 統計熱力学に基づくペプチド薬デザイン法の開発
Computational study for designing peptide drugs based on statistical thermodynamics
Shunsuke Miyamoto, Tomohiko Hayashi (*Grad. Sch. Sci. and Tech., Niigata Univ.*)

分子遺伝・遺伝情報制御／Molecular genetics & Gene expression

3Pos116 *C. elegans* のスプライシング因子 AQR の温度耐性への関与
A homolog of splicing factor AQR, *emb-4*, is involved in high and low temperature tolerance in *C. elegans*
Yuki Sato[1,2], Kazuho Isono[4], Teruaki Taji[4], Akane Ohta[1,2], Atsushi Kuhara[1,2,3] ([1]*Graduate school of Natural Science Konan University, Kobe, Japan*, [2]*Institute for Integrative Neurobiology, Konan University, Kobe, Japan*, [3]*PRIME, AMED*, [4]*Tokyo University of agriculture, Japan*)

3Pos117 Photocontrol of small GTPase Ras using its regulatory factor GEF modified with photochromic azobenzene derivative
Yuichi Imamura, Nobuyuki Nishibe, Kazunori Kondo, Shinsaku Maruta (*Grad.Sch.Sci.,Univ.Soka/Japanese*)

発生・分化／Development & Differentiation

3Pos118 (2SAP-4) グラフニューラルネットワークによる細胞間の時空間相互作用の推定
(2SAP-4) Graph-based machine learning reveals rules of spatiotemporal cell interactions in tissues
Takaki Yamamoto[1], Katie Cockburn[2], Valentina Greco[2,3], Kyogo Kawaguchi[1,4,5] ([1]*Nonequilibrium Physics of Living Matter RIKEN Hakubi Research Team, RIKEN BDR*, [2]*Department of Genetics, Yale School of Medicine*, [3]*Departments of Cell Biology and Dermatology, Yale Stem Cell Center, Yale Cancer Center, Yale School of Medicine*, [4]*RIKEN CPR*, [5]*Universal Biology Institute, The University of Tokyo*)

3Pos119 ニワトリ胚心臓の発生にエタノールが与える影響の SS-OCT 観測
Heart development of chick embryo under ethanol exposure imaged by Swept Source OCT
Taichi Furuta, Takashi Yamaoka, Keisuke Matsubara, Yuuta Moriyama, Toshiyuki Mitsui (*Dept. Phys. Sch. Sci. Aogaku Univ.*)

3Pos120 Observation of calcium and mitochondrial activity in mouse sperm state changes
Yuichi Hiramatsu, **Takashi Ijiri** (*Dept. of Lif. Sci., Fac. of Sci. and Eng., Setsunan Univ.*)

3Pos121 Analysis of the gene expression fluctuation and post-differentiation state in the differentiating human pluripotent stem cells
Kensuke Sasaki, Sayaka Yamamoto, Yasuhiro Maeda, Tomonobu Watanabe (*RIKEN Center for Biosystems Dynamics Research*)

筋肉（筋蛋白質・収縮）／Muscle

3Pos122 深層学習を利用した電子線トモグラフィー法による心筋サルコメア構造のタンパク質分類の検討
Classification of muscle tissue components elucidated by electron tomography and deep learning
Mayu Yasuda[1], Wataru Kedouin[1], Ryu Takeya[2], Takuo Yasunaga[1] ([1]*Grad. Sch. Comp. Sci. Syst. Eng., KIT*, [2]*Dept. of Pharma., Univ. of Miyazaki*)

3Pos123 滑り運動中のアクチン繊維内に沿って生じる局所的な内部コンフォメーション変化とその伝播
Local conformational changes and the propagation along an actin filament during in vitro motility assay
Kuruto Toda[1], Hirotaka Itou[1], Ichiro Nishikata[2], Kenji Kamimura[3], Ikuko Hujiwara[4], Hajime Honda[4] ([1]*Dept. of Bioeng., Nagaoka Univ. of Tech.*, [2]*Electron. and Mech. Syst. Eng. Adv. Crs., NIT, Nagaoka Coll.*, [3]*Dept. of Electron. Control Eng., NIT, Nagaoka Coll.*, [4]*Dept. of Matl. Sci. and Bioeng., Nagaoka Univ. of Tech.*)

3Pos124 温められた心筋は安定性と不安定性を併せ持った収縮リズムを刻む
The warmed myocardium creates a contractile rhythm that combines stability and instability
Seine A. Shintani[1,2] ([1]*Department of Biomedical Sciences, College of Life and Health Sciences, Chubu University*, [2]*Center for Mathematical Science and Artificial Intelligence, Chubu University*)

3Pos125 コフィリン結合によるアクチン繊維のアロステリック応答解明に向けた分子動力学計算
Molecular dynamics simulation to study the long-range allostery of an actin filament due to cofilin binding
Kyoko Shimanuki[1], Jun Ohnuki[2], Mitsunori Takano[1] ([1]*Dept. of Pure & Appl. Phys., Grad. Scl. Adv. Sci. & Eng., Waseda Univ.*, [2]*Inst. for Mol. Sci.*)

3Pos126 マウス心筋細胞で認める高静水圧誘発性緩徐収縮
High hydrostatic pressure induces slow contraction in mouse cardiomyocytes
Yohei Yamaguchi[1], Masayoshi Nishiyama[2], Hiroaki Kai[3], Toshiyuki Kaneko[1], Keiko Kaihara[3], Gentaro Iribe[1], Akira Takai[1], Keiji Naruse[3], Masatoshi Morimatsu[3] ([1]*Dept. Physio., Asahikawa Med. Univ.*, [2]*Dept. Physics, Kindai Univ.*, [3]*Dept. Cardio. Physio., Grad. Sch. Med. Dent. Pharm., Okayama Univ.*)

分子モーター／Molecular motor

3Pos127 クライオ電子顕微鏡による ATP 合成酵素 FoF1 の化学力学共役機構の解明
Molecular Basis of the Chemo-Mechanical Coupling Mechanism in the ATP-Driven Rotation of ATP Synthase FoF1
Atsuki Nakano[1], Jun-ichi Kishikawa[2], Atsuko Nakanishi[3], Ken Yokoyama[1] ([1]*Fac. of Life Sci., Kyoto Sangyo Univ*, [2]*Institute for Protein Research, Osaka University*, [3]*Research Center for Ultra-High Voltage Electron Microscopy, Osaka University*)

3Pos128 (2SCA-4) 1 分子回転操作実験によって解明されたミトコンドリア由来 ATP 合成酵素における阻害因子 IF_1 の一方向制御機構
(2SCA-4) Unidirectional regulation of ATPase factor 1 in mitochondrial ATP synthase studied by single-molecule manipulation experiments
Ryohei Kobayashi[1,2], Hiroshi Ueno[1], Kei-ichi Okazaki[2], Hiroyuki Noji[1] ([1]*Appl. Chem., Grad. Sch. Eng., Univ. Tokyo*, [2]*Inst. for Mol. Sci.*)

3Pos129 Drug binding to the mycobacterial ATP synthase – mechanistic implications
Alexander Krah[1], Gerhard Grüber[2], Peter J. Bond[1,3] ([1]*Bioinformatics Institute*, [2]*Nanyang Technological University*, [3]*National University of Singapore*)

3Pos130 Single-molecule analysis and engineering of rotary V-ATPase
Akihiro Otomo[1,2], Tatsuya Iida[1,2], Hiroshi Ueno[3], Takeshi Murata[4], Ryota Iino[1,2] ([1]*Institute for Molecular Science*, [2]*SOKENDAI*, [3]*Grad. Sch. Eng., The Univ. of Tokyo*, [4]*Grad. Sch. Sci., Chiba Univ.*)

3Pos131 Acrive structures of V/A-type rotary ATPase reveal the rotary catalytic mechanism
Jun-ichi Kishikawa[1], Atsuko Nakanishi[2], Atsuki Nakano[3], Ken Yokoyama[3] ([1]*Inst. Prot. Res., Osaka Univ.*, [2]*Res. Ctr. UHVEM, Osaka Univ.*, [3]*Dept. Adv. Life. Sci., Kyoto Sangyo Univ.*)

3Pos132 全原子分子動力学計算による KIF1A の微小管への結合過程の解析
All-atom molecular dynamics simulation analysis of KIF1A binding to microtubule
Koki Adachi, Mitsunori Takano (*Dept. of Pure & Appl. Phys., Grad. Scl. Adv. Sci. & Eng., Waseda Univ.*)

3Pos133 微小管とキネシンによる三次元のモティリティアッセイの実現
Realization of three-dimensional motility assay with microtubules and kinesin
Hisanori Saito[1], Ibuki Kawamata[1], Gikyo Usuki[2], Kohei Nishiyama[2], Shinichiro Nomura[1], Nathanael Aubert-Kato[3], Akira Kakugo[2], Satoshi Murata[1] ([1]*Grad. Sch. Eng., Univ. Hyogo*, [2]*Grad. Sch. Sci., Univ. Hokkaido*, [3]*Grad. Sch. Sci., Univ. Ochanomizu*)

3Pos134 KIF5A の ALS 関連遺伝子変異は KIF5A のオリゴマー化と凝集を促進し神経毒性を引き起こす
An ALS-associated KIF5A mutant forms oligomers and aggregates and induces neuronal toxicity
Kyoko Chiba[1], Juri Nakano[2], Shinsuke Niwa[1] ([1]*FRIS, Tohoku Univ.*, [2]*Grad. Sch. of Life Sci., Tohoku Univ.*)

3Pos135 ADP 解離の遅い変異体を用いたキネシン 1 の連続的歩行能を決める要因の研究
High-speed single molecule study of the determinant of kinesin-1's processivity using mutants with slow ADP-release
Yuta Miyazono, Hiroki Hayano, Tukasa Enomoto, Michio Tomishige (*Grad. Sch. Sci. Eng., Aoyama Gakuin Univ.*)

3Pos136 KIF1A/ダイニンが制御する軸索内小胞プールサイズ
Vesicle pool sizes controlled by axonal transport of KIF1A/dynein
Yuki Kagawa[1], Ryo Sasaki[1], Yuzu Anazawa[2], Shinsuke Niwa[3], Kumiko Hayashi[1] ([1]*Grad. Sch. Eng., Tohoku Univ.*, [2]*Grad. Sch. Life Sci., Tohoku Univ.*, [3]*FRIS., Tohoku Univ.*)

3Pos137 Dpcd ノックアウトマウスの側脳室における内腕ダイニンの遺伝子発現と脳室内の流れの解析
Analysis of inner arm dynein gene expression and intraventricular flow in the lateral ventricle of Dpcd knockout mice
Hironori Ueno[1], Daiki Yamamoto[2], Kazuhito Takeuchi[2], Yuichi Nagata[2], Fumiharu Ohka[2], Atsushi Natsume[2], Ryuta Saitou[2] ([1]*Aichi Univ. of Edu.*, [2]*Grad. Sch. of Med., Nagoya Univ.*)

3Pos138 ミュータントの S1 による F アクチンの協同的構造変化の伝播距離の推定
Estimation of propagation distance of cooperative conformational changes in F-actin induced by a mutant S1
Masahiro Miura, Taro QP Uyeda (*Department of Pure and Applied Physics, Graduate School of Advanced Science and Engineering, Waseda University*)

3Pos139 ダイニンによる細胞内輸送が細胞質動態から受ける影響について
Effect of cytoplasmic dynamics on dynein-dependent transports
Takayuki Torisawa[1,2], Akatsuki Kimura[1,2] ([1]*Cell Arch. Lab., Natl. Inst. Genet.*, [2]*Dept. Genet., SOKENDAI*)

3Pos140 減圧顕微鏡法によって測定されたバクテリア運動能
Bacterial motility measured by depressurization microscopy
Masayoshi Nishiyama (*Kindai Univ.*)

3Pos141 The relative motion of MotA around MotB in bacterial flagellar stator
Phuoc Duy Tran, Akio Kitao (*Sch. Life Sci. Tech., TokyoTech*)

3Pos142 Single particle cryo-EM of *Paenibacillus* stator complex reveals the flexibility of the pentameric MotA1 ring
Sakura Onoe[1], Tatsuro Nishikino[2], Nobuhiro Takekawa[3], Jun-ichi Kishikawa[2], Takayuki Kato[2] ([1]*FBS, Osaka Univ.*, [2]*IPR, Osaka Univ.*, [3]*Dep. Macromol. Sci., Osaka Univ.*)

3Pos143 (2SFA-6) SLC26 陰イオントランスポーターによる電気→運動エネルギー変換
(2SFA-6) SLC26 ion transporters act as electricity-driven motor proteins
Tomohiro Shima (*Grad. Sch. Sci., Univ. Tokyo*)

3Pos144 速く動く DNA ナノ粒子モーターはつくれるか？シミュレーションによる検討
How to engineer fast-moving DNA-nanoparticle motor? A simulation study
Takanori Harashima, Akihiro Otomo, Ryota Iino (*Institute for Molecular Science*)

細胞生物学的課題（接着，運動，骨格，伝達，膜）／Cell biology

3Pos145 Fimbrin の協同的相互作用による F-actin の長さの変化
Changes in actin filament length induced by the cooperative interaction of fimbrin
Ryosuke Tsunabuchi[1], Naoki Hosokawa[1], Rika Hirakawa[1], Masahiro Kuragano[1], Taro Q.P Uyeda[2], Kiyotaka Tokuraku[1] ([1]*Graduate School of Engineering, Muroran Institute of Technology*, [2]*Department of Physics, Faculty of Science and Engineering, Waseda University*)

3Pos146 魚類ケラトサイトのストレスファイバ直動回転変換メカニズム
Linear contraction of stress fibers kicks the substratum for their rotation
Chika Okimura[1], Shu Akiyama[1], Tatsunari Sakurai[2], Yoshiaki Iwadate[1] ([1]*Dept.Biol., Yamaguchi Univ.*, [2]*Dept.Math.Eng., Musashino Univ.*)

3Pos147 G146V とそのサプレッサー変異は酵母のアクチンダイナミクスに影響する
G146V and its suppressor mutations in yeast actin suggested to affect actin dynamics in vivo
Tenji Yumoto[1], Taro QP Uyeda[1], Takehiko Yoko-o[2] ([1]*Department of Pure and Applied Physics, Graduate School of Advanced Science and Engineering, Waseda University*, [2]*Cellular and Molecular Biotechnology Research Institute, AIST*)

3Pos148 気管形成におけるアクチン骨格のミクロ相分離と自己組織化構造の転移ダイナミクス
Microphase separation and transition dynamics of self-organized structures of actin cytoskeleton during tubulogenesis
Mitsusuke Tarama[1], Sayaka Sekine[2], Tatsuo Shibata[1], Shigeo Hayashi[1] ([1]*RIKEN BDR*, [2]*Grad. Sch. Life Sci., Tohoku Univ.*)

3Pos149 アクトミオシンの収縮による膜変形の再構成
Morphological transitions of lipid vesicles driven by the contraction of actomyosin networks
Makito Miyazaki[1,2,3,4], Fahmida Sultana Laboni[5], Masatoshi Ichikawa[2], Taeyoon Kim[5] ([1]*Hakubi, Kyoto Univ.*, [2]*Dept. Phys., Kyoto Univ.*, [3]*Inst. Curie*, [4]*PRESTO, JST*, [5]*Biomed. Eng., Purdue Univ.*)

3Pos150 人工細胞内アクチン光操作が可能にする細胞運動の再構成
Synthesizing motility in artificial cells by asymmetrically reconstituted actin polymerization
Hideaki Matsubayashi[1,2], Shiva Razavi[2,3], Hideki Nakamura[2,4,5], Daniel A. Kramer[6], Tomoaki Matsuura[7], Baoyu Chen[6], Takanari Inoue[2] ([1]*Frontier Research Institute for Interdisciplinary Sciences, Tohoku University*, [2]*Department of Cell Biology, School of Medicine, Johns Hopkins University*, [3]*Department of Biological Engineering, School of Engineering, Massachusetts Institute of Technology*, [4]*Hakubi Center for Advanced Research, Kyoto University*, [5]*Department of Synthetic Chemistry and Biological Chemistry, School of Engineering, Kyoto University*, [6]*Roy J. Carver Department of Biochemistry, Biophysics and Molecular Biology, Iowa State University*, [7]*Earth-Life Science Institute, Tokyo Institute of Technology*)

3Pos151 Probing the influence of geometrical constraints on collective cell dynamics in diameter-varying 3D gelatin tube structures
Mitsuru Sentoku, Kenji Yasuda (*Dept. Pure & Appl. Phys., Grad. Sch. Adv. Sci. & Eng., Waseda Univ.*)

3Pos152 プリント化したフィブロネクチン勾配に対する好中球の走触性の解析
Analysis of neutrophil haptotaxis on printed fibronectin gradients
Yoshino Tanaka[1], Gen Honda[2], Masahito Uwamichi[3], Satoshi Sawai[3] ([1]*Grad. Sch. Sci., Univ. Tokyo*, [2]*Komaba institute for science, Grad. Sch. Arts & Sci., Univ. Tokyo*, [3]*Grad. Sch. Arts & Sci., Univ. Tokyo*)

3Pos153 細胞性粘菌の運動において bleb モードへの転換は Ca^{2+}流入に依存しない
The transition to bleb mode is independent on extracellular Ca^{2+} influx in *Dictyostelium discoideum* motility
Hitomi Takeuchi, Taro QP Uyeda (*Department of Pure and Applied Physics, Graduate School of Advanced Science and Engineering, Waseda University*)

3Pos154 Velocity field dynamics under blurring in fluorescent images of dictyostelium discoideum colonies
Md Mohiuddin[7,8], Md Motaleb Hossain[1,2], Sulimon Sattari[1], Udoy S. Basak[1,3], Mikito Toda[4], Kazuki Horikawa[5], Tamiki Komatsuzaki[1,6,7] ([1]*Research Institute for Electronic Science, Hokkaido University, Japan*, [2]*University of Dhaka, Bangladesh*, [3]*Pabna University of Science and Technology, Bangladesh*, [4]*Nara Women's University, Japan*, [5]*Tokushima University Graduate School, Japan*, [6]*Institute for Chemical Reaction Design and Discovery (ICReDD), Hokkaido University, Japan*, [7]*Graduate School of Chemical Sciences and Engineering, Hokkaido University, Japan*, [8]*Mathematics Discipline, Comilla University, Bangladesh*)

3Pos155 The dominant factor of shapeshifts of collective cell migration between sheet form and clusters in flexible 3D tunnel structures
Wataru Hanamoto[1], Miki Takei[1], Masaharu Endo[2], Kaito Asahi[2], Mitsuru Sentoku[2], Kenji Yasuda[1,2] ([1]*Dept. Pure & Appl. Phys., Sch. Adv. Sci. & Eng., Waseda Univ*, [2]*Dept. Pure & Appl. Phys., Grad. Sch. Adv. Sci. & Eng., Waseda Univ.*)

3Pos156 二次元制限空間内を進行する細胞集団の流体的振る舞いの計測
Measuring the fluid-like behavior of collective cell migration in two-dimensional restricted structures
Miki Takei[1], Masaharu Endo[2], Mitsuru Sentoku[2], Kaito Asahi[2], Wataru Hanamoto[1], Kenji Yasuda[1,2] ([1]*Dept. Phys., Sch. Adv. Sci. & Eng., Waseda Univ.*, [2]*Dept. Pure & Appl. Phys., Grad. Sch. Adv. Sci. & Eng., Waseda Univ.*)

3Pos157 CheZ 局在の大腸菌走化性に及ぼす影響のキャピラリーアッセイによる解析
Analysis for the effect of CheZ localization on chemotaxis of *Escherichia coli* by capillary assay
Sawako Matsuda[1], Yong-Suk Che[1], Akihiko Ishijima[1], Masaru Kojima[2], Hajime Fukuoka[1] ([1]*Grad. Sch. Frontier Biosci. Osaka Univ*, [2]*Grad. Sch. Engineering Sci. Osaka Univ*)

3Pos158 CheB の極性局在を利用した異種走化性受容体の忌避刺激に対する応答性の比較
Comparison of responses to repellent stimulus at heterogeneous MCPs through polar localization of CheB
Shinnosuke Kawahara, Yumiko Uchida, Yong-Suk Che, Akihiko Ishijima, **Hajime Fukuoka** (*Grad. Sch. Frontier Biosci. Osaka Univ.*)

3Pos159 バクテリアの群れ運動における局所的な細胞間相互作用と運動制御
Local cell interaction and motility regulation for swarm motility of bacteria
Kodai Suzuki, Ikuro Kawagishi, Masatoshi Nishikawa (*Grad. Sch. Fun., Univ. Hosei*)

3Pos160 クラミドモナス繊毛交互打ち変異株の解析
Analysis of a *Chlamydomonas* mutant showing alternate ciliary beatings
Kazuma Sakamoto[1,2], Atsuko Isu[1], Toru Hisabori[1,2], **Ken-ichi Wakabayashi[1,2]** ([1]*Lab. Chem. Life Sci., Tokyo Tech.*, [2]*Sch. Life Sci. Tech., Tokyo Tech*)

3Pos161 海洋性ビブリオ菌におけるべん毛本数制御因子 FlhF と MS リング構成因子 FliF の相互作用解析
Interactions between the flagellar number regulator FlhF and the MS ring protein FliF in *Vibrio alginolyticus*
Yuria Fukushima, Seiji Kojima, Michio Homma (*Div. Biol. Sci., Grad. Sch. Sci., Nagoya Univ.*)

3Pos162 Functional and structural analyses of FlaK, a master regulator of the genes involved in polar flagellar formation in marine *Vibrio*
Seiji Kojima[1], Tomoya Kobayakawa[1], Yuxi Hao[1], Tatsuro Nishikino[2], Michio Homma[1] ([1]*Div. of Biol. Sci., Grad. Sch. Sci., Nagoya Univ.*, [2]*Inst. for Prot. Res., Osaka Univ.*)

3Pos163 カルシウム感受性があるクラミドモナス鞭毛内部構造のラセン配置
The Calcium Sensitive Helical Arrangement of Axonemal Structures in Chlamydomonas Flagella
Hitoshi Sakakibara[1], Kenta Ishibashi[1], Hiroyuki Iwamoto[2], Hiroaki Kojima[1], Kazuhiro Oiwa[1,3] ([1]*Bio-ICT, Nat. Inst. Inf. Com. Tech.*, [2]*SPring-8, JASRI*, [3]*Life Sci. Univ. Hyogo*)

3Pos164 大腸菌べん毛モーター間の回転方向転換同調を阻害する走化性受容体クラスター内における野生型/変異体比率の見積もり
Estimation of mutant/WT receptors ratios in receptor array that disrupts the switching coordination between flagellar motors of *E. coli*
Yumiko Uchida, Hajime Fukuoka, Akihiko Ishijima, Yong-Suk Che (*Grad. Sch. Frontier Biosci. Osaka Univ.*)

3Pos165 回転する大腸菌べん毛モーター中の GFP-FliL 局在の定量解析
Quatitative analysis of GFP-FliL localization at rotating flagellar motor of *E. coli*.
Miyuto Miyazaki, Yumiko Uchida, Hajime Fukuoka, Akihiko Ishijima, Yong-Suk Che (*Grad. Sch. Frontier Biosci. Osaka Univ.*)

3Pos166 キイロショウジョウバエの精子鞭毛の波形と鞭毛打頻度
The waveform and beat frequency of a sperm flagellum of *Drosophila melanogaster*
Sho Tamai[1,2], Kosei Sato[1,3], Hitoshi Sakakibara[1], Kazuhiro Oiwa[1,3] ([1]*Adv.ICT Res.Inst.,NICT*, [2]*Sch. Sci., Univ. Hyogo*, [3]*Grad. Sch. Sci., Univ. Hyogo*)

3Pos167 ピエゾ駆動対物レンズを用いたホヤ精子遊泳の 3 次元的解析
3D analysis of ascidian sperm swimming using a piezoelectric Z-scanner attached to a microscope objective
Kogiku Shiba, Kazuo Inaba (*Shimoda Marine Research Center, Univ. Tsukuba*)

3Pos168 蛍光共鳴エネルギー移動(FRET)によるタウ–微小管相互作用の熱力学的解析
Thermodynamic analysis of tau–MT interaction by Forster resonance energy transfer (FRET)
Riku Kiyonaka, Hideyuki Komatsu (*Dept. of Bioscience and Bioinformatics, Kyushu Inst. Tech.*)

3Pos169 FRET 計測系を用いた低濃度セリンに対する単一大腸菌受容体の協同作用による 2 種類の適応
Two behaviors of adaptation by cooperative action of a single *E. coli* receptor to low concentrations of serine using FRET measurement
Yuki Takada, Akihiko Ishijima, Hajime Fukuoka, Yong-Suk Che (*Graduate School of Frontier Biosciences Osaka University*)

3Pos170 BAR ドメインタンパク質による細胞間接着の維持
Maintenance of cell-cell adhesions by BAR domain proteins
Yosuke Senju (*RIIS, Univ. Okayama*)

3Pos171 スパイロプラズマの細胞分裂タンパク質の機能解析
Functional analysis of Spiroplasma cell division proteins
Taishi Kasai[1], Yuhei Tahara[2], Makoto Miyata[2], Daisuke Shiomi[1] ([1]*Rikkyo University, College of Science*, [2]*Osaka Metropolitan University, Graduate School of Science*)

3Pos172 細胞外小胞の受容細胞への内在化と膜融合効率の検討
Investigation of the efficiency of internalization of extracellular vesicles and their membrane fusion with recipient cells
Hisaaki Hirose, Yusuke Hirai, Shiroh Futaki (*ICR, Kyoto Univ.*)

3Pos173 レプトスピラの運動性や物性、病原性に与える外膜分子の影響
Effect of the outer membrane (OM) molecules on the motility, physical property, and pathogenicity of *Leptospira*
Keigo Abe[1], Nobuo Koizumi[2], Shuichi Nakamura[1] ([1]*Grad. Sch. Eng., Univ. Tohoku*, [2]*Dept. of Bacteriology I, National Inst. of Infectious Disease*)

3Pos174 自律拍動心筋細胞ネットワークにおける強制発火周期の記憶化
Memorization of forced firing intervals in spontaneous beating cardiomyocyte networks
Akira Nishizaki[1], Yoshitsune Hondo[2], Suguru Matsumoto[2], Kazuhumi Sakamoto[2], Kenji Yasuda[1,2] ([1]*Dept. Pure & Appl. Phys., Sch. Adv. Sci. & Eng., Waseda Univ.*, [2]*Dept. Pure & Appl. Phys., Grad. Sch. Adv. Sci. & Eng., Waseda Univ.*)

3Pos175 Plasticity of synchronized beating during connecting and separating of cardiomyocyte networks
Suguru Matsumoto[1], Kazufumi Sakamoto[1], Akira Nishizaki[2], Kenji Yasuda[1,2] ([1]*Dept. Pure & Appl. Phys., Grad. Sch. Adv. Sci. & Eng., Waseda Univ.*, [2]*Dept. Pure & Appl. Phys., Sch. Adv. Sci. & Eng., Waseda Univ.*)

3Pos176 緩やかな温度上昇による心筋細胞の拍動揺らぎの抑制
Depression of beating fluctuation in cardiomyocytes by gradual temperature rising
Kohei Oyama, Masahito Hayashi, **Tomoyuki Kaneko** (*LaRC., Dept. Frontier Biosci., Hosei Univ.*)

3Pos177 哺乳動物細胞におけるコレステロール依存的な熱吸収機構
Cholesterol-dependent mechanism underlying heat absorption in mammalian cells
Akira Murakami[1,2], Tasuku Sato[1], Kohki Okabe[1], Takashi Funatsu[1] ([1]*Grad. Sch. Pharm. Sci., Univ Tokyo*, [2]*Grad. Sch. Pharm. Sci., Univ Shizuoka*)

3Pos178 自己融解酵素によるグラム陽性細菌の溶菌過程の高速 AFM 観察
High-speed AFM observation of the lysis process of Gram-positive bacterial cell by autolysin
Yumu Ota[1], Hayato Yamashita[1], Kotaro Higashi[2], Masaya Yamaguchi[2], Shigetada Kawabata[2], Masayuki Abe[1] ([1]*Grad. Sch. of Eng. Sci., Osaka Univ.*, [2]*Grad. Sch. of Den., Osaka Univ.*)

3Pos179 Application of three-dimensional holotomography in label-free living cells
Seongsoo Lee, **Jae-Hyuk Lee** (*Korea Basic Science Institute Gwangju Center, Gwangju 61751, South Korea*)

3Pos180 細胞応答評価のためのマルチモーダル刺激可能なマイクロハンドの開発
Development of microhand with multimodal stimulus system for evaluation of cellular response
Masaru Kojima[1], Kazuma Koshide[1], Yasushi Mae[2], Tatsuo Arai[3] ([1]*Grad. Sch. Eng.Sci., Osaka Univ.*, [2]*Fac. of Eng. Sci., Kansai Univ.*, [3]*UEC*)

生体膜・人工膜：構造・物性／Biological & Artificial membrane: Structure & Property

3Pos181 皮膚線維芽細胞の長期培養による粘弾性への影響
Effect of long-term culture of skin fibroblasts on viscoelasticity
Kosuke Matsumura[1], Akira Kabasawa[1], Sayaka Miyoshi[3], Michiya Matsusaki[4], Arif Md. Rashedul Kabir[1,2], Teruki Yanagi[5], Kazuki Sada[1,2], Akira Kakugo[1,2], Kaori Shigetomi（Kuribayashi）[3] ([1]*Grad. Sch. of Chem. Sci. and Eng., Hokkaido Univ.*, [2]*Fac. of Sci., Hokkaido Univ.*,, [3]*Institute for the Advancement of Higher Education, Hokkaido Univ.*, [4]*Grad. Sch. of Eng., Osaka Univ.*, [5]*Department of Dermatology, Faculty of Medicine and Graduate School of Medicine, Hokkaido Univ.*)

3Pos182 細胞性粘菌の生細胞での膜タンパク質分子の多状態側方拡散運動の細胞膜フィールドモデルの構築
Field model for lateral diffusion of transmembrane proteins in *Dictyostelium* cells
Kazutoshi Takebayashi[1], Yoichiro Kamimura[2], Masahiro Ueda[1,3] ([1]*BDR., RIKEN*, [2]*Nara Med. Univ.*, [3]*Grad. Sch. Front. Biosci., Osaka Univ.*)

3Pos183 Unraveling the host-selective toxic interaction of cassiicolin with lipid membranes and its cytotoxicity
Kien Xuan Ngo[1], Phuong Doan N. Nguyen[1], Hirotoshi Furusho[1], Makoto Miyata[2], Tomomi Shimonaka[2], Nguyen Ngoc Bao Chau[3], Nguyen Phuong Vinh[4], Nguyen Anh Nghia[4], Tareg Omer Mohammed[1], Takehiko Ichikawa[1], Noriyuki Kodera[1], Hiroki Konno[1], Takeshi Fukuma[1], Nguyen Bao Quoc[5] ([1]*WPI-NanoLSI, Kanazawa University, Kanazawa*, [2]*Grad. Sch. Sci., Osaka City University, Osaka*, [3]*Facult. Biotech., Ho Chi Minh City Open University, Ho Chi Minh City, Vietnam*, [4]*Rubber Res. Inst. Vietnam, Ho Chi Minh City, Vietnam*, [5]*Res. Inst. Biotech. Environ., Nong Lam University, Ho Chi Minh City, Vietnam*)

3Pos184 分子動力学シミュレーションを用いた脂質膜におけるメリチンの抗菌作用の研究
Investigation for antimicrobial action of melittin on a lipid membrane using molecular dynamics simulation
Yusuke Miyazaki, Wataru Shinoda (*Research Institute for Interdisciplinary Science, Okayama University*)

3Pos185 細胞膜糖鎖構造によるウイルス感染のメカニカルな制御
Mechanical modulation of virus infection by cell membrane glycocalyx
Yoshihisa Kaizuka, Rika Machida (*National Institute for Materials Science*)

3Pos186 (2SBP-3) エンベロープ型ウイルス粒子の粗視化シミュレーション：B 型肝炎ウイルス
(2SBP-3) Coarse-grained Molecular Dynamics Study of Enveloped Virus Particle: Hepatitis B Virus
Ryo Urano, Wataru Shinoda (*Res. Inst. Interdiscip. Sci., Okayama Univ.*)

3Pos187 曲率誘導タンパク質の膜曲率応答の平均場理論
Mean field theories of curvature sensing and generation of isotropic and anisotropic curvature-inducing proteins
Hiroshi Noguchi (*ISSP, Univ. Tokyo*)

生体膜・人工膜：ダイナミクス／Biological & Artificial membrane: Dynamics

3Pos188 高分子をグラフトした脂質三成分ベシクルの膜粘度
Viscosity of polymer grafted ternary lipid vesicle
Yuka Sakuma (*Grad. Sch. Sci., Tohoku Univ.*)

3Pos189 脂質三成分ベシクルにおける膜粘度の温度依存性
Viscosity Landscape of Ternary Vesicles in Composition-Temperature Space
Juria Tanaka, Kenya Haga, Masayuki Imai, Yuka Sakuma (*Grad. Sch. Sci., Tohoku Univ.*)

3Pos190 細胞内反応拡散波の再構成に向けた膜流動性の制御手法
Improvement of the membrane fluidity to reconstitute the intracellular reaction-diffusion waves
Gen Honda[1], Nao Shimada[2], Satoshi Sawai[2,3], Miho Yanagisawa[1,2,3] ([1]*Komaba Institute for Science, Graduate School of Arts and Sciences, University of Tokyo*, [2]*Department of Basic Science, Graduate School of Arts and Sciences, University of Tokyo*, [3]*Research Center for Complex Systems Biology, Graduate School of Arts and Sciences, University of Tokyo*)

3Pos191 抗菌ペプチドの抗菌および殺菌活性の単一細胞解析
Single cell analysis for antimicrobial and bactericidal activities of antimicrobial peptides (AMPs)
Farzana Hossain[1], Masahito Yamazaki[1,2,3] ([1]*Res. Inst. Ele., Shizuoka Univ.*, [2]*Grad. Sch. Sci. Tech., Shizuoka Univ.*, [3]*Grad. Sch. Sci., Shizuoka Univ.*)

3Pos192 浸透圧ストレス下における脂質二重膜の挙動に対し、F-actin が及ぼす影響
Effect of F-actin on the behavior of lipid bilayers under osmotic stress
Ken Bessho, Moka Ito, Kingo Takiguchi (*Dept. Biol. Sci., Grad. Sch. Sci., Nagoya Univ.*)

3Pos193 クロモグリク酸ナトリウム液晶封入リポソーム上の 3 本縞様膜相分離
Three-stripe pattern of lipid domains on spindle-shaped liposome containing liquid crystal of disodium cromoglycate
Kaori Udagawa, Masahito Hayashi, Tomoyuki Kaneko (*LaRC., Dept. Frontier Biosci., Hosei Univ.*)

3Pos194 クラミドモナス含有リポソームの鞭毛運動と膜運動の高速イメージング
High-speed imaging of the flagellar beating and membrane motion of *Chlamydomonas* containing liposome
Shunsuke Shiomi, Masahito Hayashi, Tomoyuki Kaneko (*Graduate School of Science and Engineering, Hosei University.*)

生体膜・人工膜：興奮・チャネル／Biological & Artificial membrane: Excitation & Channels

3Pos195 コリネ型細菌の機械受容チャネル MscCG の人工脂質膜リポソームへの再構成と電気生理学的特性
Liposome reconstitution and electrophysiological characterization of *Corynebacterium glutamicum* mechanosensitive channel MscCG.
Yoshitaka Nakayama[1,2], Paul Rohde[1], Tomoyuki Konishi[3], Hisashi Kawasaki[3,4], Boris Martinac[1,2] ([1]*Molecular Cardiology and Biophysics Division, Victor Chang Cardiac Research Institute*, [2]*St Vincent's Clinical School, Faculty of Medicine, The University of New South Wales*, [3]*Agro-Biotechnology Research Center, Graduate School of Agricultural and Life Sciences, The University of Tokyo*, [4]*Collaborative Research Institute for Innovative Microbiology, The University of Tokyo*)

3Pos196 KcsA カリウムイオンチャネルにおける膜張力感知部位の探索
Exploring the membrane tension sensing sites in the KcsA potassium channel
Misuzu Ueki[1], Masami Miyagoshi[1], Shigetoshi Oiki[2], **Masayuki Iwamoto**[1] ([1]*Dept. Mol. Neurosci., Facul. Med. Sci., Univ. Fukui.*, [2]*Biomed. Imaging Res. Center, Univ. Fukui*)

3Pos197 KcsA カリウムチャネルゲーティングに対する膜厚と膜張力の作用
Concurrent effect of the membrane thickness and tension on the gating of the KcsA potassium channel
Yuka Matsuki[1], Masayuki Iwamoto[2], Masako Takashima[2], Shigetoshi Oiki[3] ([1]*Dept. Anesth. Reanimatol., Univ. Fukui Fac. Med. Sci.*, [2]*Dept. Anesth. Reanimatol., Univ. Fukui Fac. Med. Sci.*, [3]*Biomed. Imag. Res. Cent., Univ. Fukui*)

神経・感覚（細胞・膜蛋白質・分子）／Neuroscience & Sensory systems

3Pos198 *C.elegans* の低温耐性を制御する転写伸長因子 TCEB-3 のトランスクリプトーム解析
Transcriptome analysis of a transcription elongation factor TCEB-3 that is positive regulator of cold tolerance in *C.elegans*
Hiroaki Teranishi[1], Toshihiro Iseki[1], Natsune Takagaki[1], Yohei Minakuchi[2], Atsushi Toyoda[2], Akane Ohta[1], Atsushi Kuhara[1,3] ([1]*Grad. school of Nat. Sci., Konan Univ, Japan*, [2]*National Institute of Genetics, Japan*, [3]*PRIME, AMED*)

3Pos199 GPCR SRX は線虫の低温耐性に関わる温度受容体候補である
GPCR SRX is a thermoreceptor candidate in cold tolerance of *C. elegans*
Chinatsu Morimoto[1], Chie Miyazaki[1], Kohei Ohnishi[1], Tohru Miura[1], Akane Ohta[1], Atsushi Kuhara[1,2] ([1]*Inst. for Integrative Neurobio., Konan Univ., Japan*, [2]*PRIME, AMED*)

3Pos200 脳-腸連関によって制御された脂質代謝が線虫の温度順化を引き起こす
Lipid metabolism regulated by brain-gut interaction causes temperature acclimation in *C. elegans*
Kazutoshi Murakami[1,2], Haruka Motomura[1,2], Akane Ohta[1,2], Atsushi Kuhara[1,2,3] ([1]*rad. sch. Nat. Sci., Univ. Konan*, [2]*Inst. Integrative Neurobio., Univ Konan*, [3]*PRIME, AMED*)

3Pos201 拡散追跡による脂質膜上の初期の Aβ 凝集過程に対する開放系の効果
Effect of Open System on Early Aggregation Process of Amyloid β on Lipid Membrane by Diffusion Tracking
Akane Iida[1], Hideki Nabika[2] ([1]*Graduate School of Science and Engineering, Yamagata Univ.*, [2]*Faculty of Science, Yamagata Univ.*)

3Pos202 インスリン刺激時のモノアラガイ単離脳に対するリン酸化プロテオミクス解析
Phosphoproteomic analysis of the pond snail's CNS stimulated by insulin
Junko Nakai, Etsuro Ito (*Dept. Biol., Waseda Univ.*)

3Pos203 fMRI データに対する行列分解による脳情報コーディング
Brain information coding in fMRI data via matrix factorization
Yusuke Endo, Koujin Takeda (*Grad. Sch. Eng., Univ. Ibaraki*)

3Pos204 機能的神経クラスタ推定のためのベイズ生成モデルの一般化
Generalization of Bayesian generative model for functional neuronal ensembles inference
Shun Kimura, Koujin Takeda (*Grad. Sch. Sci. and Eng., Ibaraki Univ.*)

3Pos205 アガロースマイクロチャネル構造における単一神経突起の分化に必要な定量的条件
Quantitative requirement for single neurite differentiation of neurons in agarose microchannel structures
Ryohei Yamazaki[1], Nanami Abe[2], Yuri Kamiya[2], Kenji Yasuda[1,2] ([1]*Dept. Pure & Appl. Phys., Grad. Sch. Adv. Sci. & Eng., Waseda Univ.*, [2]*Dept. Phys., Sch. Adv. Sci. & Eng., Waseda Univ.*)

3Pos206 Evaluation of agarose microfabrication technology using Joule heat of micrometer-sized ionic current for cell network formation
Yuri Kamiya[1], Kenji Shimoda[2], Yoshitune Hondo[2], Haruki Watanabe[2], Nanami Abe[1], Ryohei Yamazaki[2], Kenji Yasuda[1,2] ([1]*Dept. Phys., Sch. Adv. Sci. & Eng., Waseda Univ.*, [2]*Dept. Pure and Appl. Phys., Grad. Sch. Adv. Sci. & Eng., Waseda Univ.*)

3Pos207 線虫の神経活動解析における擬似相関の除去
Eliminating spurious correlation in neural activity analysis of *C. elegans*
Harutaka Takeshita, Yuishi Iwasaki (*Grad. Sch. Sci. Eng., Ibaraki Univ*)

3Pos208 遺伝子発現に基づく神経回路形成のデータ駆動型解析
Data-driven analysis of the formation of neural circuit based on gene expression
Jigen Koike[1], Kana Yoshido[1], Naoki Honda[1,2,3] ([1]*Graduate School of Biostudies, Kyoto University*, [2]*Graduate School of Integrated Science for Life, Hiroshima University*, [3]*Explatory Research Center on Life and Living Systems, ExCells*)

3Pos209 ヨーロッパモノアラガイの摂食中枢ニューロン CGC 近傍における電気生理学的性質に対する緑茶由来カテキンの影響
The effect of green tea-derived catechin on electrophysiological properties around the CGC in the pond snail *Lymnaea stagnails*
Hideki Matsuoka[1], Ayaka Itoh[2], Terumasa Amano[2], Ken Lukowiak[3], Minoru Saito[2], Yoshimasa Komatsuzaki[4] ([1]*Dept. Phys., Grad. Sch. Sci. and Tech., Nihon Univ.*, [2]*Dept. Corr. Study in Phys. and Chem., Grad. Sch. Integ. Basic Sci., Nihon Univ.*, [3]*Hotchkiss Inst., Cumm. Sch. Med., Univ. of Calgary, Canada*, [4]*Dept. Phys., CST, Nihon Univ.*)

3Pos210 エピカテキンはナメクジ嗅覚中枢シナプスの長期抑圧現象を惹起する
Effects of epiatechin on synaptic plasticity of the olfactory center in the land slug *Limax valentianus*
Aya Nagata, **Yoshimasa Komatsuzaki** (*Dept. Phys., CST, Nihon Univ.*)

3Pos211 神経細胞内シナプス小胞群の光捕捉下における神経活動測定
Neuronal activity measurement under optical trapping of synaptic vesicles in neurons
Taketo Yasuda, Wataru Minoshima, Kyoko Masui, Chie Hosokawa (*Grad. Sch. Sci., Osaka Metro. Univ. / Osaka City Univ.*)

3Pos212 集光フェムト秒レーザーの短時間照射により誘発された神経活動
Neuronal activities induced by short-time irradiation of a focused femtosecond laser
Kan Otani, Yumi Segawa, Wataru Minoshima, Kyoko Masui, Chie Hosokawa (*Grad. Sch. Sci., Osaka Metro. Univ. / Osaka City Univ.*)

行動／Behavior

3Pos213 Dynamical systems model of the development of action differentiation and memory in early infancy
Ryo Fujihira, Gentaro Taga (*Grad. Sch. Edu., Univ. Tokyo*)

3Pos214 ゾウリムシの走化性はレヴィウォークを通じて現れる
Chemokinetic responses of *Paramecium tetraurelia* through Lévy walks
Azusa Kage[1], Takeru Wakano[1], Masato S. Abe[2], Takayuki Nishizaka[1] ([1]*Dept. Physics, Gakushuin Univ.*, [2]*Facl. Culture and Information Science, Doshisha Univ.*)

3Pos215 Near wall rheotaxis of ciliates, *Tetrahymena pyriformis*.
Yukinori Nishigami[1], Takuya Ohmura[2], Masatoshi Ichikawa[3] ([1]*RIES, Hokkaido Univ.*, [2]*Biozentrum, Univ. Basel*, [3]*Dept Phys., Kyoto Univ.*)

光生物：視覚・光受容／Photobiology: Vision & Photoreception

3Pos216 **Photoactive Yellow Protein** における酸性アミノ酸に置換した **52** 番目の残基のプロトン化状態
Protonation state of 52nd residue replaced by an acidic amino acid in Photoactive Yellow Protein
Kento Yonezawa[1,2], Yoichi Yamazaki[2], Mikio Kataoka[2], Hironari Kamikubo[1,2] ([1]*NAIST, CDG*, [2]*NAIST, MS*)

3Pos217 RcPYP と PBP の複合体形成に及ぼす PBP C 末端部位の役割
Role of PBP C-terminal region on the complex formation between RcPYP and PBP
Daiki Takenaka[1], Yoichi Yamazaki[1], Kento Yonezawa[1,2], Sachiko Toma-Fukai[1], Hironari Kamikubo[1,2] ([1]*NAIST, MS*, [2]*NAIST, CDG*)

3Pos218 青色光センサー TePixD の光可逆的な分子集合反応
Light-dependent reversible molecular assembly of a blue light sensor protein TePixD
Yusuke Nakasone, Yusuke Masuda, Shunrou Tokonami, Masahide Terazima (*Grad. Sch. Sci., Kyoto Univ.*)

3Pos219 深海エビ *Rimicaris hybisae* が持つオプシン類の分子特性
Molecular properties of opsins from the deep-sea hydrothermal vent shrimp *Rimicaris hybisae*
Keiichi Kojima[1], Yuya Nagata[2], Norio Miyamoto[3], Keita Sato[1], Yuji Yamanaka[4], Yosuke Nishimura[5], Susumu Yoshizawa[5], Ken Takai[3], Hideyo Ohuchi[1], Takahiro Yamashita[6], Yuki Sudo[1] ([1]*Med, Dent & Pharm Sci, Inst of Acad. & Res., Okayama Univ.*, [2]*Grad. Sch. of Med. Dent. & Pharm. Sci., Okayama Univ.*, [3]*X-STAR, JAMSTEC*, [4]*Fac. of Pharm. Sci., Okayama Univ.*, [5]*AORI, Univ. Tokyo*, [6]*Grad. Sch. Sci., Kyoto Univ.*)

3Pos220 Investigation of spectral properties and spectral tuning mechanisms of anthozoan-specific opsins from a reef-building coral
Yusuke Sakai, Mitsumasa Koyanagi, Akihisa Terakita (*Department of Biology, Graduate School of Science, Osaka Metropolitan University*)

3Pos221 光駆動型 Cl^-ポンプ・ハロロドプシンの細胞質型ハーフチャンネルにおける高速 Cl^-輸送のメカニズム解明
Probing the mechanism of fast Cl^- transport in the cytoplasmic half channel of light-driven Cl^- pump halorhodopsin
Yubo Zhai[1], Anna Shimosaka[1], Takashi Tsukamoto[1,2], Makoto Demura[1,2], Takashi Kikukawa[1,2] ([1]*Grad. Sch. Life Sci., Hokkaido Univ.*, [2]*Fac. Adv. Life Sci., Hokkaido Univ.*)

3Pos222 光駆動 Cl^-ポンプ halorhodopsin の基質放出・取込み中間体の同定
Identification of substrate release and uptake intermediates of light-driven Cl^- pump halorhodopsin
Chihaya Hamada[1], Keisuke Murabe[1], Takashi Tukamoto[1,2], Makoto Demura[1,2], Takashi Kikukawa[1,2] ([1]*Grad. Sch. Life Sci., Hokkaido Univ.*, [2]*Fac. Adv. Life Sci., Hokkaido Univ.*)

3Pos223 光駆動イオントランスポーターハロロドプシンの理論的研究
Theoretical study on molecular mechanism of a light-driven ion transport of Halorhodopsin
Tomo Ejiri, Ryo Oyama, Shigehiko Hayashi (*Grad. Sch. Sci., Univ. Kyoto*)

3Pos224 低温ラマン分光法による光駆動 Cl^-ポンプ NMR3 の発色団構造変化の研究
Low-temperature Raman study of chromophore structural changes in a light-driven Cl^- pump NMR3
Natsuki Ejima[1], Tomotsumi Fujisawa[1], Takashi Kikukawa[2], Masashi Unno[1] ([1]*Fac. Sci. Eng., Saga Univ.*, [2]*Fac. Adv. Life Sci., Hokkaido Univ.*)

3Pos225 異なるプロトン化状態のアニオンチャネルロドプシン GtACR1 とその変異体の吸収波長に関する理論的研究
Theoretical study on absorption wavelengths of anion channelrhodopsin GtACR1 in different protonation states and their mutants
Takafumi Shikakura, Cheng Cheng, Shigehiko Hayashi (*Grad. Sch. Sci., Kyoto Univ.*)

3Pos226 新奇酵素ロドプシン(NeoR)の特異な光化学特性
Unique photochemical properties of novel enzyme rhodopsin (NeoR)
Masahiro Sugiura[1], Kota Katayama[1], Leonid S. Brown[2], Satoshi Tsunoda[1], Hideki Kandori[1] ([1]*Grad. Shc. Eng., Nagoya Inst. of Tech.*, [2]*Dept. of Phys., Univ. of Guelph*)

3Pos227 近赤外光吸収型ロドプシンの波長制御機構
Color tuning mechanism of near-infrared light absorbing rhodopsins
Kazuki Ishikawa[1], Shoko Hososhima[1], Masahiro Sugiura[1], Leonid S. Brown[2], Satoshi Tsunoda[1], Hideki Kandori[1] ([1]*Grad. Sch. Eng., Nagoya Inst. Tech.*, [2]*Dept. Phys., Univ. Guelph*)

3Pos228 表面増強赤外分光法を用いた Heliorhodopsin の O 中間体構造変化解析
Structural change upon O intermediate formation of Heliorhodopsin analyzed by using SEIRA spectroscopy
Soichiro Kato[1], Jingyi Tang[1], Insyeerah Binti Muhammad Jauhari[2], Hideki Kandori[1,3], Yuji Furutani[1,3] ([1]*Graduate School of Engineering, Nagoya Institute of Technology*, [2]*Nagoya Institute of Technology*, [3]*OptoBio, Nagoya Institute of Technology*)

光生物：光合成／Photobiology: Photosynthesis

3Pos229 ヘリオバクテリア反応中心における Chl-a_F から BChl-g への励起エネルギー移動速度の理論的解析
Theoretical analysis of rate of excitation energy transfer from Chl-a_F to BChl-g in heliobacterial reaction center
Wataru Shimooka[1], Akihiro Kimura[1], Hirotaka Kitoh[2], Shigeru Itoh[1] ([1]*Grad. Sch., Nagoya Univ.*, [2]*Fac. Sci. and Engi., Kindai Univ.*)

3Pos230 ヘリオバクテリアにおける cyt *bc* 複合体から光合成反応中心への電子伝達反応の分子機構
Molecular mechanism of the electron transfer reaction from cyt *bc* complex to the photosynthetic reaction center in heliobacteria
Hirozo Oh-oka[1,2], Hiraku Kishimoto[2], Yuki Makino[2], Risa Kojim[1], Akihiro Kawamoto[3], Hideaki Tanaka[3], Genji Kurisu[3] ([1]*CELAS, Osaka Univ.*, [2]*Grad. Sch. Sci., Osaka Univ.*, [3]*Inst. Protein Res., Osaka Univ.*)

3Pos231 緑色光合成硫黄細菌における Rieske/cyt*b* 複合体と *c* 型シトクロムとの構造機能相関
Structure-function relationships between the Rieske/cyt*b* complex and *c*-type cytochromes in photosynthetic green sulfur bacteria
Hiraku Kishimoto[1], Ryoga Kawanami[1], Chihiro Azai[2], Risa Mutoh[3], Hideaki Tanaka[4], Yohei Miyanoiri[4], Genji Kurisu[4], Hirozo Oh-oka[1] ([1]*Grad. Sch. Sci., Osaka Univ.*, [2]*Col. Life Sci., Ritsumeikan Univ.*, [3]*Fac. Sci., Toho Univ.*, [4]*Inst. Protein Res., Osaka Univ.*)

3Pos232 低温顕微鏡による藻類細胞内光捕集調節機構の空間・波長・時間分解解析
Study on light-harvesting regulation mechanism in algal cells by space-wavelength-time-resolved analysis by cryogenic microscope
Yuki Fujita, XianJun Zhang, Shen Ye, **Yutaka Shibata** (*Grad. Sch. Sci., Tohoku Univ.*)

3Pos233 紅色光合成細菌の辺縁アンテナタンパク質の B800 バクテリオクロロフィル *a* の改変：色素酸化と色素置換
Conversion of B800 bacteriochlorophyll *a* in peripheral antenna proteins of purple photosynthetic bacteria by oxidation and reconstitution
Yoshitaka Saga, Kohei Hamanishi, Yuji Otsuka, Madoka Yamashita (*Fac. Sci. Eng., Kindai Univ.*)

3Pos234 タンパク質間相互作用による光合成集光システムの調節
Regulation of light-harvesting systems by protein-protein interactions in plants
Eunchul Kim, Jun Minagawa (*National Institute for Basic Biology*)

3Pos235 紅藻 *Porphyridium purpureum* のフィコビリソームロッドにおける最低第 1 励起状態をもつ発色団の特定
Identification of chromophores with the lowest first excited state in the phycobilisomal rod of the red alga *Porphyridium purpureum*
Hiroto Kikuchi (*Dept. of Phys. Nippon Med. Sch.*)

3Pos236 太古岩石試料中の光合成色素の顕微分光分析
Microspectroscopic analysis of photosynthetic pigments in ancient rock samples
Tomohiro Ishikawa[1], Ryosuke Saito[2], Toru Kondo[1] ([1]*Dept. of Life Sci. and Tech. Tokyo Tech.*, [2]*Dept. of Earth Sci., Yamaguchi Univ.*)

3Pos237 反復回分培養による紅色非硫黄細菌の光合成を利用した水素生成能について
Photosynthetic hydrogen production performance of purple non-sulfur bacteria in repeated batch culture
Masahiro Hibino, Sota Suzuki (*Div. Sust. Enviro. Eng., Muroran Inst. Tech.*)

光生物：光遺伝学・光制御／Photobiology: Optogenetics & Optical Control

3Pos238 Photo-control Small GTPase Ras Using Photochromic Peptide inhibitor
Nobuyuki Nishibe, Yuichi Imamura, Kazunori Kondo, Shinsaku Maruta (*Department of Bioinformatics, Soka University Graduate School of Engineering, Hachioji, Japan*)

3Pos239 陸生アクチノバクテリア由来の新規微生物ロドプシン群
A novel clade of microbial rhodopsins in terrestrial *Actinobacteria*
Mako Ueno[1], Fumio Hayashi[2], Takashi Kikukawa[3], Masashi Sonoyama[1,4,5] ([1]*Grad. Sch. Sci. Tech., Gunma Univ.*, [2]*Ctr. Inst. Anal., Gunma Univ.*, [3]*Fac. Adv. Life Sci., Hokkaido Univ.*, [4]*GIAR, Gunma Univ.*, [5]*GUCFW, Gunma Univ.*)

3Pos240 Gs 共役型オプシンを用いた二状態安定型光操作ツールの作製
Development of bistable optical control tools based on a Gs-coupled opsin
Akinari Sakayori[1], Yusuke Sakai[2], Mitsumasa Koyanagi[2], Akihisa Terakita[2], Hisao Tsukamoto[1] ([1]*Department of Biology, Kobe University*, [2]*Department of Biology, Osaka Metropolitan University*)

3Pos241 光活性化転写因子「光ジッパー」の分子機構
Molecular mechanism of a light-activatable transcription factor, Photozipper
Osamu Hisatomi, Yuta Nagano, Yumiko Adachi (*Grad. Sch. of Sci., Osaka Univ.*)

3Pos242 高速原子間力顕微鏡による光制御型転写因子 Photozipper の二量体形成過程の観察
Dimerization processes of a light-regulated transcription factor, Photozipper, observed by high-speed atomic force microscopy
Akihiro Tsuji[1], Hayato Yamashita[1], Osamu Hisatomi[2], Masayuki Abe[1] ([1]*Grad. Sch. Eng. Sci., Osaka Univ.*, [2]*Grad.Sch. Sci., Osaka Univ.*)

3Pos243 光受容タンパク質を用いた液液相分離の光制御システムの作製
Creation of a light-control system for liquid-liquid phase separation using a photoreceptor protein
Mizuki Takasugi[1], Yoichi Yamazaki[1], Kento Yonezawa[1,2], Sachiko Toma-Fukai[1], Hironari Kamikubo[1,2] ([1]*NAIST, MS*, [2]*NAIST, CDG*)

放射線生物／活性酸素／Radiobiology & Active oxygen

3Pos244 集束超音波による生体分子への影響
Focused ultrasound induced denaturation of biomolecules
Takumi Akiu[1], Kotarou Takeda[2], Wakako Hiraoka[1] ([1]*Grad. Sch. Sci. & Tech., Meiji Univ.*, [2]*Sch. Sci. & Tech., Meiji Univ.*)

3Pos245 Elucidation of intracellular temperature changes induced by external stress using fluorescent nano diamonds
Kiichi Kaminaga, Chihiro Suzuki, Yanagi Tamami, Hiroshi Abe, Takeshi Ohshima, Ryuji Igarashi (*Institute for Quantum Life Science, Quantum Life and Medical Science Directorate, QST*)

3Pos246 ヒトプリオンタンパク質オクタリピート領域におけるレドックス調節
Redox regulation in octarepeat region of human prion protein
Wakako Hiraoka[1], Osamu Inanami[2], Satoru Tsuri[3] ([1]*Grad. Sch. Sci. & Tech., Meiji Univ.*, [2]*Grad. Sch. Vet. Med., Hokkaido Univ.*, [3]*Sch. Sci. & Tech., Meiji Univ.*)

生命の起源・進化／Origin of life & Evolution

3Pos247 Coexistence of crystals and membraneless polyester microdroplets in a primitive complex system
Chen Chen[1], Ruiqin Yi[1], Motoko Igisu[2], Afrin Rehana[1], Takazo Shibuya[2], Yuichiro Ueno[2,3], Anna Wang[4], Andre Antunes[5], Kuhan Chandru[6], Tony Z. Jia[1,7] ([1]*Earth-Life Science Institute, Tokyo Institute of Technology, Japan*, [2]*Institute for Extra-cutting-edge Science and Technology Avant-garde Research (X-star), Japan Agency for Marine-Earth Science and Technology (JAMSTEC), Japan*, [3]*Department of Earth Science and Planetary Sciences, Tokyo Institute of Technology, Japan*, [4]*School of Chemistry, UNSW Sydney, Australia*, [5]*State Key Laboratory of Lunar and Planetary Sciences, Macau University of Science and Technology, China*, [6]*Space Science Center (ANGKASA), Institute of Climate Change, Level3, Research Complex, National University of Malaysia (UKM), Malaysia*, [7]*Blue Marble Space Institute of Science, USA*)

3Pos248 Exploring ancient origins of the circadian clock system through molecular evolution
Atsushi Mukaiyama[1,2], Yoshihiko Furuike[1,2], Shuji Akiyama[1,2] ([1]*Inst. for Mol. Sci. CIMoS*, [2]*SOKENDAI*)

3Pos249 Development of a translational field in the artificial cell by the shell of multiphase droplets
Kanji Tomohara, Yoshihiro Minagawa, Hiroyuki Noji (*Dept. Appl. Chem., Grad. Sch. Eng., Univ. Tokyo*)

3Pos250 アミノ酸熱重合物を用いた代謝様反応
Metabolism-like reactions using proteinoid
Shunsuke Ito[1], Shigeru Sakurazawa[2] ([1]*Future University Hakodate*, [2]*Department of Complex and Intelligent Systems, Future University Hakodate*)

3Pos251 触媒反応ネットワークにおけるコンパートメントの進化的獲得
Catalytic reaction networks evolve compartmentalization and compartment-specific reactions
Shunsuke Ichii[1], Yusuke Himeoka[1], Chikara Furusawa[1,2] ([1]*Grad. Sch. Sci., Univ. of Tokyo*, [2]*BDR, RIKEN*)

3Pos252 緩慢凍結融解サイクルによるベシクル融合実験：原始細胞生成過程への示唆
Vesicle fusion via slow freeze-thaw cycles and its implications for the emergence of a protocell
Natsumi Noda[1], Tatsuya Shinoda[1], Kazumu Kaneko[1], Yoshikazu Tanaka[2], Yasuhito Sekine[1], Tomoaki Matsuura[1] ([1]*ELSI, Tokyo Tech.*, [2]*Grad. Sch. Life Sci., Tohoku Univ.*)

ゲノム生物学：ゲノム構造／Genome biology: Genome structure

3Pos253 核スペックルの構造形成・動態のシミュレーション
Simulations of structural dynamics of nuclear speckle
Shingo Wakao, Masashi Fuji, Akinori Awazu (*Graduate School of Integrated Sciences for Life, Univ. Hiroshima*)

3Pos254 Hi-C データからの直感的なヘテロクロマチンとユークロマチンの識別法
An intuitive discrimination method of heterochromatin and euchromatin from Hi-C data
Takashi Sumikama[1,2], Takeshi Fukuma[2] ([1]*JST, PRESTO*, [2]*WPI-NanoLSI, Kanazawa Univ.*)

3Pos255 Modeling heterogeneous chromatin structure ensembles using metainference from Hi-C data
Chenyang Gu, Giovanni Brandani (*Grad. Sch. Sci., Univ. Kyoto*)

生命情報科学：構造ゲノミクス／Bioinformatics: Structural genomics

3Pos256 改良 MSA を用いたアブラナ科植物の SRK/SP11 複合体構造のハプロタイプ網羅的な予測
Haplotype exhaustive prediction of SRK/SP11 complex structure in Brassicaceae using a modified MSA
Tomoki Sawa[1], Yoshitaka Moriwaki[1], Tohru Terada[1], Kohji Murase[2], Seiji Takayama[2], Kentaro Shimizu[1] ([1]*Dept. of Biotechnol., Grad. Sch. of Agri. and Life Sci., Univ. of Tokyo*, [2]*Dept. of Appl. Biol. Chem., Grad. Sch. of Agri. and Life Sci., Univ. of Tokyo*)

3Pos257 深層学習を用いた、電子顕微鏡画像からの骨格筋小胞形態判別
Skeletal muscle vesicle morphology discrimination from electron microscope images using deep learning method
Natsuki Kezuka[1], Shiho Kasaya[1], Kenji Etchuya[1], Jun Nakamura[3], Chikara Sato[2], **Makiko Suwa**[1,2] ([1]*Aoyamagakuin Univ. Sci. and Eng.*, [2]*Grad. Sch., Sci. and Eng., Aoyamagakuin Univ.*, [3]*Health and Medical Res. Inst., AIST.*)

3Pos258 新しいタンパク質立体構造がミスセンスバリアントの評価に与える影響の評価
Evaluating the impact of new three-dimensional structures for interpretation of missense variants in human genome
Matsuyuki Shirota[1,2], Kengo Kinoshita[2,3] ([1]*Grad. Sch. Med., Tohoku Univ*, [2]*ToMMo, Tohoku Univ*, [3]*Grad. Sch. Inform. Sci., Tohoku Univ*)

3Pos259 Structural characteristics of coregulated phosphorylation sites
Hafumi Nishi[1,2,3] ([1]*Grad. Sch. Info. Sci., Tohoku Univ.*, [2]*Fac. Core Res., Ochanomizu Univ.*, [3]*ToMMo, Tohoku Univ.*)

生命情報科学：機能ゲノミクス／Bioinformatics: Functional genomics

3Pos260 微生物群集は普遍的に極めて安定な形質組成を持つ
Microbial communities are universally characterized by extremely stable trait compositions
Takao K Suzuki[1], Motomu Matsui[1], Susumu Morigasaki[2], Iwao Ohtsu[2], Yuki Doi[2], Hisayoshi Hayashi[3], Naoki Takaya[4], Wataru Iwasaki[1] ([1]*Graduate School of Frontier Sciences, the University of Tokyo*, [2]*School of Life and Environmental Science, University of Tsukuba*, [3]*Tsukuba-Plant Innovation Research Center, University of Tsukuba*, [4]*Microbiology Research Center for Sustainability, University of Tsukuba*)

3Pos261 乳腺組織のがん化により染色体内相互作用を維持する遺伝子の遺伝子オントロジーの特定
Identification of gene ontologies of genes with intra-chromosomal interactions in the breast cancer tissue
Yuta Shintani (*Fac. Adv. Math. Sci., Meiji Univ*)

3Pos262 出芽酵母プロテオームからの新規 PLP 結合タンパク質の予測
Prediction of novel PLP-binding proteins from budding yeast proteome
Masafumi Shionyu[1], Momoka Nakamoto[1], Atsushi Hijikata[2], Yukio Mukai[1] ([1]*Grad. Sch. Biosci., Nagahama Inst. Bio-Sci. Tech.*, [2]*Sch. Life Sci., Tokyo Univ. Pharm. Life Sci.*)

数理生物学／Mathematical biology

3Pos263 膜タンパク質クラスター形成とそのシグナル伝達系における機能的意義に関する数理的研究
A Mathematical study for membrane protein cluster formations and its functional significance in signal transduction systems
Hiroaki Takagi (*Sch. Med., Nara Med. Univ.*)

3Pos264 主成分分析を用いた希少/遺伝性疾患に対する human phenotype ontology からの特徴抽出
Feature extraction from human phenotype ontology for rare/hereditary disease using principal component analysis
Yoshino Jibiki[1], Toyofumi Fujiwara[2], Takanori Sasaki[1] ([1]*Fac. Adv. Math. Sci., Meiji Univ.*, [2]*DBCLS*)

3Pos265 クロマチンポリマーモデルにおける結合分子によるクラスターの寿命
Lifetime of Bridging Induced Cluster in Chromatin Polymer Model
Ryo Nakanishi[1], Koji Hukushima[1,2] ([1]*Graduate School of Arts and Sciences, The University of Tokyo*, [2]*Komaba Institute for Science*)

3Pos266 遺伝子発現制御ネットワークモデルの応答ダイナミクス次元圧縮
Dimensional compression of response dynamics on a gene regulatory network model
Masayo Inoue[1], Kunihiko Kaneko[2] ([1]*Grad. Sch. Eng., Kyushu Inst. Tech.*, [2]*Niels Bohr Inst.*)

3Pos267 細胞配置替え過程におけるアクトミオシンケーブルの剥離と接着の数理モデル
Mathematical model for detachment and attachment of cortical actin cable in cell rearrangement
Shuji Ishihara[1,2], Keisuke Ikawa[3], Kaoru Sugimura[2,4] ([1]*Grad. Sch. Arts. Sci., Univ. Tokyo*, [2]*UBI, Univ. Tokyo*, [3]*Grad. Sch. Sci., Nagoya Univ.*, [4]*Grad. Sch. Sci., Univ. Tokyo*)

3Pos268 Which asymmetry leads to genitalia rotation: Direction-dependent interfacial tension vs effective cellular torque
Sonja Tarama[1,2], Sayaka Sekine[3], Erina Kuranaga[3], Tatsuo Shibata[2] ([1]*Col Life Sci, Ritsumeikan Univ*, [2]*Riken BDR*, [3]*Grad Sch Life Sci, Tohoku Univ*)

3Pos269 生態・進化ダイナミクスにおける一般的な速度制限
General constraint on speeds in ecological and evolutionary dynamics
Kyosuke Adachi[1,2], Ryosuke Iritani[2,4], Ryusuke Hamazaki[2,3] ([1]*RIKEN BDR*, [2]*RIKEN iTHEMS*, [3]*RIKEN CPR*, [4]*Grad. Sch. Sci., Univ. Tokyo*)

3Pos270 ヒト血中インスリンによるアミノ酸および脂質代謝制御機構のモデルベース同定
Model-based identification of the regulation of amino acid and lipid metabolism by insulin in human blood
Suguru Fujita[1], Yasuaki Karasawa[2], Ken-ichi Hironaka[1], Akiyoshi Hirayama[3], Tomoyoshi Soga[3], Shinya Kuroda[1] ([1]*Dept. of Biol. Sci., Grad. Sch. of Sci., Univ. of Tokyo.*, [2]*Dept. of Neur., Grad. Sch. of Med., Univ. of Tokyo.*, [3]*Inst. for Adv. Biosci., Keio Univ.*)

3Pos271 ネットワーク解析に基づく乳がんのバイオマーカー予測
Biomarker prediction of breast cancer based on network analysis
Saito Torii (*Fac. Adv. Math. Sci., Meiji Univ.*)

非平衡・生体リズム／Nonequilibrium state & Biological rhythm

3Pos272 A general approach to chemical thermodynamics and constraints for growing systems
Yuki Sughiyama, **Atsushi Kamimura**, Dimitri Loutchko, Tetsuya J. Kobayashi (*IIS, The University of Tokyo*)

3Pos273 動物の老化に伴う活動速度の指数減衰とトランスポゾン駆動老化仮説の検証
Exponential decline of *C. elegans* behavioral activity along with aging and experimental test of the transposon-driven aging hypothesis
Yukinobu Arata, Jurica Peter, Sako Yasushi (*RIKEN, CPR, Cell Info*)

3Pos274 Overpotential Estimation in Enzymatic Reactions of Mitochondrial Respiratory Chains
Nuning Anugrah Putri Namari[1], Kotaro Takeyasu[2,3], Junji Nakamura[3,4] ([1]*Graduate School of Science and Technology, University of Tsukuba*, [2]*Department of Materials Science, Faculty of Pure and Applied Sciences, University of Tsukuba*, [3]*Tsukuba Research Center for Energy Materials Science, University of Tsukuba*, [4]*Mitsui Chemicals, Inc.-Carbon Neutral Research Center, International Institute for Carbon-Neutral Energy Research, Kyushu University*)

3Pos275 細胞内微小管の物理的性質
Probing physical properties of intracellular microtubules
Ryota Ori, Hirokazu Tanimoto (*Grad. Sch. Nanobioscience., Univ. Yokohama City*)

計測／Measurements

3Pos276 磁気刺激による細胞活動制御のための磁気レシーバー・磁気刺激システムの開発
Development of novel technique for magnetic activation of living-cell functions
Shunki Takaramoto[1], Hiromu Yawo[1], Yujiro Nagasaka[1], Hikaru Yoshioka[2], Masaki Sekino[2], Keiichi Inoue[1] ([1]*ISSP Univ. Tokyo*, [2]*Sch. Eng., Univ. Tokyo*)

3Pos277 (2SGA-3) Decoding single-cell transcriptomic phenotypes from cell images enabled by robotic data acquisition and deep learning
Jianshi Jin[1], Taisaku Ogawa[1], Nozomi Hojo[1], Kirill Kryukov[2], Kenji Shimizu[3], Tomokatsu Ikawa[4], Tadashi Imanishi[2], Taku Okazaki[3], Shiroguchi Katsuyuki[1] ([1]*BDR, RIKEN*, [2]*Dept. of Mol. Life Sci., Tokai Univ. Sch. of Med.*, [3]*Inst. for Quant. Biosci., Univ. of Tokyo*, [4]*Res. Inst. for Biomed. Sci., Tokyo Univ. of Sci.*)

3Pos278 Plunus Lanessiana から抽出した蛍光色素の解析と水素化アモルファスシリコン薄膜上での特性
Characterization of fluorescent pigment extracted from Plunus Lanessiana and the properties on hydrogenated amorphous silicon film
Kazunori Takada[1], Mao Izumi[1], Satomi Kimura[1], Koyu Akiyama[1], Hiroshi Masumoto[2], Yutaka Tsujiuchi[1,2] ([1]*Material Science and Engineering, Akita University*, [2]*Frontier Research Institute for Interdisciplinary Sciences, Tohoku University*)

3Pos279 センサシステム研究のための水素化アモルファスシリコンで増強された脂肪酸とクマリンの複合分子薄膜
Composite molecular film of fatty acid and coumarin for sensor system enhanced by hydrogenated amorphous silicon
Koyu Akiyama[1], Kazunori Takada[1], Hiroshi Masumoto[2], Yutaka Tsujiuchi[1,2] ([1]*Material Science and Engineering, Akita University*, [2]*Frontier Research Institute for Interdisciplinary Sciences, Tohoku University*)

3Pos280 光退色後蛍光寿命回復法の開発と応用
Fluorescence Lifetime Recovery After Photobleaching (FLRAP): Concept and application
Ikumi Mori, Miyuki Sakaguchi, Shoichi Yamaguchi, Takuhiro Otosu (*Grad. Sch. Sci. Eng. Saitama Univ.*)

3Pos281 光ファイバ型蛍光相関分光装置の開発と性能評価
Development of a fiber-optic based fluorescence correlation spectroscopy and its performance evaluation
Johtaro Yamamoto[1], Akira Sasaki[2] ([1]*Health & Med. Res. Inst., AIST*, [2]*Biomed. Res. Inst., AIST*)

3Pos282 Measuring the heat flux of intracellular reactions using differential scanning calorimetry
Tasuku Sato[1], Akira Murakami[1], Kohki Okabe[1,2], Takashi Funatsu[1] ([1]*Graduate School of Pharmaceutical Sciences, The University of Tokyo*, [2]*PRESTO, JST*)

3Pos283 Measurement of the physical properties in a cell with optical method
Yasuhiro Maeda[1], Sonja Tarama[2], Mitsusuke Tarama[2], Junichi Kaneshiro[1], Tatsuo Shibata[2], Tomonobu Watanabe[1] ([1]*Laboratory for Comprehensive Bioimaging , RIKEN BDR*, [2]*Laboratory for Physical Biology, RIKEN BDR*)

3Pos284 ゼブラフィッシュ心臓における細胞外マトリックスの弾性率の AFM 測定と細胞運命制御機構
AFM analysis of the stiffness of extracellular matrix of zebrafish heart and its contribution to cell fate determination
Sho Matsuki, Ryuta Watanabe, Yuuta Moriyama, Toshiyuki Mitsui (*Grad. Sch. Sci., Univ. Aogaku*)

3Pos285 High-Speed AFM revealed dynamic behavior of antibody
Norito Kotani, Takashi Morii, Takao Okada (*Research Institute of Biomolecule Metrology Co.,Ltd.*)

3Pos286 シロザケ椎骨の骨質解析
Assessment of Bone Quality in Chum Salmon Vertebrae
Shota Hironaka, Chihiro Kawamoto, Humiya Nakamura, Hiromi Kimura-Suda (*Graduate School of Science and Engineering, Chitose Institute of Science and Technology*)

3Pos287 Application of a bench-top NMR instrument for omics studies of gut microbiota metabolites
Zihao Song[1], Yuki Ohnishi[1], Seiji Osada[2], Li Gan[1], Jiaxi Jiang[1], Zhiyan Hu[1], Hiroyuki Kumeta[1], Yasuhiro Kumaki[1], Kiminori Nakamura[1], Tokiyoshi Ayabe[1], Kazuo Yamauchi[3], Tomoyasu Aizawa[1] ([1]*Grad. Sch. Life Sci., Hokkaido Univ.*, [2]*Nakayama Co.,Ltd.*, [3]*IAS, OIST*)

3Pos288 Research on metabolomics of human breast milk samples by benchtop NMR and high field NMR
Zhiyan Hu[1], Jiaxi Jiang[1], Li Gan[1], Zihao Song[1], Yuki Ohnishi[1], Seiji Osada[2], Hiroyuki Kumeta[1], Yasuhiro Kumaki[1], Kazuo Yamauchi[3], Tomoyasu Aizawa[1] ([1]*Grad. Sch. Life Sci., Hokkaido Univ.*, [2]*Nakayama Co.,Ltd.*, [3]*IAS, OIST*)

3Pos289 大腸菌一遺伝子欠損株におけるラマンスペクトルとオミクスデータの対応
Correspondence between Raman spectra and omics data in *E. coli* single gene deletion strains
Genta Chiba[1], Ken-ichiro Kamei[2], Arisa Oda[2,3], Kunihiro Ohta[2,3], Yuichi Wakamoto[2,3] ([1]*Dept. Integ. Sci., Univ. Tokyo*, [2]*Grad. Sch. Art Sci., Univ. Tokyo*, [3]*UBI, Univ. Tokyo*)

3Pos290 アクチン繊維の QCM 測定における独特の周波数シフト
Unique frequency-shifts in QCM measurement on binding biomolecules having filamentous shape
Naoki Matsumoto[1], Honoka Kobayashi[2], Taiki Nishimura[1], Yuki Sakurai[1], Kaito Kobayashi[1], Kaho Yokomuro[1], Kazuya Soda[1], Ikuko Fujiwara[2], Hajime Honda[2] ([1]*Dept. of Bioeng. Nagaoka Univ. of Tech.*, [2]*Dept. of Matl. Sci. and Bioeng., Nagaoka Univ. of Tech.*)

3Pos291 交流電場による細胞の回転運動を利用した，非標識に細胞の誘電特性を計測する電極デバイスの開発
Development of Simultaneous Electrorotation Device with Microwells for Non-Labeled Characterization of Cellular Dielectric Properties
Masato Suzuki[1], Mio Tsuruta[1], Shee Chean Fei[2], Seiichi Uchida[2], Tomoyuki Yasukawa[1] ([1]*Grad. Sch. Sci., Univ. Hyogo*, [2]*Grad. Sch. Info. Sci. Elect. Eng., Kyushu Univ.*)

バイオイメージング／Bioimaging

3Pos292 RNA ポリメラーゼによる転写開始素過程の一分子解析
Probing processes in transcription initiation by *Escherichia coli* RNA polymerase using single-molecule methods
Shingo Fukuda, Toshio Ando (*WPI Nano Life Science Institute (WPI-NanoLSI), Kanazawa University*)

3Pos293 水中測定におけるサブミクロン分解能赤外分析法（O-PTIR）の汎用性拡大に向けた検討
Expanding the versatility of sub-micron resolution infrared analysis method (O-PTIR) in underwater measurement
Naoki Baden (*Nihon Thermal Consulting, Co., Ltd.*)

3Pos294 Importance of annexin V N-terminal for 2D crystal formation revealed by HS-AFM
Trang Ngoc Tran[1], Ryusei Yamada[2], Holger Flechsig[3], Toshiki Takeda[4], Noriyuki Kodera[3], Hiroki Konno[3] ([1]*Graduate School of Frontier Science Initiative, Kanazawa University, Kakuma-machi, Kanazawa 920-1192, Japan*, [2]*Graduate School of Natural Science & Technology, Kanazawa University, Kanazawa 920-1192, Japan*, [3]*WPI Nano Life Science Institute (WPI-NanoLSI), Kanazawa University, Kakuma-machi, Kanazawa 920-1192, Japan*, [4]*College of Science and Engineering, School of Natural system, Kanazawa University, Kakuma-machi, Kanazawa 920-1192, Japan*)

3Pos295 蛍光タンパク質型高感度温度センサーを用いた小胞体での微小な熱発生計測
Extremely sensitive measurement of thermogenesis in the endoplasmic reticulum using a FRET-based thermosensor with huge dynamic range
Shun-ichi Fukushima, Takeharu Nagai (*SANKEN, Univ. Osaka*)

3Pos296 超広視野顕微鏡の安価版(SeMATERAS)の開発
Inexpensive development of ultra-wide-field microscope SeMATERAS
Masashi Ohmach, Hiromichi Wakebe, Yuichi Inoue (*SIGMA KOKI Co.,LTD.*)

3Pos297 Protein Unfolding Dynamics during Translocation through a Solid-state Nanopore
Hirohito Yamazaki, Sotaro Uemura (*The University of Tokyo, Department of Biological Science*)

3Pos298 チラコイド膜中に存在する光化学系 II 超複合体の高速 AFM による可視化
Visualization of photosystem II super complex in thylakoid membrane by HS-AFM
Daisuke Yamamoto (*Fac. Sci., Fukuoka Univ.*)

3Pos299 Nanoscale visualization of cell membrane exposed to non-thermal atmospheric pressure plasma
Han Gia Nguyen[1], Linhao Sun[2], Tatsuya Kitazaki[3], Shinya Kumagai[3], Shinji Watanabe[2] ([1]*Grad. Sch. Nano Life Sci., Univ. Kanazawa*, [2]*WPI NanoLSI, Univ. Kanazawa*, [3]*Univ. Meijo*)

3Pos300 ナノレベルの精度を持つ光電子相関顕微鏡の要素開発：無冷媒クライオスタットを用いたサンプルホルダーのサブミリケルビン安定化
Sub-milliKelvin stabilization of sample holders with closed-cycle cryostat for correlative light and electron microscopy with nm accuracy
Takuma Yorita, Michio Matsushita, Satoru Fujiyoshi (*Department of Physics,Tokyo Institute of Technology*)

3Pos301 (2SBA-6) 細胞内の一分子を三次元でナノレベルの分解能で観察できる「クライオ三次元ナノスコピー」の開発
(2SBA-6) Cryo-3D Nanoscopy to localize three-dimensional position of individual fluorophore with nanometer precision in the cell
Kanta Naruse[1], Tsuyoshi Matsuda[1], Yuta Mizouchi[1], Takeshi Shimi[2], Hiroshi Kimura[2], Eiji Nakata[3], Takashi Morii[3], Michio Matsushita[1], Satoru Fujiyoshi[1] ([1]*Department of physics, Tokyo institute of technology*, [2]*Cell Biology Center, Institute of Innovative Research, Tokyo institute of technology*, [3]*Institute of Advanced Energy, Kyoto University*)

3Pos302 SARS-CoV-2 スパイク（S）タンパク質の時空間追跡と ACE2 受容体および小さな細胞外小胞との相互作用
Spatiotemporal tracking of SARS-CoV-2 spike (S) protein and its interaction with ACE2 receptor and small extracellular vesicles
KeeSiang Lim[1], Goro Nishide[2], Takeshi Yoshida[4], Takahiro Watanabe-Nakayama[1], Akiko Kobayashi[3], Masaharu Hazawa[1,3], Rikinari Hanayama[1,4], Toshio Ando[1], Richard W. Wong[1,3] ([1]*Kanazawa University., WPI-Nano Life Science Institute*, [2]*Kanazawa University., Division of Nano Life Science in the Graduate School of Frontier Science Initiative, WISE Program for Nano-Precision Medicine, Science and Technology*, [3]*Kanazawa University., Cell-Bionomics Research Unit, Institute for Frontier Science Initiative (INFINITI)*, [4]*Kanazawa University., Department of Immunology, Graduate School of Medical Sciences.*)

3Pos303 細胞内一分子ナノスコピーのための近赤外蛍光標識技術の開発
Near-infrared fluorescent labeling technique for cryogenic single molecule nanoscopy in cell
Kazuki Kuramoto[1], Kei Muto[2], Ryuya Miyazaki[2], Junichiro Yamaguchi[2], Kanta Naruse[1], Naoki Kamiya[1], Hidekazu Aramaki[1], Michio Matsushita[1], Haruka Oda[3,4], Takeshi Shimi[3,4], Hiroshi Kimura[3,4], Satoru Fujiyoshi[1] ([1]*Department of Physics, Tokyo Institute of Technology*, [2]*Department of Applied Chemistry, Waseda University,*, [3]*Bioscience and Biotechnology, Tokyo Institute of Technology*, [4]*Cell Biology Center, Institute of Innovative Research, Tokyo Institute of Technology,*)

3Pos304 局在化する高分散化表面修飾ナノダイヤモンドの開発とその細胞移行に関する研究
Research on the development of localized highly dispersed surface modified nanodiamond and their cellular uptake
Hirotaka Okita[1], Shingo Sotoma[1], Shunsuke Chuma[1,2], Madoka Suzuki[1], Yoshie Harada[1,3] ([1]*IPR., Osaka Univ.*, [2]*Grad. Sch. Sic., Osaka Univ.*, [3]*QIQB., Osaka Univ.*)

3Pos305 (2SBA-5) High-resolution mapping of chromatin compaction and dynamics in live cells by label-free interference microscopy
Yi-Teng Hsiao, Chia-Ni Tsai, Fasih Bintang Ilhami, Chia-Lung Hsieh (*Institute of Atomic and Molecular Sciences (IAMS), Academia Sinica / Taiwan*)

3Pos306 A new technique for detecting single biomolecule fluctuations using surface distance-dependent spectral changes in the QD emission
Kaoru Okura, Hitoshi Tatsumi (*Department of Applied Bioscience, Kanazawa Inst. of Technol., Ishikawa, Japan*)

3Pos307 Gaussian Weighted Background Correction For Raman images with application to hydrogel samples
Jean-Emmanuel Clement (*Institute for Chemical Reaction Design and Discovery (ICReDD), Hokkaido University*)

3Pos308 一分子イメージングを用いた生細胞内 RNA ポリメラーゼⅡの様々な転写サイクル段階におけるダイナミクス解析
RNA Polymerase II dynamics analysis at different stages of the transcription cycle in living cells using single-molecule imaging
Ryo Akita, Yuma Ito, Makio Tokunaga (*Sch. Life Sci. Tech., Tokyo Inst. Tech.*)

3Pos309 A green color fluorescence lifetime-based biosensor for quantitative imaging of intracellular ATP in multicellular system

Cong Quang Vu[1], Taketoshi Kiya[2], Toshinori Fujie[3], Tetsuya Kitaguchi[4], Satoshi Arai[1] ([1]*Grad. Sch. NanoLS., Kanazawa Univ.*, [2]*Grad. Sch. of Nat. Sci. Tech., Kanazawa Univ.*, [3]*Sch. of Life Sci. and Tech., Tokyo Tech.*, [4]*Inst. of Inno. Res., Tokyo Tech.*)

3Pos310 膜受容体と脂質ドメインの共クラスター化を評価するための 3 色 SMLM 解析ワークフロー

Workflows of triple-color single-molecule localization microscopy analysis to assess co-clustering of membrane receptors and lipid domains

Masataka Yanagawa[1,2], Mitsuhiro Abe[1], Yasushi Sako[1] ([1]*Riken CPR*, [2]*JST PRESTO*)

3Pos311 NIR-triggered vesicles to manipulate spatial and temporal dynamics of a neurotransmitter in skeletal muscle and Drosophila brain

Takeru Yamazaki[1], Satya Sarker[1], Taketoshi Kiya[2], Satoshi Arai[1] ([1]*Grad. Sch. NanoLS., Kanazawa Univ.*, [2]*Grad. Sch. of Nat. Sci. Tech., Kanazawa Univ*)

3Pos312 (1SEP-3) Triple-color photothermal dye-based nanoheaters to generate multiple heat spots within a single cell

Md Monir Hossain, Takeru Yamazaki, Kayoko Nomura, Satoshi Arai (*Grad. Sch. NanoLS., Kanazawa Univ.*)

3Pos313 可逆的ターンオン型蛍光標識技術の開発とライブセル蛍光イメージングへの応用

Development of reversible turn-on fluorescent labeling technology and its application to live cell fluorescence imaging

Shigeyuki Namiki, Daisuke Asanuma, Hiroki Ishikawa, Shinkuro Kobayashi, Kenzo Hirose (*Department of Pharmacology, Graduate school of Medicine, The University of Tokyo*)

バイオエンジニアリング／Bioengineering

3Pos314 DNA で作るナノミウラ折り

Nano Miura fold fabricated with DNA

Daisuke Ishikawa, Masahiko Hara (*Sch. Mater. Chem. Tech., Tokyo Tech*)

3Pos315 相分離液滴をテンプレートとした DNA オリガミカプセルの構築

Construction of DNA origami capsules using phase-separated droplets as templates

Nagi Yamashita[1], Marcos Masukawa[2], Mayumi Chano[3], Yusuke Sato[4], Masahiro Takinoue[1,3] ([1]*Department of Life Science and Technology, School of Life Science and Technology, Tokyo Institute of Technology.*, [2]*Department of Chemistry, Johannes Gutenberg University Mainz.*, [3]*Department of Computer Science, School of Computing, Tokyo Institute of Technology.*, [4]*Department of Systems Design and Informatics, School of Computer Science and Systems Engineering, Kyushu Institute of Technology.*)

3Pos316 DNA ハイドロゲルの形成と変形の光制御

Photocontrol of DNA hydrogel formation and deformation

Yoshiaki Sano[1], Masahiro Takinoue[1,2] ([1]*Department of Life science and Technology, Tokyo Institute of Technology, Japan*, [2]*Department of Computer Science, Tokyo Institute of Technology, Japan*)

3Pos317 電子線照射が微生物細胞に及ぼす影響

Effects of an electron beam irradiation on living bacterial cells

Junya Katai[1], Yuta Nagano[1], Kenshi Suzuki[2], Kazuki Yasuike[1], Ryoya Hayashi[1], Asahi Tanaka[3], Tetsuo Narumi[1], Masaki Shintani[1], Yosuke Tashiro[1], Wataru Inami[4], Yoshimasa Kawata[4], Fumihiro Sassa[5], Hiroyuki Futamata[6] ([1]*Dept. Appl. Chem. Biological Eng., Univ. Shizuoka*, [2]*Grad. Sch. Scie. Tech., Univ. Shizuoka*, [3]*Coop. Major. Med. Photo., Univ. Shizuoka.*, [4]*Res. Inst. Elect., Univ. Shizuoka*, [5]*Grad. Sch. Fac. Inf. Sci. Elect. Eng.,Unv. Kyushu*, [6]*Res. Inst. Green. Sci. Tech., Univ. Shizuoka*)

3Pos318 サブテラヘルツ照射によるタンパク質および核酸の構造変化の溶液 NMR 解析
Structural changes of proteins and nucleic acids induced by sub-terahertz radiation investigated by using solution NMR spectroscopy
Yuji Tokunaga[1], Masahiko Imashimizu[2], Koh Takeuchi[1] ([1]*Grad. Sch. Pharm. Sci., UTokyo*, [2]*CMB, AIST*)

3Pos319 Medusavirus の局所構造解析によるウイルス粒子形成に伴う構造変化の可視化
Visualization of structural changes associated with virus particle formation by local structural analysis of Medusavirus
Ryoto Watanabe[1,2], Chihong Song[1,2,3], Kazuyoshi Murata[1,2,3], Masaharu Takemura[4] ([1]*National Institute for Physiological Sciences (NIPS)*, [2]*The Graduate University for Advanced Studies (SOKENDAI)*, [3]*The Exploratory Research Center on Life and Living Systems (ExCELLS)*, [4]*Tokyo University of Science*)

3Pos320 人工多細胞の自動生産に関する研究
Toward automated production of lipid-based multi-compartment assemblies
Ryo Shimizu[1], Richard James Archer[1], Gen Hayase[2], Satoshi Murata[1], Shin-Ichiro Nomura[1] ([1]*Grad. Sch. Eng., Univ. Tohoku/Japanese*, [2]*WPI-MANA*)

3Pos321 表面微細構造上における付着珪藻の増殖挙動
The growth of marine benthic diatoms on micro patterned surfaces
Takayuki Murosaki[1], Taiki Kishigami[2], Yuji Hirai[3], Yasuyuki Nogata[4] ([1]*Department of Chemistry, Asahikawa Medical University*, [2]*Graduate School of of Science and Engineering, Chitose Institute of Science and Technology*, [3]*Department of Applied Chemistry and Bioscience, Faculty of Science and Engineering, Chitose Institute of Science and Technology*, [4]*Sustainable System Research Laboratory, Central Research Institute of Electric Power Industry*)

3Pos322 Magnetic induced assembly of anisotropic structures for reversible lipid compartment deformations
Richard Archer, Shinichiro M. Nomura (*Tohoku University, Department of Robotics*)

3Pos323 超撥水表面上の水滴の跳ね返り挙動に関する理論的考察
Theoretical Consideration on Bouncing Behavior of Water Droplet on Superhydrophobic Surface
Hiroyuki Mayama (*Department of Chemistry, Asahikawa Medical University*)

3Pos324 Self-assembly of DNA origami blocks into two-dimensional crystalline structures with designed geometries
Yuki Suzuki[1], Ibuki Kawamata[2] ([1]*Grad. Sch. Eng., Mie Univ.*, [2]*Grad. Sch. Eng., Tohoku Univ.*)

1SAA-1 TIA-1 プリオン様ドメインの ALS 変異は高度に凝縮した病原性構造体を形成する
ALS mutations in the TIA-1 prion-like domain trigger highly condensed pathogenic structures

Naotaka Sekiyama[1], Kiyofumi Takaba[2], Saori Maki-Yonekura[2], Ken-ichi Akagi[3], Yasuko Ohtani[1], Kayo Imamura[1], Tsuyoshi Terakawa[1], Keitaro Yamashita[4], Koji Yonekura[2], Takashi Kodama[1], Hidehito Tochio[1] ([1]*Dept. of Biophysics, Grad Sch. of Science, Kyoto Univ.*, [2]*RIKEN SPring-8 Center*, [3]*NIBIO*, [4]*MRC Laboratory of Molecular Biology*)

T-cell intracellular antigen-1 (TIA-1) plays a central role in stress granule (SG) formation by self-assembly via the prion-like domain (PLD). In TIA-1 PLD, amino acid mutations associated with neurodegenerative diseases such as amyotrophic lateral sclerosis (ALS) or Welander distal myopathy (WDM) have been identified. However, how these mutations affect PLD self-assembly properties has remained elusive. In this study, we uncovered the implicit pathogenic structures caused by the mutations by NMR, Molecular dynamics simulations and 3D electron crystallography. These results suggest that ALS mutations increase the likelihood of irreversible amyloid fibrillization following phase-separated droplet formation, and this process may lead to pathogenicity.

1SAA-2 流れが駆動するタンパク質のアミロイド線維化機構
Mechanism of amyloid fibrillation of a protein driven by a flow

Kenji Sugase[1], Daichi Morimoto[2], Erik Walinda[3] ([1]*Division of Applied Life Sciences, Graduate School of Agriculture, Kyoto University*, [2]*Department of Molecular Engineering, Graduate School of Engineering, Kyoto University*, [3]*Department of Molecular and Cellular Physiology, Graduate School of Medicine, Kyoto University*)

Inside living organisms is a non-equilibrium environment in which, for example, blood flow exists. From the viewpoint of fluid mechanics, flow in a confined space is accompanied by forces that distort molecules. The flow equivalent to that in neurons causes amyloid fibrillation. Hence the effect of physical perturbation by the flow on amyloid fibrillation is of interest. However, existing instruments cannot analyze molecules in a flow at the atomic level. Recently, we developed a highly sensitive Rheo-NMR instrument that can perform NMR measurements while generating flow in a sample. In this presentation, I will show the results of real-time Rheo-NMR measurement of the amyloid fibrillation process and the effects of the flow on each step of amyloid fibrillation.

1SAA-3 生体分子のための動的溶媒和理論の開発
Development of Dynamic Solvation Theory for Biomolecules

Norio Yoshida (*Grad. Sch. Info., Nagoya Univ.*)

Biomolecules maintain structure and exhibit functions through interactions with solutions. We have used 3D-RISM theory, one of the solvation theories of molecular liquids, to study the molecular recognition, transport, and chemical reactions of proteins. 3D-RISM theory is formulated as a DFT of liquids in equilibrium state. In addition, solvation dynamics associated with changes in the states of biomolecules are involved in the control of their dynamics. Recently, a formulation based on time-dependent DFT has been proposed to describe solvation dynamics. This theory enables to describe the solvation dynamics associated with changes in protein states, such as electron transfer. In this presentation, the developments and the applications of the theory will be reported.

1SAA-4 リン酸化による HP1α の液-液相分離機構の解明
Phase separation mechanism of HP1α by phosphorylation

Ayako Furukawa[1], Kento Yonezawa[2,3], Tatsuki Negami[4], Yuriko Yoshimura[5], Aki Hayashi[5], Jun-ichi Nakayama[5,6], Naruhiko Adachi[2], Toshiya Senda[2], Kentaro Shimizu[4], Tohru Terada[4], Nobutaka Shimizu[2], Yoshifumi Nishimura[1,7] ([1]*Grad. Sch. Med. Life Sci., Univ. Yokohama City*, [2]*IMSS, KEK,*, [3]*NAIST, CDG*, [4]*Grad. Sch. Agr. Life Sci., Univ. Tokyo*, [5]*NIBB*, [6]*SOKENDAI*, [7]*Grad. Sch. Integ. Sci. Life, Univ. Hiroshima*)

Heterochromatin is a highly condensed state of chromatin, and liquid-liquid phase separation (LLPS) is suggested to be involved in the formation of this higher-order chromatin structures. HP1α, one of major components of heterochromatin, HP1α consists of N-terminal disordered tail (N-tail), chromodomain (CD), central flexible hinge region, and chromo shadow domain (CSD); CD recognizes the lysine9-methylated histone H3 tail in the nucleosome and HP1α forms a dimer via CSD. The phosphorylation of the N-tail forms LLPS of HP1α. To elucidate the LLPS mechanism by the phosphorylation, integrative structural analyses of NMR, SEC-SAXS, and MD simulations were performed. We found important interactions in the LLPS formed by the phosphorylated HP1α.

1SAA-5 タンパク質の変性状態における構造ダイナミクスと溶媒環境依存性の理論的解析
Theoretical study on the conformational dynamics of proteins in disordered states under different solvent environments

Toshifumi Mori (*Inst. Mat. Chem. Eng., Kyushu Univ.*)

Molecular dynamics (MD) simulations have been a powerful tool in revealing the microscopic structure and dynamics of proteins. Yet, proteins in disordered states remain challenging to study using MD, since the conventional force fields were optimized to describe folded states. Many studies thus have been performed to update the MD force fields, and succeeded in refining static properties such as radius of gyration. On the other hand, how these changes in force fields affect the dynamic aspects, which may be critical for aggregation and condensation, are often overlooked. Here, I will describe how the conformational dynamics of proteins in disorder states can be characterized, and discuss how these dynamics are affected by altering the force fields.

1SAA-6 ポリマーコートされたダイヤモンドナノ粒子によるバイオセンシング
Biosensing Using Diamond Nanoparticles Coated with Polymers

Shingo Sotoma, Yoshie Harada (*IPR, Osaka Univ.*)

I will show our recent achievement in the FND-based technologies including surface chemical coating, specific cell labeling, and temperature sensing inside a cell. Using a nanoheater/nanothermometer hybrid based on a polydopamine shell encapsulating an FND, we measured the intracellular thermal conductivity of the HeLa cell with a spatial resolution of about 200 nm. Its mean value of 0.11 Wm-1K-1 determined for the first time is significantly smaller than that of water. Finally, I present a simple and scalable wet-chemistry route to uniformly conjugate GNPs on the surface of FNDs by exploiting thin PDA layers for intracellular controlled nanoheating.

1SAA-7 (2Pos051) 蝶々型金ナノデバイスが可能にするタンパク質液液相分離過程の制御
(2Pos051) Control of protein condensation by butterfly-shaped gold nanodevices

Tomohiro Nobeyama[1], Koji Takata[2], Tatsuya Murakami[2], Kentaro Shiraki[1,2] ([1]*Pure and Appli.Sci., Univ.Tsukuba*, [2]*Grad. Sch. Sci. Toyama Pref. Univ*)

Protein droplets caused by liquid-liquid phase separation（LLPS) are a key concept to comprehending dynamic phenomenon in cells. The droplets would form and change their shape through interactions with other molecules. We hypothesize that the butterfly-shaped gold nanomaterial (GNB) works as a controller of protein droplets due to the concave curved shape. We investigated the droplet formation of ATP and poly-Lysine, which is a model of protein droplets, in high concentrations with gold nanomaterials (GNs). GNBs induced large droplets. The comparative analysis of GNB and ball and rod shapes of GNs imply that the shape of GNs is critical to form the droplets. Details of the mechanism will be discussed at this meeting.

1SAA-8 (1Pos054) GGGGCC-RNA は、TDP43 およびそのカルボキシ断片の凝集を抑制する
(1Pos054) GGGGCC-RNA prevents aggregation of TDP43 and its carboxy terminal fragments

Ai Fujimoto[1], Masataka Kinjo[2], Akira Kitamura[2] ([1]*Grad. Sch. of Life Sci., Hokkaido. Univ*, [2]*Fac. Adv. Life Sci., Hokkaido. Univ*)

TDP-43 is an abnormally aggregation-prone protein associated with amyotrophic lateral sclerosis (ALS), and its 25 kDa carboxy-terminal fragments (CTFs), TDP25, are highly aggregation-prone. TDP25 aggregation is started by RNA elimination [Kitamura A. *et al.*, ***Sci. Rep.*** 6, 19230 (2016)]. We focus on the GGGGCC repeat sequence (rG4) as an RNA interacting with TDP25 and analyzed the interaction between them using fluorescence cross-correlation spectroscopy (FCCS). rG4 directly interacts with both TDP25 and TDP-43. Furthermore, rG4 expression in Neuro2a cells decreased the aggregates of both TDP25 and TDP-43. However, UG repeat RNA interaction with TDP43 did not inhibit aggregation. These results suggest that rG4 prevents the aggregate formation of ALS-associated TDP-43.

1SBA-1 X 線 1 分子追跡法によるヘモグロビン・アロステリーの再検討
Allosteric Transition Dynamics in Hemoglobin Reconsidered by Diffracted X-ray Tracking

Hiroshi Sekiguchi[1], Naoki Yamamoto[2], Naoya Shibayama[2], Yuji Sasaki[1,3] ([1]*JASRI/SPring-8*, [2]*Dept. Physiology, Jichi Med. Univ.*, [3]*Grad. Sch. Front. Sci., Univ. Tokyo*)

Allosteric conformational transitions underlie the biological functions of many multimeric proteins. The best-studied allosteric protein is hemoglobin in red blood cells, which carries oxygen effectively through large-scale conformational changes. The two-state model without intermediates is presented in a textbook to describe the allosteric behavior of hemoglobin. However, the model has been reconsidered by recent experimental breakthroughs [Shibayama, BBA 1864:129335 (2020)]. We applied the diffracted X-ray tracking (DXT) method to monitor single-molecule allosteric transitions in hemoglobin at a sub-milliseconds scale. We succeeded in observing the twisting motions upon oxygen detachment from hemoglobin and will discuss the recent DXT results in the presentations.

1SBA-2 Internal dynamics of intrinscially disordered protein as studied by neutron scattering

Rintaro Inoue (*Institute for Integrated Radiation and Nuclear Science, Kyoto University*)

Since instrinscially diordered protein (IDP) plays significant roles especially for Eukaryotes, they are still attracting attention. Because of the limitation of applicability of existing conventional method to IDP, the relationship between function and structure has remined to be unknown. To overcome such a situation, it is essential to apply the solution scattering method than can directly solve the flexible structure of the IDPs and extract the dynamical information. In this presentation, we introduce the application of small-angle X-ray/neutron scattering and quasielastic neutron scattering to investaige both the structure and dynmaics of IDP utilizing Hef-IDR, an intrinsically disordered region of the archaeal protein Hef, as a sample.

1SBA-3 (2Pos050) タンパク質ケージ内における芳香環相互作用ネットワークの熱力学・分子動力学的解析
(2Pos050) Thermodynamic and Molecular Dynamic Analysis of Aromatic Interaction Networks in Protein Cages

Yuki Hishikawa[1], Noya Hiroki[1], Asuka Asanuma[1], Basudev Maity[1], Satoru Nagatoishi[2], Kouhei Tsumoto[2,3], Satoshi Abe[1], Takafumi Ueno[1] ([1]*Sch. Life Sci. Technol., Tokyo Inst. Technol.*, [2]*Inst. Med. Sci., Univ. Tokyo*, [3]*Sch. Eng., Univ. Tokyo*)

Non-covalent interactions involving aromatic amino acids are ubiquitous in nature and play essential roles in biological systems. Multiple aromatic residues assemble to form higher ordered structures – aromatic clusters or aromatic interaction networks, which govern protein folding, thermal stability and molecular recognition. The current challenge is to assess thermophysical and dynamic properties of aromatic interaction networks and relevance to their structural correlation at the atomic level. To address these issues, we constructed Phe/Tyr/Trp residue clusters using protein cages and examined their thermodynamic features and dynamic behaviors by circular dichroism (CD) spectroscopy, differential scanning calorimetry (DSC) and molecular dynamics (MD) simulations.

1SBA-4 (1Pos076) 3D structural determination of proteins from fluctuation X-ray scattering data

Wenyang Zhao[1], Osamu Miyashita[1], Florence Tama[1,2] ([1]*Center for Computational Science, RIKEN*, [2]*Grad. Sch. Sci., Univ. Nagoya*)

Fluctuation X-ray scattering (FXS) can investigate the nanoscale structure of proteins in near-physiological conditions and consequently help understand protein dynamics. The technique measures thousands of 2D coherent diffraction images of multiple non-crystalized biological particles at random orientations using an X-ray free-electron laser (XFEL). Computation methods are required for reconstructing the 3D structure from the set of 2D images. The present research proposes an efficient reconstruction algorithm based on comparing the double, triple, and quadruple angular correlations of the 2D images. In this report, the computational pipeline is demonstrated and examples with simulated image data are given. Impacts of experimental parameters are also discussed.

1SBA-5 Microscopic Mechanisms of Stable Amyloid β (1-42) Oligomer Formation

Ikuo Kurisaki, Shigenori Tanaka (*Graduate School of System Informatics, Kobe University*)

Stable formation of amyloid β (1-42) ($A\beta_{42}$) oligomer is a critical step toward the amyloid fibril formation, while the physicochemical mechanisms are still elusive at the microscopic level. Aiming to provide deeper insights into this important process, we performed atomistic molecular dynamics simulations for $A\beta_{42}$ oligomer dimers, $A\beta_{42}$(d). We found that configurational fluctuation of $A\beta_{42}$(d) affects thermodynamic stability of dimerization. Such stability is enhanced by increase of $A\beta_{42}$(d) size and $A\beta_{42}$ pentamer dimer shows remarkable suppression of dimer dissociation. Meanwhile, dissociation of $A\beta_{42}$ monomer from the growth edge can be prevented by interaction with $A\beta_{42}$ aggregates, suggesting that $A\beta_{42}$ oligomers stable form in $A\beta_{42}$ aggrecate milieu.

1SBA-6 非干渉性中性子散乱で観測するアミロイド構造多形体及びリン脂質分子のサブナノ秒ダイナミクス
Sub-nanosecond dynamics of amyloid polymorphs and phospholipid molecules observed by incoherent neutron scattering

Tatsuhito Matsuo[1,2,3], Alessio De Francesco[2], Aline Cissé[2,3], Dominique Bicout[2,3], Judith Peters[2,3,4] ([1]*iQLS, QST*, [2]*Institut Laue-Langevin, France*, [3]*Université Grenoble Alpes, France*, [4]*Institut Universitaire de France*)

Incoherent neutron scattering (iNS) is a powerful technique to study biomacromolecular dynamics at the sub-nanosecond timescale. In this talk, we will first describe our recent iNS study on lysozyme amyloid polymorphs called LP27 and LP60, which show high and low levels of cytotoxicity, respectively. LP60 was found to show enhanced molecular dynamics compared with LP27, implying that LP60 promotes binding to lipid membranes underlying cytotoxicity. Next, a newly developed Matryoshka-model, which describes various types of motions manifest in phospholipid molecules based on iNS data, will be introduced. Our findings and model will be useful to elucidate the molecular mechanism of interactions between amyloid and lipids, and eventually amyloid cytotoxicity.

1SBA-7 アミロイド線維前駆中間体の構造発達とその阻害
Structural development of amyloid prefibrillar intermediates and its inhibition

Naoki Yamamoto (*Sch. Med. Jichi Med. Univ.*)

Amyloid fibrils are abnormal protein aggregates associated with several amyloidoses and neurodegenerative diseases. Prior to the fibril formation, prefibrillar intermediates usually emerge, and thus thought to play an important role in the fibril formation. In this study, the structural development of prefibrillar intermediates of insulin-derived model peptide was monitored by transmission electron microscopy and small-angle X-ray scattering. We demonstrated that prefibrillar intermediates were wavy rod-like structures with low β-sheet content, and grew in a multistep manner toward the nucleation for protofilament formation. We also found that a blood clotting protein, fibrinogen, inhibited the amyloid fibril formation via interacting with prefibrillar intermediates.

1SCA-1 遊離鉄およびヘム蛍光プローブのライブセルイメージングへの応用
Fluorescence probes for labile iron and heme and their applications to live-cell imaging

Tasuku Hirayama (*Lab. Pharm. Med. Chem., Gifu Pharm. Univ.*)

Iron is the most abundant transition metal species in our body and is essential to maintaining our lives. Iron overload readily triggers cell damage via overproduction of highly reactive oxygen species. Because of its dual nature - essential but not too much- iron homeostasis is strictly controlled by sophisticated systems in cells to keep the iron levels constant.
To monitor the dynamics and alteration of labile iron species, including Fe(II) and heme, we have made much effort to develop selective fluorescent probes for each of labile Fe(II) and labile heme. In this symposium, I will present two topics a highly sensitive fluorescent probe for Fe(II) compatible with high-throughput screening and a new heme-selective fluorescent probe and its applications.

1SCA-2 細胞内遊離亜鉛イオンの定量解析を可能とする小分子蛍光プローブの開発
Development of small-molecule fluorescent probes for the quantitative analysis of labile Zn^{2+} in cells

Toshiyuki Kowada (*Institute of Multidisciplinary Research for Advanced Materials, Tohoku University*)

Zinc ion (Zn^{2+}) has important physiological roles in living cells, such as an enzyme cofactor, a protein structural modulator, and a signaling mediator. To investigate the intracellular Zn^{2+} fluctuations, fluorescence microscopy with a fluorescent Zn^{2+} probe is a powerful tool. However, there remains a lack of consensus on the labile Zn^{2+} concentrations in several organelles, as the fluorescence properties and zinc affinity of probes are greatly affected by the pH and redox environments in organelles. In this study, we developed small-molecule fluorescent Zn^{2+} probes with low pH sensitivity and organelle-targetability using HaloTag labeling. By using the probes, we achieved the quantitative analysis of labile Zn^{2+} in various organelles.

1SCA-3 コンディショナルプロテオミクスによる金属関連タンパク質のイメージングとプロファイリング
Imaging and profiling of metal-related proteins by conditional proteomics strategies

Tomonori Tamura (*Grad. Sch. Eng., Univ. Kyoto*)

Zinc signaling and dynamics play significant roles in many physiological responses and diseases. To understand the physiological roles of zinc, comprehensive identification of proteins under high concentrations of mobile zinc ion is crucial. We developed a ‘conditional proteomics’ approach to identify proteins involved in zinc homeostasis based on a chemical proteomic strategy that utilizes designer zinc-responsive labeling reagents to tag such proteins and quantitative mass spectrometry for their identification. Furthermore, our efforts have been dedicated to extending this approach to profile proteins involved in other metals and biological metabolites, such as copper, nitric oxide, and hydrogen peroxide. This presentation will report on these latest researches.

1SCA-4 量子ビームによる生命金属シングルセルイメージング
Single cell imaging by quantum beam elemental analyses for dynamics of cellular distribution of bio-metals

Shino Takeda (*National institute of Radiological Sciences, National Institutes for Quantum Science and Technology*)

Chemical information of cellular elements, such as elemental distribution, localization, composition, and chemical status, is required for understanding bio-metals. In the present symposium, intracellular distribution of bio-metals with cultured cells derived from mouse renal proximal tubules by quantum beam-based elemental analyses, such as PIXE (particle induced X-ray emission) and SR- XRF (X-ray fluorescence spectrometry using high energy synchrotron radiation) will be introduced. The chemical status of a localized bio-metal in a cell by XAFS (X-ray absorption fine structure) will be also presented.

1SCA-5 蛍光イメージングで解き明かす細胞内マグネシウムイオンの役割
The roles of intracellular magnesium ion revealed by fluorescence imaging

Yutaka Shindo (*Dept. Biosci. Info., Keio Univ.*)

Mg^{2+} is the most abundant divalent cation in mammalian cells. Recent studies have demonstrated that changes in intracellular Mg^{2+} concentration are involved in the regulation of cellular functions such as energy metabolism, intracellular signaling, and cell division. Although the changes in intracellular Mg^{2+} concentration have small amplitude, it has large effects on cellular functions. To detect the fluctuation of Mg^{2+} concentration in detail, our group developed highly selective fluorescent Mg^{2+} probes, KMG series. These probes were applied to simultaneous imaging of multiple intracellular signals and Mg^{2+} imaging in the intracellular local area, demonstrating the effect of Mg^{2+} on cellular energy metabolisms and intracellular signals.

1SCA-6 H_2S 検出蛍光プローブの開発とそれを用いた活性イオウ分子産生酵素の阻害剤スクリーニングへの応用
Development of a fluorescence probe for H_2S and its application to the inhibitor screening of reactive sulfur species-producing enzymes

Kenjiro Hanaoka (*Grad. Sch. Pharm. Sci., Keio Univ.*)

For detailed studies of the physiological functions of the reactive sulfur species such as H_2S and sulfane sulfur, a detection method is required. We previously developed a fluorescence probe for H_2S, HSip-1, utilizing macroazacyclic complex chemistry with copper ion (II) (*J. Am. Chem. Soc.* **2011**, *133*, 18003). We applied HSip-1 to HTS of a chemical library containing 160,000 compounds from The University of Tokyo, Drug Discovery Initiative, and found selective inhibitors for 3-mercaptopyruvate sulfurtransferase (3MST) (Sci. Rep. **2017**, 7:40227) and cystathionine γ-lyase (CSE). More recently, we newly developed a fluorescence probe for H_2S, which was especially aimed for in vitro assay, and enabled the inhibitor screening of cystathionine-β-synthase (CBS).

1SDA-1 Viral glycosylation: HIV-1 to SARS-CoV-2

Max Crispin (*School of Biological Sciences, University of Southampton, UK*)

Membranous viruses can exploit host-cell glycosylation for a variety of structural and functional roles. One aspect shaping viral glycosylation is immune evasion. Numerous human pathogens are heavily glycosylated including HIV-1, Lassa virus, influenza virus and SARS-CoV-2. In this talk, I will discuss viral glycosylation in the context of the efforts to develop an HIV-1 vaccine and contrast this to the glycosylation of a range of other human pathogenic viruses. I will assess to what extent recombinant glycoproteins mimic the viral spikes of native virions and the implications for vaccine design.

1SDA-2 Integrative methods in structural glycobiology

Jon Agirre (*University of York*)

Graphical software has enabled novice structural biologists to build protein models rapidly. In contrast, up until recently carbohydrates were in a different situation: scant automation existed, and users frequently tripped over issues such as incorrect dictionaries, forcing all refinement programs to produce high-energy conformations at low resolution. Recently, AlphaFold has delivered accurate but glycan-less structures of human glycoproteins, once again widening the gap between protein and sugars. To bring structural glycobiology up to protein standards, we are implementing a methodological overhaul, integrating prior knowledge from multiple techniques to help produce correct atomic models. The methods are part of Privateer, the software I will discuss in my talk.

1SDA-3 GLYCO: a tool to quantify glycan shielding of glycosylated proteins

Myungjin Lee (*National Institutes of Health*)

Glycans play important roles in protein folding and cell–cell interactions—and, furthermore, glycosylation of protein antigens can dramatically impact immune responses. While there have been attempts to quantify the glycan shielding of a protein surface, none of the publicly available tools analyzes glycan shielding computationally. Here, we developed an *in silico* approach, GLYCO (GLYcan COverage), to quantify the glycan shielding of protein surfaces. The software provides insights into glycan-dense/sparse regions of the entire protein surface or subsets of the protein surface. GLYCO calculates glycan shielding from a single coordinate file or multiple coordinate files. Overall, GLYCO provides fundamental insights into the glycan shielding of glycosylated proteins.

1SDA-4 Psme3 の部位特異的な *O*-GlcNAc 修飾は、P-body の恒常性の阻害を介してマウス ES 細胞の多能性維持に関与する
Site-specific *O*-GlcNAcylation of Psme3 maintains mouse embryonic stem cell pluripotency by impairing P-body homeostasis

Shoko Nishihara (*Glycan & Life System Integration Center (GaLSIC), Soka University*)

Recently, we have revealed that *O*-GlcNAc modification inhibits P-body formation and maintains mouse ES cell (mESC) pluripotency. P-bodies, membrane-less cytoplasmic organelles, are produced by liquid-liquid phase separation and regulate stem cell identity. *O*-GlcNAc on Ser111 of the proteasome activation subunit 3 (Psme3) promotes the degradation of DEAD box polypeptide 6 (Ddx6) required for P-body assembly, consequently reducing P-body amount. As a result, mRNAs encoding core transcription factors involved in the maintenance of pluripotency, such as Klf4 and Klf2, are translated and the pluripotency state is maintained. These findings establish *O*-GlcNAcylation at Ser111 of Psme3 as a critical switch that regulates mESC pluripotency via control of P-body homeostasis.

1SDA-5 Description of the dynamic conformation of oligosaccharides by combining NMR spectroscopy and molecular simulation

Takumi Yamaguchi[1,2] ([1]*School of Materials Science, Japan Advanced Institute of Science and Technology*, [2]*Graduate School of Pharmaceutical Sciences, Nagoya City University*)

To gain insights into the molecular basis of the biological functions of oligosaccharides, it is important to describe their conformational dynamics. The combination of NMR spectroscopy and molecular simulations is an effective way for providing the dynamical structural views of oligosaccharides. The quantitative description of their conformational spaces provides the dynamic views of oligosaccharide–lectin interactions, which complemented static insights from crystallographic analyses. We also attempted to develop a methodology for non-linear multivariate analyses of oligosaccharide conformational data to extract key structural features relevant to express their biological functions.

1SDA-6 病原性細菌における付着因子の糖鎖認識機構
Analyses of recognition mechanism and structure of bacteria FimH adhesin

Kaori Ueno-Noto (*Coll. Lib. Arts Sci., Kitasato Univ.*)

FimH is a surface protein of bacterial fimbrial tip, which mediates mannose-specific, multivalent, and shear-dependent binding to glycans. It is also involved in allosteric recognition due to its conformational changes. The glycan recognition mechanism of FimH and its structure, with and without shear force, were analyzed by molecular dynamics simulation based on its crystal structures. The interaction energies between FimH and glycans were also calculated by quantum chemical method, and they qualitatively agreed well with the experimentally obtained thermodynamic data. Furthermore, the interaction energies varied with the conformations of two tyrosine residues and an aspartic acid of the active site, suggesting their important role in the interaction.

1SEA-1 1800 nm フェムト秒ファイバーレーザーを用いた多光子蛍光顕微鏡
Multi-photon fluorescence microscopy using a 1800 nm femtosecond fiber laser system

Takao Fuji[1], Hideji Murakoshi[2,3], Hiromi Ueda[2,3], Kosuke Hamada[1], Ryuichiro Goto[4] ([1]*Toyota Technological Institute*, [2]*National Institute for Physiological Sciences*, [3]*The Graduate University for Advanced Studies*, [4]*Fiberlabs Inc.*)

We have developed a 1.8 μm 150 fs fiber laser system for multi-photon microscopy. The system starts from a commercially available erbium doped silica fiber laser and the wavelength is converted to 1.8 μm using a Raman shift fiber. The 1.8 μm pulses are amplified with a chirped pulse amplifier based on a two-stage thulium doped fluoride fiber amplifier. The final output power is about 0.5 W at the repetition rate of 500 kHz. The generated pulses are used for multi-photon fluorescence microscopy with which biological samples expressing red and green fluorescent proteins are observed through three- and four-photon excitation processes respectively. We also observed 0.8 mm deep inside the cortex of a living mouse using the system.

1SEA-2 高機能超短パルスファイバレーザーを用いた第 3 の生体の窓における生体深部イメージング
Deep tissue imaging using highly functional ultrashort pulse fiber laser in the third NIR optical tissue window

Norihiko Nishizawa[1], Masahito Yamanaka[2] ([1]*Department of Electronics, Nagoya University*, [2]*Department of Applied Physics, Osaka University*)

Optical coherence tomography (OCT) is non-invasive cross-sectional imaging technique with um resolution based on incoherent interferometer. One of the important tasks in OCT is the improvement of penetration depth in tissue samples. Recent studies showed that the use of the third NIR optical tissue window (1550-1850 nm) is useful for deep tissue imaging because of the low light scattering and local minima of water absorption. In our group, we developed three-dimensional, high resolution OCT and optical coherence microscopy (OCM) using a high power supercontinuum fiber laser source with 300 nm spectral bandwidth. The deep tissue imaging at a depth up to 1.8 mm was demonstrated successfully using the developed systems.

1SEA-3 非線形光学過程を利用した 2 種類の赤外超解像顕微鏡による生体試料の観察
Selective IR super-resolution imaging of biological samples by micro-spectroscopies based on non-linear optical process

Hirona Takahashi, Makoto Sakai (*Faculty of Sci., Okayama Univ. of Sci.*)

Keratin is one of the most important structural proteins. We have studied the distribution and orientation of keratins inside the feather, animal hairs and human nails by an IR micro-spectroscopy based on the vibrational sum-frequency generation (VSFG). VSFG is proportional to the second-order susceptibility and allows us to selectively detect only molecules located on the interfaces. Recently, we developed a new IR super-resolution micro-spectroscopy based on the 4-wave mixing, which is the third-order non-linear optical process, to detect keratin proteins in the bulk area. The IR imaging of secondary structures of keratin proteins will be presented with the features of the two IR super-resolution micro-spectroscopies.

1SEA-4 ロドプシンをモデルとした膜タンパク質の表面増強赤外分光計測による構造変化解析
Structural changes of rhodopsin studied by surface-enhanced infrared spectroscopy as a model system of membrane proteins

Yuji Furutani[1,2] ([1]*Grad. Sch. Eng., Nagoya Inst. Tech.*, [2]*OptoBio, Nagoya Inst. Tech.*)

Surface-enhanced infrared (SEIRA) spectroscopy has been applied to analyze protein structure and function with tiny amount of sample immobilized on the gold surface. Especially, it would be a powerful tool for the biophysical study of membrane proteins because it can imitate physiological condition of cell membrane to monitor protein-ligand and protein-protein interactions. Thus, it is expected to extend the SEIRA technique more widely in the field of biophysics. Rhodopsins have many functions such as light-driven pump, light sensors, light-gated channel and light-regulated enzyme, which are ideal for models of membrane proteins. In this talk, I would like to talk application of SEIRA on rhodopsins for discussing their protein structural changes.

1SEA-5 高速中赤外分光および顕微鏡
High-speed mid-infrared spectroscopy and microscopy

Takuro Ideguchi (*IPST, Univ. Tokyo*)

Mid-infrared spectroscopy is an essential tool in molecular science, and Fourier-transform infrared (FT-IR) spectroscopy is the gold standard for measuring broadband vibrational spectra. Although FT-IR spectrometers have been widely used in various fields for decades, recent rapid advancements in mid-infrared optical technology have enabled the development of advanced spectroscopy and microscopy techniques. In this talk, I will introduce high-speed mid-infrared spectroscopy and microscopy techniques that our group has developed in the last several years.

1SGA-1 DNA ナノテクノロジーを軸に挑む人工分子システム構築
Toward the construction of cell-like molecular systems based on DNA nanotechnology

Yusuke Sato (*Fac. Comp. Sci. and Sys. Eng., Kyushu Inst. Tech.*)

The construction of cell-like structures is one of the biggest challenges in science. It can contribute to developing technologies and revealing the origin of life. DNA nanotechnology provides a promising approach to the challenge because of programmable base-pairing, allowing for designing nanostructures and chemical reaction networks. Recently, controllable liquid-liquid phase separation (LLPS), a recent hot topic in biology, was demonstrated using sequence-designed DNAs. Here, I will show the DNA-based LLPS system and discuss its potential. Dynamic function and the formation of higher-order structures can be achieved by varying the structural design and molecular interaction. The DNA-based LLPS system will shed light on a new way to construct cell-like structures.

1SGA-2 (2Pos120) 人工核酸 PNA を用いた DNA の液ー液相分離制御
(2Pos120) Regulation of liquid-liquid phase separation of DNA using peptide nucleic acid (PNA)

Rikuto Soma, Yuichiro Aiba, Masanari Shibata, Shinya Ariyasu, Osami Shoji (*Graduate School of Science, Nagoya University.*)

The phenomenon of liquid-liquid phase separation (LLPS) in cells has attracted much attention, and it has become clear that nucleic acids also undergo LLPS. In this study, we developed a novel method to control the LLPS of DNA by using peptide nucleic acid (PNA), a type of artificial nucleic acid. PNA, which has a neutral peptide backbone, can form a stable duplex with complementary DNA, and its charge can be easily modulated by introducing amino acids into PNA. Therefore, PNA can potentially be applied to LLPS, where electrostatic interaction is one of the major driving forces. When PNA was mixed with target DNA, droplet formation was observed. Furthermore, we have succeeded in controlling the LLPS of DNA in a sequence-selective manner.

1SGA-3 Investigating the role of membrane biophysical properties on protein folding and sorting

Neha Kamat[1,2] ([1]*Department of Biomedical Engineering, Northwestern University*, [2]*Center of Synthetic Biology, Northwestern University*)

Membranes play a vital role in a variety of physiological processes. Recapitulating these processes outside of the cell may allow us to better understand them as well as design an entirely new class of materials that can sense, transport, or target important biological signals and molecules. In this talk, I will present our recent work using model membranes (ex. liposomes and polymersomes) and cell-free expression systems to: 1) uncover the role of membrane mechanical properties on the folding of model membrane proteins and 2) uncover how these properties impact protein sorting and interactions. Our approach bridges synthetic biology techniques and model membrane assembly to probe the role of membrane composition and biophysical properties on protein dynamics.

1SGA-4 脂質を合成する人工細胞
Lipid synthesis in artificial cell

Yutetsu Kuruma[1,2], Yasuhiro Shimane[1], Rumie Matsumura[1] ([1]*JAMSTEC*, [2]*JST PRESTO*)

One of the borders that separate life and non-life is the phenomenon of self-reproduction, which has not yet been reproduced within the frame of artificial cells. The construction of growing-and-dividing cells is an urgent mission in the fields of origin of life and synthetic biology. Here, we developed a fully reconstructed lipid synthesis system. The system produces phospholipids by synthesizing fatty acids and membranous enzymes. Because the system is an autonomous and sustainable system, it can be expected to function in the closed space of membrane vesicles. In this talk, I will discuss the way to build a self-propagating system and a possible scenario in which a life system has emerged from non-living objects.

1SGA-5 RNA 複製と進化のための区画構造
Compartmentalization for RNA replication and evolution

Ryo Mizuuchi[1,2] ([1]*Komaba Inst. Sci., Univ. Tokyo*, [2]*JST, PRESTO*)

Sustained replication and evolution of genetic molecules such as RNA are probable requisites for the emergence of life, but these steps are easily affected by the appearance of parasitic molecules that replicate by exploiting others. Compartmentalization, a means that restricts molecular interactions, is a way to prevent the complete dominance of parasites. In this talk, I will first describe how an RNA can undergo continuous evolution, using a reconstituted RNA replication system enclosed in water-in-oil droplets. Then I will report the use of liquid–liquid phase-separated droplets toward RNA replication and evolution while enabling the interaction with the environment. Finally, I will discuss primitive RNA replication that does not require compartmentalization.

1SGA-6 エクソソームが司る、がん転移の新しいストーリー
Exosomes, new players in the field of metastasis

Ayuko Hoshino (*Tokyo Institute of Technology*)

Exosomes, first thought to function only as cellular garbage disposal, are secreted by all cells and have recently been discovered that they also function as a cell-cell communication tool. We have previously shown that cancer cells send "exosomes" to the future site of metastasis to alter the environment to a favorable place where cancer cells can successfully metastasize. In this presentation, I will discuss how exosomes define the metastatic sites, potential of exosomes as a disease detection tool and how other type of disease could also be influenced by exchange of exosomes between the organs.

1SHA-1 骨格筋ミオシン，心筋ミオシン分子集団の自律特性が骨格筋，心臓収縮を作り出す
Autonomous characteristics of skeletal and cardiac myosin ensembles are essential for contractile functions of skeletal muscle and heart

Motoshi Kaya (*Grad. Sch. Sci., Univ. Tokyo*)

Skeletal or cardiac myosins form filaments of 300 molecules and interact with actin filaments to cause contraction in skeletal muscle or heart. Since the amino acid homology between these myosins is high, it has been thought that the contraction mechanisms are essentially the same. However, the morphological changes and functional requirements of skeletal muscle and heart are very different, and we investigated the molecular properties of these myosins. We found the significant differences in these properties and the autonomous functions expressed when they are ensembled. In this talk, I will discuss how the molecular properties of these myosins contribute to the autonomous functions of their ensembles, which characterize the contractile functions of each tissue.

1SHA-2 人工細胞による細胞動態の再構築：自発運動から波動現象の力学的理解へ向けて
Artificial cells: Reconstruction of cell-like behaviors from spontaneous migration to wave dynamics toward understanding cell mechanics

Ryota Sakamoto[1,2], Ziane Izri[3], Yuta Shimamoto[4], Makito Miyazaki[5,6,7,8], Yusuke Maeda[2] ([1]*Dept. Biomed. Engr., Yale Univ.*, [2]*Dept. Phys., Kyushu Univ.*, [3]*Dept. Phys., Minessota Univ.*, [4]*Natl. Inst. Genetics*, [5]*Hakubi Ctr., Kyoto Univ.*, [6]*Dept. Phys., Kyoto Univ.*, [7]*Institut Curie*, [8]*JST PRESTO*)

Precise control of cellular force generation is essential to achieve biological functions from cell migration to intracellular material transport. Such cellular force generation is mainly driven by the actin cytoskeleton, however, underlying mechanics is challenging to identify in living cells because of the overlapping complex signaling pathways. To overcome this bottleneck, we constructed an *in vitro* 'artificial cells' encapsulating cytoplasmic actin cytoskeleton into water-in-oil droplets to decouple the mechanics from biochemical signaling. In this talk, we outline our recently developed artificial cells showing cell-like behaviors from spontaneous droplet migration to actin wave dynamics and discuss how this growing paradigm expands our knowledge of cell mechanics.

1SHA-3 紡錘体の自己組織化ダイナミクスと微小管の集団運動メカニクス
Morphological growth dynamics and active microtubule mechanics underlying spindle self-organization

Yuta Shimamoto (*National Institute of Genetics*)

The spindle, needed for error-free segregation of chromosomes during cell division, is a dynamic structure self-organized from microtubules and microtubule-associated proteins. Whereas the cataloguing of molecules that build the spindle is essentially complete, how the molecules of nanometer-sized give rise to the defined cell-sized architecture remains a mystery. We use a combination of high-resolution imaging, machine learning, morphological profiling, and physical and chemical perturbations to study how this fundamental structure is built within a subcellular space. I'll share our recent findings on the multistable nature of spindle self-organization and the underlying microtubule mechanics, which explain how varied shape morpholgies emerge from a set of components.

1SHA-4 時計回りの組織形成を支える集団細胞移動の作動原理
Mechanical perspective of collective cell movement in epithelial morphogenesis

Erina Kuranaga (*Grad. Sch. Life Sci., Tohoku Univ.*)

The collective cell migration is a key process involved in epithelial morphogenesis. How migrating cells are able to maintain its collectivity and how it synchronizes multiple cells remained largely unknown as to its in vivo mechanisms. The male *Drosophila* external genitalia undergo a dynamic morphological change during the pupal stage, a 360° rotation. We have shown that this rotational movement is accomplished by a clockwise collective migration of the epithelial cells surrounding the external genitalia, which is driven by the continuous induction of the adherence junctions remodeling by actomyosin associated with the asymmetric planar polarity of individual epithelial cells. I would like to discuss the mechanism by which continuous junction remodeling is maintained.

1SHA-5 魚類表皮ケラトサイト集団ではリーダー細胞とフォロワー細胞が協調的かつ強制的にフォロワーをリーダーに昇進させる
Cooperative but forcible promotion of follower cells to leaders in collective migration of fish keratocytes

Yoshiaki Iwadate (*Dept. Biol., Yamaguchi Univ.*)

In the collective migration of keratocytes, the epidermal cells of fish responsible for wound repair, all the cells at the front row have polarized lamellipodia that are characteristic of leader cells, and are interconnected with each other via actomyosin cables. The leading edge of the collective becomes gradually longer while maintaining the same shape as it advances, regardless of the cell-to-cell connections. In this study, we will show the unique interaction of follower cells with their neighbouring two leader cells that enable elongation of the leading edge. A mechanical interaction between two leader cells and a single follower cell forcibly breaks the connection between the two leader cells and promotes the follower cell into a leader cell.

1SHA-6 Interaction rules within multicellular dynamics and biological condensates

Kawaguchi Kyogo (*RIKEN CPR/BDR*)

An outstanding theme of biophysics is to understand the rules of the collective dynamics at multiple scales, ranging from multicellular tissues to biomolecules. For the tissue level dynamics, we have been studying how cultured neural progenitor cells (NPCs), which undergo self-propelled motion with liquid-crystal-like cell-to-cell interactions, can exhibit large structures with handedness by controlling the initial seeding condition. Here we will describe our recent results on estimating the interactions between the cells that consistently explain such macroscopic behavior. If time allows, we will also describe our recent work on estimating the rules of subcellular localization of intrinsically disordered regions in proteins.

1SAP-1 超高周波超音波照射下での分子動力学シミュレーションによるタンパク質-医薬品結合プロセスの加速
Hypersound-perturbed molecular dynamics to accelerate slow protein-ligand binding processes

Mitsugu Araki, Yasushi Okuno (*Grad.Sch.Med., Kyoto Univ.*)

We developed a method to accelerate MD simulations by high-frequency ultrasound (hypersound) perturbation. The binding events between the protein CDK2 and its small-molecule inhibitors were nearly undetectable in 100-ns conventional MD, but the method successfully accelerated their slow binding rates by up to 10-20 times. Hypersound-accelerated MD simulations revealed a variety of microscopic kinetic features of the inhibitors on the protein surface, such as the existence of different binding pathways to the active site. Moreover, the simulations allowed the estimation of the corresponding kinetic parameters and exploring other druggable pockets. This method can thus provide deeper insight into the microscopic interactions controlling biomolecular processes.

1SAP-2 スーパーコンピューター「富岳」による創薬へ向けた自由エネルギー摂動法の開発
Development of the free-energy perturbation method toward drug discovery on supercomputer Fugaku

Hiraku Oshima[1], Yuji Sugita[1,2,3] ([1]*RIKEN BDR*, [2]*RIKEN R-CCS*, [3]*RIKEN CPR*)

The free energy perturbation (FEP) method is one of the most essential tools to predict the binding affinity. When the particle mesh Ewald is used, conventional FEP requires additional fast Fourier transformations (FFT) to calculate electrostatic interactions, which largely decreases the computational performance. To overcome this problem, we propose a modified FEP scheme by introducing non-uniform scaling parameters into the Hamiltonian, which does not require additional FFT calculations. We implemented modified FEP into “GENESIS”. Modified FEP greatly improves the computational performance, which is marked for large biomolecular systems. Using supercomputer Fugaku, modified FEP might be applied to drug discovery in large biosystems, which are impossible before.

1SAP-3 Binding Kinetics of Kinase Complexes by PaCS-MD/MSM

Kazuhiro Takemura, Akio Kitao (*SLST, TokyoTech*)

We applied a sampling method, dissociation parallel cascade selection-MD (dPaCS-MD), combined with the Markov state model (dPaCS-MD/MSM), to several kinase complexes to calculate the binding free energy and association/dissociation rate constants. By repeating cycles of multiple parallel short MD simulations combined with initial structure selection having larger inter-molecular distances, dPaCS-MD efficiently simulated the dissociation of kinase-inhibitor complexes. The binding free energies of all complexes and parts of association/dissociation constants were accurately calculated by dPaCS-MD/MSM. The suitable selection of collective variables improved the evaluation of association/dissociation rate constants.

1SAP-4 MD シミュレーションで考える抗原-抗体界面：合理的な抗体医薬品設計に向けて
A molecular dynamics study on the antigen-antibody interface: Toward rational antibody drug design

Takefumi Yamashita (*The University of Tokyo*)

Antibodies recognize foreign substances (antigens) to trigger the immune response. Due to this feature, high-affinity antibodies have been used as drugs. Recently, we have investigated an antibody (B5209B) targeting ROBO1, which is expressed in liver cancer. We found that the stabilization of the salt bridge between ROBO1 and B5209B is an important factor in the design of the antibody. Then, we developed a constitutive analysis to identify the factors governing the stability of the salt bridge and found that the hydrophobic interactions of tryptophan and tyrosine are also important. Using these MD simulation-based analyses, we will be able to efficiently discover structural motifs for antibody modification and hints on how to modify them.

1SAP-5 大規模分子動力学シミュレーションを用いた上皮成長因子受容体キナーゼの活性化メカニズムの研究
A study of activation mechanism of epidermal growth factor receptor kinase using large-scale molecular dynamics simulations

Masao Inoue[1], Toru Ekimoto[1], Tsutomu Yamane[2], Mitsunori Ikeguchi[1,2] ([1]*Grad. Sch. Med. Life Sci., Yokohama City Univ.*, [2]*RIKEN R-CCS*)

The epidermal growth factor receptor (EGFR) has been studied extensively as a drag target because its mutations have been known to cause various kinds of cancer. The kinase domain of the EGFR forms an asymmetric dimer in its activation process. We study the activation mechanism of the EGFR kinase dimer by large-scale molecular dynamics (MD) simulations using the supercomputer Fugaku. Using the obtained MD trajectories, we build the Markov state model (MSM). This MSM analysis provides us with deep insight into the intermediate structures via which the EGFR kinase structure changes from the inactive state to the active one. Particularly, we focus on the structural change of the dimer interface and the relation between the kinase activation and dimerization.

1SAP-6 Extracting protein dynamics from experimental cryo-EM maps using a machine learning technique combining with MD simulations

Shigeyuki Matsumoto[1], Shoichi Ishida[2], Kei Terayama[2], Yasushi Okuno[1,3] ([1]*Grad. Sch. Med., Kyoto Univ.*, [2]*Grad. Sch. Med. Life Sci., Yokohama City Univ.*, [3]*RIKEN R-CCS*)

Technical breakthroughs in single-particle analysis based on cryo-electron microscopy (cryo-EM) have solved the three-dimensional structures of numerous proteins. However, the analysis of their dynamics is often challenging because of their large molecular sizes and complex structural assemblies. Here, we have developed a molecular dynamics (MD) simulation-combined deep learning approach to directly extract the dynamics that are hidden in cryo-EM density maps, named as DEFMap. Using only cryo-EM density data, DEFMap provides dynamics that correlate well with data obtained from MD simulations and experimental approaches. Furthermore, DEFMap successfully detects changes in dynamics that are associated with molecular recognition.

1SBP-1 ナトリウムポンプのつくりかた
How to make a sodium pump

Kazuhiro Abe (*CeSPI, Nagoya Univ*)

P-type 2 ATPases are a family of ion pumps that build ionic gradients across biological membranes in all phyla. The sodium pump (NKA) transports three Na^+ ions in exchange for two K^+ ions per ATP hydrolyzed. This electrogenic transport contrasts with the electroneutral transport of non-gastric (ngHKA) proton pumps. The molecular basis for their distinctly different selectivity remains unknown. Here we combine functional measurements with cryo-EM structures to demonstrate that substituting four NKA residues in the ion-binding-site region of the ngHKA catalytic subunit is necessary and sufficient to convert the electroneutral ngHKA into a canonical electrogenic NKA. Our results resolve a decades long enigma of how these close relatives perform their distinct functions.

1SBP-2 光可逆的蛋白質ラベル化システムによる細胞内蛋白質動態と細胞機能の光制御
Optical control of intracellular protein dynamics and cellular functions using a photoreversible protein labeling system

Shin Mizukami (*IMRAM, Tohoku Univ.*)

Spatiotemporal control of intracellular protein networks helps clarify intracellular molecular networks. Thus, optogenetics and caged compounds have received significant attention. Currently, we are developing a small molecule-protein hybrid system that optically controls cellular functions. For the applications, we have developed a photoreversible protein labeling system based on a photochromic ligand. By applying this technology to protein dimerization systems, we achieved the quick and repetitive regulation of subcellular protein localization by alternating different-wavelength light irradiation. Using this system, we attempted the photoinduction of mitophagy by controlling a protein network on the mitochondrial outer membrane.

1SBP-3 分離した RNP ミセルとしてのパラスペックル核内構造体の構築機構
Construction mechanism of nuclear paraspeckle as an isolated RNP micell

Tetsuro Hirose[1,2], Takakuwa Hiro[1,3], Yamamoto Tetsuya[4], Yamazaki Tomohiro[1] ([1]*Grad. Sch. Front. Biosci., Osaka Univ*, [2]*OTRI, Osaka Univ*, [3]*Grad. Sch. Med., Hokkaido Univ*, [4]*ICReDD, Hokkaido Univ*)

Paraspeckles are membranless nuclear bodies constructed by NEAT1_2 architectural lncRNA. Paraspeckles exhibit characteristic cylindrical shapes with an internal shell/core organization and a distinct size. These features can be explained by our recent model that paraspeckles behave as block copolymer micelles assembled through a type of microphase separation, micellization. In the nucleus, various nuclear bodies separately exist in the interchromatin space. We unexpectedly found that the paraspeckles formed with specific NEAT1_2 mutants were engulfed by another nuclear body, nuclear speckle. This observation suggests the existence of the mechanism to maintain the isolated state of paraspeckle in the nuclear space, which is operated by the specific NEAT1_2 domain.

1SBP-4 細胞内における酵母プリオン伝播のクロススケール解析
Cross-scale analyais of yeast prion propagation in cells

Motomasa Tanaka (*RIKEN Center for Brain Science*)

Disaggregation of amyloid fibrils is a fundamental biological process required for amyloid propagation. Here, we established a robust in vitro reconstituted system of yeast prion propagation and found that heat-shock protein 104 (Hsp104), Ssa1 and Sis1 chaperones are essential for efficient disaggregation of Sup35 amyloid. Real-time imaging of single-molecule fluorescence coupled with the reconstitution system revealed that amyloid disaggregation is achieved by ordered, timely binding of the chaperones to amyloid. These findings provide a physical foundation for otherwise puzzling in vivo observations and for therapeutic development for amyloid-associated neurodegenerative diseases.

1SBP-5 原子間力顕微鏡を用いた生きた細胞のメゾスケール表面構造体及び内部構造体観察方法の開発
Development of the method for observing mesoscale structures outside and inside living cells using atomic force microscopy

Takehiko Ichikawa[1], Marcos Penedo[2], Keisuke Miyazawa[1,3], Hirotoshi Furusho[1], Mohammad Shahidul Alam[1], Kazuki Miyata[1,3], Chikashi Nakamura[4], Takeshi Fukuma[1,3] ([1]*NanoLSI, Kanazawa Univ.*, [2]*Inst. Bioeng., EPFL*, [3]*Frontier Eng., Kanazawa Univ.*, [4]*CMB, AIST*)

Direct observation of the mesoscopic protein complexes is essential for understanding life phenomena and diseases. So far, electron microscopy and fluorescence microscopy have been used to observe these scale structures. However, electron microscopy cannot observe living cells, and fluorescence microscopy does not have enough resolution to observe the mesoscopic structures. Atomic force microscopy (AFM) has a high enough resolution and can observe living cells, but it has not been adopted for living cells at this resolution. Here, we report the two novel methods to observe the mesoscale structures on the cell surface and inside the living cells using AFM.

1SBP-6 Structure modeling of protein complex from experimental data using molecular dynamics simulation

Takaharu Mori (*RIKEN CPR*)

Recently, single particle analysis, cryo-electron tomography, and high-speed AFM have enabled us to observe the structure and dynamics of protein complexes at high resolution or in real time. On the other hand, experimental data usually contains dynamic effects, noise, or low local resolution, which must be carefully dealt in the structure modeling. We have developed the molecular dynamics (MD) program GENESIS and have been working on the development of the MD-based protocols for structure modeling of biomolecular complexes from experimental data such as cryo-EM flexible fitting. In the presentation, we introduce our recent developments and applications in experimental data analysis and discuss prospects for reliable structural modeling.

1SBP-7 Ferritin phase separation driven by NCOA4 promotes two types of ferritin autophagy, macro-autophagy and endosomal micro-autophagy

Hayashi Yamamoto (*Grad. Sch. Med., Univ. Tokyo*)

Ferritin is an iron storage protein that forms cage-like particles and plays a key role in iron homeostasis. To reuse the stored iron ions, ferritin particles are transported to lysosomes via two different pathways, autophagy (macro-autophagy) and ESCRT-dependent MVB-like pathway (endosomal micro-autophagy). Here, we show that ferritin particles assemble to form mesoscopic condensates through LLPS driven by NCOA4. The liquid-like ferritin condensates are degraded by macro-autophagy and endosomal micro-autophagy, thus both of which are considered a type of "fluidophagy". In this symposium, we would like to discuss how liquid-like mesoscopic condensates are commonly recognized by two different organelles, autophagosomes and endosomes.

1SCP-1 ネットワーク構造に基づく細胞運命の制御
Controlling cell fate specification system based on network structure

Atsushi Mochizuki (*Inst. Life Med. Sci, Kyoto Univ.*)

In modern biology, we have many examples of large networks describing regulatory interactions between biomolecules. On the other hand, we have a limited understanding of dynamics of such complex systems. We developed the Linkage Logic theory, by which key molecules to identify/control the dynamics of a whole system can be determined from the information of the network alone. We applied the theory to the gene regulatory network for the fate specification of seven tissues in ascidian embryos, including more than 90 genes. The analysis showed that dynamical attractors possibly generated by the network should be identified/controlled by only 6 genes. We verified that all the seven tissues could be induced deterministically by experimental manipulations of these 6 genes.

1SCP-2 摂動後の発現時系列データを用いた遺伝子制御ネットワーク推定法
Estimating gene regulatory network using time-series expression data following gene perturbation

Masato Ishikawa[1], Mototsugu Eiraku[2], Kosuke Yusa[2], Yuhei Yamauchi[2], Hisanori Kiryu[1], Atsushi Mochizuki[2] ([1]*Grad. Sch. Front. Sci., UTokyo*, [2]*Inst. Life Med. Sci., Kyoto Univ.*)

Gene expression dynamics during cell differentiation are driven by gene regulatory networks (GRNs). The most reliable way to estimate the correct GRNs is to perturb gene expression and investigate its effects. The recently developed pooled CRISPR screen has made it possible to measure changes in expression after knocking out each of many genes. However, existing methods for GRN estimation have not taken full advantage of such data.
We developed RENGE, a method to estimate GRNs using time-series gene expression data following gene perturbation. RENGE models how perturbation effects propagate through a GRN. We applied our method to the simulated data and human iPS cell data, showing that it performs better than the other methods.

1SCP-3 ネットワーク構造から生化学反応の摂動応答を決める
Network architecture determines sensitivity of biochemical reaction systems

Takashi Okada[1], Je-Chiang Tsai[2], Atsushi Mochizuki[1] ([1]*Inst. Life Med. Sci, Kyoto Univ.*, [2]*National Tsing Hua University, Taiwan*)

In metabolic networks, biochemical reactions connect and form complex networks. One experimental approach to studying them is sensitivity experiment, which measures the responses under enzymatic perturbations. However, because detailed kinetics are unknown, it has been unclear how the experimental results can be explained theoretically. In this talk, we introduce our original mathematical method, called structural sensitivity analysis, which determines responses only from the information of network structures. We also find a mathematical theorem that explains responses in terms of network topology. We discuss how our theoretical method can be utilize to understand biological functions of real metabolic networks.

1SCP-4 複雑な化学反応ネットワークを単純化する
Simplifying complex chemical reaction networks

Yuji Hirono (*Asia Pacific Center for Theoretical Physics*)

Chemical reactions form a large web of networks inside living cells and they are responsible for physiological functions. Understanding the behaviors of complex reaction networks is a challenging and interesting task. In this talk, I will introduce a systematic method for simplifying chemical reaction networks. We identify the structural condition under which a subnetwork can be eliminated without altering the steady-state properties of the remaining parts. The condition is solely determined by the structural information and is insensitive to the details of reactions, because of which the method is widely applicable. The techniques of homological algebra are found to be useful in deriving the result.

1SCP-5 開放系トポロジカル相
Topological phases in open systems

Masatoshi Sato (*Yukawa Institute for Theoretical Physics, Kyoto University*)

The concept of topological phases, which distinguishes "states" by the difference in the way they are connected, is now one of the fundamental principles for the development of materials. Traditionally, the theory of topological phases has been developed based on the Hermite Hamiltonian, which describes isolated systems, but recently it has been discovered that new topological structures exist in open systems that have lost their Hermitian nature due to environmental effects and dynamic structures. This finding has led to expanding the target systems of topological phases. This talk will review the basic idea of open system topological phases (=non-hermitian topological phases) and their possible applications to complex systems.

1SDP-1 圧力ジャンプ法による液液相分離の速度論解析：RNA 結合タンパク質 FUS
Pressure-jump kinetics of liquid-liquid phase separation (LLPS) : The RNA-binding protein fused in sarcoma (FUS)

Ryo Kitahara[1,2], Shujie Li[2], Takuya Yoshizawa[3] ([1]*Coll. Pharm. Sci., Ritsumeikan Univ.*, [2]*Grad. Sch. Pharm. Sci., Ritsumeikan Univ.*, [3]*Coll. Life Sci., Ritsumeikan Univ.*)

Liquid droplets, namely, LLPS, of the FUS protein transform into reversible hydrogels and into more irreversible and toxic aggregates. We demonstrated the pressure-jump kinetics of phase transition between the 1-phase and FUS-LLPS states observed at low pressure (<2 kbar, LP-LLPS) and high pressure (>2 kbar, HP-LLPS) using high-pressure UV-Vis spectroscopy. Turbidity changes were reproduced repeatedly using pressure cycles, indicating that the transitions are reversible. The HP-LLPS formation and vanishing rates were 2-fold and 20-fold slower, respectively, than those of LP-LLPS. We also found that the longer FUS remained on HP-LLPS, the harder it was to transform into 1-phase. These results indicate that the liquid-to-solid phase transition is accelerated in HP-LLPS.

1SDP-2 アミノ酸の溶解性に基づくタンパク質の液- 液相分離
Liquid-liquid phase separation of proteins based on the solubility of amino acids

Akira Nomoto, Kentaro Shiraki (*Pure and Appl. Sci., Univ. Tsukuba*)

Liquid-liquid phase separation (LLPS) of proteins is regulated by multivalent interactions between amino acids. However, there are no parameters that can compare the strength of interaction between amino acids in aqueous solution. Here we examined the solubility of amino acids in amino acid solvents and calculated the transfer free energy (ΔG_{tr}) of amino acids from water to amino acid solvents. The ΔG_{tr} of aromatic amino acids and glycine varied significantly depending on the type and pH of amino acid solvent. The ΔG_{tr} can represent how favorable the affinity between amino acids is for the aqueous solvents. We believe that the ΔG_{tr} is the simplest parameter for understanding the propensity of LLPS of proteins based on the solution property of each amino acid.

1SDP-3 Raman and Brillouin microscopy as a tool for quantitative study of LLPS

Shinji Kajimoto[1,2] ([1]*Grad. Sch. Pharm. Sci., Tohoku University*, [2]*JST PRESTO*)

Liquid-liquid phase separation (LLPS) of proteins and other biomolecules has been attracted great interests of cell biologists. Since LLPS is a phenomenon resulting from the net balance of weak inter- and intramolecular interactions, label-free methods are desirable for its observation. In this presentation, we propose Raman and Brillouin microscopy as a promising tool for study of LLPS, which offers quantitative *in-situ* observation of single droplets in label-free manner. From the simultaneous Raman and Brillouin imaging of a single droplet, we can analyze the quantitative molecular distribution and molecular structures, as well as the stiffness of the droplet.

1SDP-4 液–液相分離会合体の分子取り込みと並進拡散運動に関する分子文法解析
Molecular grammar characterization of recruitment and translational dynamics of guest proteins in liquid droplets

Kiyoto Kamagata (*IMRAM, Tohoku Univ.*)

Despite the continuous discovery of host and guest proteins in membraneless organelles, complex host–guest interactions hinder the understanding of the molecular grammar governing liquid–liquid phase separation (LLPS). In this study, we characterized the recruitment and dynamic properties of guest proteins in liquid droplets using single-molecule fluorescence microscopy and molecular dynamics simulation (Sci. Rep. 2021, 2022). The recruitment property was significantly affected by host proteins and determined by intermolecular interactions and/or void-size in droplets. The diffusion of guests did not depend on host proteins, but depended on structural types: folded and disordered. These results provide molecular grammar used in cellular LLPS.

1SDP-5 分子動力学シミュレーションと機械学習を組み合わせたペプチド凝集予測
Prediction of peptide aggregation by combining molecular dynamics simulation and machine learning

Tomoshi Kameda (*AIRC, AIST*)

Machine learning is an effective method for evaluating the physical properties of proteins and peptides. However, it requires a large amount of training data through experiments. In this study, instead of experiments, we combined machine learning and molecular dynamics (MD) simulations to predict the physical properties of mutants. We apply the methods to predict the aggregation property of four amino acid peptides with a sequence space of 160,000 (=20^4). All-atom MD simulations of 319 peptides were performed, which were used as training data for machine learning. Our method predicted the peptides with N-terminal proline have a high aggregation tendency. We have proved that these peptides crystallize by experiments and succeed in getting the steric structure.

1SEP-1 マイクロ・ナノ加工技術を用いた 3D 腫瘍組織構築と新しいがん創薬開発にむけて
Construction of 3D tumor tissue using micro/nano processing technology and toward to development of new drug discovery

Kaori Kuribayashi-Shigetomi (*Inst. Adv. High. Edu., Hokkaido Univ.*)

We develop a micro/nano-sized pattern substrate in which cancer cells spontaneously construct three-dimensional tumors. Nano-sized surface roughness is created inside the micro-sized pattern. In this research, we are able to form the tumors that are closer to the one in the living body *in vitro*. This has made it possible to observe living tumor in real time, which was not possible until now. Furthermore, as a result of seeding cells with differences in malignancy on the substrate, we found that their behaviors were different. Since the substrate can be created by simply dappling a surface treatment to a glass substrate, it is considered possible to achieve high throughput that can be applied to future new drug development.

1SEP-2 Crosstalk between myosin II and formin in the regulation of force generation and actomyosin dynamics in stress fibers

Yukako Nishimura[1,2], Shidong Shi[2], Virgile Viasnoff[2,3], Alexander Bershadsky[2,4] ([1]*IGM, Hokkaido Univ.*, [2]*MBI, NUS, Singapore*, [3]*Dept.of Biol.Sci., NUS*, [4]*Dept. of Mol. Cell Biol., Weizmann Inst.*)

The coordination of contractile activity with its molecular turnover is crucial for many cellular functions. Here, we developed a methodology that enabled the simultaneous measurement of mechanical forces exerted by actomyosin stress fibers and the high-resolution dynamics of actin and myosin in REF52 cells. We revealed that 1) stress fiber turnover depends on myosin II activity, and 2) generation of traction forces requires not only myosin II activity but also formin functions. This previously overlooked function of formins in maintenance of the actin cytoskeleton connectivity could be the main mechanism of formin involvement in traction force generation. Our data revealed new features of the crosstalk between actomyosin contractility and stress fiber dynamics.

1SEP-3 (3Pos312) Triple-color photothermal dye-based nanoheaters to generate multiple heat spots within a single cell

Md Monir Hossain, Takeru Yamazaki, Kayoko Nomura, Satoshi Arai (*Grad. Sch. NanoLS., Kanazawa Univ.*)

Nano-heating technology enables spatiotemporal temperature control for the investigation of thermal effects on the subcellular microenvironment. Here, we designed a photothermal dye-based nanoheater that allows to create the subcellular sized heat spot with concurrent fluorescent thermometry. Specifically, three different photothermal dyes were embedded into the polymeric particles, respectively. An individual nanoheater could be operated by a relevant near-infrared laser at 808, 855, and 980 nm. When three nanoheaters were applied to a live cell, we could achieve to produce multi-heat spots within a single cell at the same time. We further attempted to alter energy metabolism and muscle contractions locally by the combination of three nanoheaters and different lasers.

1SEP-4 Evaluation of the physicochemical properties of biomolecules using microdroplets

Ryo Iizuka (*Dept. of Biol. Sci., Grad. Sch. of Sci., The Univ. of Tokyo*)

Microfluidics allows ultrarapid production of monodisperse microdroplets such as water-in-oil microdroplets. Each microdroplet serves as a nano/picoliter-volume test tube, enabling the isolation and parallel processing of thousands of individual molecules and cells under defined conditions. Here, I will demonstrate that microdroplets can be used to evaluate the physicochemical properties of biomolecules. First, I will present a method for screening single microbial cells that secrete hydrogel-degrading enzymes using deformability-based microfluidic microdroplet sorting. Second, I will show the effect of the microenvironments created by microdroplets on polynucleosome condensation. I hope my talk provides you with a hint on what you are planning next.

1SEP-5 (3Pos093) Control of small G-protein Ras using calmodulin-based ionochromic molecular device.

Yassine Sabek, Nobuyuki Nishibe, Kazunori Kondo, Shinsaku Maruta (*Graduate school of science and engineering , department of biosciences , soka university, Hachioji TOKYO*)

A small G-protein (RAS) which leads to the stimulation of downstream pathways, playing an important role in cell proliferation, and differentiation among others may also promote tumorigenesis. We have been studying to control Ras function using photochromic molecular devices. In this study, we used Calmodulin as an ionochromic molecular device to control Ras with Ca^{2+} ions. Calmodulin fusion protein with inhibitory peptide for Ras and M13 calmodulin target peptide (CAM-I-M13) was designed and prepared by the E.coli expression system. CAM-I-M13 exhibited different inhibitory activities for Ras GTPase between the conditions in the presence and absence of Ca^{2+}. Ca^{2+}-dependent reversible binding of CAM-I-M13 was also examined by size-exclusion-HPLC

1SEP-6 (1Pos283) Centromere-kinetochore structures revealed by 12x modified expansion microscopy

Yasuhiro Hirano[1], Aussie Suzuki[2], Yasushi Hiraoka[1], Tatsuo Fukagawa[1] ([1]*Graduate School of Frontier Biosciences, Osaka University*, [2]*McArdle Laboratory for Cancer Research, University of Wisconsin-Madison*)

The kinetochore is essential for faithful chromosome segregation during mitosis and is assembled on centromeres through dynamic processes involving numerous kinetochore proteins. However, the orientation of the kinetochore proteins remains elusive because of the limitation of fluorescence microscopy resolution despite super-resolution microscopies enabling us to resolve 50-100 nm structure. In this study, we applied 12x modified expansion microscopy (mExM) and obtained a diffraction-limited resolution in the expanded sample that corresponds to ~30 nm resolution in the original sample under conventional microscopy. By using the mExM, we found that constitutive centromere-association network proteins, CENP-T and CENP-C, formed a different structure in the kinetochore.

1SEP-7 ボトムアップポリマーナノテクノロジーを用いたミクロレベル・マクロレベルの液液相分離制御
Control of the microscopic and macroscopic liquid-liquid phase separation based on bottom-up polymer nanotechnology

Akihiro Kishimura (*Department of Applied Chemistry, Faculty of Engineering, Kyushu University*)

Coacervates are a well-known liquid-liquid phase separation state, and their relevance to biological systems, e.g., biomolecular condensates or membraneless organelles, has been intensively discussed. Our project aimed to control the micro- and macroscopic structure of complex coacervates using bottom-up molecular technology. We developed the method for microstructure control of complex coacervates based on synthetic-polypeptide-based block copolymers, which are typically composed of charge-neutral polymer, PEG, and poly(aspartic acid)s. Next, we tried to obtain hierarchical structures and successfully developed novel (sub)micron-sized structures. Also, unique multiphase coacervates were developed, in which the arrangement of different droplets was controlled.

1SEP-8 発色団補助光不活化法 (CALI) の基礎と利用
Basics and applications of chromophore-assisted light inactivation (CALI)

Akira Kitamura (*Fac. Adv. Life Sci., Hokkaido Univ.*)

Chromophore-assisted light inactivation (CALI) enables the destruction of proteins of interest through reactive oxygen species (ROS) that are produced by photosensitizer fluorescent probes. However, the photophysical characterization remains elusive, and its application has not been fully established. Here, we present an understanding of the wavelength selectivity of photosensitizers and their application to the inactivation of cellular condensates. Our talk will provide an insight into the cutting-edge availability of photosensitizers for CALI.

1SFP-1 Uptake mechanisms of cell-penetrating peptides

Christian Widmann (*University of Lausanne, Switzerland*)

Cell-penetrating peptides (CPPs) are used in research and for therapeutic purposes to carry a variety of cargos into cells and tissues. These peptides can enter cells in two ways: through direct translocation of the plasma membrane or via endocytosis. In this presentation, I will describe how ~2nm-wide water pores in the plasma membrane are formed to allow CPPs to access the cytosol by direct translocation. I will also describe our findings that CPPs are taken up by a previously uncharacterized endocytic pathway that moves material to non-acidic Lamp1-positive late endosomes in a Rab14-dependent manner but that is fully independent of Rab5 and Rab7. Finally, I will show that CPPs have a very limited endosomal escape capacity.
Website: https://wp.unil.ch/widmannlab/

1SFP-2 Roles of membrane lipids in the organization of cell-cell adhestion structure

Junichi Ikenouchi (*Grad. Sch. Sci., Kyushu Univ.*)

Lipids have the ability to self-organize. However, the significance of this phenomenon in the organization of membrane structures remains unknown. Tight junctions (TJs) are cell-adhesion structures responsible for the epithelial barrier. We previously reported that accumulation of cholesterol at TJs is required for TJs formation. However, it is unclear whether cholesterol enrichment at apical junctions precedes or follows the assembly of cell adhesion molecules (claudins). To answer this question, we recently established an epithelial cell line (claudin-null cells) that lacks TJs by suppressing the expression of claudins. In this presentation, I would like to discuss a novel mechanism for TJ formation that is dependent on cholesterol.

1SFP-3 (2Pos198) Mechanism study of antimicrobial peptide synergistic effects at the molecular level by combining spectroscopy and electrochemical methods

Yuge Hou, Kaori Sugihara (*Institute of Industrial Science, The University of Tokyo,*)

In 2020, Sugihara Group has reported that antimicrobial peptides LL37 and HNP1 cooperatively protects mammalian cell membranes from lysis for minimizing the cytotoxicity in contrast to known synergistic effect against bacteria. Previous study also showed that the synergy among LL37 and HNP1 would greatly increase the killing ability to E. coli. In this project, we study why the LL-37/HNP1 cooperativity enhances the cytotoxicity of E. coli? How the changes in the electric property and composition of membrane will affect the interaction with peptides. Black lipid membrane, circular dichroism, dynamic light scattering and isothermal titration calorimetry measurements will be employed to further understand the interaction mechanism.

1SFP-4 Biofunctional peptide-modified exosomes for intracellular delivery

Ikuhiko Nakase (*Grad. Sch. Sci., Osaka Metropolitan Univ.*)

We have been developing exosomes (extracellular vesicles, EVs)-based therapeutic technologies by effective usage of peptide chemistry to deliver therapeutic/diagnostic molecules into targeted cells. With pharmaceutical advantages of the EVs as carriers for intracellular delivery, our research team has been developing techniques for easily modifying biofunctional peptides on EV's membranes for receptor targeting (e.g., artificial coiled-coil peptides), enhanced cellular uptake (e.g., cell-penetrating peptides), and cytosolic release (e.g., membrane fusion peptides). The experimental techniques of EV-based delivery with modification of biofunctional peptides and crucial points for controlling EVs uptake via macropinocytosis will be introduced and discussed.

1SFP-5 Membrane shaping by the BAR domain superfamily proteins and the extracellular vesicles by the shedding of filopodia

Shiro Suetsugu[1,2,3] ([1]*Biological Science, Nara Institue of Science and Technology*, [2]*Data Science Center, Nara Institue of Science and Technology*, [3]*Digital Green-Innovation, Nara Institue of Science and Technology*)

There are various membrane curvatures of the cellular membrane. The Bin-Amphiphysin-Rvs (BAR) family domain proteins are the scaffolds for membrane curvatures. Typically, BAR domain proteins are involved in endocytic pit formation and vesicle formation. In contrast, the I-BAR domain proteins, including Missing-in-metastasis (MIM), promote filopodia formation. However, the involvement of the BAR domain proteins in extracellular vehicles (EVs) generation remains unclear. We found that the filopodia that are induced by the I-BAR domain proteins are susceptible to being shredded into EVs. Interestingly, the shedding was promoted by *in vivo* equivalent external forces. These results indicated that some populations of EVs are generated from I-BAR-domain-dependent filopodia.

1SFP-6 Investigating the mechano-osmotic regulation of cell membrane tension using fluorescent membrane tension probes

Aurelien Roux[1,2] ([1]*Department of Biochemistry, CH-1211, University of Geneva*, [2]*NCCR Chemical Biology, CH-1211, University of Geneva*)

Because plasma membrane rupture leads to lysis, regulating plasma membrane tension is thus a question of life and death for cells. Many players are actively controlling cell membrane tension during events that pertub its functions: osmotic shocks, cell migration or tissue morphogenesis. But because tools to monitor membrane tension in space and time were lacking, the quantitative analysis this regulation remained poor. Together the group of Stefan Matile, University of Geneva, we have developped and characterized membrane tension probes called flippers. Using these tools, I will review recent work from our group showing how membrane tension is being regulated during osmotic shocks and morphogenesis, and participate in the control of many cell functions.

1SGP-1 高次構造体の協奏的機能を合理的に制御することを目指して
Toward rational control of concerted functions by supramolecular assemblies

Takahiro Kosugi[1,2,3,4] ([1]*IMS*, [2]*SOKENDAI*, [3]*ExCELLS*, [4]*PRESTO, JST*)

Concerted functions of supramolecular assemblies (protein complexes) in biomolecular systems are exerted by orchestrating the cooperative works between the constituent subunits. No study on rational control of concerted functions have been reported, although recently several protein design methods have been developed and native proteins have been successfully redesigned to regulate or change the functions. Here, I show an approach to designing allosteric sites which provide novel orchestration into protein complexes and report a concerted function, rotation rate, of a molecular motor V_1-ATPase was successfully regulated by the approach. Moreover, I will talk about recent applications and future potentials of the approach.

1SGP-2 タンパク質合成を司る高次構造体を操る：リボソームの光制御
Controlling a supra-assembly dedicated to protein synthesis: optogenetic control of ribosomes in the cell

Takeshi Yokoyama[1,2,3] ([1]*Grad. Sch. Lif. Sci., Tohoku Univ.*, [2]*INGEM, Tohoku Univ.*, [3]*JST PRESTO*)

Ribosomes translate genetic information encoded on mRNA to the corresponding amino acid sequences, the essential machinery in gene expression. This presentation will discuss how to control this fascinating supra-assembly dedicated to protein synthesis in situ. An optogenetic approach was employed to control ribosomal function freely, controlling ribosomes inside cells by the light to medium. RNA moieties comprise the structural core of the ribosome that also plays an essential role functionally, which was used as the target of the optogenetic tool for binding. This presentation will show the recent achievement of this research project.

1SGP-3 両親媒性αヘリックスが操るオートファジー関連分子 ATG3 の機能
Amphipathic α-helix Manipulates ATG3 Function

Taki Nishimura[1,2,3], Gianmarco Lazzeri[4], Noboru Mizushima[2], Roberto Covino[4], Sharon Tooze[3] ([1]*JST PRESTO Researcher*, [2]*Dept. of Biochem & Mol. Biol., Faculty of Med., The Univ. of Tokyo*, [3]*The Francis Crick Institute*, [4]*Frankfurt Institute for Advanced Studies*)

Autophagy is a dynamic membrane process which is driven by ATG proteins in response to nutrient starvation. Among ATG proteins, ATG3 catalyzes LC3-phosphatidylethanolamine conjugation by binding highly curved membranes via its N-terminal amphipathic α-helix (AH_{ATG3}). Yet, it remains obscure how the LC3 lipidation reaction is controlled by AH_{ATG3}. Here, we report that the membrane binding is not the sole function of AH_{ATG3}. By comparative analysis of various AHs, we find several key features of AH_{ATG3} essential for LC3 lipidation *in vivo*. Together with all-atom MD simulation analysis, I will talk about our working hypothesis regarding AH_{ATG3}-dependent LC3 lipidation and discuss a possible application of various AHs for manipulating protein functions.

1SGP-4 ヘテロクロマチン形成高次構造体の解明と制御
Understanding and reconstructing small RNA mediated heterochromatin formation

Yuka Iwasaki (*Keio Univ. Sch. Med.*)

Heterochromatin is vital to sustaining stable chromosome structure and gene expression patterns, and its dysregulation can cause various diseases. Some classes of small RNAs can regulate their target genes via heterochromatin formation. PIWI-interacting RNAs (piRNAs) are germline-specific small RNAs that form effector complexes with PIWI proteins to preserve genomic integrity by repressing transposable elements (TEs). Among PIWI-clade proteins in *Drosophila*, Piwi transcriptionally silences its targets via heterochromatin formation characterized by H3K9me3 marks and the linker histone H1. Here, by reconstructing piRNA-mediated silencing, we characterize higher-order nuclear architectural change induced upon small RNA-guided heterochromatin formation in a stepwise manner.

1SGP-5 操ることで見えてきた細胞内相分離現象の時空間デザイン原理
Spatio-temporal design principles of intracellular phase separation

Shunsuke Shimobayashi (*CiRA, Kyoto University*)

In recent years, LLPS has taken the biology world by storm, with this process now thought to drive the formation of dozens of intracellular biomolecular condensates. However, we are still largely in the dark about the design principles that decide **where and when these condensates form** in living cells. Here, we quantitatively show that despite the complex nature of the intracellular environment, the kinetics of condensate nucleation occurs through a physical process similar to that in inanimate materials, but the efficacy of nucleation sites can be tuned by their biomolecular features. This quantitative framework sheds light on the intracellular nucleation landscape, and paves the way for engineering synthetic condensates precisely positioned in space and time.

1SGP-6 合成生物学で生きた細胞内の動的構造体を操り、デザインし、理解する
Manipulation, design, and analysis of dynamic intracellular structures with synthetic biology tools

Hideki Nakamura[1,2] ([1]*Hakubi Center, Kyoto University*, [2]*Grad. Sch. Eng., Kyoto University*)

Cells are filled with diverse structures ranging from protein complexes, classical organelles, to membraneless organelles. Recent studies revealed dynamic nature of the intracellular structures. They undergo constant trafficking, deformation, or diffusion, with incessant turnover of their components. To understand biological roles and biophysical mechanisms of the dynamics, conventional methods often suffer from lack of spatio-temporal resolutions. Tools in synthetic biology field often provide promising solutions to such difficulties. In the talk, I will introduce my recent trials to develop tools that manipulate, design, or analyze various intracellular structures with high resolution. Related works, as well as future perspectives of the field will also be presented.

1SHP-1 筋収縮・制御機構に関する研究の現在と将来について
About the present and future of research on muscle contraction/regulation mechanism

Shin'ichi Ishiwata (*Fac. Sci. & Engn., Waseda Univ.*)

In the 1950s, a "sliding mechanism" was proposed based on structural analysis by electron/light microscopy and physiological research. It was then established that the myosin molecule is a chemo-mechanical energy conversion molecular motor. In the 1980s, single-molecule research emerged, and it became possible to elucidate the structural changes of myosin molecules and actin filaments at the single-molecule level. In particular, the details of the molecular mechanism of non-muscle myosin have been elucidated, whereas unclear points still exist about muscle myosin mainly because it is difficult to capture the moment of force generation due to the short binding time to actin. I will give an overview of the current state of muscle research and talk about the future.

1SHP-2 高輝度シンクロトロン放射光に照らされる筋肉研究の明るい未来
Rosy future of muscle research illuminated by bright synchrotron radiation X-rays

Hiroyuki Iwamoto (*SPring-8, JASRI*)

For structural scientists, “imaging” and “diffraction/scattering” have been opposing notions. The former deals this the real space that we can see easily, while the latter deals with the reciprocal space that requires prohibitively difficult diffraction theories. Recently, however, novel computational tools are filling the gap between the two notions, and started to provide googles to see “diffraction/scattering” information in the real space. Here we explain two of them: the 3-D extended version of coherent diffractive imaging (CDI), and 3-D structure restoration based on Patterson method. Application of these methods for muscle structure research will be explained.

1SHP-3 局所熱パルスによる横紋筋の細いフィラメントの活性化
Microscopic heat pulses induce activation of striated muscle thin filaments

Shuya Ishii[1], Norio Fukuda[2] ([1]*QST*, [2]*Dept Cell Physiol, Sch Med, Jikei Univ.*)

Sarcomeres in striated muscle are activated via structural changes of thin filaments, i.e., from the “off” state to the “on” state, in response to Ca^{2+} binding to troponin (Tn). We investigated the effects of rapid heating by infra-red (IR) laser irradiation on the sliding movements of thin filaments reconstituted with cardiac or fast skeletal tropomyosin-Tn complex in the *in vitro* motility assay. IR laser irradiation caused sliding of thin filaments in the absence of Ca^{2+} at body temperature (37°C). Likewise, sarcomeres shortened at body temperature in skeletal myofibrils. These findings suggest that the “on-off” equilibrium of the thin filament state is partially shifted toward the “on” state under the relaxing condition at physiological body temperature.

1SHP-4 3 次元バイオプリントで作られた和牛ステーキ：未来の肉？
3D-Bioprinted Wagyu Steak: Meat of the future?

Michiya Matsusaki (*Grad. Sch. Eng., Osaka Univ.*)

Since there will be an insufficient supply of protein in the future (protein crisis), in recent years, alternative meats such as plant-derived meats and cell-based cultured meats have been attracting much attention in the world. There is thus still a high demand for artificial steak-like meat. We demonstrate in vitro construction of engineered steak-like wagyu tissue assembled of three types of bovine cell fibers (muscle, fat, and vessel). Our developed tendon-gel-assisted 3D-bioprinting might be a promising technology for "tailor-made structured wagyu meat". In this lecture, we would also like to discuss the meat of the future.

1SHP-5 光熱変換を利用した局所熱パルス法による筋肉の熱暴走メカニズムの解明
Thermal runaway in muscles studied using a local heat pulse method

Madoka Suzuki (*Inst. Protein Res., Osaka Univ.*)

Muscle has been studied intensively as a contractile system in biophysics. However, thermogenesis is the other important role of muscle. Due to its strong heat power when activated, it becomes fatal if not correctly regulated. Malignant hyperthermia is an unstoppable thermogenesis in skeletal muscle due to abnormal Ca^{2+} homeostasis. We have recently found using an optically controlled local heat pulse method that a Ca^{2+} release channel in skeletal muscles ryanodine-receptor-type-1 (RyR1) is activated by heating, and RyR1 mutants implicated in malignant hyperthermia is more heat sensitive than their WT. Recent results obtained in cellular and animal model systems will be introduced.

2SAA-1 Solid-State NMR spectroscopic approaches to investigate membrane-bound peptide structure

Izuru Kawamura (*Grad. Sch. Eng. Sci., Yokohama Natl. Univ.*)

Solid-state NMR spectroscopy is frequently used to investigate the dynamic structure of membrane-bound peptides in phospholipid bilayers. A pore-forming peptide, named SV28, has been de novo designed so that a β-hairpin structure assembles to form a stable nanopore in a bilayer lipid membrane. The conformation-dependent chemical shifts and interatomic distance about the site-specific isotope-labeled SV28 were investigated. Consequently, our solid-state NMR approach has demonstrated the formation of β-turn-β structure in the DOPC membrane [1]. The membrane-bound structure is corresponding to a stable nanopore by peptide self-assembly in the membrane.

[1] K. Shimizu, K. Usui, I. Kawamura, R. Kawano, et al. (2022) *Nat. Nanotech.* 17, 67-75.

2SAA-2 Mobility, location, and kinetics of membrane binding and cell entry of peptides by solution-state ^{19}F and ^{1}H NMR

Emiko Okamura (*Faculty Pharm. Sci., Himeji Dokkyo Univ.*)

Drug delivery to lipid membranes is crucial as a primary stage of bioactivities. We proposed a strategy to quantify the drug binding and mobility in membrane *in situ* by applying solution-state ^{19}F and ^{1}H NMR in combination with the pulsed-field-gradient technique. Mobility, location, the kinetics of membrane binding, and the bound fraction of the drug including peptides were quantified by using vesicles as model membranes.

The analysis was also applied to real-time, non-endocytic cell entry of membrane-permeable octaarginine (R8). By ^{19}F labelling of R8, the ^{19}F NMR method revealed why and how the cationic peptide showed an ability to go across hydrophobic cell membrane, and how the introduction of neutral amino acids modified the membrane-permeable properties.

2SAA-3 Sec 非依存性膜蛋白質膜挿入における大腸菌由来糖脂質 MPIase の役割解明
Role of a bacterial glycolipid MPIase in Sec-independent membrane protein integration

Kaoru Nomura (*Suntory Foundation for Life Sciences*)

An endogenous glycolipid MPIase in the *Escherichia coli* membrane regulates membrane protein insertion cooperatively with proteinaceous translocons. Here, we focused on the Sec translocon-independent pathway and examined the mechanisms of MPIase-facilitated protein insertion using physicochemical techniques. Diacylglycerol reduced the acyl chains mobility and inhibited the insertion, whereas MPIase restored them. Intermolecular interactions between MPIase-basic amino acids in the protein suggested that the MPIase pyrophosphate attracts the basic amino acids near the membrane surface, which acts as a trigger of the insertion. This study demonstrated MPIase support membrane insertion by using its unique molecular structure in various ways.

2SAA-4 Solid-state NMR measurements of amphotericin B, a natural product that interacts with lipid bilayers

Yuichi Umegawa (*Grad. Sch. Sci., Osaka Univ.*)

Amphotericin B is a polyene macrolide antibiotic isolated from *Streptomyces nodosus* and widely used to treat fungal infections. In the 1970s, a barrel plate model was proposed as a mechanism of this activity, in which AmB molecules self-assemble and interact with ergosterol in the fungal cell membrane to form an ion-permeable channel complex. Although this model structure was widely accepted, it was difficult to elucidate the structure of complex formed by natural products in lipid membrane, and the details remained unknown for more than 40 years. In order to elucidate the structure of this channel complex, we combined solid-state NMR and molecular dynamics calculations to elucidate the structure.

2SAA-5 Revealing Novel Polymorphs and Cross Propagation for 42-residue Amyloid beta by Solid-state NMR

Yoshitaka Ishii[1,2] ([1]*Tokyo Institute of Technology, School of Life Science and Technology*, [2]*RIKEN, BDR*)

We discuss our progress in structural examination of misfolded amyloid-β (Ab) by solid-state NMR (SSNMR). Increasing evidence suggests that formation and propagation of misfolded aggregates of 42-residue Aβ42, rather than the more abundant 40-residue Aβ40, provokes the Alzheimer's cascade. Here, we discuss our ongoing efforts to examine the feasibility of characterizing the structure of trace amounts of brain-derived and synthetic amyloid fibrils by sensitivity-enhanced ^{1}H-detected SSNMR under ultra-fast magic angle spinning. The data reveals the presence of new polymorphs for Ab42 fibrils, including ones from an AD brain. Our SSNMR data also indicate possibility that cross propagation from Ab42 fibrils to Ab40 fibrils may be modulated by structures of Ab42 fibril.

2SBA-1 Chromatin mobility of X-linked loci and its epigenetic regulation

Yuko Sato[1,2], Yuma Ito[2], Satoshi Uchino[2], Makio Tokunaga[2], Hiroshi Kimura[1,2] ([1]*IIR, Tokyo Tech*, [2]*Sch. Life Sci. Tech., Tokyo Tech*)

Single molecule imaging studies of histones have revealed that individual nucleosomes exhibit local dynamic behavior on milliseconds to seconds timescales, depending on gene expression state. In this study, the mobility of three X-linked loci, detected using sgRNA-dCas9 system, were analyzed to compare the difference between active and inactive X chromosomes (Xa and Xi) in mouse female embryonic carcinoma cell line MC12. The mobilities of all three loci on Xi were lower compared to those on Xa. We are investigating the impact of RNA polymerase II-mediated transcription and individual epigenetic marks using inhibitors and knockout cell lines. We will discuss the chromatin plasticity regulated by epigenetic modification and its relationship with gene expression.

2SBA-2 (2Pos303) ヒト生細胞の局所クロマチン動態は細胞周期を通して一定である
(2Pos303) Single-nucleosome imaging reveals steady-state motion of interphase chromatin in living human cells

Shiori Iida[1,2], Soya Shinkai[3], Yuji Itoh[1], Sachiko Tamura[1], Masato Kanemaki[2,4], Shuichi Onami[3], Kazuhiro Maeshima[1,2] ([1]*Genome Dynamics Lab., Natl. Inst. of Genet.*, [2]*Dept. of Genet., Sch. of Life Sci., SOKENDAI*, [3]*RIKEN BDR*, [4]*Mol. Cell Eng. Lab., Natl. Inst. of Genet.*)

Dynamic chromatin behavior plays a critical role in various genome functions. However, it remains unclear how chromatin behavior changes during interphase, where the nucleus enlarges and genomic DNA doubles. We unveil that local chromatin motion captured by single-nucleosome imaging remained steady throughout interphase in live human cells. A defined genomic region also behaved similarly. Our results of Brownian dynamics modeling suggest that this steady-state chromatin motion was mainly driven by thermal fluctuations. Steady-state motion temporarily increased following a DNA damage response. The observed steady-state chromatin motion allows cells to conduct housekeeping functions, such as transcription and DNA replication, under similar environments during interphase.

2SBA-3 DNA の量とクロマチン構造による核のサイズ制御機構
DNA quantity and chromatin structure contribute to nuclear size control in *Xenopus laevis*

Yuki Hara (*Fac. Sci., Yamaguchi Univ.*)

Cells adapt to drastic changes in the genome during evolution and cell cycle by adjusting the nuclear size to exert genomic functions. However, the mechanism by which DNA content and chromatin structure within the nucleus contribute to controlling the nuclear size remains unclear. Here, we experimentally evaluated the effects of DNA quantity and chromatin structure by utilizing cell-free Xenopus egg extracts. Upon perturbating DNA properties, expansion dynamics of the nucleus and structure of the nuclear membrane correlated with DNA physical properties. These results demonstrate a novel model in which the physical properties of the chromatin, rather than the coding sequences themselves, contribute to generating forces for controlling nuclear size.

2SBA-4 (2Pos116) 細胞核内における underwound DNA の蛍光イメージング
(2Pos116) Fluorescence imaging of underwound DNA in the cell nucleus

Jumpei Fukute[1,2], Koichiro Maki[1,3], Taiji Adachi[1,2,3] ([1]*Inst. Life & Med. Sci., Kyoto Univ.*, [2]*Grad. Sch. Biostudies, Kyoto Univ.*, [3]*Grad. Sch. Eng., Kyoto Univ.*)

In the cell nucleus, underwound DNA is known to affect key biological processes such as gene transcription. In this study, we aimed to reveal the intranuclear distribution of underwound DNA by developing a fluorescence imaging method. We utilized biotinylated-psoralen (bio-psoralen), which binds to underwound DNA. Based on this new method, we found that underwound DNA was predominantly distributed in the nucleolus, where ribosomal RNA was transcribed by RNA polymerase I. Our novel imaging technique could be useful to explore DNA underwinding-mediated mechanisms.

2SBA-5 (3Pos305) High-resolution mapping of chromatin compaction and dynamics in live cells by label-free interference microscopy

Yi-Teng Hsiao, Chia-Ni Tsai, Fasih Bintang Ilhami, Chia-Lung Hsieh (*Institute of Atomic and Molecular Sciences (IAMS), Academia Sinica / Taiwan*)

We present a novel optical microscope technique to resolve the chromatin organization in the unlabeled live cell nuclei. A highly sensitive interference microscopy, coherent brightfield microscopy (COBRI), is used to directly record the dynamic scattering signal of chromatin at a high speed. The chromatin density and the level of chromatin compaction are estimated with sub-micrometer spatial resolutions by analyzing the temporal fluctuation of the scattering signal. The reconstructed chromatin density map is highly correlated to the fluorescence image of chromatin. In addition, the chromatin compaction changes by chemical drugs are successfully detected. Using our methods, we investigate the chromatin remodeling of local DNA damage induced by laser microirradiation.

2SBA-6 (3Pos301) 細胞内の一分子を三次元でナノレベルの分解能で観察できる「クライオ三次元ナノスコピー」の開発
(3Pos301) Cryo-3D Nanoscopy to localize three-dimensional position of individual fluorophore with nanometer precision in the cell

Kanta Naruse[1], Tsuyoshi Matsuda[1], Yuta Mizouchi[1], Takeshi Shimi[2], Hiroshi Kimura[2], Eiji Nakata[3], Takashi Morii[3], Michio Matsushita[1], Satoru Fujiyoshi[1] ([1]*Department of physics, Tokyo institute of technology*, [2]*Cell Biology Center, Institute of Innovative Research, Tokyo institute of technology*, [3]*Institute of Advanced Energy, Kyoto University*)

Biological phenomena are regulated by many biomolecules in the cell. In order to study them, it is needed to observe the individual molecules and three-dimensional network of them in the cell. For such purpose, we developed “cryo-3D nanoscopy” to determine three-dimensional position of individual fluorophore with nm precision in the cell. We have already achieved precision of 1 nm in lateral direction, but about 17 nm in axial direction. The z-localization precision was worse than the theoretical limit 1 nm. It is because of the blinking noise and the background noise. To improve the precision, we developed “cryo-3D nanoscopy” and achieved precision of 0.5 nm in lateral direction and 1.9 nm in axial direction. These are less than 2 times the theoretical limit.

2SBA-7 新しいクロマチン基盤ユニットである **H3-H4** オクタソームのクライオ電子顕微鏡解析
Cryo-electron microscopic analysis reveal a novel structural unit of chromatin

Kayo Nozawa[1], Yoshimasa Takizawa[2], Kazumi Saikusa[3], Satoko Akashi[4], Hitoshi Kurumizaka[2] ([1]*Tokyo Institute of Technology, School of Life Science and Technology*, [2]*The University of Tokyo, Institute for Quantitative Biosciences*, [3]*National Institute of Advanced Industrial Science and Technology*, [4]*Yokohama City University, Graduate School of Medical Life Science*)

Genetic information is stored in chromatin with nucleosomes as the basic unit. A typical nucleosome comprises a DNA segment wrapped around a histone octamer core, consisting of two copies of histone H2A-H2B and histone H3-H4 dimers. In the present study, we determined the structures of a novel nucleosome, the H3-H4 octasome, composed of four H3-H4 dimers without H2A-H2B. *In vivo* crosslinking experiments supported the existence of the H3-H4 octasome in yeast cells. The discovery of the unique structural characteristics of the H3-H4 octasome will have major impacts on topics ranging from chromatin structure and dynamics to epigenome regulation in eukaryotes.

2SBA-8 斥力相互作用する溶質混合系における相分離：クロマチン高次構造の視点から
Phase separation in soft-repulsive mixtures: implication for chromatin organization

Takahiro Sakaue, Naoki Iso, Yuki Norizoe (*Dep. Phys. Aoyama Gakuin Univ.*)

The large-scale chromatin organization in interphase nucleus is characterized by phase separation to form A/B compartments. A recent study has indicated that the repulsion but not the attraction among coarse-grained chromatin monomers is essential for the large-scale chromatin phase separation [1].
Here we propose a simple mean-field model for the phase separation in solute mixtures, which interact through soft-repulsive interactions. We analyze the phase behavior of the model, and its dependence on the nature of repulsive interactions among components. We will also discuss its implication for chromatin phase separation.
[1]S. Fujishiro and M. Sasai, BioRxiv 441596 (2021).

2SBA-9 1 細胞全ゲノム DNA 複製解析からゲノム三次元構造動態を探る
Unraveling the dynamic 3D genome architecture through single-cell DNA replication profiling

Ichiro Hiratani (*Laboratory for Developmental Epigenetics, RIKEN Center for Biosystems Dynamics Research (RIKEN BDR)*)

Hi-C technology has revolutionized genome biology, revealing that mammalian chromosomes are partitioned into megabase-sized topologically associating domains (TADs). TADs can be in either A (active) or B (inactive) nuclear compartments, which exhibit early and late DNA replication timing (RT), respectively. In parallel, we recently developed a single-cell DNA replication sequencing (scRepli-seq) method, which has allowed us to monitor genome-wide RT dynamics and infer A/B compartment dynamics in single cells. I will discuss our ongoing efforts to utilize scRepli-seq to understand the regulatory principles of 3D genome organization, including its dynamics during mammalian development and cell cycle, as well as the mechanisms underlying RT/compartment regulation.

2SCA-1 アクティブマターが示す秩序形成の幾何的設計原理
Geometric design principle for active ordering

Kazusa Beppu[1], Yusuke T. Maeda[2] ([1]*Appl. Phys., Aalto Univ. Sch. of Sci.*, [2]*Phys., Kyushu Univ.*)

Highly concentrated motile agents tend to exhibit turbulent collective dynamics, named active turbulence, where many transient interacting vortices are intermingled. We previously demonstrated that co-rotational and anti-rotational vortex pairs inherent in active turbulence are ruled by the ratio of the distance between vortices to their radius. However, what properties in active systems overcome this constraint and whether the geometric rule is universal have been challenges. We show that the chirality of bacteria allows them to form larger rotational flows, which provides a novel strategy to control active turbulence by chirality. Moreover, we present the geometric universality of active ordering, which is established from swimming bacteria to active cytoskeletons.

2SCA-2 (1Pos217) Conversion of light-driven outward proton pump rhodopsin into inward proton pump

Maria Del Carmen Marin Perez[1], Masae Konno[1,2], Himoru Yawo[1], Keiichi Inoue[1] ([1]*ISSP, Univ. Tokyo*, [2]*PRESTO, Japan Science and Technology Agency*)

Microbial rhodopsins are retinal-binding membrane proteins which function as ion-transporters, photo-sensors, and light-regulated enzymes. The most ubiquitous microbial rhodopsins are the outward-directed light-driven H^+ pumps. However, new sub-families of microbial rhodopsins exhibited an inwardly and unidirectionally H^+ transport. Although structural studies provide insight into their ion transporting mechanism, the key elements which determinate the direction of the H^+ transport pathway were not revealed. We report the H^+ transport activity of site-directed mutations of *Psp*R (outward H^+ pump) from *Pseudomonas putida*, to successfully convert *Psp*R into an inward H^+ pump by site-specific replacement of their amino acid residues involve in the H^+ transport pathway.

2SCA-3 フッ素化人工チャネルによる膜間物質輸送
Transmembrane material transport by fluorinated channels

Kohei Sato (*Sch. Life Sci. Tech., Tokyo Tech.*)

Membrane proteins that transport ions across cellular membranes play essential roles in various biological events, including energy conversions. To mimic their structures and functions, our research group has developed a series of amphiphilic molecules that can self-assemble within the hydrophobic layer of lipid bilayer membranes to form supramolecular transmembrane channels. More recently, we have discovered that aromatic fluorination of such amphiphiles can expand their transmembrane material transport properties and their response to external stimuli. Details of their molecular design and functions will be presented at the conference.

2SCA-4 (3Pos128) 1 分子回転操作実験によって解明されたミトコンドリア由来 ATP 合成酵素における阻害因子 IF_1 の一方向制御機構
(3Pos128) Unidirectional regulation of ATPase factor 1 in mitochondrial ATP synthase studied by single-molecule manipulation experiments

Ryohei Kobayashi[1,2], Hiroshi Ueno[1], Kei-ichi Okazaki[2], Hiroyuki Noji[1] ([1]*Appl. Chem., Grad. Sch. Eng., Univ. Tokyo*, [2]*Inst. for Mol. Sci.*)

IF_1 is a regulatory protein for mitochondrial ATP synthase (F_oF_1), which inserts its N-terminus into the $\alpha_3\beta_3$ interface of F_1. One of the unique features of IF_1 is the unidirectional regulation: it inhibits ATP hydrolysis but does not inhibit ATP synthesis. To elucidate how IF_1 is released from F_1, we have performed single-molecule manipulation experiments of IF_1-inhibited F_1. The "stall-and-release" experiment showed the strong angle dependence of IF_1 release in the clockwise direction, but no activation in the counter-clockwise direction. Further, to explore the origins of the unidirectionality, we have conducted experiments with the N-terminal truncated IF_1, suggesting that the entrance part of the long helix of IF_1 contributes most to the unidirectionality.

2SCA-5 1 分子計測・活性測定・タンパク質工学による回転型 V-ATPase の統合的研究
Integrated research on rotary V-ATPase approached by single-molecule observation, biochemical assay, and protein engineering

Akihiro Otomo[1,2], Ryota Iino[1,2] ([1]*Institute for Molecular Science*, [2]*The Graduate University for Advanced Studies*)

V-ATPases (V_oV_1) are ion pumps consisting of two rotary motor proteins V_o and V_1, and actively transport ions across the cell membrane by using chemical energy of ATP. However, energy transduction and ion transporting mechanisms of V_oV_1 remain elusive. Recently, we directly visualized rotational pauses and steps of V_o and V_1 motors of *Enterococcus hirae* V-ATPase (EhV_oV_1) which pumps Na^+, and revealed rigid coupling between Vo and V_1. In addition, we succeeded in change the ion selectivity of EhV_oV_1 from Na^+ to H^+ by engineering ion-binding site. Here, we discuss the details of the rotational mechanism involving ion transportation of EhV_oV_1 and introduce our ongoing efforts to engineer a new ion-binding site in V-ATPase to double the number of transported ions per turn.

2SCA-6 ミトコンドリア呼吸鎖における熱産生の物理化学的メカニズム
Physicochemical mechanism of heat generation in mitochondrial respiratory chain

Kotaro Takeyasu[1,2,3], Nuning Namari[4], Junji Nakamura[2,5] ([1]*Fac. Pure and Appl. Sci., Unive. Tsukuba*, [2]*TREMS, Univ. Tsukuba*, [3]*Zero-CO2, Univ. Tsukuba*, [4]*Grad. Sch. Sci. Technol., Univ. Tsukuba*, [5]*I2CNER, Kyushu Univ.*)

In mitochondrial respiratory chain, heat is generated under not only uncoupled condition but also coupled condition. Several groups measured that the local temperatures in the vicinity of mitochondria are more than 40 ℃, though physicochemical mechanism of the heat generation and the flow has not been established. Herein, we hypothesized that the redox potential difference between the oxidation of NADH ($FADH_2$) and oxygen reduction reaction is also used for the overpotentials in the consecutive electrochemical reactions in the complex I-IV as well as for the proton pumping. We have analyzed the reported experimental data for the reaction rates and estimated the overpotentials, which is converted to heat finally, at each complex as a first step.

2SCA-7 キラル液晶の自己組織化ナノ構造を利用した力学センシングと応答速度設計
Mechanical sensor using chiral liquid crystals with self-organized nanostructures and tuning of molecular recovery response

Kyohei Hisano[1,2], Atsushi Shishido[2], Osamu Tsutsumi[1] ([1]*Col. of Life Sci., Ritsumeikan Univ.*, [2]*Lab. for Chem. & Life Sci., Tokyo Tech*)

Chiral liquid crystals (CLCs) have attracted much attention because form a self-organized nanostructure of a helically twisted molecular orientation with the spatial distribution of refractive index, showing reflection color. Especially, CLC elastomers, with a strong coupling of molecular orientation and polymer networks, change their reflection wavelength under external stimuli such as mechanical force. This enables to realize flexible mechanical sensors. However, a molecular recovery response after stimulus removal is relatively slow. In this study, we propose a rational route for designing the optical and mechanical properties of CLC elastomers, and demonstrate the arbitrary tuning of the recovery of molecular-level response (< 1 s or > months).

2SCA-8 Structural stability and dynamics of de novo designed transmembrane peptide barrels

Ai Niitsu[1], Jaewoon Jung[2], Yuji Sugita[1,2] ([1]*Wako Inst., Riken*, [2]*Kobe Inst., Riken*)

Natural voltage-dependent ion channels convert the electrostatic potential across membranes into mechanical energy, expressing an ion-permeating function. Inspired by such proteins, our goal is to design transmembrane peptide channels that open/close in a voltage-dependent manner as “Molecular Engines”. A series of membrane coiled-coil peptide barrels has recently been de novo designed, which exhibit dynamic conformational/stoichiometry changes in single-channel current recordings. Using all-atom molecular dynamics simulations, we investigate the structural dynamics of the barrels under an external electric field and demonstrate possible molecular mechanisms of their large conformational change. This will guide further designs toward controllable peptide ion channels.

2SDA-1 Toward broadly accessible, highly scalable solid-state nanopore research

Kyle Briggs (*University of Ottawa, Department of Physics*)

Nanopores are at the core of a technology revolutionizing sequencing and are poised to transform medicine and digital data storage. Recently, the T.-Cossa Lab reported a breakthrough in nanopore fabrication that allows automated pore fabrication, becoming the gold standard in labs around the world. Here, we present advances in scientific tools to accelerate solid-state nanopore research. We present parallel nanopore sensing at high bandwidth, including fully automated tools and workflows for producing many solid-state nanopores in parallel, multi-channels millifluidic flow cells, and multi-membrane chips. We also present software tools to analyze nanopore data that simplifies and automates common nanopore analysis tasks, facilitating collaboration and reproducibility.

2SDA-2 プローブ型人工細胞システムの応用展開
Application of Probe-Type Artificial Cell Membrane Systems

Kan Shoji (*Nagaoka Univ. Tech.*)

Stochastic nanopore sensors are a powerful analytical tool for understanding single biomolecular properties. Our group developed probe-type artificial cell membrane systems and applied the probe systems for high-throughput nanopore sensors, scanning probe microscopy, and analysis of transmembrane proteins. Additionally, we proposed electrode-threaded DNA nanopore systems to develop DNA nanopore-based sensors. This paper describes the development of our probe-type artificial cell membrane systems and the latest research results obtained with our probe systems.

2SDA-3 ナノポアシーケンサと nanoDoc を用いた DNA/RNA 修飾解析
Detection of DNA/RNA modification using nanopore sequencer and nanoDoc

Ueda Hiroki (*Biological Data Science, RCAST, Univ. of Tokyo*)

Advances in Nanopore single-molecule sequencing have presented the possibility of detecting comprehensive chemical modifications of DNA/RNA. However, the accuracy of informatics method need to be improved. Here, we presented a new software, nanoTune and nanoDoc. nanoTune is sequence to signal assignment (resquiggling) software designed for running on cloud. nanoTune uses trace value (probability output from basecaller) to realign the signal to the reference. We have also developed nanoDoc, for detecting DNA/RNA using a deep neural network. Current signal deviations caused by modifications are analyzed by Deep One-Class Classification. By using, nanoTune and nanoDoc generic DNA/RNA modifications could be detected without a training dataset.

2SDA-4 (2Pos290) Nanopore direct determination of DNA methylation and demethylation intermediates

Ping Liu[1], Masayuki Honda[1], Ryuji Kawano[2] ([1]*Department of Food and Energy Systems Science, Tokyo University of Agriculture and Technology*, [2]*Institute of Engineering, Tokyo University of Agriculture and Technology*)

This paper describes a nanopore sensing approach method for 5-methylcytosine (5mC) positions with numbers and demethylation intermediates directly. Methylation-demethylation processes are crucial for mammalian development and aberrant methylation patterns could lead to human diseases. However, the general modification methods need chemical conversion or enzymatic reaction and the incomplete reaction may reduce the reliability of the epigenetic analysis. In this work, we utilized the epigenetic modulation of cytosine dynamics in dsDNA which destabilizes the Watson-Crick base pair to allow modified cytosine to interact with the acidic anion acids in nanopore for determining the position with the number of 5mC and three other modifications at the single-nucleotide level.

2SDA-5 (2Pos315) ATP を検出可能な DNA ナノポアセンサの開発
(2Pos315) ATP-detectable DNA nanopore sensor

Hiromu Akai, Kan Shoji (*Nagaoka University of Technology*)

Nanopore sensors, that can electrically detect target molecules, are a powerful tool for single molecular analysis. However, the molecular selectivity and usable conditions of biological nanopores were limited. Thus, DNA-based nanopores are expected as alternative nanopores because of their high designability and robustness. Here, we proposed DNA nanopores, that can repeatedly open and close in response to ATP, as a model for molecular-selective DNA nanopores. DNA aptamers, which specifically bind to a molecule, were applied as a molecular-recognition domain of the molecular-responsive DNA nanopore. In this study, we investigated the molecular response-ability of the DNA nanopore by measuring the channel currents through the nanopore with multiple ATP concentrations.

2SDA-6 Integrating nanopore sensing and artificial intelligence for multiplex single-virus identification

Akihide Arima (*IIFS, Nagoya Univ.*)

Nanopores can be used to detect and characterize bio-molecules and -particles, however discriminating target species with similar physical properties is difficult, limiting the wider application. Here, we present virus identification based on a combination of solid-state nanopore sensing and machine-learning. In the discrimination, various characteristic features were extracted from resistive pulse waveforms of virus particles and utilized for the classification in a high-dimensional feature space. This approach enables us to demonstrate over 99% accuracy for five different virus species. The present findings would offer the prospect of a novel diagnostic system for rapid screening of viruses including new strains.

2SDA-7 Probing the Effect of Ubiquitinated Histone on Mononucleosomes through solid-state nanopores

Hu Rui, Wei Guanghao, Wang Zhan, **Qing Zhao** (*Peking University, School of Physics*)

Recently, solid-state nanopore sensors have emerged as a versatile technique for label-free single-molecule detection. Here we leverage the advantages of mechanically stable solid-state nanopores and detect the effect of a ubiquitinated histone on mononucleosomes at the single-molecule level. We found that a turning point of voltage corresponds to the onset of nucleosome rupture. More importantly, we reveal that ubH2A stabilizes the nucleosome by shifting the turning point to a larger value and investigated the effect of ubiquitination on different histones (ubH2A and ubH2B). These findings open promising possibilities for developing a miniaturized and portable device for the fast screening of PTMs on nucleosomes.

2SDA-8 Light Enhanced Solid-state Nanopore for Single Molecule Sensing

Yamazaki Hirohito (*The University of Tokyo, Department of Biological Science*)

Nanopore sensing become an attractive sensing platform to characterize single biological molecules. When lights irradiate on solid-state materials, additional modality into nanopore sensing can be employed because the energy of absorbed light cause verities of phenomena such as fluorescence, heating, and chemical reactions. In this talk, we present how optical technologies can integrate into nanopore sensing. First, we show a method to probe single molecule thermal melting using a localized thermal gradient at a pore. Second, we introduce controlled laser-induced fabrication that allow to have 1−2 nm in diameter and thickness in silicon nitride membrane. Further, we present how these technologies can be used for single molecule studies.

2SEA-1 アクチン線維において顕在化する時空アロステリー
Spaciotemporal allostery in the actin filament

Akihiro Narita (*Grad. Sci, Nagoya Univ.*)

There are many biological phenomena of molecular systems such as cilia motility, self-excited vibration of muscle and a circadian clock cycle by KaiABC, whose mechanism has not yet been understood. We named “spaciotemporal allostery” that a molecule changes its properties in a population of molecules depending on the surrounding environment, and as a result, the rate constant changes. When we include it in simulation, typical patterns of molecular system phenomena can be reproduced easily. Therefore, it is crucial to understand spaciotemporal allostery to understand a wide range of biological phenomena. I will discuss the spaciotemporal allostery using the actin filament as an example.

2SEA-2 細菌べん毛モーター回転制御機構の理解の進展
Recent understanding of the control mechanism of the bacterial flagellar motor rotation

Katsumi Imada (*Grad. Sch. Sci., Osaka Univ.*)

The torque of the bacterial flagellar motor is generated by the interaction between the stator and the rotor, which are assembly of several hundreds of protein subunits. The number of the stators and their ion channel activities are regulated in response to the rotational load and environmental conditions to optimize the output efficiency of the motor. The rotational direction of the motor is switched by binding of phosphorylated CheY (CheY-P) to the rotor, which triggers the cooperative structural change of the rotor. Recently, CryoET analysis revealed that CheY-P binding changes the rotor diameter. Here we will show and discuss the recent understanding of the mechanism of both phenomena, which include cooperative structural change that propagates over long distances.

2SEA-3 膜と細胞骨格の動態制御におけるダイナミンのヘクトスケール分子集団のアロステリー変化
Allosteric changes of hecto-scale population of dynamin GTPases provide in dynamic regulation of membranes and cytoskeletons

Kohji Takei, Tadashi Abe, Tetsuya Takeda, Hiroshi Yamada (*Fac. Med. Dent. Pharma. Sci., Okayama Univ.*)

Dynamin GTPases is an endocytic protein, which polymerizes into helical ring at the neck of endocytic pit, and the ring severs the membrane upon GTP hydrolyses. Dynamin helical ring is 45 nm in diameter and made up of 26-30 molecules. A few dynamin rings form a cluster in the fission process. Dynamin also regulates cytoskeletons. Dynamin polymerizes around F-actin forming actin bundles, which are rapidly disassembled upon GTP hydrolysis. Dynamin GTPase activity is drastically enhanced by the presence of F-actin. Dynamin also bundles and unbundles microtubules in a similar manner. These findings indicate that the functional unit of dynamin is comprised of a hecto-scale population of molecules, and their conformational change upon GTP hydrolyses need to be synchronized.

2SEA-4 夜明けに自律離散する概日時計システム
Autonomous Disassembly of Circadian Clock System at Dawn

Shuji Akiyama[1,2] ([1]*CIMoS, IMS, NINS*, [2]*SOKENDAI*)

In general, when a biomolecular complex that is deeply involved in a biological phenomenon is discovered, research on the formation and structure of the complex tends to progress, while research on the dissociation of the complex lags behind. The same is true for the circadian clock system of cyanobacteria. The disassembly process of a ternary complex accumulated at night, in which three Kai proteins (KaiA, KaiB, and KaiC) are bound, has not received much attention from researchers. In this presentation, we will discuss how the "three physiological properties of the circadian clock" emerge in the dawn phase when KaiC ATPase is conjugated with an autocatalytic disassembly reaction, and its relevance to other circadian clock systems, which also dissociates at dawn.

2SEA-5 高速 **AFM** による **100-nm** サイズの分子集団の直接観察
Direct observation of 100 nm-sized molecular systems by high-speed AFM

Noriyuki Kodera (*WPI-NanoLSI, Kanazawa Univ.*)

High-speed AFM (HS-AFM) is a unique microscopy that allows us to directly observe the structural dynamics of biomolecules in action, under near physiological condition, at nanometer spatial and sub-second temporal resolution. In particular, interesting information can be obtained from the HS-AFM observations on relatively large molecular assemblies of ~100 nm-sized or composed of ~100 molecules. In this presentation, typical observation results obtained from such molecular assemblies will be shown. Furthermore, I will show our recent efforts on the functional extensions of HS-AFM, such as development of concave/convex substrates and HS-AFM system with a manipulator that would be useful to reveal the function and structural mechanisms of such molecular assemblies.

2SEA-6 長距離アロステリーの物理基盤としてのクーロン結合ネットワーク
Coulomb bond network as a physical basis for long-range allostery

Mitsunori Takano (*Grad. Sch. Sci. Eng., Waseda Univ*)

The physical basis of allostery was first given by Perutz who explained the cooperativity of oxygen binding in Hemoglobin by a series of local structural changes. The allosteric input in one subunit transmits to an adjacent subunit. Although hemoglobin is composed of only four subunits, the allosteric input in a certain subunit may go beyond the nearest neighbors in the case of a protein assembly composed of more subunits (several tens or more). Then, what physical mechanism could underlie such a long-range allostery? In this talk, the concerted rearrangement of Coulomb bond network in protein will be discussed as a physical basis of the long-range allostery, keeping in mind a dielectric material in which a number of micro-dipoles concertedly respond to a doped charge.

2SEA-7 (3Pos013) Optineurin の E50K 緑内障変異はオリゴマー粒径を増大させる (3Pos013) The E50K mutation of optineurin increases the oligomer size

Rintaro Kawamura[1], Soya Uetsuki[1], Takehito Tanzawa[2], Takayuki Kato[2], Masataka Kinjo[3], Akira Kitamura[3] ([1]*Grad. Sci. Life Sci., Hokkaido Univ.*, [2]*Inst., for Proteins Res., Osaka Univ.*, [3]*Fac. Adv. Life sci., Hokkaido Univ.*)

Optineurin (OPTN) is a coiled-coil-rich oligomerization protein. E50K mutant of OPTN (EK), associated with glaucoma, forms larger foci in the cytoplasm than its wild type (WT). However, little is known about their oligomerizing mechanism. The oligomeric states of purified recombinant WT and EK were analyzed using Native-PAGE, Dynamic light scattering (DLS), and negative stain transmission electron microscopy (TEM). Native-PAGE showed that WT mainly formed pentamers, whereas EK was heptamers. DLS showed that EK formed oligomers of larger and diverse particle size than WT. Furthermore, ring-like structures of OPTN were observed using TEM. Consequently, the higher order of EK oligomers may be because the assemble angle between intermolecular coiled-coils would be shifted.

2SFA-1 Torque Generation Mechanism of F_1-ATPase

Hiroyuki Noji, Hiroshi Ueno (*Grad. Sch. Eng., Univ. Tokyo*)

F_1-ATPase is the catalytic domain of ATP synthase, and functions as a rotary motor driven by ATP hydrolysis when isoloated. Rotational dynamics as well as chemomechanical coupling scheme have been well characterized by single-molecule studies on the F_1-ATPase from thermophilic *Bacillus* (TF_1). However, the structural studies of TF_1 have been restricted because TF_1 is not suitable for crystallization, which has hampered the elucidation of torque generation mechanism of F_1. Recently, we succeeded in cryo-EM analysis of TF_1 and revealed the structures of almost all catalytic states of F_1 in rotational catalysis. In this presentation, I will discuss the torque generation mechanism of F_1 based on the structural study as well as our previous single-molecule studies.

2SFA-2 Regulation of Motors by Microtubule-Associated Proteins

Ahmet Yildiz (*University of California Berkeley*)

The microtubule (MT)-associated protein, MAP7 is a required cofactor for kinesin-1 driven transport of intracellular cargoes. Using cryo-electron microscopy and single-molecule imaging, we investigated how MAP7 binds MTs and facilitates kinesin-1 motility. Unexpectedly, MAP7 partially overlapped with kinesin-1's binding site and inhibited kinesin-1 motility. However, by tethering kinesin-1 to the MT, the projection domain of MAP7 prevented dissociation of the motor and facilitated its binding to available neighboring sites. The inhibitory effect of microtubule binding is dominated as MTs became saturated with MAP7. Our results reveal biphasic regulation of kinesin-1 by MAP7 in the context of their competitive binding to MTs.

2SFA-3 Cholesterol in the cargo membrane amplifies the inhibitory effects of tau on kinesin-1-based transport

Qiaochu Li[1], James Ferrare[2], Jonathan Silver[2], John Wilson[1], Luis Arteaga-Castaneda[1], Weihong Qiu[3], Michael Vershinin[4], Stephen King[5], Keir Neuman[2], **Jing Xu**[1] ([1]*Physics, University of California, Merced, CA, USA*, [2]*Laboratory of Single Molecule Biophysics, National Heart, Lung and Blood Institute, National Institutes of Health, Bethesda, MD, USA*, [3]*Physics, Oregon State University, Corvallis, OR, USA*, [4]*Physics and Astronomy, University of Utah, Salt Lake City, UT, USA*, [5]*Burnett School of Biomedical Sciences, University of Central Florida, Orlando, FL, USA*)

Intracellular cargos are often membrane-bound and transported by microtubule-based motors (such as kinesin-1) in the presence of microtubule-associated proteins (MAPs). Whereas increasing evidence reveals how MAPs impact the interactions between motors and microtubules, critical questions remain about the impact of the cargo membrane on transport. Here we show that attaching kinesins to a fluid lipid membrane decreases the inhibitory effect of tau in comparison to membrane-free cargos in vitro. Adding cholesterol, which reduces kinesin diffusion in the cargo membrane, amplifies the inhibitory effect of tau on kinesin in a dosage-dependent manner. Our study establishes a direct link between the physical properties of cargo membrane and MAP-based regulation of kinesin-1.

2SFA-4 Ultralong-Term, Real-Time Tracking of Single Cargoes in Living Neurons

Sam Peng (*Stanford University*)

Single-molecule fluorescence microscopy has enabled numerous novel findings in biology. However, its full potential has been limited by the photo-instability of current probes. I will describe our development of rare-earth ion doped upconversion nanoparticles whose non-blinking luminescence is extremely stable, allowing single-particle imaging for several hours. I will demonstrate how the photostable probes enable ultralong-term single-particle tracking in living neurons and allow us to address fundamental questions regarding axonal transport. First, I will describe how we measure the number of active dynein motors driving the transport. Second, I will describe our proposed chemomechanical model for dynein which requires the hydrolysis of two ATP molecules per step.

2SFA-5 (1Pos137) Plus and minus ends of microtubules respond asymmetrically to kinesin binding by a long-range directionally driven allosteric mechanism

Huong T Vu[1], Zhechun Zhang[2], Riina Tehver[3], Dave Thirumalai[4] ([1]*University of Warwick*, [2]*Harvard University*, [3]*Denison University*, [4]*University of Texas*)

Although it is known that the majority of kinesin motors walk predominantly toward the plus end of microtubules (MT) in a hand-over-hand manner, the structural origin of the stepping directionality is not understood. To resolve this issue, we modelled the structures of kinesin-1 (Kin1), MT, and the Kin1-MT complex using the elastic network model and calculated the residue-dependent responses to a local perturbation in the constructs. Kin1 binding elicits an asymmetric response, opening the clefts of multiple plus end tubulin heterodimers, creating binding-competent conformations which are required for processivity. Our findings explain the directionality of stepping and the long-range communication of kinesin.

2SFA-6 (3Pos143) SLC26 ion transporters act as electricity-driven motor proteins

Tomohiro Shima (*Grad. Sch. Sci., Univ. Tokyo*)

Outer hair cells in the inner ear of vertebrates greatly change their cell length in response to membrane potentials and amplify sound signal. The energy conversion efficiency from electricity to physical motion by the outer hair cells is approximately 10,000 times higher than that of man-made piezoelectric devices. Prestin, a unique member of SLC26 anion transporter family, is the motor protein responsible for this highly efficient energy conversion. By combining sensitive electrophysiological assays with light microscopy techniques, we found that prestin and other SLC26 proteins share voltage-sensing and motile abilities. Based on our results, we would like to discuss the currently conceivable mechanism that drives the large movement of outer hair cells.

2SGA-1 シンギュラリティ現象を直接観るトランススケールスコープ AMATERAS
Trans-scale scope AMATERAS for direct observation of singularity phenomena

Taro Ichimura[1], Taishi Kakizuka[2], Hitoshi Hashimoto[1,3], Takeharu Nagai[1,2] ([1]*OTRI, Osaka Univ.*, [2]*SANKEN, Osaka Univ.*, [3]*Grad. Sch. Pharm., Osaka Univ.*)

Optical imaging plays the vital role in the studies of singularity phenomena. In order to find important cells that trigger a state transition of a multicellular system, it is desirable for an optical imaging tool to have both a wide field-of-view (FOV) to see the state of the entire system in the millimeter/centimeter scale and high spatial resolution to see the dynamics of all the element cells in the micrometer scale. We have been developing a “trans-scale scope” to cover the scale range from the micrometer to centimeter beyond the limitation of conventional microscopy, which we named AMATERAS. In the presentation, we will introduce the latest status of AMATERAS including technical impact, imaging performance, and application study.

2SGA-2 Chemical probes for detecting enzyme activities in living cells with single cell resolution

Mako Kamiya (*Dep. Life Sci. Tech., Tokyo Tech.*)

Selective imaging of targeted cells in living samples with chemical probes remains highly challenging. We have developed functionalized activatable fluorescence probes for β-galactosidase to selectively label lacZ-positive cells at single-cell resolution in living organisms or tissues. This design strategy based on intramolecular spirocyclization and quinine methide chemisty, in which fluorescence and biding ability to intracellular nucleophiles are simultaneously activated upon reaction with the enzyme, can be expanded to prepare analogues with different colors, or to target different enzymes and with photosensitizing abilities. In this symposium, I would also like to introduce our recent effort in developing chemical probes with new functionalities.

2SGA-3 (3Pos277) Decoding single-cell transcriptomic phenotypes from cell images enabled by robotic data acquisition and deep learning

Jianshi Jin[1], Taisaku Ogawa[1], Nozomi Hojo[1], Kirill Kryukov[2], Kenji Shimizu[3], Tomokatsu Ikawa[4], Tadashi Imanishi[2], Taku Okazaki[3], Shiroguchi Katsuyuki[1] ([1]*BDR, RIKEN*, [2]*Dept. of Mol. Life Sci., Tokai Univ. Sch. of Med.*, [3]*Inst. for Quant. Biosci., Univ. of Tokyo*, [4]*Res. Inst. for Biomed. Sci., Tokyo Univ. of Sci.*)

Predicting marker-gene-defined phenotypes of cells from microscopy images by deep learning has had a great impact on biological studies and medical applications. Here, we developed a robot named ALPS (Automated Live-imaging and cell Picking System), and performed whole transcriptome analysis (RNA-seq) for microscopically observed single cells, *e.g.*, peripheral blood mononuclear cells. Using these datasets, we predicted the transcriptome-defined (unbiased) cell types or states of the same cell type from the label-free live cell images (dynamics) by deep learning. Furthermore, we found that the deep learning had the ability to predict RNA expression levels of individual genes, which opened a new window to challenge the image-based prediction of all genes.

2SGA-4 局所かつ任意のタイミングで摂動を与える光操作技術 CALI 法とその応用
A light manipulation technology by CALI that provides localized and arbitrarily timed perturbations

Kiwamu Takemoto (*Mie University, Graduate School of Medicine*)

The dynamics of molecular activity involves not only a simple on/off switch, but also the spatiotemporal nature of when and where it is activated. However, due to the lack of techniques to manipulate molecular activity spatially and locally, little is known about the physiological functions and in vivo importance of the spatiotemporal nature of molecular activity. If such techniques are realized, they are also expected to be an important tool in new approaches such as Singularity Biology, which focuses on a very small number of cells. In this session, we will present a new elemental technology for CALI (Chromophore-assisted light inactivation) for localized and arbitrary deactivation of molecules. We also hope to discuss future applications of the CALI technology.

2SGA-5 最小の発光酵素「**picALuc**」の開発とその応用
Development of the smallest luciferase “picALuc” and its applications

Yuki Ohmuro[1], Sung Bae Kim[2], Hayato Matsui[1], Masaki Kanai[1], Tadaomi Furuta[3] ([1]*Shimadzu Corporation*, [2]*AIST*, [3]*Sch. Life Sci. Tech., Tokyo Tech*)

Luciferases have been isolated and improved for use as sensitive reporters in bioassays and molecular imaging. Among them, Artificial Luciferase (ALuc) is known as a superluminescent optical readout, derived from copepod. In this study, we successfully miniaturized ALuc, named “picALuc” (13 kDa), which has excellent bioluminescence (BL) activity and thermostability. This size is the smallest among the bright luciferases (1/5 the size of firefly luciferase and 2/3 of NanoLuc). picALuc was successfully applied to BRET-based assay and protein-fragment complementation assay. Moreover, picALuc showed unique substrate specificity and red-shifted BL spectra with some substrate analogs. Our development invites the wider applications to bioassays and molecular imaging.

2SGA-6 時空間トランススケールイメージングを可能にするケージドルシフェリンの開発
Development of caged luciferin enabling spatiotemporal trans-scale imaging

Yuki Hiruta (*Fac. Sci. Tech., Keio Univ.*)

Bioluminescence imaging (BLI) is widely used in the investigation of biological events in living cells and animals. Among the BL systems, combining the enzyme NanoLuc/the substrate Furimazine (FMZ) has attracted attention because of its high brightness. However, FMZ is easily decomposed by spontaneous oxidation causing auto-luminescence. In addition, due to the fast catalytic reaction of FMZ, the signal decays rapidly. The chemical and signal instability of FMZ limits the sensitivity and the duration available for monitoring. In this work, we developed FMZ derivatives enabling longer BLI of life phenomena at single cell level[1]. Long-term BLI using developed FMZ derivatives has the potential to find out rare biological phenomena at the single cell level.

2SHA-1 光熱変換を利用した細胞操作に向けた試み
Toward cell manipulation through photothermal conversion

Hiromi Imamura (*Graduate School of Biostudies, Kyoto University*)

The light energy absorbed by chromoproteins is dissipated as heat (photothermal conversion). In this research, we aim to create a new technology that enables the manipulation of living cells with a long-wavelength light by using the principle of photothermal conversion. Using Sirius fluorescent protein, whose fluorescence is highly sensitive to temperature, as a nano-size thermometer, we observed that ShadowR chromoprotein dissipated detectable heat when it was irradiated by laser light. We are now testing whether it is possible to manipulate intracellular calcium handling by opening a thermosensitive ion channel by the heat dissipated from ShadowR.

2SHA-2 高効率光熱変換タンパク質ヒーター創出に向けた分子内熱伝導機構の解明
Elucidation of intramolecular heat transfer mechanism for construction of highly effective photothermal protein heaters

Misao Mizuno (*Grad. Sch. Sci., Osaka Univ.*)

Controlled cell heating creates new bio-manipulation technologies. We aim to elucidate the mechanism of energy flow in proteins to construct highly efficient photothermal protein heaters. We focus on heme proteins as a prototype protein heater for observation of intramolecular energy flow, because heme undergoes the instantaneous nonradiative relaxation after photoexcitation so as to deposit large excess vibrational energy on heme. The migration of excess energy released by heme was observed using time-resolved anti-Stokes Raman scattering of a tryptophan residue in a protein moiety which is a probe for the excess energy. By utilizing three-dimensional structures of proteins, the distance and orientation dependence of energy diffusion was comprehensively investigated.

2SHA-3 BMI のための高密度皮質脳波電極の開発
Development of high-density ECoG array for BMI

Takafumi Suzuki[1], Taro Kaiju[1], Masayuki Hirata[1,2] ([1]*Center for Information and Neural Networks (CiNet), NICT & Osaka Univ.*, [2]*Osaka Univ. graduate school of medicine*)

Electrocorticogram (ECoG) has recently been attracting increased attention as a source signal for clinical Brain-machine interface (BMI) because it offers a good balance of features: less invasive than penetrating electrode methods, and a higher spatial resolution than EEG.
In this presentation we introduce our high density electrode array for ECoG recording, and its application for BMI.

2SHA-4 深部神経活動磁場操作に向けた新規分子ツール開発
Development of molecular tools for magnetic manipulation of neural activity in the deep tissue

Keiichi Inoue (*Inst. Solid State Phys., Univ. Tokyo*)

Optogenetics enabled us to manipulate neuronal activity in the brain by light illumination and led new understandings of the causal correlation between the activity of the specific neural group and biological responses. However, due to the limitation of the wavelength of light to the visible region, which can activate optogenetic actuators, ion channeling, and pumping rhodopsins, it is difficult to avoid strong scattering of manipulating light by the tissue and to manipulate neural activity in the deep tissue. To overcome this difficulty, we are developing new molecular tools to manipulate neural activity by magnetic field which can penetrate into much deeper tissue than visible light. Also, new magnetic-field application systems for magnetogentics will be introduced.

2SHA-5 生体内磁性粒子を操るための磁気力場の設計と最適化
Design and optimization of magnetic force field for manipulating magnetic particles in living bodies

Masaki Sekino[1], Hikaru Yoshioka[1], Keiichi Nakagawa[1], Keiichi Inoue[2] ([1]*Grad. Sch. Eng., Univ. Tokyo*, [2]*ISSP, Univ. Tokyo*)

Recent developments of biomolecular engineering enable us to manipulate neuronal firing using ion channels combined with magnetic particles and externally applied low-energy fields. Designing the distribution of magnetic force field is an important technique for realizing spatially selective cell manipulation. We propose a theoretical framework to design a force field in a target region. The coefficient of each harmonic component was optimized to generate a field as close to the target distribution as possible. Numerical solutions were obtained for several test cases. The target distributions were well reproduced for physically reasonable ones. Even when target fields do not satisfy Maxwell equations, the proposed scheme lead to a solution giving the closest solution.

2SAP-1 多細胞系の情報物理学
Information Physics of multi-cellular systems

Tetsuya J. Kobayashi (*IIS, UTokyo*)

Physical understanding of multi-cellular systems is the unexplored frontier in biophysics.
Sparked by the rapid advancements in bioimaging, bioinformatics, synthetic biology and so on,
multi-cellular systems are becoming a promising target of biophysics.
In this talk, we outline our attempts to investigate the design principles of multi-cellular systems by using or integrating the methods of physics, informatics, and other disciplines.

2SAP-2 内皮細胞集団動態と血管新生
Collective endothelial cell migration and angiogenesis

Naoko Takubo (*Isotope Science Center, The University of Tokyo*)

Although vascular endothelial cells (ECs) in angiogenesis exhibit inhomogeneous collective cell migration, how ECs collectively form complex vessels remains largely unknown. To quantitatively clarify the relationship between EC movements and angiogenesis, we created an in vitro angiogenesis model using extracellular matrix precision processing technics. Taking advantage of the quantitative analysis of EC movements, macroscopic cellular orientation was observed in the ECs in the vicinity of the base of the sprouting vessels. We also found a relationship between cellular orientation of ECs flow and vascular elongation. These findings suggest that collective endothelial cell migration is a key factor in angiogenesis.

2SAP-3 細胞間コミュニケーションの操作による多細胞パターンのデザイン
Programming multicellular pattern formation with synthetic cell-cell signaling

Satoshi Toda (*NanoLSI, Kanazawa Univ.*)

In developing embryos, cells communicate with each other to control the behaviors of cell populations and assemble multicellular tissues. However, due to the extreme complexity of cell-cell interactions in vivo, how communicating cells organize complex tissue structures precisely and robustly remains unclear. Here, to explore key mechanisms of tissue formation, we design new cell-cell communication rules between cultured cells and test multicellular behaviors to understand a logic of how cells organize multicellular structures and patterns. In this talk, I will introduce our synthetic biology technologies to create tissue patterning processes and discuss the mechanisms of multicellular pattern formation.

2SAP-4 (3Pos118) グラフニューラルネットワークによる細胞間の時空間相互作用の推定
(3Pos118) Graph-based machine learning reveals rules of spatiotemporal cell interactions in tissues

Takaki Yamamoto[1], Katie Cockburn[2], Valentina Greco[2,3], Kyogo Kawaguchi[1,4,5] ([1]*Nonequilibrium Physics of Living Matter RIKEN Hakubi Research Team, RIKEN BDR*, [2]*Department of Genetics, Yale School of Medicine*, [3]*Departments of Cell Biology and Dermatology, Yale Stem Cell Center, Yale Cancer Center, Yale School of Medicine*, [4]*RIKEN CPR*, [5]*Universal Biology Institute, The University of Tokyo*)

Robustness in developing and homeostatic tissues is supported by various types of spatiotemporal cell-to-cell interactions. Although live imaging and cell tracking are powerful in providing direct evidence of cell coordination rules, extracting and comparing these rules across many tissues requires a versatile framework of analysis. We demonstrate that graph neural network (GNN) models are suited for this purpose, by showing how they can be applied to predict cell fate in tissues and utilized to infer the cell interactions. Analyzing the live mammalian epidermis data, where spatiotemporal graphs constructed from cell tracks and cell contacts are given as inputs, GNN discoveres distinct neighbor cell fate coordination rules that depend on the region of the body.

2SAP-5 線虫の神経回路における多重情報コードの情報物理学的解析
Analyisis of multiplexed information coding in the nervous system of C.elegans

Yu Toyoshima, Ayaka Matsumoto, Yuichi Iino (*Grad. Sch. Sci., Univ. of Tokyo*)

The Nervous system of *C.elegans* is one of multi-cellular systems and provides unique opportunities to understand their dynamics because all the neurons and their connections had been identified. *C. elegans* migrates toward NaCl concentrations at which it was cultivated in the presence of food. During the chemotaxis behavior, two different tactic strategies are used separately depending on the direction of NaCl concentration gradient. The information of the direction will be encoded as a temporal pattern of activities of sensory neurons, and the information will be decoded by downstream neural networks. We have been studying the decoding mechanisms of this information processing system and would like to report and discuss our latest results.

2SAP-6 器官形態形成プロセスの種間スケーリング
Scaling of organ morphogenetic process between species

Yoshihiro Morishita (*RIKEN Center for Biosystems Dynamics Research*)

It is known that the concentration distributions of secreted molecules and the spatial patterns of different gene expressions in tissues during development and the skeletal morphology already formed after development can scale between species with different sizes. Do these scaling relationships also hold for organ developmental/morphogenetic process? To address this issue, we reconstructed tissue deformation dynamics for chick and Xenopus limb development from cell lineage data and compared the morphogenetic processes between species. We defined an appropriate coordinate system to directly compare tissue deformation dynamics of homologous organs of different sizes/outlines, and found that the tissue dynamics were well scaled between species.

2SBP-1 富岳と超並列分子動力学を用いたタンパク質の構造変化、会合と解離
Protein conformational change, association and dissociation observed using Fugaku and massively parallel molecular dynamics simulations

Akio Kitao (*Scl. Life Sci. Tech., Tokyo Tech*)

Protein conformational change, association and dissociation are closely related to protein functions. However, it is not straightforward to experimentally observe these processes at atomic resolution. All-atom molecular dynamics (MD) can simulate atomic behavior of proteins and other biomolecules in silico, but accessible time scale of standard MD is still limited to microsecond order. In this talk, investigation of protein conformational change, association and dissociation which was enabled by using more advance conformational sampling methods, such as parallel cascade selection molecular dynamics (PaCS-MD), was introduced.

2SBP-2 Molecular dynamics study of multidrug efflux transporter complex embedded in lipid bilayer: Role of membrane lipids in the transporter

Keiko Shinoda, Hisashi Kawasaki (*AgTECH, GSALS, UTokyo*)

The multidrug efflux transporter AcrA-AcrB-AcrZ-TolC complex is a multidrug efflux transport system in Escherichia coli and plays a major role in the intrinsic resistance of Gram-negative bacteria. The complex is a large modular-built protein complex composed of AcrB, which is responsible for the pump function, TolC of the external channel, AcrZ reported being involved in substrate selectivity and AcrA that connects AcrB and TolC. In this work, we examined the interaction of each amino acid of AcrB with the three types of membranes using Molecular dynamics simulation. We will report how the different properties of membrane lipids affect their interaction with the transporter complex.

2SBP-3 (3Pos186) エンベロープ型ウイルス粒子の粗視化シミュレーション：B 型肝炎ウイルス
(3Pos186) Coarse-grained Molecular Dynamics Study of Enveloped Virus Particle: Hepatitis B Virus

Ryo Urano, Wataru Shinoda (*Res. Inst. Interdiscip. Sci., Okayama Univ.*)

Coarse-grained molecular dynamics simulation has been performed for Hepatitis B virus (HBV) particle to investigate the structure and dynamics of the enveloped capsid at molecular level. The envelope is a lipid membrane containing viral membrane proteins, though which structure was not determined at the molecular level. Thus, the structural role of viral membrane protein in the envelope is unclear. By constructing a reasonable HBV envelope model, our simulations clarified the role of envelope protein in the interaction with capsid spike and surrounding lipids. The details will be reported on the day.

2SBP-4 Binding free energy landscapes of Src Kinase to its inhibitors sampled by two-dimensional replica exchange molecular dynamics simulations

Ai Shinobu[1], Suyong Re[1,2], Yuji Sugita[1] ([1]*RIKEN*, [2]*National Institutes of Biomedical Innovation, Health, and Nutrition*)

Protein kinases (PKs) play important roles in cellular signal transduction. Their dysfunction leads to disease such as cancer thus they are considered attractives drug targets. To design a selective PK inhibitor, we must elucidate the regulatory mechanism at the atomic level, which is difficult to obtain solely by experiments.
Here, we use the two-dimensional replica-exchange molecular dynamics simulation method gREST/REUS to sample the binding free energy landscapes of Src kinase to its inhibitors of varying sizes and flexibilities. We collected over 600 microseconds of trajectory data using the supercomputer Fugaku, from which we obtained multiple un/binding pathways and structures of poses along them.

2SBP-5 REST シミュレーションによるタンパク質やペプチドリガンドの活性制御機構の解析
Applications of REST simulation to understanding regulation mechanism of protein activation and peptide ligands

Toru Ekimoto[1], Tsutomu Yamane[2], Mitsunori Ikeguchi[1,2] ([1]*Grad. Med. Life Sci., Yokohama City Univ.*, [2]*R-CCS, Riken*)

To regulate protein activation by small compounds or peptide ligands, dynamical information about both dynamic interaction modes between protein and ligands, and conformational changes of protein induced by ligand binding are necessary. In addition, drug design should consider kinetics such as membrane permeation, and for peptide ligands, e.g., middle-molecule drug cyclosporin A, it is necessary to understand how conformational stability changes in the surrounding environment. Such long time-scale conformational changes, which are difficult to capture in conventional MD simulations, can be obtained by enhanced sampling methods using multiple replica systems, such as replica exchange with solute tempering (REST) method. We will introduce applications of REST simulation.

2SBP-6 (1Pos027) Automated Density Extraction of Isomorphous Difference map and Occupancy-estimation for Conformer Fitting

Sriram Srinivasa Raghavan[1], Florence Tama[1,2,3], Osamu Miyashita[1] ([1]*RIKEN Center for Computational Science, Kobe, Japan.*, [2]*Institute of Transformative Biomolecules (WPI-ITbM), Nagoya University, Aichi, Japan.*, [3]*Department of Physics, Graduate School of Science, Nagoya University, Aichi, Japan.*)

TR-SFX allows capturing of time-evolved residual motion within crystal structure thereby enabling the visual inspection of reaction kinetics. The changes in fractional density of intermittent states are estimated from isomorphous difference density map (ISM). The discrete density observed from ISM are then interpreted as minor states corresponding to various intermittent time steps. ISM map interpretations are generally time-consuming and methodologically inaccurate during manual density estimation. Here, we employ clustering and SVD based approaches to extract and evaluate residues corresponding to isomorphous difference density. Fractional occupancy corresponding to the change in map density is estimated and the conformers of the minor states are fitted using MD trajectory.

2SBP-7 スーパーコンピュータ「富岳」を用いたテンプレートマッチング法による生体分子のマルチコンフォメーション解析
Multi-conformational analysis of biomolecule by the template-matching method using the supercomputer Fugaku

Atsushi Tokuhisa (*R-CCS, Riken*)

My current research theme is constructing a next-generation drug discovery platform that considers the flexibility of biomolecules by fusion of "Experiment x AI x Simulation". To clarify the multi-conformational state of biomolecules, I am focusing on single-particle structural analysis experiments. A new scheme called the template-matching method with the data assimilation concept and AI techniques can estimate a plausible structural model with a high resolution from individual experimental images. This enables us to evaluate a wide variety of conformational states. In my presentation, I will introduce the development status of the integrated workflow for multi conformational analysis on the supercomputer Fugaku and our efforts to apply it to individual applications.

2SCP-1 タンパク質構造の人工設計
De novo design of novel protein structures

Nobuyasu Koga (*NINS, ExCELLS*)

The structural diversity of proteins underlies their functional variety. We have developed principles for designing protein structures from scratch. The developed design principles describe favorable backbone geometries, lengths of secondary structures and loop torsion patterns, for design target topologies. Using the developed principles, we have succeeded in various protein structures, including novel topologies not observed in nature, with atomic-level accuracy. Moreover, most of the designed proteins exhibited high thermal stability: the melting temperatures were more than 100 °C. The super-stable designed protein structures should be used as scaffolds for engineering functions.

2SCP-2 Towards the de novo design of binding proteins through beta-sheet folds

Enrique Marcos (*Molecular Biology Institute of Barcelona (IBMB-CSIC), Protein Design and Modeling Lab*)

The recent revolution of de novo protein design is transforming the protein engineering field. Instead of searching and modifying natural proteins, de novo protein design crafts new proteins from physical principles with sequences and geometries not restricted to those seen in nature. We have identified key principles for the de novo design of a variety of protein folds containing beta-sheets, which are attractive structural motifs for building ligand- and protein-binding sites such as antibody frameworks, and used these principles for computationally designing hyperstable proteins in excellent agreement with their experimental structures and new functionalities.

2SCP-3 Protein engineering for biogeeks; practical examples of structural redesigns of a model protein and therapeutic antibody designs

Koki Makabe (*Grad. Sch. Sci. and Eng., Yamagata univ.*)

Protein engineering is a method to genetically engineer the protein sequences to investigate the structures and functions of proteins or construct useful proteins. The falling price for artificial gene synthesis has enabled biogeeks to make a variety of modified proteins based on protein engineering skills within a limited budget. Here, I will show practical examples of protein engineering approach for redesigns of a β-sheet rich model protein and antibody engineering applications. Based on the experimental findings, I will discuss the current state of the technique.

2SCP-4 非環状型人工核酸による天然核酸認識の設計
Understanding the design of acyclic artificial nucleic acids that recognize natural nucleic acids

Yukiko Kamiya (*Grad. Sch. Eng., Nagoya Univ.*)

Artificial nucleic acids have potential for use in nucleic acid drugs and as orthogonal genetic biopolymers and prebiotic precursors. Although few acyclic-type nucleic acids can stably bind to RNA and DNA, SNA and L-*a*TNA stably bind to them. However, it is unclear how, if at all, RNA hybridizes with these acyclic nucleic acids. Our team was able to determine crystal structures of RNA hybridizing with SNA and with L-aTNA. We found that intra-molecular interactions are important for keeping the helical double-stranded structures formed of acyclic nucleic acids and RNA stable. The unique structural features of the RNA-recognizing mode of L-*a*TNA and SNA should prove useful in nanotechnology, biotechnology, and basic research into prebiotic chemistry.

2SCP-5 Engineering RNA-protein interactions by directed evolution

Keisuke Fukunaga, Yohei Yokobayashi (*Nucleic Acid Chemistry and Engineering Unit, OIST*)

RNA-binding proteins (RBPs) and their RNA ligands are useful for various applications in cell biology and synthetic biology. However, re-engineering novel and orthogonal RNA-RBP pairs from natural components remains challenging while such synthetic RNA-RBP pairs could significantly expand the RNA-RBP toolbox for various applications. In this symposium, I will present a novel library-vs-library *in vitro* selection strategy based on Phage Display coupled with Systematic Evolution of Ligands by EXponential enrichment (PD-SELEX). Evolved two RNA-RBP pairs exhibited a binding selectivity greater than 4000-fold.

2SCP-6 DNA ナノ構造によるデザインされた人工細胞と人工オルガネラの実現へ向けて
Toward DNA nanostructure-based designed artificial cells and artificial organelles

Masahiro Takinoue (*Sch. Computing, Tokyo Tech*)

The construction of artificial cells and organelles has been attracting much attention because of the possibility of revealing the construction principle of molecular dynamical systems like cells from a physics point of view. DNA nanostructures can be precisely designed in a computer-aided manner; thus, artificial cells and organelles with various functions such as molecular sensors and molecular computation have recently been constructed. In this presentation, DNA nanostructure-based coacervate droplets and microcapsules, called DNA droplets and DNA-origamisomes, respectively, will be introduced. The capability of DNA design in this field will be shown, and the integration of designed DNA systems with designed protein systems will be discussed in this symposium.

2SDP-1 酵素反応における弱い金属イオン結合の意義
Significance of weak metal-ion binding in enzymatic reactions

Oda Masayuki (*Grad. Sch. Life Environ. Sci., Kyoto Pref. Univ.*)

The cutinase-like enzyme, Cut190, could depolymerize polyethylene terephthalate (PET). One of the unique features of Cut190 is that its catalytic function and thermal stability are increased upon Ca^{2+} binding. Ribonuclease HI (RNase HI) catalyzes the specific cleavage of RNA strands of RNA/DNA hybrid duplexes in the presence of Mg^{2+}. Both enzymes in common bind to divalent cations such as Ca^{2+}, Mg^{2+}, Mn^{2+}, and Zn^{2+}, and express the catalytic function most efficiently, in the presence of low-affinity binders, Ca^{2+} for Cut190 and Mg^{2+} for RNase HI. I will present a brief introduction of the conformational characteristics of the two enzymes and their thermodynamic evaluation for the effects of weak metal-ion binding in terms of enzymatic reactions.

2SDP-2 PET 分解酵素 Cut190 における弱く結合した Ca^{2+}イオンを介したアロステリック制御
Allosteric regulation of PET-degrading enzyme Cut190 through the weakly bound Ca^{2+} ion

Nobutaka Numoto (*Med. Res. Inst., Tokyo Med. Dent. Univ.*)

Cutinase-like enzyme Cut190 from *Saccharomonospora viridis* AHK190 has been shown to hydrolyze polyethylene terephthalate (PET). We have previously demonstrated the Ca^{2+} dependent enzymatic reaction cycle based on the crystal structures of Cut190 complexed with the two substrates of straight-chain esters. Recently, we have obtained the mutants of improved thermal stability and enzymatic activity, and determined the crystal structures of complexes with the substrate analogues containing aromatic ring, which closely mimic a monomeric or dimeric unit of PET. Our structures and MD analysis suggest that the allosteric regulation via Ca^{2+} binding loop is finely adjusted by a fast binding/dissociation of Ca^{2+} ion.

2SDP-3 RNaseHI の触媒反応機構：必須金属は 1 個か 2 個か？
Catalytic mechanism of RNaseHI: one metal or two metals?

Kosuke Morikawa (*Kyoto Univ.*)

RNaseHI is the endonuclease, which specifically cleaves the RNA strand only of a DNA/RNA hybrid duplex. This activity plays essential roles in gene expression and genome stability from prokaryotes to eukaryotes. The activity seems to be related to degradation of R-loop structures. Since the first crystal structure determination in 1990, its catalytic mechanism remains controversial and elusive particularly on the essential number of Mg^{2+} or Mn^{2+} ions. More importantly, the requirement of divalent metal ions such as Mg^{2+} appears to be conserved in almost all of nucleases, thus tempting us to elucidate the general catalytic scheme in terms of molecular evolution. In the symposium, I would like to discuss this longstanding yet important problem in the biological world.

2SDP-4 エレクトロスプレーイオン化質量分析法による活性型リボヌクレアーゼ HI：RNA/DNA:金属イオン複合体の検出
Active ternary complex of ribonuclease HI: RNA/DNA hybrid: metal ions probed by ESI mass spectrometry

Toshifumi Takao[1], Tomoshige Ando[1], Hiromi Hayashi[1], Nujarin Jongruja[2], Nobuaki Okumura[1], Kosuke Morikawa[3], Shigenori Kanaya[2] ([1]*Inst. Protein Res., Osaka Univ.*, [2]*Grad. Sch. Eng., Osaka Univ.*, [3]*Grad. Sch. Biostudies, Kyoto Univ.*)

Ribonuclease HI requires divalent metal ions for its enzymatic activity. However, the mechanistic details of the activity and its interaction with divalent metal ions remains unclear. We here performed real-time monitoring of the enzyme–substrate complex in the presence of divalent metal ions (Mn^{2+} or Zn^{2+}) using ESI-MS. The findings provide clear evidence that the enzymatic activity of the ternary complex requires the binding of two divalent metal ions. The Zn^{2+} ions bind to both the enzyme itself and the enzyme:substrate complex more strongly than Mn^{2+} ions to form the ternary complex even after the hydrolysis of the substrate, suggesting how Zn^{2+} ions confer inhibitory properties on the activity of this enzyme by forming a highly stable complex with the substrate.

2SDP-5 (2Pos026) Structural basis of the significant metal-histidine coordination in *E. coli* RNase HI

Zengwei Liao[1], Takuji Oyama[2], Yumi Kitagawa[3], Katsuo Katayanagi[4], Kosuke Morikawa[5], Masayuki Oda[3] ([1]*Grad. Sch. Agri. and Life Sci., the Univ. of Tokyo*, [2]*Faculty of Life and Environ. Sci., Univ. of Yamanashi*, [3]*Grad. Sch. Life Environ. Sci., Kyoto Pref. Univ.*, [4]*Grad. Sch. Integrated Sci. for Life, Hiroshima Univ.*, [5]*Grad. Sch. Biostudies, Kyoto Univ.*)

RNase HI is an endonuclease that cleaves the RNA strand of a DNA/RNA hybrid by a canonical metal cation catalytic mechanism. Its activity is the highest in the presence of Mg^{2+}, while it is limited in the presence of other metal cations such as Mn^{2+} and Zn^{2+}. Biophysical experiments have shown that the carboxyl groups of the conserved DEDD motif creates a delicate field at the active center. Moreover, an adjacent His may also be one piece of the puzzle yet not well-defined. Our crystallographic analyses of *E. coli* RNase HI-Mg^{2+} showed two Mg^{2+} binding in the absence of substrate. The structural features of the imidazole ring of His124, along with the RNase HI-Zn^{2+} structures, provided significant insights into the pivotal metal dependent enzymatic mechanism.

2SDP-6 Metal interaction and Conformational Changes in HIV-1 Reverse Transcriptase

Rieko Ishima (*University of Pittsburgh School of Medicine*)

HIV-1 Reverse transcriptase (RT) is a bi-functional enzyme, having two activities: a DNA polymerase that converts HIV genomic RNA into DNA and an RNase H that selectively degrades the RNA, both with divalent ions as co-factors. We have mainly used NMR to investigate the RT conformational or chemical changes. However, the highly sensitive NMR instrumentation can elucidate data artifacts, caused by minor pathways and systematic errors, in addition to detecting the desired signals. For this reason, we have made efforts toward identification of such artifacts with respect to RT metal interaction, inhibitor interaction, and RT maturation, by combining NMR-based observations with those from other biophysical methods (Ilina et al, Int J Mol Sci, 2020).

2SDP-7 High-resolution and time-resolved insights into an RNA-cleaving DNA catalyst

Manuel Etzkorn[1,2] ([1]*Heinrich Heine University Düsseldorf*, [2]*Research Center Jülich*)

RNA-cleaving DNAzymes carry a great therapeutic potential. However, they are facing a number of limitations, which coincide with an insufficient understanding of their mode of action.
Using an integrative approach combining NMR-based methods with FRET, EPR, and MD simulations we could obtain detailed insights into one of the most active DNAzymes (1,2). Our data capture an unexpected but highly efficient structure and provide information about the essential role of metal-ion cofactors.
Overall, our insights highlight the importance of dynamic processes in DNA-mediated catalysis and demonstrate the faesability of rational-design strategies aiming to unravel the full potential of the DNAzyme technology.
Borggräfe et al. *Nature* 2022 Rosenbach et al. *Biol Chem* 2021

2SEP-1 Novel repressive role of eIF4A1 during mTORC1 inhibition

Yuichi Shichino (*RIKEN CPR*)

Eukaryotic translation initiation factor (eIF) 4A — a DEAD-box RNA helicase — plays an essential role in translation initiation. Given the recent reports of helicase-dependent and independent function of the protein, the multifaceted roles of eIF4A have been suggested but not fully explored. Here we found a novel function of eIF4A1 that facilitates translational repression during inhibition of the mechanistic target of rapamycin complex 1 (mTORC1). eIF4A1 preferentially binds to terminal oligopyrimidine (TOP) mRNAs depending on a LARP1. The deletion of *EIF4A1* rendered the translation of TOP mRNAs resistant to mTOR inactivation. eIF4A1 enhances the affinity between TOP mRNAs and LARP1. Our data provide a unique example of the repressive role of a translation activator.

2SEP-2 (1Pos121) 自由エネルギー地形から探る開始コドン認識機構
(1Pos121) Computational Analysis of the Start Codon Recognition Mechanism Based on Free Energy Landscape

Takeru Kameda[1], Katsura Asano[2,3,4], Yuichi Togashi[1,5] ([1]*Coll. Life Sci., Ritsumeikan Univ.*, [2]*Div. Biol., Kansas State Univ.*, [3]*HiHA, Hiroshima Univ.*, [4]*Grad. Sch. Integ. Sci. Life, Hiroshima Univ.*, [5]*RIKEN BDR*)

Eukaryotic translation usually initiates at the AUG codon in mRNA. Alternatively, CUG is reported to play the role of start codons at a low frequency, and thus attention has been paid to the frequency and mechanism of translation initiation at non-AUG codons. Recently, we have studied start codon recognition mechanisms in eukaryotic ribosomes based on free-energy evaluation using computer simulations, and discussed them from the molecular dynamics viewpoint. We also reported the effects of chemically modified nucleotides (e.g. pseudouridine) on translation initiation. In this presentation, we will introduce these studies and discuss future directions of computational research on translation initiation.

2SEP-3 (2Pos109) RNase T2 のリボソームへの結合を介した翻訳阻害機構
(2Pos109) Regulation mechanism of translation through the interaction of RNase T2 with ribosome

Atsushi Minami[1], Takehito Tanzawa[2], Zhuohao Yang[3], Takashi Funatsu[3], Takayuki Kato[2], Tomohisa Kuzuyama[1,4], Hideji Yoshida[5], Tetsuhiro Ogawa[1,4] ([1]*Grad. Sch. Agri. and Life Sci., Univ. Tokyo*, [2]*IPR, Osaka Univ.*, [3]*Grad. Sch. Pharm. Sci., Univ. Tokyo*, [4]*CRIIM, Univ. Tokyo*, [5]*Fac. Med., Osaka Med. Pharm. Univ.*)

RNase T2 is a conserved ribonuclease found in almost all organisms. Although the enzymatic activity is quite simple that it cleaves single-stranded RNA nonspecifically, it is involved in diverse and important biological events, e.g. tumor suppressor in mammals and biofilm formation in *Escherichia coli*.
It is known that *E. coli* RNase T2 interacts with ribosomes, but the physiological role remains elusive. During our analysis of the biofilm formation mechanism, we found that RNase T2 interacts with ribosomes that are not engaged in translation. Moreover, the ribosome bound to RNase T2 cannot initiate translation. Together with the Cryo-EM structure of RNase T2 complexed with ribosome, we will discuss the mechanism of translation impairment in this presentation.

2SEP-4 High-speed AFM visualizes translational GTPase factor pool formed around the ribosomal P-stalk

Hirotatsu Imai[1,2], Toshio Uchiumi[3], Noriyuki Kodera[2] ([1]*Fac. Med., Univ. Ryukyus*, [2]*Nano-LSI, Kanazawa Univ.*, [3]*Fac. Sci., Niigata Univ.*)

Translation of genetic information by the ribosome is a core biological process in all organisms. The ribosomal stalk is a multimeric ribosomal protein complex which plays an essential role in translation elongation. However, the working mechanism of the ribosomal stalk still remains unclear. Here, we applied high-speed atomic force microscopy (HS-AFM) to investigate the working mechanism of the archaeal ribosomal P-stalk. HS-AFM movies demonstrate that the P-stalk collects two translational GTPase factors (trGTPases), aEF1A and aEF2, and increases their local concentration near the ribosome. These direct visual evidences show that the multiple arms of the ribosomal P-stalk catch the trGTPases for efficient protein synthesis in the crowded intracellular environment.

2SEP-5 The mechanical stability of SecM translation arrest

Zhuohao Yang[1], Ryo Iizuka[2], Takashi Funatsu[1] ([1]*Grad. Sch. Pharm. Sci., The Univ. Tokyo*, [2]*Dept. Biol. Sci., Grad. Sch. Sci., The Univ. Tokyo*)

SecM, a secretion monitor protein of E. coli, contains an arrest sequence that interacts with the ribosomal tunnel to arrest its translation. It is considered that the pulling force of the Sec apparatus releases the translation arrest and resumes its translation. However, the mechanical stability and the release process of SecM translation arrest have not been fully elucidated. In this study, we developed a single-molecule force measurement system using magnetic tweezers and applied force to SecM-ribosome-mRNA arrested complexes to artificially resume its translation. We found that SecM translation arrest is sensitive to a force of a few pN. Here, we would like to discuss SecM translation arrest and its release process from a mechanical point of view.

2SEP-6 Attempt to visualize the synthetic polypeptide during translational arrest

Takehito Tanzawa (*IPR., Osaka Univ.*)

Protein synthesis on ribosome is very systematically controlled. Polypeptide chains synthesized at the peptidyl transferase center of the 50S ribosomal subunit during translation elongation passes through the ribosome exit tunnel. When the polypeptide chain is released from the tRNA after translation termination, it is precisely folded via chaperones and finally becomes a functional molecule “protein”. Recent studies have provided indirect experimental evidence suggesting that the polypeptide in the exit tunnel may take on some secondary structures rather than maintaining a complete primary structure. Here, we discuss the structure of polypeptide chain in the exit tunnel by using a translational arrest sequence that temporarily-paused elongation of the nascent chain.

2SEP-7 The final step of protein synthesis; the capture of an unfolded polypeptide by chaperonin GroEL

Kevin Mac Alister Stapleton (*Grad. Sch. Frontier BioSci., Osaka Univ.*)

The final step of information transfer within the cell requires folding newly synthesized nascent polypeptide chains into biologically active conformations. Bacterial chaperonin GroEL from *E. coli* is a molecular chaperone responsible for folding nonnative (unfolded) polypeptides into uniquely folded active proteins required for maintaining cellular homeostasis. This study investigates the fortuitous structure complex formation of a human protein construct (UGT1A) permanently bound to GroEL during expression and stalled at the start of the GroEL-mediated protein folding reaction cycle. From this unexpected event captured by cryoEM, we can address the question: *At the terminal end of protein synthesis, what features of nascent polypeptides identify GroEL-assisted folding?*

2SEP-8 ER Redox shift through the ribosome translation

Ryo Ushioda[1,2] ([1]*Fac. of Life Sci., Kyoto Sangyo Univ.*, [2]*Inst. for Protein Dynamics, Kyoto Sangyo Univ.*)

The endoplasmic reticulum (ER) is an organelle for the maturation of secretory and membrane proteins synthesized from ribosomes, and various molecular chaperones and oxidoreductases exist to assist the folding. Disulfide bond formation for protein maturation is favorably promoted by the oxidative environment of the ER lumen. On the other hand, We identified disulfide reductase in the ER and revealed that its reducing activity contributes to protein quality control and calcium ion control and is important for maintaining ER homeostasis.
Here, we would like to introduce a unique ER Redox environmental shift according to the translation of nascent polypeptides by the ribosome as a homeostasis maintenance strategy.

2SFP-1 Phase separation provides a reaction chamber for autophagy progression

Yuko Fujioka (*Institute for Genetic Medicine, Hokkaido Univ.*)

Autophagy is an intracellular degradation system that contributes not only to securing nutrient source upon starvation, but also to intracellular clearance, especially in brain, under normal conditions. To elucidate the autophagy mechanisms, we have been performing the structural and biochemical analyses of autophagy-related proteins. After a decade of struggle on the Atg1 complex, a scaffold protein complex mediating autophagy initiation, we found that the Atg1 complex undergoes phase separation to form liquid-like droplets, which function as the reaction chamber for enzymatic reactions important for autophagy progression. In this talk, I will summarize the regulation and function of the Atg1 complex droplets and discuss why droplet formation is required for autophagy.

2SFP-2 蛋白質ミスフォールディング病における蛋白質凝集の分子機構
The molecular mechanism of protein aggregation in protein misfolding disease

Young-Ho Lee[1,2,3] ([1]*Research Center for Bioconvergence Analysis, Korea Basic Sci. Inst., Korea*, [2]*Bio-Analytical Sci., Uni. of Sci. and Tech., Korea*, [3]*Grad. Sch. of Analytical Sci. and Tech., Chungnam National Uni., Korea*)

Disruption of protein homeostasis by protein misfolding and aggregation causes aggregopathy including Alzheimer's disease and Parkinson's disease. Despite of numerous efforts, much remains to be elucidated on underlying principles of protein misfolding and aggregation. Today, I will show the molecular mechanisms of protein aggregation, especially, amyloid fibrillation, and its unique property such as context-dependent and polymorphic amyloidogenesis and cross seeding. Impacts of biological membranes on amyloidogenicity in neurodegenerative diseases will be also described. Finally, amyloid formation based on the amyloidogenic structure and solubility/supersaturation will be explained using the structure and phase diagrams.

2SFP-3 脳神経疾患研究における１分子イメージング研究の現状・課題・可能性
Current status, problems, and potential of single molecule imaging studies in neurological disease research

Hiroko Bannai (*Fac. Sci. Eng., Waseda Univ.*)

Single-molecule imaging is a powerful tool for understanding the principles of action of neurons at the molecular level. Recently, single molecule imaging has attracted much attention as a method to detect abnormalities in disease model cells with high sensitivity and to contribute to our understanding of the mechanisms of pathology. In this symposium, we will discuss what is currently possible with single molecule imaging research, problems that need to be overcome, and proposed solutions. In addition, we will discuss the temporal control of biological events that are necessary for neurological disorder research.

2SFP-4 超分子ペプチドゲルを用いた損傷脳再生
Injured brain regeneration using supramolecular peptide hydrogels

Itsuki Ajioka[1,2] ([1]*Center for Brain Integration Research (CBIR), Tokyo Medical Dental Univ (TMDU)*, [2]*KISTEC*)

The artificial hydrogels mimicking the extracellular matrix enhances injured tissue regeneration. Although the brain is thought to be a non-regenerative tissue, the injured brain has regenerative potential. A supramolecular peptide forms a hydrogel by non-covalent bonds. The biodegraded products of a supramolecular peptide are the original peptide, thereby fitting for medical application as far as the original peptide is biocompatible. Moreover, the viscoelasticity of a supramolecular peptide hydrogel can be modulated by tuning hydrophilic and hydrophobic interactions. In this symposium, I would like to outline the supramolecular peptides developed by combining computational physics and supramolecular chemistry and their application to injured brain regeneration.

2SFP-5 相反する匂い価値の脳内表現と神経回路基盤
Representations and circuits for opposing odor values in the brain

Hokto Kazama (*RIKEN Center for Brain Science*)

Odors are intrinsically associated with values ranging from positive to negative as they induce innate behaviors such as attraction and aversion. However, how opposing, innate values of odors are represented and computed in the brain remains unclear. Here we addressed these questions in fruit fly *Drosophila* and found that the lateral horn (LH), the brain region implicated for innate behavior, encoded the value of odors. Subsets of LH neurons were tuned to either positive or negative odor values and were differentially clustered in space. Simulation based on a network model constructed from the connectome data suggested that the representation of opposing odor values emerge through distinct circuits with the former involving stronger recurrent interactions.

2SGP-1 Putting prions in context: towards in vivo structural biology using DNP NMR

Kendra King Frederick (*UT Southwestern*)

The prion domain of Sup35 adopts (at least) two different conformations which result in heritable stop-codon read-through phenotypes of varying strength (strong or weak). The strong and weak prion conformations of Sup35PrD are beta-sheet rich amyloid folds that differ both in size and organization and, in purified settings, the regions that are not sequestered in the amyloid core are intrinsically disordered although they adopt alternative conformations in cellular milieu. We examined the amyloid cores of prions assembled in cellular milieu and found that amyloids assembled in cellular milieu are more ordered than those in purified settings, possibly because of specific interactions with cellular components and/or selective amplification of a conformation.

2SGP-2 The single-particle cryo-electron microscopic analysis of amyloid disaggregation reaction

Takashi Nomura[1], Yoshiko Nakagawa[1], Yusuke Komi[1], Shingo Tamai[1,2], Masako Yamazaki[1], Motomasa Tanaka[1]
([1]*CBS, RIKEN*, [2]*Biomed. Sci. & Eng., Grad. Sch. of Med. &Dent. Sci., TMDU*)

Amyloid fibrils, β-sheet rich fibrillar protein aggregates, are associated with many neurodegenerative diseases. However, the molecular basis of how amyloid fibrils are formed and disaggregated is poorly understood. Here we revealed the two types of Sup35NM amyloid structures and the disaggregation intermediates, Sup35NM/Ssa1/Sis1 complex, by single-particle cryo-electron microscopy (cryo-EM) and micro-scale IR spectroscopy that we have recently developed. These findings have helped us to decipher disaggregation mechanisms of the two types of amyloids at the molecular level. Our results will provide insights into how amyloid fibrils elicit neurodegenerative disorders by their cell-to-cell propagation.

2SGP-3 Critical Jamming and gel rheology of droplet suspensions in living cells

Daisuke Mizuno (*Kyushu University*)

Mechanical properties of living cells are determined by soft glassy materials and gels. Weak non-specific interactions between these constituents drive the formation of microscopic droplets which takes place under non-equilibrium situation. In this study, we aim to investigate the mechanics of the activated cytoplasm, by comparing with various dense disordered materials. The viscoelastic properties typically predicted for critically-jammed materials were generally observed in cells and dense suspensions driven out of equilibrium by metabolic activities, but they are hidden by the gel-like elasticities in inactive suspensions. Liquid droplets in cells also showed similar critical behavior in the beginning, but it disappeared with time after the formation of droplets.

2SGP-4 レオロジー NMR 法による SOD1 アミロイド形成の多状態その場観察
Multiple-state *in situ* observation of SOD1 amyloid formation by Rheo-NMR spectroscopy

Daichi Morimoto[1], Erik Walinda[2], Masahiro Shirakawa[1], Ulrich Scheler[3], Kenji Sugase[4] ([1]*Grad. Sch. Eng., Kyoto Univ.*, [2]*Grad. Sch. Med., Kyoto Univ.*, [3]*IPF*, [4]*Grad. Sch. Agr., Kyoto Univ.*)

Amyloid fibril formation entails the conversion of soluble native protein monomers via multiple molecular states. However, no spectroscopic techniques have succeeded in capturing the transient molecular-scale events of fibril formation *in situ*. In this study, we have established high-sensitivity Rheo-NMR spectroscopy to monitor residue-specific fibril formation of an ALS-related protein SOD1. Under moderately denaturing conditions where NMR signals of folded and unfolded SOD1 are simultaneously observable, the folded species was found to decrease faster than the unfolded species; especially, a 3_{10}-helix in folded SOD1 was shown to be deformed prior to global unfolding. These observations provide insights into local and global unfolding events in SOD1 fibril formation.

2SGP-5 TDP43-LC ドメインの病原性変異と線維形成能の網羅的解析
Comprehensive studies of disease-related mutations on cross-β polymerization of TDP43-LC domain

Nobuo Maita[1], Yuko Kajino[1], Masato Kato[1,2] ([1]*National Institutes for Quantum Science and Technology*, [2]*UT Southwestern Medical Center*)

Low-complexity (LC) domains of some RNA-binding proteins, such as FUS and TDP43, assemble as cross-β polymers and form liquid-like droplets. These assemblies are known to efficiently promote many biochemical reactions. In cells, cross-β polymers of wild-type TDP-43 LC domains are labile, while those of disease-related mutants become abnormally stable and, as a result, accumulate inside of brain cells, leading to neurodegenerative diseases.
To examine the relationship between the mutations and severity of the neurodegenerative diseases, we have prepared 47 disease mutants of TDP43-LC and investigated cross-β polymerization propensities by hydrogel-binding assays. We also performed biophysical analysis on the mutants that show high-level polymerization propensities.

2SHP-1 mRNA の翻訳制御を 1 分子解像度で in situ イメージングする
Translational regulation visualized at single-molecule resolution in cells

Hotaka Kobayashi[1,2] ([1]*JST PRESTO*, [2]*IQB, The University of Tokyo*)

Translation, the process of protein synthesis, is regulated by various RNA-binding proteins (RBPs) that target mRNAs. For decades, translational regulation by RBPs has been monitored by ensemble methods, where a bulk collection of mRNAs is analyzed outside cells. Thus, the behavior of each mRNA during translational regulation, as well as its spatiotemporal control inside cells, remains unclear. To overcome the limitation of canonical methods, I have developed a novel method to image translational regulation at single-mRNA resolution in cells, where translational and RBP-binding status of each mRNA can be analyzed quantitatively in situ. At the meeting, I will discuss the latest findings revealed by this method, which illuminate novel “facets” of protein synthesis.

2SHP-2 SARS-CoV-2 nsp1 はホスト翻訳系をどう乗っ取るのか？
SARS-CoV-2 nsp1: how do they hijack the host translation?

Shun Sakuraba[1], Qilin Xie[2], Kota Kasahara[3], Junichi Iwakiri[4], Hidetoshi Kono[1] ([1]*Natl. Inst. Quantum Sci. & Tech.*, [2]*Grad. Sch. Life Sci., Ritsumeikan Univ.*, [3]*Col. Life Sci., Ritsumeikan Univ.*, [4]*Grad. Sch. Frontier Sci., Univ. Tokyo*)

Nonstructural protein 1 (nsp1) of severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2) is a 180-residue protein that modulates the translation of the host cell infected by SARS-CoV-2. Nsp1 of SARS-CoV-2 blocks the translation of the host mRNA, while that of virus RNA remains unblocked. It has been reported that stem loop 1 (SL1) of SARS-CoV-2 RNA, which resides at the very beginning of the viral RNA, is essential to the evasion, but its mechanism is unknown. Through a computer simulation of SARS-CoV-2 nsp1 and SL1, we found that SL1 binds to both nsp1's N-terminal globular region and C-terminal disordered region. Simulation results suggest a selective translation hijacking mechanism through the nsp1-RNA-ribosome interaction.

2SHP-3 神経変性疾患を引き起こすアミロイド線維のクライオ電顕解析
Cryo-EM analyses of the amyloid fibrils causing neurodegenerative diseases

Atsushi Yamagata (*RIKEN Center for Biosystems Dynamics Research*)

Neurodegenerative diseases, such as Alzheimer's disease, ALS, and Parkison's disease are caused by amyloid-like aggregates of the misfolded proteins. The recent advances in cryo-EM have provided the high-resolution structures of these fibrils and shed light on the relationship between structure and pathology. Moreover, recent studies indicate that amyloid fibril formation is dynamically controlled by unique cellular mechanisms, such as RAN translation, self-propagation, and chaperone-mediated disaggregation. Here I show our high-resolution cryo-EM structure of amyloid-beta fibril carrying the familial Alzheimer's disease mutation. I would also present our recent trials to visualize the cellular mechanisms for the amyloid filament assembly using cryo-EM.

2SHP-4 (2Pos260) 新規遺伝子の誕生と機能獲得の進化メカニズムに迫るゲノム計算科学：バイオインフォマティクスのその先に遺伝子の本質を探求する
(2Pos260) How do *de novo* genes evolve and acquire function?: Computational genomics to revisit the nature of genes beyond bioinformatics

Shun Yamanouchi[1], Wataru Iwasaki[1,2] ([1]*Grad. Sch. Sci., Univ. Tokyo*, [2]*Grad. Sch. Front. Sci., Univ. Tokyo*)

It has recently been shown that novel genes arise from scratch (*de novo* gene birth). Previous studies have focused on identifying and describing *de novo* genes, but their molecular functions and underlying evolutionary mechanisms remain poorly understood. Thus, we systematically evaluated the functional potential of non-coding regions of the yeast and fly genomes. We found that functional motif-like peptides were enriched in some "alternative reading frames" of coding sequences, while they were rarely conserved even at genus level. We then hypothesized that genomes can potentially pool the source of genes, which may contribute to short-term adaptation in microevolution. Here, we aim to obtain new insights that go beyond bioinformatics.

2SHP-5 Multifaceted view of protein diffusion

Eiji Yamamoto (*Dept. Syst. Des. Eng., Keio Univ.*)

In the classical Stokes-Einstein relationship the diffusivity of tracers is determined by their radius and by the liquid's viscosity. However, this relationship is assumed on a scale longer than the relaxation time of the fluctuation of the radius and viscosity. Although proteins or polymers exhibit a constant change in their morphology in a dilute solution or condensed matter, the effect of the fluctuating conformation on the molecular diffusivity has been unclear. Here we perform molecular dynamics simulations of proteins isolated in solute or a membrane-less droplet formed via liquid-liquid phase separation. We will show how the fluctuation of the protein conformations and the interaction with other molecules affect the diffusion process of proteins.

2SHP-6 生体分子の 1 分子解析とその応用
Single-molecule analysis of bio-molecules and its applications

Rikiya Watanabe (*CPR, RIKEN*)

Micron/nano technologies enable highly sensitive and quantitative bioassays at the single-molecule level, which are widely used for ultra-sensitive biomedical applications, e.g., digital PCR. Here, we developed a novel microsystem "SATORI" with emerging CRISPR-Cas13a technologies that allows an accurate, rapid, and fully automated detection of single-stranded RNA (ssRNA) at single-molecule level. SATORI detected a target ssRNA with a LoD of ~1.4 copies/μL in <9 min, thereby enabling the rapid detection of viral ssRNA, i.e., SARS-CoV-2. In addition, SATORI discriminated between SARS-CoV-2 variants of concern, e.g., omicron, with 98% accuracy. Collectively, we expect that SATORI can serve as a rapid and convenient diagnostic platform for various viral infections.

3SAA-1 定量的な蛍光顕微鏡計測に向けて - FCS を用いた顕微鏡ベンチマーク -
Toward traceable quantitative fluorescence microscopy - Benchmarking microscope using FCS technique -

Akira Sasaki (*BMRI, AIST*)

Fluorescence microscopy is a broadly used technique within a variety of different fields and its quantitative aspects are becoming emphasized. The challenge now lies in improving the accuracy, precision and reproducibility of the measurements obtained from fluorescence microscopy. In this presentation, recent advances of standardization procedures, including the benchmarking of the instrument performance and the standardization of the image itself, as well as the reference materials for calibration which can realize traceability of the obtained data are introduced. Also, an overview of the usefulness of FCS techniques for standardizing quantitative confocal fluorescence imaging by evaluating the microscope system performance will be presented.

3SAA-2 Supporting cellular analysis by quantitative imaging with standards and reference materials

Michael Halter, Ed Kwee, Alexander Peterson, John T Elliott (*National Institute of Standards and Technology (NIST), USA*)

We have developed methods to benchmark the analytical performance of an epifluorescence microscope using photostable reference materials and provided guidance for performing quantitative fluorescence intensity measurements (ASTM F3294-18). Our more recent efforts have focused on transmitted light reference materials for quantitative phase microscopy (QPM) for label-free cellular analysis. We evaluated polymer bead and immersion media combinations to identify robust reference preparations with optical pathlength differences similar to cultured cells. Ongoing work includes the fabrication of etched glass targets for QPM. The reference materials and protocols described can help ensure the accuracy and reproducibility of quantitative imaging used for cellular analysis.

3SAA-3 細胞を用いた分析・製造分野における細胞形態計測の信頼性向上を目指して～ISO 標準化活動の紹介
Towards improvement of the reliability of cell morphometry for analysis and manufacturing of cells - Role of ISO standardization

Yoshiko Nomi (*Chiyoda Corporation*)

Microscopy is a widely practiced technique for characterization of cells, morphological evaluation of cell is widely employed in basic research, drug discovery, and release testing for cell manufacturing in the fields of biological products. However, in view of the current situation, characteristics of cell morphology obtained from microscopic images are frequently described qualitatively in expressions such as "unevenness around", "elongated", "rounded" and the like. When characterizing cell morphological parameters are measured and quantified from the cell image, it is necessary to establish a common understanding of language and formulae. In this presentation, the background of this standardization activity and outline of the standard will be introduced.

3SAA-4 (1Pos289) Morphological Analysis of Hydrogel Induced Cancer Stem Cells in Synovial Sarcoma Model Cells

Zannatul Ferdous[1], Masumi Tsuda[1,3,4], Jean-Emmanuel Clément[3], Jian Ping Gong[1,3,6], Shinya Tanaka[3,4,6], Tamiki Komatsuzaki[2,3,5], Koji Tabata[2] ([1]*Graduate School of Life Science, Hokkaido University*, [2]*Research Center of Mathematics for Social Creativity, Research Institute for Electronic Science, Hokkaido University, Sapporo, Japan*, [3]*Institute for Chemical Reaction Design and Discovery (WPI-ICReDD), Hokkaido University, Sapporo, Japan*, [4]*Department of Cancer Pathology, Hokkaido University Faculty of Medicine, Sapporo*, [5]*Graduate School of Chemical Sciences and Engineering, Hokkaido University, Sapporo, Japan*, [6]*Global Station for Soft Matter, Global Institution for Collaborative Research and Education (GI-CoRE), Hokkaido University, Sapporo, Japan*)

Cancer tissues are composed of the heterogenous population composed of small numbers of cancer stem cells (CSCs), progenitor cells, and differentiated non-CSCs. CSCs cause therapy-resistance and recurrence, thus CSCs should be a therapeutic target for eradicating cancer. However, The identification of CSCs is extremely difficult because of the quite small number and only few markers. In this study, we studied the of morphological changes of the cancer cells on hydrogels in terms of stemness marker elevation. In this study, we studied the of morphological changes of the cancer cells on hydrogels in terms of stemness marker elevation.

3SAA-5 Quantification of receptor clustering and activation at the cell surface using correlation and lifetime-based methods

Andrew Harry Albert Clayton (*Cell Biophysics, Optical Sciences Centre, Swinburne University of Technology, Hawthorn, Australia*)

Cell surface receptor clustering is a key biological control mechanism. However, in the presence of complex oligomerization processes and activation/deactivation cycles it is challenging to identify a link between receptor clustering and receptor activation. To attempt to resolve this issue, we present an analytical approach, which combines fluorescence lifetime-detected Forster resonance energy transfer as a measure of receptor biochemical fate (i.e. activation or adaptor binding) with image correlation spectroscopy, as a measure of receptor clustering. The analytical approach enables quantification of the density of activated receptors, the density of inactive receptors, and the oligomerization ratio between the activated and inactivated receptors.

3SAA-6 (1Pos288) Size determination of cytoplasmic condensates of optineurin using spatial image correlation spectroscopy (SICS)

Yuta Hamada[1], Masataka Kinjo[2], Akira Kitamura[2] ([1]*Grad. Sch. Sci. of Life Sci., Hokkaido Univ.*, [2]*Fac. of Adv. Life Sci., Hokkaido Univ*)

Optineurin (OPTN) regulates many cellular processes and plays a neuroprotective role. Neurodegenerative diseases-associated mutations in OPTN make its cytoplasmic condensates to various sizes. However, since a standard procedure to quantify the sizes of the protein condensates has not been established, we establish an integrated analysis procedure using spatial image correlation spectroscopy (SICS), which determines the average sizes of foci from a single fluorescence microscopic image. The larger foci of E50K mutant of OPTN than its wild type were successfully determined in a single processing from the original microscopic fluorescence images. Our established procedure would contribute to standardize to determine other intracellular condensates.

3SAA-7 絶対発光量計測技術に基づく生物発光反応の量子収率解析とバイオ分析機器標準化
Absolute light measurement for the investigation of bioluminescence quantum yield and standardization of bioanalysis instruments

Kazuki Niwa (*National Metrology Institute of Japan (NMIJ), National Institute of Advanced Industrial Science and technology (AIST)*)

Fluorescence and bio/chemiluminescence are widely applied in analytical methods in the field of biotechnology and medicine. Since the lights are diffusively emitted from the samples, “integrating sphere spectrometer” technique was adopted to measure the absolute light values of energy (W) or the number of photons. The absolute sensitivity of the apparatus was calibrated using a standard lamp that was traceable to the “national standards”. Based on this technique, quantum yield values of bioluminescence reactions were investigated, which provided the basic information of light production efficiency by the reaction. The technique also helps to provide reference light sources for calibrating bioanalysis instruments (e.g. luminometer, microscope, plate reader).

3SAA-8 定量的 in vivo, ex vivo 生物発光イメージング
Quantitative bioluminescence imaging in vitro and ex vivo

Yoshihiro Ohmiya[1,2] ([1]*AIST*, [2]*Osaka Institute of technology*)

Bioluminescence imaging (BLI) demonstrates cellular events as a light signal from the single cell to tissue levels. However, BLI signals are relative values and cannot be compared directly. Thus, we established a reference LED light source that was characteristic of the total flux and light distribution and calibrated the BLI system as an absolute light signal. This calibrated BLI system revealed that the average light signal of beetle luciferase was at an attowatt level per sec at the single cell level [T. Enomoto et.al.: Biotechniques 64 (2018) 270-274.]. Furthermore, we applied a quantitative detection method for immunohistochemistry and can convert a relative light unit to target-antigen count [K. Wang et.al.: Biotechniques 69 (2020) 302-304].

3SBA-1 ポールシェーラー研究所でのいろいろな実験手法を組み合わせた時分割シリアル結晶学への取り組み
Time resolved serial crystallography with various methods at the Paul Scherrer Institut

Takashi Tomizaki, Tsujino Soichiro (*Paul Scherrer Institut*)

At the Paul Scherrer Institut, beamlines for serial crystallography are dedicated to academic/proprietary users at a free-electron laser facility, SwissFEL, and a synchrotron, SLS. Users can perform diffraction experiments to observe conformational changes in the three-dimensional structure of proteins with a wide range of time resolution, from femtosecond to minutes.
In this talk, we will mainly introduce the diffraction experiment methods using the ultrasonic levitation diffractometer (ALD), developed by our team, and describe how to combine the methods to clarify the structural change with a wide range of time resolutions.

3SBA-2 分子動力学シミュレーションによるタンパク質の構造ダイナミクス研究
Structural dynamics of proteins studied using molecular dynamics simulations

Mitsunori Ikeguchi[1,2] ([1]*Grad. Sch. Med Life Sci., Yokohama City Univ.*, [2]*R-CCS, RIKEN*)

Structural dynamics is key to protein function. Molecular dynamics simulation is a computational method to study structural dynamics. With the development of computational capabilities, the scope of its application is expanding year by year. In this talk, I will present examples of research on molecular dynamics simulation in collaboration with experimental researchers. For example, molecular dynamics simulations can be used to observe phenomena that are difficult to capture experimentally, such as how a protein responds to modifications such as phosphorylation. Also, conformational dynamics is also important in in-silico screening, and I would like to introduce examples of such studies.

3SBA-3 生体分子の動的構造解析のためのマイクロ流体デバイスの開発
Development of microfluidic devices for structural dynamics measurement of biomolecules

Masatoshi Maeki[1,2,3] ([1]*Faculty of Engineering, Hokkaido University*, [2]*JST PRESTO*, [3]*Institute of Materials Structure Science, High Energy Accelerator Research Organization (KEK)*)

Structural dynamics of biomolecules are essential for understanding the biological function and drug discovery. Microfluidic devices provide many advantages for the measurement of biomolecules, such as low consumption of valuable samples, time-resolved measurement, and precise control of reaction time. We have developed several types of microfluidic devices to produce biomimetic materials, diagnostics, and biomolecular analysis, including the measurement of structural dynamics. In this study, we will introduce our microfluidic devices and microfluidic-based approaches coupled with X-ray synchrotron facilities to measure biomolecular structural dynamics.

3SBA-4 Serial Femtosecond Crystallography reveals structural intermediates during CO-dissociation process in ba3-type Cytochrome c Oxidase

Swagatha Ghosh[1,2], Cecilia Safari[1], Rebecka Andersson[1], Jonatan Johannesson[1], Peter Dahl[1], Eriko Nango[3], Rie Tanaka[3], So Iwata[3], Richard Neutze[1], Gisela Brändén[1] ([1]*Dept. Chem. and Mol. Bio, Gothenburg University, Sweden*, [2]*Dept. Appl.Physics, Nagoya University, Japan*, [3]*RIKEN Spring-8 Center, Hyogo, Japan*)

Cytochrome *c* oxidases (C*c*O) is an integral membrane protein that act as terminal acceptor of electrons and catalyzes the reduction of molecular oxygen to water. The free energy stored in this process is used for proton transport across the biological membrane and ATP synthesis. In this study, I will present the time-resolved serial femtosecond crystallography (Tr-SFX) changes during the disscociation of carbon monoxide (CO) from the active site of *ba3*- type C*c*O from *Thermus thermophilus*. In addition to the Tr-SFX study of C*c*O, I will also present results from serial crystallography at synchrotrons performed by using in-house developed simple and cost-effective sample- delivery techniques for routine data-collection.

3SBA-5 光化学系ＩＩ酸素発生中心における V185 の役割についての QM/MM-MD 解析
QM/MM-MD study of the role of valine 185 in the oxygen-evolving center of photosystem II

Mitsuo Shoji[1,2], Koichi Miyagawa[1], Kenji Mishima[1], Kizashi Yamaguchi[3], Yasuteru Shigeta[1] ([1]*CCS, U.Tsukuba*, [2]*JST-PRESTO*, [3]*Osaka Univ.*)

Photosynthetic water oxidation occurs at the Mn cluster of the oxygen-evolving complex in photosystem II (PSII). Valine 185 in the D1 protein (V185) located at the close position of the Mn cluster is a highly conserved amino acid and is important for the water splitting reaction. In order to elucidate the explicit role of the V185, hybrid quantum mechanics/molecular mechanics molecular dynamics (QM/MM-MD) simulations were performed for the wild type and threonine mutant (V185T). We found that the hydrogen bond network around T185 is changed upon the V185T mutation by the hydrophilic side chain. The present QM/MM results suggest that the hydrophobic covering of the Mn cluster by V185 is one of the key elements for PSII to achieve the efficient water-splitting reaction.

3SBA-6 光活性化アデニル酸シクラーゼ OaPAC の動的構造解析による反応機構の解明
Reaction mechanisms of photoactivated adenylate cyclase OaPAC using dynamic structural analysis

Naito Ishimoto[1], Yasufumi Umena[3], Sofia Trampari[2], Soichiro Tsujino[2], Takashi Tomizaki[2], Sam-Yong Park[1] ([1]*Grad. Sch. MLS, Yokohama City Univ. / Japanese*, [2]*Paul Scherrer Institute / Switzerland*, [3]*Synchrotron Radiation Research Center, Nagoya University / Japanese*)

Cyclic AMP (cAMP) is a second messenger which regulates intracellular responses such as axonal elongation and gene expression. OaPAC (Photoactivated Adenylate Cyclase from cyanobacteria) is an enzyme which catalyzes ATP into cAMP using light and has potential for optogenetics applications. The structure of OaPAC has been elucidated, however light-induced conformational change and the mechanism of catalytic activity remains unknown.
To unravel the reaction mechanisms of OaPAC, dynamic structural changes are captured as molecular movie over a wide range of time scale using X-ray Free Electron Laser (XFEL) and synchrotrons.

3SCA-1 Myosin molecular motors convert information into motion

Toshio Yanagida[1,2,3,4] ([1]*NICT*, [2]*Grad. Sch. Info. Sci. Tech., Osaka Univ.*, [3]*Grad. Sch. Front. Biosci., Osaka Univ.*, [4]*iFReC*)

We have used single molecule detection techniques to show that muscle myosin motors and vesicle-transporting myosin motors work using Brownian motion. In the lecture, based on Szilard's engine, I propose a model that myosin motors convert the information about the direction of Brownian motion into mechanical energy.

3SCA-2 The network of microtubule integrates the spatial information provided by the actin network along the cell periphery

Manuel Thery (*CEA (French Atomic Energy Reserch Center)*)

In this presentation I will discuss how the microtubule and actin networks in cells can be compared to human nervous and muscle systems. I will describe how the actin network act as sensor along the cell periphery, how it senses and adapts to external cues by self-organizing into various structures, such as thick bundles or thin layers of branched filaments, depending on the local adhesiveness. I will then describe how the microtubule network interact with these actin structures, in terms of mechanical and biochemical interplays. I will then discuss how the outcome of these interplays produces mechanical forces in the **microtubule** networks that define the position of the microtubule organizing center, either at the cell center or at the cell periphery.

3SCA-3 Molecular mechanisms of the chaperones that assist in the folding of actin and tubulin

Masafumi Yohda (*Grad. Sch. Eng., Tokyo Univ. Agr. Tech.*)

Molecular chaperones mediate the folding of various proteins. Chaperonin-containing TCP-1 (CCT) is a molecular chaperone found in the cytoplasm of all eukar yotes. CCT was first identified as a chaperone required to fold the major cytoskeletal proteins actin and tubulin. Later, a heterohexameric chaperone protein, prefoldin, was identified. Prefoldin captures an unfolded actin or tubulin and then transfers it to CCT. The formation of actin and tubulin requires the support of these chaperones. Because of the complex structures of these chaperones, the detailed mechanism was poorly revealed. However, recent studies, including structure determination by cryoEM, enabled us to access the mechanism. I will talk about the molecular mechanism for the chaperones.

3SCA-4 多細胞動物ヒトの筋適応の素過程：ストレス因子カルシウム、微小管及び分子シャペロン αB-クリスタリン
Elementary processes of slow muscle adaptation in multicellular human: calcium, microtubules and the molecular chaperone αB-crystallin

Yoriko Atomi (*Tokyo University of Agriculture and Technology*)

The elementary process of striated muscle contraction is the interaction of actin and myosin due to the influx of calcium. This is structured by the cytoskeleton in a sarcomere, and the change in sarcomere length caused by contraction is transmitted as tension to the extracellular matrix via the Z band causing joint and physical movement. Upright and bipedal humans have maximally adapted and evolved the slow-twitch skeletal muscles to maintain their own weight, thus supporting healthy longevity. The process of responding to calcium is the main mechanism of plasticity in the nervous system and skeletal muscles. This presentation will introduce the elementary process of adaptation by the stressor calcium and αB-crystallin, which sustains microtubule dynamic instability.

3SCA-5 骨格筋幹細胞の活性化・分化と筋再生のサーカディアン制御
Circadian regulation of skeletal muscle stem cell activation differentiation, and muscle regeneration

Atsushi Asakura (*Stem Cell Institute, University of Minnesota Medical School*)

The circadian rhythm, with a 24-hour cycle, is a highly conserved biological system common to almost all living species on earth. Many physiological functions, including sleep and wakefulness, are directly linked to circadian rhythms oscillated by the biological clock system. Circadian rhythms also regulate cell proliferation and differentiation by a transcriptional feedback loop centered on the master clock transcription factors Bmal1/Clock and Per/Cry, and isolated cells have a 24-hour rhythm just like living organisms. Here, we show that the circadian master regulators Per1 and Per2 and myogenic master regulator MyoD are integral components defining the efficiency of skeletal muscle stem cell (satellite cell) activation, differentiation, and muscle regeneration.

3SCA-6 ヒトの不安定な立位姿勢における頭部-体幹部の構造的冗長性の制御
Control of structural redundancy from head to trunk during unstable upright standing in humans

Tomoaki Atomi (*Health Sci., Univ. Kyorin*)

The human being dynamically and highly controls the head–trunk, which has a high mass ratio in the whole body with redundant mechanical structures to maintain a stable, inherently unstable upright standing in the central nervous system, including the higher cerebral functions. However, it is unclear how the head–trunk segmental properties are altered to respond to situations that require appropriate changes in standing posture control strategies. Our findings suggested that the structural redundancy of the head–trunk must be adjusted adaptively by control of the central nervous system according to the different conditions of the sensory input to stabilize upright standing in human-specific bipeds.

3SDA-1 Mechanism of sulfide/supersulfide sensing in bacteria

Shinji Masuda (*Grad. Sch. Life Sci. & Technol., Tokyo Inst. Tech.*)

Sulfide impacts on bacterial growth positively and negatively; it is utilized as an electron donor, and it also contributes to antibiotic resistance. Thus, bacteria need sulfide-responsive mechanisms for survival. We have studied bacterial transcription factor controlling sulfur assimilation and detoxification. The transcription factor family, SqrR/BigR homologs, were found in both sulfur and non-sulfur bacteria such as purple photosynthetic bacteria and *E. coli*. SqrR/BigR homologs sense sulfide and/or supersulfide directly; they form an intramolecular tri- or tetra-sulfide bond between two conserved cysteine residues, which influences their affinity to target promoters. The mechanism of how the transcription factors sense sulfide/supersulfide will be discussed.

3SDA-2 Intramolecular disulfide bond switches enzymatic activity of SOD1

Shinya Tahara[1], Kousuke Yamazaki[1], Takumi Ohyama[1], Kunisato Kuroi[2], Takakazu Nakabayashi[1] ([1]*Grad. Sch. Pharm. Sci., Tohoku Univ.*, [2]*Dept. Pharm. Sci., Kobe Gakuin Univ.*)

Cu, Zn superoxide dismutase (SOD1) is an antioxidant enzyme. Aggregations of SOD1 in motor neurons have been considered to induce the onset of amyotrophic lateral sclerosis for the last few decades, but recent studies showed that SOD1 oligomers show stronger cytotoxicity than aggregates. However, details on the toxicity of the oligomers remain elusive. In this presentation, we report that disulfide-linked oligomers of SOD1 exhibit pro-oxidant property that generates reactive oxygen species from hydrogen peroxide. We also found that dimers and trimers show stronger pro-oxidant activity than large oligomers and aggregates. We concluded that this non-native enzymatic activity arises from cleavage of the intramolecular disulfide bond associated with the oligomerization.

3SDA-3 Reaction mechanism of tRNA sulfur modifying enzyme using a cofactor iron-sulfur cluster

Min Yao (*Fac. Adv. Life Sci., Hokkaido Univ.*)

Enzymatic posttranscriptional modifications regulate tRNA function after its transcription. Sulfur modification (thiolation) is universal and has various cellular roles, such as codon recognition, sensing UV radiation stress and stabilizing the ternary structure of tRNA for growth at high temperatures. Several thiolation enzymes have been identified that require an inorganic cofactor, an iron-sulfur cluster.
We recently analyzed the structure-function relationship of a tRNA thiolation enzyme TtuA with its sulfur donor protein TtuB, showing that TtuA employs [4Fe-4S] as a cofactor for receiving sulfur from TtuB. Combing electron paramagnetic resonance (EPR) spectroscopy, we characterized the [4Fe-4S] bond to TtuA and proposed the thiolation mechanism of TtuA.

3SDA-4 2 つの異なるタイプの PLP 依存型システイン脱硫酵素と基質 L-システインおよび阻害剤との反応
Actions of two distinct types of PLP-dependent cysteine desulfurase enzymes with substrate L-cysteine and inhibitors

Takashi Fujishiro (*Grad. Sch. Sci. Engeneer., Saitama Univ.*)

Cysteine desulfurases, such as IscS, SufS, and NifS, found in Fe-S cluster biosynthesis, are PLP-dependent enzymes catalyzing mobilization of inorganic sulfur from substrtate L-cysteine. Recently, two sub-types (type I: IscS and NifS, type II: SufS) of the cysteine desulfurases have been of great interest for understanding the structural diversity and evolution of these enzymes. We herein report X-ray crystallographic, biochemical and mutational analyses of NifS (type I) and SufS (type II) for unveiling molecular basis of the common and distinct features of two types, which contribute to enrich the PLP enzyme chemistry and to develop a novel inhibitor targeting one type or the other.

3SDA-5 Structural and functional analyses of *E. coli* SufBCD complex involved in iron-sulfur clusters biogenesis

Kei Wada[1,2], Yoshikazu Tanaka[3], Yasuhiro Takahashi[4] ([1]*Department of Medical Sciences, University of Miyazaki*, [2]*Frontier Science Research Center, University of Miyazaki.*, [3]*Graduate School of Life Sciences, Tohoku University*, [4]*Graduate School of Science and Engineering, Saitama University*)

Biogenesis of iron-sulfur (Fe-S) clusters is an indispensable process in living cells. In *Escherichia coli*, the SUF biosynthetic system is composed of six proteins among which SufB, SufC and SufD form the SufBCD complex, which serves as a scaffold for *de novo* assembly of a nascent Fe-S cluster. We have determined the crystal structure of *Escherichia coli* SufBCD complex, which exhibits the common architecture of ABC proteins: two ABC ATPase components (SufC) with function-specific components (SufB-SufD protomers). Biochemical and physiological analyses have provided critical insights into Fe-S cluster assembly and revealed a dynamic conformational change driven by ABC ATPase activity and the pathway for the sulfur migration in the complex.

3SDA-6 アミノ酸とナノカーボンの相互作用：物理吸着およびシステインの化学反応
Interactions of carbon nanomaterials with amino acids: physical adsorption and chemical reaction with cysteine

Atsushi Hirano (*NMRI, AIST*)

Protein adsorption onto nanoparticles governs the first stage of nanoparticle uptake into biological systems and is associated with biological impacts such as cytotoxicity. This presentation focuses on the mechanism of the interactions—physical adsorption and chemical reaction—between proteinogenic amino acids and carbon nanomaterials including graphene and carbon nanotubes. Physical adsorption is striking for arginine as well as aromatic amino acids. Chemical reaction is observed for cysteine, which involves electron transfer from sulfhydryl groups to the carbon nanomaterials. This reaction is facilitated by transition metal ions originating from the material impurities. These findings are useful for understanding and predicting protein–nanoparticle interactions.

3SEA-1 微生物電気化学を活用した二酸化炭素資源化技術
CO_2 utilization technologies based on microbial electrochemistry

Souichiro Kato (*BPRI, AIST*)

CO_2 utilization technology using living organisms has the advantage of being able to synthesize diverse and complex organic compounds (polymer materials, liquid fuels, foods, etc.), compared to those based on material sciences. However, the current biotechnology using photosynthetic organisms (plants, algae, etc.) has problems such as low productivity, competition with food, and demand for a large amount of clean water. In this presentation, a novel biotechnology based on microbial electrochemistry, which uses non-photosynthetic microorganisms that can fix CO_2 using electricity as the energy source, as a new technology that can solve above mentioned problems.

3SEA-2 気相微生物反応
Microbial gas-phase reaction

Katsutoshi Hori (*Grad. Sch. Eng., Nagoya Univ.*)

Since I found a super-sticky bacterium and its adhesive protein AtaA, I have been developing the process of material transformation by immobilized bacteria. By the way, it has been a common sense that most of microbial reactions are performed using microbial cells suspended in an aqueous phase, such as media and buffer solutions. Then, I conceived a game-changing idea that microbial reactions may be more efficient in a gas-phase due to much faster diffusion velocity than in an aqueous phase. For the gas-phase reaction, bacterial cells must be immobilized because of no suspension medium. Bubbling or agitation should not be required in energy-saving passive reactions. In this symposium, I introduce several examples for the proof of this concept.

3SEA-3 資源循環の最適化による農地由来の温室効果ガスの排出削減
Mitigation of greenhouse gas emissions from agricultural lands by optimizing nitrogen and carbon cycles

Kiwamu Minamisawa (*Graduate School of Life Sciences, Tohoku University*)

Nitrous oxide (N2O) is a powerful greenhouse gas. Agriculture accounts for 59% of global anthropogenic N2O emissions. Paddy rice fields are also a source of methane (CH4) emissions, accounting for 11% of the global anthropogenic CH4 emissions. Thus, it is essential to mitigation of greenhouse gases from agriculture. Although modern agriculture has succeeded to increase food production using nitrogen fertilizers, N2O emission from agricultural soil is increasing rapidly. Some rhizobia and soil bacteria can reduce N2O to N2. Methanotrophs are known to oxidize CH4 to CO2. Such microbial processes could be maximized at the field scale by optimizing nitrogen and carbon cycles via plant-microbe-soil systems.

3SEA-4 土壌団粒構造と微生物
Soil aggregate structure and microorganisms

Rota Wagai (*NARO/NIAES*)

Soil is arguably the highest biodiversity zone on earth. It also represents the largest carbon (C) and nitrogen (N) reservoirs on land that are largely present as organic matter (OM). Yet soil microbial activity is generally C limited. These are achieved by highly porous, physical structure called aggregates that consist of mineral particles of 100 nm to 2 mm sizes and OM of both plant and microbial origins. Aggregate pores are the habitable space for microbes while acting as the highway for O2 diffusion and H2O transport. Here I introduce our research on how aggregates are assembled in soil and how microbially-driven C and N dynamics (including N2O) are linked to aggregate structure.

3SEA-5 ウシルーメンマイクロバイオーム制御による消化管メタンの削減をはかる新しい家畜生産システム開発に向けて
Toward a new livestock production system to reduce enteric methane through controlling bovine rumen microbiome

Yasuo Kobayashi (*Research Faculty of Agriculture, Hokkaido University*)

Methane gas produced by the fermentation in cows' stomach (rumen) is released into the atmosphere as burp, which not only affects global warming but also results in the loss of feed energy. By 2050, we aim to reduce this methane gas by 80%, thereby curbing global warming and improving the efficiency of cow's production by 10%. We take on the challenge for developing an individualized feeding system that minimizes methane from cattle. First, we will develop new feeds that control rumen microbiome to strongly inhibit methane synthesis. The efficacy of these will be evaluated using a new device (smart pill) that is placed in the rumen and transmits the fermentation status outside the body in real time.
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3SEA-6 牛ルーメンからのメタン低減に向けた微生物利用の可能性
Potential microbial target for mitigating enteric methane production in the rumen of cows

Takumi Shinkai (*Institute of Livestock and Grassland Science, National Agricultural and Food Research Organization*)

Ruminants have a unique digestive system in their foregut that is beneficial to both ruminant and rumen microbes. Feed carbohydrates are fermented, and convert into short-chain fatty acids (SCFA) while generating metabolic hydrogen during rumen fermentation. Enteric methane works as a main sink for metabolic hydrogen, and is released into the air.
In the symposium, we will provide physiological and ecological information of a novel bacterial target for rumen manipulation that was found in low methane and high propionate producing cows. Our challenge can provide a novel biological material and better understand mechanisms of the low methane and high propionate rumen fermentation which is important for improving methane mitigation and animal productivity.

3SFA-1 Structure-function relationship of pump-like cation channelrhodopsins

Koichiro Kishi[1], Yoon Seok Kim[2], Masahiro Fukuda[1], Masatoshi Inoue[2], Tsukasa Kusakizako[3], Peter Wang[2], Toshiki Matsui[1], Keitaro Yamashita[4], Takashi Nagata[5], Masae Konno[5], Tomoko Uemura[6], Kehong Liu[6], Mikihiko Shibata[7], Norimichi Nomura[6], So Iwata[6], Osamu Nureki[3], Keiichi Inoue[4], Karl Deisseroth[2], **Hideaki Kato[1]** ([1]*Komaba Inst. Sci., Grad. Sch. Arts. Sci., Univ. Tokyo*, [2]*Stanford Univ.*, [3]*Grad. Sch. Sci., Univ. Tokyo*, [4]*MRC*, [5]*ISSP, Univ. Tokyo*, [6]*Grad. Sch. Med., Kyoto Univ.*, [7]*Kanazawa Univ.*)

The experimental technique to optically control the excitability of cells, optogenetics, has revolutionized neuroscience. More and more ion-translocating rhodopsins (ion pump-type rhodopsins and ion channel-type rhodopsins) have been engineered or discovered from nature to broaden the application of optogenetics. Recently, a new type of channelrhodopsins, pump-like cation-conducting channelrhodopsins or bacteriorhodopsin-like channelrhodopsins (PLCRs or BCCRs), have been discovered and attracted broad attention because of their unique properties (e.g. large photocurrents, high light sensitivity, high ion selectivity). In this talk, I will present the cryo-EM structure of one of the recently-discovered PLCRs, ChRmine, and discuss the structure-function relationship.

3SFA-2 III-E 型 CRISPR-Cas7-11 エフェクター複合体の立体構造と分子改変
Structure and engineering of the type III-E CRISPR-Cas7-11 effector complex

Hiroshi Nishimasu (*The University of Tokyo*)

The type III-E CRISPR-Cas effector Cas7-11, with dual RNase activities for precursor crRNA processing and crRNA-guided target RNA cleavage, is a new platform for bacterial and mammalian RNA targeting. We report the 2.5-Å resolution cryo-electron microscopy structure of Cas7-11 in complex with a crRNA and its target RNA. Cas7-11 adopts a modular architecture comprising seven domains (Cas7.1–Cas7.4, Cas11, INS, and CTE) and four interdomain linkers. This study expands our mechanistic understanding of diverse CRISPR-Cas effector complexes and establishes a framework for the development of new RNA-targeting technologies.

3SFA-3 (2Pos003) クライオ電子顕微鏡による高分解能解析によって明らかになってきた二成分毒素の膜透過機構
(2Pos003) High-resolution Cryo-EM analysis reveals the mechanism of binary toxin translocation

Tomohito Yamada[1], Yukihiko Sugita[2,3], Takeshi Noda[2], Hideaki Tsuge[1] ([1]*Graduate School of Life Science, Kyoto Sangyo University*, [2]*Laboratory of Ultrastructural Virology, Institute for Life and Medical Sciences, Kyoto University*, [3]*Hakubi Center for Advanced Research, Kyoto University*)

Binary toxin is bacterial protein toxin which is composed of enzymatic A-component, and B-component which forms membrane spanning pore to translocate A-component into the cell. To study the translocation mechanism, we tried reconstituting *C. perfringens* iota toxin Ib-pore into liposome to mimic in vivo environment. However, the product was not proteo-liposomes, but clusters which are formed by radially assembled Ib-pores in lipid micelle (Ib-rosette). Surprisingly, single particle analysis of Ib-rosette produced Ib-pore map at 2.38Å resolution, revealing whole structure of membrane spanning β-barrel. This map exhibited hydrated water on the β-barrel, and clearly revealed the structures of the constriction-site which are located on A-component translocation pathway.

3SFA-4 IscB–ωRNA 複合体による RNA 依存性 DNA 切断の構造基盤と Cas9 への進化的洞察
Structure of the IscB–ωRNA ribonucleoprotein complex, the likely ancestor of CRISPR-Cas9

Kazuki Kato[1], Sae Okazaki[1], Soumya Kannan[2], Feng Zhang[2], Hiroshi Nishimasu[1] ([1]*RCAST, Univ. Tokyo*, [2]*MIBR, MIT*)

IscB is an RNA-guided nucleases, and likely ancestors of Cas9 in the type II CRISPR-Cas adaptive immune system. IscB associates with ωRNA to form a ribonucleoprotein complex that cleaves DNA targets complementary to an ωRNA guide segment. Here, we report the cryo-EM structure of an IscB–ωRNA–target DNA complex. The structure shows how the IscB protein assembles with the ωRNA and mediates RNA-guided DNA cleavage. The ωRNA structurally and functionally compensates for the nucleic-acid recognition lobe of Cas9, and participates in the recognition of the guide RNA–target DNA heteroduplex. These findings provide insights into the mechanism of the programmable DNA cleavage by the IscB–ωRNA complex and the evolution of the type II CRISPR-Cas9 effector complexes.

3SFA-5 ミトコンドリアのリボソームの成熟過程から翻訳開始過程に至る構造解析
Structural analysis of the late assembly states of mitochondorial ribosome to the translation initiation

Yuzuru Itoh[1,2], Anas Khawaja[3], Joanna Rorbach[3], Alexey Amunts[2] ([1]*Dept. BioSci., Grad. Sch. Sci., Univ. Tokyo*, [2]*SciLifeLab, DBB, Stockholm University*, [3]*Karolinska Institutet*)

Mitochondria have their specific ribosome (mitoribosome). Here, we knocked out two assembly factors, purified mitoribosome from the cells and performed electron cryo-microscopy. We determined 6 states of the late assembly and two initiation states of the mammalian mitoribosomal. The methyltransferase TFB1M binds to the partially unfolded rRNA, induced by the protein factor RBFA. The specific RBFA C-terminal extension blocks the mRNA channel. A large conformational change of RBFA allows another methyltransferase METTL15 to bind, which is then replaced by the initiation factor mtIF3. The specific mitoribosomal protein mS37 replaces RBFA to complete the assembly and starts a pre-initiation state. Finally, mRNA, fMet-tRNA^{Met} and mtIF2 bind and complete the initiation state.

3SFA-6 膜タンパク質と非翻訳 RNA の分子機構の構造基盤
Structural basis for molecular mechanisms of membrane proteins and non-coding RNA

Osamu Nureki (*Grad. Sch. Sci., Univ. Tokyo*)

Membrane and membrane-spanning proteins, and non-coding RNA are biomolecules to play central roles in beginning of life and distinguishing higher-order eukaryotes. We have determined the structures of membrane protein-lipids complexes and non-coding RNA-protein complexes by Cryo-EM single particle analysis, and combined with complementary functional analyses, elucidate their molecular mechanisms at atomic resolutions, to promote creating drugs and medical technologies with two venture companies. In this symposium, I will talk on recent topics in our labotratory.

3SGA-1 ポリマー化脂質膜と天然脂質膜からなるパターン化人工膜
Micropatterned model membrane composed of polymerized and natural lipid bilayers

Kenichi Morigaki[1,2] ([1]*Biosignal Res. Cen., Kobe Univ.*, [2]*Grad. Sch. Agrobio., Kobe Univ.*)

We have developed a patterned model system of the biological membrane on a solid substrate by combining a polymerized lipid bilayer and natural (fluid) lipid bilayers. The polymeric bilayer acts as a framework to define the geometry of the fluid bilayers and enhance their stability. The fluid bilayers comprise natural lipids and membrane proteins, and retain the physicochemical properties the biological membrane. The model membranes can be confined in a nanometric aqueous space to reduce the background noise and enable sensitive detection of membrane-bound molecules. Patterned model membrane in combination with a nanometric confinement provide promising platforms for biophysical studies of the biological membrane as well as biomedical applications.

3SGA-2 メカノクロミック生体膜を用いたペプチド－脂質相互作用の検出
Mechanochromic biomembranes for studying peptide-lipid interactions

Kaori Sugihara (*IIS, Univ. Tokyo*)

A mechanochromic lipidic polymer, polydiacetylene, changes color upon ligand binding, being a popular material in biosensing. However, whether it can also detect ligand functions in addition to binding is left understudied. In this work, we report that the polydiacetylene can be used to determine the net charges and the mode of actions (carpet model, toroidal pore model etc.) of antimicrobial peptides and detergents via EC_{50} and Hill coefficients from the colorimetric response dose curves. Taking advantage of this properties, we will screen and study a phenomenon called “antimicrobial peptide cooperative effect”, where a mixture of different types of peptides present a super power to potentially combat the current crisis of antibiotic resistance.

3SGA-3 多価不飽和脂質によって形成される脂質ドメイン
Lipid domains generated by polyunsaturated lipids

Melvin Wei Shern Goh, **Ryugo Tero** (*Dept. Appl. Chem. Life Sci., Toyohashi Univ. Tech.*)

Lipid domain formation is a fundamental process of biomembrane reactions. Ternary mixtures of a lipid with a high transition temperature (High-T_m), that with Low-T_m, and cholesterol have been studied as a raft-mimicking system. Recently, we found that polyunsaturated lipids generate domains in lipid bilayers comprising a polyunsaturated Low-T_m lipid, a monounsaturated Low-T_m lipid, and cholesterol. Lipid microdomains are observed in fluorescence images and AFM topographies. The area fraction of the microdomains depends on the number and *sn*-position of double bonds in the unsaturated lipids. The microdomains functions as membrane fusion site, and thus is applicable to reconstitution of membrane proteins to artificial lipid bilayer systems through proteoliposome fusion.

3SGA-4 リキッドマーブル：粒子膜で安定化された液滴
Liquid marble: Droplet covered by particulate membrane

Syuji Fujii (*Osaka Institute of Technology*)

Liquid marbles (LMs) are liquid droplets stabilized by solid particles adsorbed at the gas-liquid interface. LMs can be artificially fabricated by coating the liquid droplets with hydrophobic solid particle layer and can move easily on various solid surfaces because of their nonwetting nature. Here, I will give a talk on our recent research related to LMs that are stabilized solely with functional particles.

3SGA-5 (2Pos188) DNA ゲル骨格が決定する人工細胞の力学特性
(2Pos188) Cytoskeletons of self-assembled DNA regulate the mechanical properties of artificial cells

Kazutoshi Masuda[1], Fuyu Ohno[2], Miho Yanagisawa[1,2] ([1]*College of Arts and Sciences, The University of Tokyo*, [2]*Graduate school of Arts and Sciences, The University of Tokyo*)

Artificial cells composed of lipid membranes are more fragile than living cells due to the lack of cytoskeletons, making their application problematic. We previously reported that self-assembled DNA networks under the membrane stabilize the artificial cells. However, it was unclear what kind of DNA structure would improve the mechanical properties of cells. Here, we tested the correlation between the viscoelasticity of cells and the structure of the DNA network by using two types of DNA nanostructures, Y- and X-shaped, with different lengths of the sticky-ends. Our results show Y-shaped DNA can stabilize membranes better than X-shaped DNA. The reasons based on the morphology of DNA networks and the potential applications of DNA-stabilized artificial cells are discussed.

3SGA-6 生体膜表面を模倣した高分子自己集合体
Self-assembled polymer aggregates with mimetic cell membrane surface

Shin-ichi Yusa (*Department of Applied Chemistry, Graduate School of Engineering, University of Hyogo*)

A pair of oppositely charged diblock copolymers with biocompatible polyphosphobetaine (PMPC) block bearing phosphorylcholine groups were prepared via controlled radical polymerization method. The pendant phosphorylcholine group in the PMPC block is the same chemical structure of the surface of cell membrane. When the oppositely charged diblock copolymers were mixed, polyion complex (PIC) aggregates which covered with hydrophilic PMPC shells were formed in water. The shape of the PIC aggregates such as spherical micelle, rod-like micelle, and vesicle strongly depends on the polymer chain length ratio of polyelectrolyte and PMPC blocks. If the PMPC block was short, the shape of PIC aggregates was vesicle. If the PMPC block was long, the shape was spherical micelle.

3SGA-7 合成高分子によって形成される最小モデル膜としての脂質ナノディスク
Lipid nanodisc as a minimal model membrane formed with synthetic polymers

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Lipid nanodisc is a homogeneous molecular assembly with a discoidal shape encompassing a lipid bilayer that provides the smallest model cell membrane to investigate membrane proteins and various membrane-active agents. We have previously designed nanodisc-forming polymers inspired by the amphiphilic structure of apolipoprotein A-I, which is known to form discoidal assembly with phospholipids *in vivo*. The designed polymer can spontaneously form lipid bilayer nanodiscs through the fragmentation of the membrane. In this presentation, we will introduce our previous studies including the design principle of the nanodisc-forming polymer, the physicochemical characteristics of the nanodisc, and their applications in the field of biophysics as well as cell biology.

3SHA-1 Constructing an in vitro gene screening system for membrane proteins and its application

Tomoaki Matsuura (*ELSI, Tokyo Tech*)

An *in vitro* transcription and translation (IVTT) systems have been used not only for protein synthesis but also for various applications including *in vitro* directed evolution of proteins. However, not much has been reported on the evolution of membrane proteins because of the lack of the hydrophobic environment essential for the membrane protein folding. We succeed in supplying such environment by adding nanodisc to the reconstituted IVTT system. In this way, G-protein-coupled receptors, one of the representatives of membrane proteins, was displayed in their functional form and selected for its agonist binding using ribosome display. We foudn that the choice of the phospholipid for the nanodisc preparation was essential for the functional GPCR expression.

3SHA-2 人工金属酵素を用いた触媒システムの構築
Artificial enzymes towards systems catalysis

Yasunori Okamoto (*FRIS, Tohoku Univ.*)

Artificial metalloenzymes, resulting from the incorporation of a synthetic metal complex within a protein matrix, have been developed to combine attractive features of both homogeneous catalysis and enzymatic catalysis. Thanks to their complementarity to natural enzymes, artificial metalloenzymes are promising building blocks to implement new-to-nature chemical transformations in a biochemical reaction network. In this presentation, we will show catalytic systems comprised of a natural enzyme and an artificial metalloenzyme: (i) the creation of new cascade reactions and (ii) an enzymatic cross-regulation system.

3SHA-3 2 次元ナノ材料界面を利用した高感度バイオセンサの開発
Development of Highly Sensitive Biosensor Using Two-Dimensional Nanomaterial Interface

Yuhei Hayamizu (*Sch.Mater, Tokyo Tech*)

Two-dimensional (2D) materials, such as graphene and MoS_2, have gained broad interest in their applications for developing biosensors due to their high surface area and unique electronic properties. We have developed engineered peptides that can functionalize the surfaces of 2D materials in the manner of self-assembly. These peptides can form a monomolecular-thick thin film on the surface and modulate the electronic properties of 2D materials. The presentation introduces the series of peptides we have developed so far and their application for highly sensitive biosensors. This work was supported by the Cabinet Office (CAO), Cross-ministerial Strategic Innovation Promotion Program (SIP), “Intelligent Processing Infrastructure of Cyber and Physical Systems”.

3SHA-4 分子進化によるタンパク質集合体の構築
Directed evolution of protein assembly

Naohiro Terasaka[1], Hiroaki Suga[1], Donald Hilvert[2] ([1]*Grad. Sch. Sci., The Univ. of Tokyo*, [2]*Laboratory of Organic Chemistry, ETH Zurich*)

Living organisms are maintained by a network of a wide variety of biomolecules with various functions. Recent developments in biotechnology have enabled engineering the functions of single proteins and nucleic acids, but engineering biomolecule assemblies remains challenging.
Recently, we have developed an mRNA-encapsulating protein capsule (nucleocapsid) that mimics a natural virus by directed evolution from lumazine synthase of *Aquifex aeolicus* (AaLS). During the course of evolution, the structure of both mRNA and protein was changed to efficiently package mRNA into 240-mer protein capsule. This study showed the powerful potential of simultaneous molecular evolution of RNA and proteins, and that artificial nucleocapsids are promising virus alternatives.

3SHA-5 人工細胞膜システム：デノボ設計ナノポアの構築
Artificial Cell-membrane system: the construction of *de novo* nanopores

Ryuji Kawano (*Dept. Biotech&Life Sci., Tokyo University of Agriculture and Technology*)

Artificial cell membranes have emerged as biomimetic tools in such areas as membrane protein study, synthetic biology, and drug discovery. Planar lipid bilayers are used for functional studies of ion channels and nanopore sensing. We have proposed a stable and reproducible preparation procedure for the planar lipid bilayer using the “droplet contact method”, and it is applied to measure pore-forming peptides with *de novo* design and the nanopore sensing.

3SHA-6 合理設計による機能性タンパク質集合体の構築
Rational design of protein assembly

Yuta Suzuki (*Hakubi Center, Kyoto University*)

If chemist can serve as a “designer” to modify and control protein functions and structures more freely, the era might come soon, when smart bionanorobots, which are programmed to perform multiple tasks, play active roles in the field of medicine and biotechnology. In this presentation, I will discuss my work 1. Novel design to create 2D protein assembly, 2. Analysis of unique structural changes of 2D protein assembly, and 3. Implementation of new design to control structure changes 4. Additional functions onto 2D protein assembly, 5. Recent discovery. Further development of this research concept should contribute to the fabrication of functional materials for biomedical and biotechnological applications.

1Pos001 珪藻 *Thalassiosira pseudonana* 由来ルビスコの構造解析及び新規ピレノイドタンパク質との相互作用解析
Structural study of RubisCO from diatom *Thalassiosira pseudonana* and its interaction with novel pyrenoid proteins

Taiki Fukuzawa[1], Rei Tohda[1], Nawely Hermanus[2], Natumi Morishima[2], Ryosuke Okubo[2], Yoshinori Tsuji[2], Akihiro Kawamoto[1], Hideaki Tanaka[1], Gerle Christogh[1], Yusuke Matsuda[2], Genji Kurisu[1] ([1]*Institute for Protein Research, Osaka University*, [2]*School of Biological and Environmental Sciences, Kwansei Gakuin University*)

Photosynthetic organisms use RubisCO in chloroplasts for carbon fixation to convert CO_2 into organic compounds. Algae-specific organelles, pyrenoids, accumulate RubisCO in their interior to enhance the efficiency of carbon fixation. Our previous study revealed that a new protein named Pyshell from *Thalassiosira pseudonana*, forms hollow tube structures under physiological conditions. These results indicate that the easily assembled Pyshell protein may play an important role in the accumulation of RubisCO. Therefore, we aimed to elucidate the interaction between RubisCO and Pyshell from *T. pseudonana* using cryo-EM structural analysis. In this meeting, we will discuss about a model for RubisCO accumulation in pyrenoids based on both structures.

1Pos002 ヒト B 細胞抑制性共受容体 CD72 の構造解析
Structure analysis of human B cell inhibitory co-receptor CD72

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CD72, a 45 kDa type II transmembrane protein containing a C-type lectin-like domain (CTLD) in the extracellular part, is expressed as a homodimer in B cells, and functions as a negative regulator of BCR signalling. The polymorphism of CD72 is associated with lupus in both human and mice. CD72 CTLD (15kDa) binds to lupus-associated self-antigens including Sm/ribonucleoprotein (RNP), regulating B cell response to the self-antgens. We have determined the crystal structure of the CTLD of human CD72^{4g}, a deletion construct where the insertion region is replaced with four glycines, at 2.95 Å resolution. The shape and charge distribution at the putative ligand binding site are different from those of previously reported mouse CD72, which may affect ligand binding.

1Pos003 Generation of protein distance matrices and novel structures utilizing Generative Adversarial Networks(GAN)

Taihei Yamaguchi (*Grad. Sch. Agr. Life Sci., Univ. Tokyo*)

Protein design has been conducted to understand the structure-function relationships. Various computational methods have been developed to generate novel proteins and machine learning has made great progress in structural biology. Here we applied Generative Adversarial Networks (GAN), one of the popular machine learning models, to protein design. GAN is known for the superiority of generating fake data that is like real data. It may be possible to generate novel proteins utilizing GAN that are similar to native proteins. We generated novel distance matrices of α-carbons utilizing GAN and reconstructed 3D structures based on the matrices utilizing AlphaFold networks. We will discuss the structural novelty in comparison with proteins registered on PDB and AlphaFold DB.

1Pos004 ヒト由来電位依存性カリウムイオンチャネルのクライオ電子顕微鏡単粒子解析
Cryo-EM single particle analysis of a human voltage-gated potassium channel

Natsuko Sekido[1], Tomona Iizuka[2], Tomoyasu Aizawa[2], Makoto Sasaki[1], Haruhiko Fuwa[3], Mari Yotsu-Yamashita[4], Keiichi Konoki[4], Takeshi Yokoyama[1], Yoshikazu Tanaka[1] ([1]*Grad. Sch. Life Sci., Tohoku Univ.*, [2]*Grad. Sch. Life Sci., Hokkaido Univ.*, [3]*Fac. Sci. & Eng., Chuo Univ.*, [4]*Grad. Sch. Agri Sci., Tohoku Univ.*)

Marine toxins produced by dinoflagellates have potent biological activities. In this study, we attempted cryo-electron microscopy (cryo-EM) single-particle analysis of the voltage-gated potassium ion (K_V) channel, one of the targets of these marine toxins. Human K_V channels composed of K_V1.2 and K_V beta 2.1 was overexpressed and purified by affinity chromatography and size exclusion chromatography. Micrographs of the purified sample were collected under cryogenic conditions using a transmission electron microscope (CRYO ARM300II) equipped with a direct electron detector. By single particle analysis with the program cryoSPARC, a 3D cryo-EM map showing four-fold assembly of K_V1.2 and K_V beta 2.1 were obtained.

1Pos005 電子線クライオトモグラフィーで可視化したスピロプラズマの細胞骨格リボン
Cytoskeletal ribbon of *Spiroplasma* revealed by cryo electron tomography

Yuya Sasajima[1], Takayuki Kato[2], Tomoko Miyata[3], Akihiro Kawamoto[2], Fumiaki Makino[3,4], Keiichi Namba[3,5,6], Makoto Miyata[1,7] ([1]*Grad. Sch. Sci., Osaka Metropolitan Univ.*, [2]*IPR., Osaka Univ.*, [3]*Grad. Sch. Front. Biosci., Osaka Univ.*, [4]*JEOL Ltd.*, [5]*BDR & SPring-8 Center, Riken*, [6]*JEOL YOKOGUSHI Res. Alliance. Lab. Osaka Univ.*, [7]*OCARINA, Osaka Metropolitan Univ.*)

Spiroplasma has a unique cytoskeletal ribbon. The ribbon is composed of *Spiroplasma*-specific Fibril protein which evolved from a bacterial nucleosidase. Previously, we clarified the atomic structure of the Fibril filament by using single particle cryoEM. In this study, we analyzed the ribbon by using cryo electron tomography and discuss the organization of the ribbon based on the fibril atomic structure.Cryo-ET visualized the ribbon along the inner part of the helical cell body. To analyze the detail structures of the ribbon, we performed subtomogram averaging of the extracted density including three protofilaments. The result suggested that fibril filaments are aligned by iom interaction between positive and negative molecular surfaces of adjacent protofilaments.

1Pos006 左巻き *βαβ* モチーフをもつタンパク質のデノボデザインに向けて
Toward *de novo* design of left-handed *βαβ*-motif-containing proteins

Hiroto Murata, George Chikenji (*Dept of Appl. Phys., Grad. Sch of Eng., Nagoya Univ.*)

De novo design is one of the most useful and well-known methods for designing proteins.
However, the left-handed *βαβ*-motif, which is so rare motif, containing proteins has not been designed yet.
To solve this problem, we generated a large number of *βαβ*-motifs with Rosetta simulation and analyzed their structural features.
This analysis revealed that the left-handed *βαβ*-motif requires a structure-specific *βα*-loop that is not present in the right-handed *βαβ*-motif.
Using this structural feature, we designed the left-handed-containing proteins.
In some Ferredoxin-like fold samples, that stability and foldability are validated by the alpha fold and GROMACS MD simulation.
This result indicates that it is possible to design left-handed *βαβ*-motif-containing proteins.

1Pos007 CRISPR-Cas7-11 の構造とエンジニアリングによる RNA ノックダウンツールへの応用
Structure and engineering of the type III-E CRISPR-Cas7-11 effector complex

Kazuki Kato[1], Wenyuan Zhou[2], Sae Okazaki[1], Yukari Isayama[1], Tomohiro Nishizawa[3], Jonathan S. Gootenberg[2], Omar O. Abudayyeh[2], Hiroshi Nishimasu[1] ([1]*RCAST, Univ. Tokyo*, [2]*MIBR, MIT*, [3]*Grad. Sch. Med. Life Sci., Univ. Yokohama City*)

The type III-E CRISPR-Cas effector Cas7-11, with dual RNase activities for precursor CRISPR RNA (pre-crRNA) processing and crRNA-guided target RNA cleavage, is a new platform for bacterial and mammalian RNA targeting. We report the cryo-EM structure of Cas7-11 in complex with a crRNA and its target RNA. Cas7-11 adopts a modular architecture comprising seven domains (Cas7.1–Cas7.4, Cas11, INS, and CTE) and four interdomain linkers. The Cas7.1 domain process pre-crRNAs to produce mature crRNA, while the Cas7.2 and Cas7.3 domains cleave target RNA at two defined positions for programmable cleavage. We rationally engineered a compact Cas7-11 variant for single-vector AAV packaging for transcript knockdown in human cells, enabling *in vivo* Cas7-11 applications.

1Pos008 疑似電子顕微鏡画像を機械学習することにより生体分子の同定手法を開発する
Deep learning of computer-generated electron microsopy images to identify biomolecules

Atsushi Matsumoto (*Institute for Quantum Life Science, National Institutes for Quantum Science and Technology*)

We are developing a computational method to identify biomolecules in electron microscopy (EM) images utilizing the neural network or deep learning. One of the important steps in the deep learning is to prepare training datasets. Previously, we have developed a technique to make negative-stained EM images from atomic models computationally. Using this technique, we generated a few thousand EM images from each model in Protein Data Bank (PDB). We selected relatively large ~20,000 models from PDB. One thing that should be considered was that PDB stored similar models in shape, which gave similar EM images which were difficult to be distinguished. Thus, we classified the models into groups by their shapes and gave the same label or ID to the EM images in the same group.

1Pos009 Time-resolved X-ray crystallography of *E. coli* MutT, a Nudix hydrolase

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E. coli MutT hydrolyzes mutagenic 8-oxo-dGTP in the presence of Mg^{2+} or Mn^{2+} ions and prevents transversion mutations. MutT is also the most studied enzymes in the Nudix hydrolase superfamily, which is widely distributed in living organisms. However, the catalytic mechanisms of Nudix hydrolases, including two- or three-metal-ion mechanisms, remain elusive. We have followed the hydrolysis process of 8-oxo-dGTP by MutT using time-resolved X-ray crystallography. The intermediate structures and electron densities show that MutT hydrolyzes 8-oxo-dGTP via binding of three metal ions in the active site. We discuss the three-metal-ion mechanism observed in this study and propose that some Nudix hydrolases share this mechanism.

1Pos010 X 線自由電子レーザーを用いた単粒子解析における分子サイズ効果
Molecular size effect on the single-particle analysis using X-ray free electron laser

Miki Nakano[1], Osamu Miyashita[1], Florence Tama[1,2,3] ([1]*RIKEN Center for Computational Science*, [2]*Grad. Sch. Sci., Nagoya Univ.*, [3]*ITbM, Nagoya Univ.*)

The high coherent light source of X-ray free electron laser, XFEL, provides an approach to obtaining diffraction data without crystallization. The high transmittance of X-ray allows us to observe the inner structure of thicker samples, more than 500 nm without multiple scattering events. However, how the restored molecular structure depends on the molecular size has not been studied. To clarify this issue, we simulated XFEL single particle analysis for five biological molecules of different sizes with the same experimental conditions. Using the simulated data, we compared the difficulty of restoring molecular structures. Our results bring useful information for the experimental design and the selection of the target samples.

1Pos011 クライオ電子顕微鏡を用いた繊毛軸糸ダイニンコンポーネント Calaxin の機能解析
Cryo-electron tomography revealed that Calaxin stabilizes the docking of outer arm dyneins onto ciliary doublet microtubule in vertebrate

Hiroshi Yamaguchi, Masahide Kikkawa (*Grad. Sch. Med., Univ. Tokyo*)

Outer arm dyneins (OADs) generate the main force of ciliary beating, however, the docking mechanism of OADs onto ciliary doublet microtubule remains elusive in vertebrate. We analyzed the functions of Calaxin/Efcab1 and Armc4, both of which are the components of vertebrate OAD-DC (docking complex), using zebrafish spermatozoa and cryo-electron tomography. Mutation of armc4 caused complete loss of OADs, whereas calaxin mutant showed only partial loss of OADs. Detailed structural analysis revealed that retained OADs are tethered to doublet microtubule through DC components other than Calaxin, and that recombinant Calaxin can spontaneously rescue the deficient DC structure. Our data provide the distinct roles of Calaxin and Armc4 as vertebrate DC components.

1Pos012 スーパーフォールドを区別する構造ルールの探索:フェレドキシン構造とリバースフェレドキシン構造の解析
The structural rule distinguishing a superfold: A case study of ferredoxin fold and the reverse ferredoxin fold

Takumi Nishina, George Chikenji (*Dept of Appl. Phys., Grad. Sch. of Eng., Nagoya Univ.*)

Superfolds are folds commonly observed among evolutionarily unrelated multiple superfamilies of proteins. Since discovering superfolds almost two decades ago, structural rules distinguishing superfolds from the other ordinary folds have been explored but remained elusive. Here, we analyzed a typical superfold, the ferredoxin fold (FR), and the fold which reverses the N to C terminus direction from the FR as a case study to find the rule to distinguish superfolds from the other folds. The database analyses revealed the structural preferences of ab/ba-units distinguish a superfold from ordinary folds. Threrefore, this result indicates that superfolds and normal folds can be distinguished based on topological information, not on amino acid sequence.

1Pos013 ネフローゼ症候群原因タンパク質 podocin の調製と結晶化
Preparation and crystallization of podocin, associated with nephrotic syndrome

Koki Ando[1], Hideshi Yokoyama[2] ([1]*Grad. Sch. Pharm. Sci., Tokyo Univ. Sci.*, [2]*Fac. Pharm. Sci., Tokyo Uni. Sci.*)

Slit diaphragm (SD), a cell-cell junction of podocytes, plays an essential role in the glomerular filtration barrier. Podocin is encoded by *NPHS2* that was identified as a causative gene of autosomal recessive steroid-resistant nephrotic syndrome. Podocin is exclusively expressed in the podocytes and composes the SD with the other SD components, such as nephrin, CD2AP and TRPC6. Little is known about details of its function, and its structure has not also been solved.
In order to determine the structure by X-ray crystallography, we have prepared podocin and crystallized it. Podocin has been expressed in *E. coli*, highly purified by size exclusion chromatography, and then crystallized by sitting-drop vapor-diffusion method.

1Pos014 TMD シミュレーションを用いたギャップ結合ファミリータンパク質のクローズ機構及び周囲の脂質分子の流動性の解析
Analysis on the closing mechanism of gap junction family proteins and fluidity of surrounding lipid molecules by TMD simulation

Ikuma Kaneshiro[1], Florence Tama[1,2], Osamu Miyashita[2] ([1]*Grad. Sch. Sci., Univ. Nagoya*, [2]*Kobe Inst., Riken*)

Innexin-6 exists as a transmembrane hemichannel and forms a gap junction channel by binding to the corresponding on an adjacent cell. Pannexin-1 has a weak homology with the innexin family and functions as a single transmembrane channel. Recent analysis suggests that conformational changes in N-terminal allow surrounding lipids to interact with the protein and flow in the channel pathway to block it. However, its details or the actual process is not observed yet, in spite of its physiological importance. We generated systems including innexin-6 or pannexin1 and the lipid bilayer, run targeted molecular dynamics (TMD) simulations, and tried to confirm that the lipids show interaction with the protein when it shifts from the open to the closed state.

1Pos015 レジリン蛋白質における自己組織化能の評価
Evaluation of Self-Assembling Ability in Resilin Proteins

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Fibron, a structural protein of spider silk, had been shown to self-assemble to form nanoscale fiber structures. In this study, to verify that the formation of higher-order structures by self-assembly is a property of structural proteins in general, we focus on resilin, another structural protein, and examine its self-assembling ability. In addition to the full-length resilin, domains corresponding to Exon I and III were cloned, and an expression system was constructed to obtain 25 mg of protein per liter of culture. All obtained samples showed the concentration-dependent formation of secondary structure, where Exon III aggregates upon the secondary structure formation. From these results, it can be assumed that resilin also has a self-assembling ability.

1Pos016 代謝安定型作動薬と LysoPS 受容体 LPS1 の構造解析
Cryo-EM structure of LysoPS Receptor LPS1 in complex with Metabolically Stable Agonist

Ryo Kawahara[1], Fumiya Sano[1], Akiharu Uwamizu[2], Luying Chen[2], Tomohiko Ohwada[2], Junken Aoki[2], Wataru Shihoya[1], Osamu Nureki[1] ([1]*Grad. Sch. Sci., Univ. Tokyo*, [2]*Grad. Sch. Pharm., Univ. Tokyo*)

Lysophosphatidylserine (LysoPS) is a type of lysophospholipids containing a serine moiety. LysoPS activates LysoPS receptors LPS1-3, which belong to G-protein-coupled receptors. Activation of LPS1 enhances innate and acquired immunity and anti-cancer effects. Thus, LPS1 has attracted attention as a drug target. Compound M1 is a derivative of LysoPS in which an acyl group is replaced with aromatic groups. M1 is an agonist with high agonist activity and metabolic stability than intrinsic LysoPS. In this presentation, we report the cryo-electron microscopy structure of the M1-bound LPS1-Gi complex.

1Pos017 免疫受容体 LILRA2 の ANGPTL6 認識機構
Molecular mechanism of ANGPTL6 recognition by immune activation receptor LILRA2

Jiaqi Wang[1], Atsushi Furukawa[1,2], Rika Yamazaki[1], Kouyuki Hirayasu[3,4], Tsuyoshi Kadomatsu[5], Yuichi Oike[5], Hisashi Arase[3], Katsumi Maenaka[1] ([1]*Pharm. Sci. Hokkaido Univ.*, [2]*Pharm. Kanazawa Univ.*, [3]*Res. Inst. Microbial Diseases, Osaka Univ.*, [4]*Adv. Preventive. Med. Sci. Res. Center., Kanazawa Univ.*, [5]*Med., Kumamoto Univ.*)

Leukocyte immunoglobulin-like receptor (LILR) family are type I transmembrane glycoproteins with extracellular Ig-like domains. Among the LILRs, LILRA2 attracts attention as a novel innate immune receptor. As reported, LILRA2 binds to Angiopoietin-like protein 6 (ANGPTL6) which contributes to angiogenesis. This study investigates the molecular mechanism of the interaction. The two proteins were purified by size exclusion chromatography (SEC). The interaction was analyzed by surface plasmon resonance (SPR). SPR result shows a specific binding with weak affinity (K_D ~ 14 μM) and fast kinetics. This binding mode is similar to typical cell-cell recognition, which provides novel insights into the molecular regulation of LILRA2-mediated immune responses targeting ANGPLT6.

1Pos018 gREST 法による VHH 構造の効率的サンプリング
Enhanced Conformational Sampling of VHH by Generalized Replica-Exchange with Solute Tempering

Ren Higashida, Kouhei Yamaguchi, Yasuhiro Matsunaga (*Grad. Sch. Sci. Eng., Saitama Univ.*)

The variable domains of a heavy-chain antibody are known as VHH or nanobody. VHH is a small domain composed of approximately 125 amino acid residues, but shows similar affinities to antigens compared with conventional antibodies. Here, we apply an enhanced sampling method, the generalized replica-exchange with solute tempering (gREST) (Kamiya and Sugita J. Chem. Phys 2018), to sample or predict CDR H3 loop structures of VHHs and their binding poses to an antigen. In the sampling of unbound VHHs, the gREST efficiently found correct structures of CDR H3 loops that are hard to access with conventional simulations. In the poster, we will report the details of binding pose sampling with the gREST.

1Pos019 毛髪ダメージに伴う毛髪繊維の変形とその分光学的解析
Deformation of hair fibers due to hair damage and its spectroscopic analysis

Kazuki Kobayashi, Atsushi Baba, Kazuyuki Suzuta, Len Ito (*MILBON Co.,Ltd.*)

It is important to study hair damage in order to maintain a beautiful hair design. The irregular deformation of hair fibers occurs locally with hair damage caused by some cosmetic procedures such as coloring, perming, ironing, and combing. In order to approach the mechanism of local deformation of hair fibers, we focused on the cortex which composing most of the hair fiber. Analysis of the secondary structure of cortical protein by microscopic IR measurement revealed that the signal intensity based on the α-helix structure was locally decreased and non-uniformly distributed in the hair cross section at the deformed site. Details including the SAXS analysis will be discussed at the poster session on the day.

1Pos020 ミトコンドリア蛋白質搬入ゲート TOM 複合体の高速原子間力顕微鏡解析
High-speed atomic force microscopy analysis of the mitochondrial protein import gate TOM complex

Yuhei Araiso[1], Nanako Kobayashi[1], Kana Kuzasa[1], Hirotatsu Imai[2], Aimi Makino[2], Akihiro Inazu[1], Noriyuki Kodera[2], Toshiya Endo[3,4] ([1]*Dept. of Clin. Lab. Sci., Div. of Health Sci., Kanazawa Univ.*, [2]*WPI-NanoLSI, Kanazawa Univ.*, [3]*Fac. of Life Sci., Kyoto Sangyo Univ.*, [4]*Inst. of Protein Dynamics, Kyoto Sangyo Univ.*)

The translocase of the outer mitochondrial membrane (TOM) complex is the main entry gate for mitochondrial proteins. The TOM complex is a multi-subunit membrane protein complex in equilibrium with several oligomerization states on the mitochondrial surface, which consists of the β-barrel channel Tom40 and six α-helical subunits. Based on the cryo-EM structure of the TOM complex, we are trying to analyze the dynamic behaviors of the TOM complex at a nm spatial resolution by High-speed atomic force microscopy (HS-AFM) in order to understand the protein translocation mechanism. Here we report the HS-AFM analysis showing that the TOM complex is a mixture of a trimer and a dimer, and the trimeric TOM complex tends to dissociate into the dimer and a peripheral monomer.

1Pos021 カイコ storage protein の単粒子解析
Single particle analysis of silkworm storage proteins

Shunsuke Kita, Yuki Anraku, Cong Tian, Katsumi Maenaka (*Faculty of Pharmaceutical Sciences, Hokkaido University*)

The accumulation and utilization of storage proteins (SPs) are essential for insect metamorphosis. SPs are synthesized, secreted into larvae blood and stored in fatbody when the insect begins wandering. During the development from pupa to adult, SPs are proteolyzed and utilized as amino acids resource for adult development. SPs are composed of SP1, SP2 and SP3. SP1 is rich in methionine, while SP2 and SP3 are rich in aromatic amino acids. Insect SPs belong to hexamerin superfamily and form heterohexamer. In this study, *Bombyx mori* SPs were isolated from hemolymph. The purified sample was plunge frozen with Vitrobot Mark IV and datasets were collected with Glacios and Krios. The structure showed hexameric protein with one N-linked glycosylation in each protomer.

1Pos022 狂犬病ウイルスの P 蛋白質が宿主の JAK-STAT 経路を阻害する分子機構の解明
Molecular dissection on how rabies virus P-protein inhibits JAK-STAT pathway of host

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Rabies is one of the zoonosis caused by rabies virus (RABV). RABV can invade host cells through its ability to antagonize host immune system. The molecular target of RABV immune evasion is transducer and activator of transcription (STAT) molecules which have a crucial role in inducing antiviral gene expression. In recent research, it has been revealed that RABV P-protein C-terminal domain (RVPC) is able to interact with STAT and inactivates this system. Although our interaction analysis shows that the domain of STAT recognized by RVPC, the details of the interaction region are still unclear. we aim to reveal how RABV counteracts host immunity using RVPC at molecular level by analyzing the interaction between these molecules as well as complex structures.

1Pos023 一分子蛍光測定を目指した SARS-CoV2 の N 蛋白質の精製及びラベル化
Purification and fluorophore labeling of SARS-CoV2 N protein aiming at single molecule fluorescence measurements

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SARS-CoV2 N protein binds to viral genomic RNA(gRNA) forms "beads on a string" structure with gRNA in virion, and is involved in replication, transcription, and packaging of gRNA in host cells.To understand the structure shanges of N protein upon the binding to RNA, we plan to use single molecule fluorescence spectroscopy, and are preparing N protein labeled with donor and acceptor fluorophores. We oconstructed a plasmid encoding a single cysteine mutant pf N protein, transformed it into E.coli, and clustered the cells. The expressed N protein was purified by using His-tag column. To emiliminate contaminants of nucleic asids, the purification was conducted in the presence of urea. We are currently labeling the purified mutant with Alexa488 and Alexa647.

1Pos024 高分解能中性子構造解析によるペプチド結合の平面性の再検討
Revisiting the peptide bond planarity by high-resolution neutron structure

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The peptide bond has a partial double-bond character because of its resonance stabilization. However, several high-resolution X-ray structures and computational analyses have shown the distortion of the peptide bond. The deviations of the position of the amide protons are not well understood because of the lack of structural data for hydrogen atoms. To investigate the peptide bond planarity, we determined a 1.2 Å resolution neutron structure of high-potential iron-sulfur protein (Hanazono *et al.*, *Sci. Adv.*, 8, eabn2276, 2022). The high-resolution neutron structure shows that the amide protons deviate from the peptide plane and shift toward the acceptors. The planarity of the H-N-C=O plane is strongly dependent on the pyramidalization of the nitrogen atom.

1Pos025 大腸菌由来 ribonuclease HI の金属イオン結合熱力学解析と活性との相関
Metal-ion binding and folding thermodynamics of *Escherichia coli* ribonuclease HI in correlation with its activity

Yumi Kitagawa[1], Zengwei Liao[1], Kosuke Morikawa[2], Masayuki Oda[1] ([1]*Grad. Sch. Life Environ. Sci., Kyoto Pref. Univ.*, [2]*Grad. Sch. Biostudies, Kyoto Univ.*)

Ribonuclease HI (RNase HI) hydrolyzes the RNA strands of RNA/DNA hybrids in the presence of divalent metal-ions. In addition to the negatively charged electrostatic field formed by Asp and Glu, DEDD motif, which coordinates the divalent cation at the active site, His124 adjacent to the active site is a key player in RNase HI function. In this study, we analyzed the metal-ion binding thermodynamics to RNase HI wild-type and H124A mutant and their folding thermodynamics in the absence or presence of metal-ions, Mg^{2+}, Mn^{2+}, Ca^{2+}, and Zn^{2+}, using isothermal titration calorimetry, circular dichroism, and differential scanning calorimetry. Based on the results, we discuss the change of structural dynamics of RNase HI upon metal-ion binding and its correlation with function.

1Pos026 大規模な薬剤データセットにおける心筋イオンチャネル-薬剤間の結合自由エネルギー計算
Calculation of the binding free energies between cardiac ion channels and drugs on a large data set

Tatsuki Negami, Tohru Terada (*Grad. Sch. Agr. Life Sci., Univ. Tokyo*)

All drug candidates are tested for cardiotoxicity. Predicting interactions between drugs and cardiac channels, especially hERG, $Na_V1.5$, and $Ca_V1.2$, is important for the proarrhythmia assessment. We are developing a method to predict the channel-drug binding affinity by combining the ligand docking simulation and the MP-CAFEE method. Previously, we have shown that the calculated binding free energies to the hERG, $Na_V1.5$, and $Ca_V1.2$ channels were correlated with experimental data for several drugs. In this study, we applied the method to a large data set. We calculated binding free energies of 27 drugs to the three cardiac channels and compared the results with experimental data. We will discuss the accuracy of the calculated binding free energies.

1Pos027 (2SBP-6) Automated Density Extraction of Isomorphous Difference map and Occupancy-estimation for Conformer Fitting

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TR-SFX allows capturing of time-evolved residual motion within crystal structure thereby enabling the visual inspection of reaction kinetics. The changes in fractional density of intermittent states are estimated from isomorphous difference density map (ISM). The discrete density observed from ISM are then interpreted as minor states corresponding to various intermittent time steps. ISM map interpretations are generally time-consuming and methodologically inaccurate during manual density estimation. Here, we employ clustering and SVD based approaches to extract and evaluate residues corresponding to isomorphous difference density. Fractional occupancy corresponding to the change in map density is estimated and the conformers of the minor states are fitted using MD trajectory.

1Pos028 HIV-1 の Nelfinavir 耐性プロテアーゼ D30N/N88D 変異体に対する動的残基間相互作用ネットワーク解析
Dynamic Residue Interaction Network Analysis of the Protease D30N/N88D Mutant Conferring Nelfinavir Resistance in HIV-1

Ayaka Ojima, Norifumi Yamamoto (*Chiba Tech*)

Human immunodeficiency virus type 1 (HIV-1) is the pathogen of acquired immunodeficiency syndrome (AIDS), a disease that can be controlled in the long term by anti-HIV drugs. However, there are serious concerns about the emergence of viral mutants that are resistant to anti-HIV drugs. The D30N mutant of the HIV-1 protease is known to be resistant to Nelfinavir. In adittion, the D30N/N88D dual mutation is known to restore the enzyme activity that is reduced by the D30N mutation. In this study, we investigated the dynamic correlation between the binding of D30N/N88D mutant HIV-1 protease to Nelfinavir using dynamic residue interaction network (dRIN) analysis based on molecular dynamics simulation.

1Pos029 Elucidating the Mechanisms of the Bacterial Flagella ATPase Subcomplex

Thomas Stefan Davies[1,2], Peter John Bond[1], Alexander Krah[1], Chrystala Constantinidou[2] ([1]*A*STAR Singapore*, [2]*University of Warwick*)

The formation of the flagellum, considered an important virulence factor, is a vital process for many pathogenic bacteria. Its formation entails a complex mechanism that utilises protein export apparatus and ATP hydrolysis. Unfolding of nascent flagella proteins is understood to be driven by successive ATP hydrolysis reactions of a hexameric ATPase assembly which rotates a central stalk protein. Unfolded proteins can then be incorporated into the growing flagellum. We are using molecular dynamics (MD) simulations of the type three secretion system ATPase subcomplex to elucidate structural features and the associated mechanism.

1Pos030 Molecular dynamics study of phase behaviors of heat-resistant obscure proteins and their anti-aggregation functions

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Liquid-liquid phase separation (LLPS) has been proposed as a general mechanism for the dynamic compartmentalization of biomolecules. Recent studies of the heat-resistant obscure (Hero) proteins revealed their ability to prevent the pathological aggregation of LLPS-prone peptides. Here, we utilize molecular dynamics simulations to investigate the phase behavior of Hero11 and its interplay with TDP-43. We carried out residue-level coarse-grained simulations of Hero11 and its KR-less mutant, in which all the positively-charged residues are mutated to glycine. Our results show that the intermolecular electrostatic repulsion dominantly determines the phase equilibrium thermodynamics of Hero11, while the secondary structure also contributes to its anti-aggregation function.

1Pos031 インバース共溶媒分子動力学法による分子プローブ周辺アミノ酸残基環境の可視化
Inverse Mixed-Solvent Molecular Dynamics for Visualization of Amino Acid Residue Interaction Profile of Molecular Probes

Keisuke Yanagisawa[1], Ryunosuke Yoshino[2,3], Genki Kudo[4], Takatsugu Hirokawa[2,3] ([1]*Comput. Sci., Sch. Comput., Tokyo Tech*, [2]*Faculty Med., Univ. Tsukuba*, [3]*TMRC, Univ. Tsukuba*, [4]*Appl. Sci., Grad. Sch. Sci. Tech., Univ. Tsukuba*)

The computational methods used in lead optimization to improve activity and reduce the toxicity of compounds are still evolving. In this study, we propose a method to construct the residue interaction profile of the chemical structure used in the lead optimization by performing "inverse" mixed-solvent molecular dynamics (MSMD) simulation. We constructed a protein residue interaction profile. It indicates us the preferred protein environments of probes without co-crystallized structures. The residue interaction profiles obtained by MSMD were a reasonable physicochemical description of the general non-covalent interaction. Moreover, comparison with the X-ray structure shows that the interaction profile matches the arrangement of amino acid residues in the structure.

1Pos032 タイプⅠインターフェロン経路を阻害する麻疹ウイルスⅤタンパク質の機能解析
Mechanistic analysis of type I interferon pathway inhibition by Measles virus V protein

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Measles is an acute systemic infectious disease caused by measles virus, which has high infectivity for human. Its infectivity derives from counteracting host immunity. The type I Interferon (IFN) pathway is one of the major host innate immune system. In this pathway, the recognition of type I IFN induces tyrosine kinase JAK1 and TYK2 to phosphorylate STAT1/2. Phosphorylated STAT1/2 recruits IRF9 and they form the heterotrimer, ISGF3, which works as a transcription factor and promotes antiviral gene expression. Measles virus V protein (MeV-V) inhibits this pathway. Previous our study showed that MeV-V competes with IRF9-IFN associated domain and inhibits ISGF3 formation. We are now focusing on the detailed inhibition mechanism using ultracentrifuge, ITC, and SEC.

1Pos033 SMN タンパク質のプロリン残基異性化による機能変化
Functional changes in SMN proteins by isomerization of proline residues

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SMN is a causative gene of spinal muscular atrophy and its protein product localized in both cytoplasm and nucleus, however, SMN is mainly localized at subnuclear bodies called Cajal body (CB) in nucleus. We found a compound that induces dispersion of CB and that is accompanied with proline isomerization of SMN. Then, we focuss on how the proline isomerization affects the protein function of SMN.
The amino acid substitution mutant of the proline residue (SMN-PA) showed altered localization in cultured cells compared to wild-type SMN. Furthermore, in vitro studies showed that the SMN-PA mutant had a reduced dimerization capacity compared to wild-type SMN.
Thus, the isomerization of a specific proline residue of SMN has a potential role to maintain the property of SMN.

1Pos034 MD シミュレーションとクライオ電顕を用いた p97 の構造変化の研究
Conformational change of p97 by MD simulations and experimental data

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p97 is a hexameric AAA+ adenosine triphosphatase (ATPase) that is an attractive target for cancer drug development. Multiple conformations of p97 have been observed. However, the detail of its function and conformational change are unknown. In addition, p97 has three domains, each plays a role in conformational change but its detail is unknown. We investigated conformational change of p97 and role of each domain by integrating simulations and experimental data.

We used all-atom MD simulations to sample p97 conformational states. Representative structures from MD simulations were compared to 2D electron microscopy images in order to elucidate details of the conformational change. In addition, MD simulation and experimental data elucidated role of each domain.

1Pos035 ホソイトスギ由来パンアレルゲン、ポルカルシンの組換え発現と NMR 構造
Recombinant expression and NMR structural analysis of a pan-allergen, polcalcin from European cypress

Peiwen Fan, Shaokai Zhao, Tomona Iizuka, Jingkang Zheng, Mitsuki Shibagaki, Tomoyasu Aizawa (*Grad. Sch. Life Sci., Hokkaido Univ.*)

Polcalcin is a calmodulin-like protein mainly expressed in pollen. Polcalcin has pan-allergenic potential, which leads to IgE cross-activity due to sharing a highly conserved sequence region called the EF-hand domain. Previous studies have focused on 2EF-hand polcalcins. In this study, based on next-generation sequencing RNA-seq results of European cypress (*Cupressus sempervirens*), a new 4EF-hand polcalcin was discovered, named Cup s 4. Cup s 4 is an intracellular protein with three cysteines, and its oxidation state may affect allergenicity. Therefore, we expressed wild-type and mutant recombinant proteins in E. coli, analyzed their solution structures by NMR, and investigated the effect of disulfide cross-linking on their allergenicity.

1Pos036 STAT2 との相互作用に必要な麻疹ウイルス V 蛋白質最小領域の同定と相互作用特性
Characterization of the minimum region of measles virus V protein to interact with STAT2

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Measles is a highly contagious infectious disease characterized by fever, rash, and koplik spots. Measles virus V protein (MeV-V) is known to be a pathogenic factor that inactivates innate immunity and increases the severity of other infectious diseases. MeV-V interacts with STAT1 using the N-terminal domain (MeV-V_{NT}) and STAT2 using the C-terminal one (MeV-V_{CT}). Previously, we reported that MeV-V inhibits the formation of the STAT1/STAT2/IRF9 heterocomplex, ISGF3, by blocking the interaction between STAT2 and IRF9, thereby inhibiting the type I interferon pathway. We have been focusing on the interaction between MeV-V_{CT} and STAT2 using ITC, SPR, SEC, NMR, and cystography. The preparation, characterization of MeV-V_{CT}, and interaction analysis of them will be discussed.

1Pos037 ストレスファイバーにおけるアクチンサブユニットの張力依存的な構造状態
Tension-dependent structural state of actin subunits in stress fibers

Yuki Karan, Taro Q.P. Noguchi (*National Institute of Technology, Miyakonojo College*)

It has been suggested that applying force to F-actin changes the structure of actin subunit. In a previous meeting, we also reported that actin structure in cells changes by mechanical stimulation. In this study, we aimed to confirm whether actin structures are also affected by the force generated inside a cell. FRET actin, in which two dyes are attached, was introduced into cells, and FRET intensity was compared between peripheral and central SFs. The peripheral SF generates stronger tension than the central SF. The analysis suggested that each actin in these SFs has different molecular structures. Furthermore, the addition of Y27632, myosin inhibitor, changed actin structure in both SFs. These are suggesting that tension to F-actin in cells affects actin structures.

1Pos038 Structural dynamics and *in silico* design of pyrazolopyran-based inhibitors against *Plasmodium* serine hydroxymethyltransferases

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The clinical efficacy of antimalarial drugs has been reduced due to drug resistance. Herein, 500-ns MD simulations were carried out to investigate the mode of action of pyrazolopyran(+)-85 and pyrazolopyran(+)-86 on *Plasmodium* serine hydroxymethyltransferases (SHMTs), *P. falciparum,* and *P. vivax* SHMTs. The binding free energy results indicated the binding affinity of pyrazolopyran(+)-86, which is more favorable than pyrazolopyran(+)-85 by ~2 kcal·mol^{-1}. By the rational drug design, some parts of pyrazolopyran(+)-86 were modified to promote the interaction with the surrounding residues. Therefore, our findings provide insights into the inhibition mode of pyrazolopyran-based inhibitors and rational ideas for designing novel antimalarial drugs targeting *Plasmodium* SHMTs.

1Pos039 SARS-CoV-2 スパイク蛋白質と NTD 結合抗体との糖鎖を介した相互作用の解析
Investigation of interactions between SARS-CoV-2 spike and NTD-binding antibody through glycans

Mao Oide[1], Yuji Sugita[1,2,3] ([1]*RIKEN CPR*, [2]*RIKEN BDR*, [3]*RIKEN R-CCS*)

Spike protein of severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2) has many glycosylation sites. The decollating glycans shield the protein surface and prevent antibodies from binding. In 2021, a specific antibody was reported to enhance infectivity of SARS-CoV-2. This enhancing antibody binds to N-terminal domain (NTD) of spike, and does not directly interact with receptor binding domain (RBD), which binds to receptor in active up form. Since some of the glycans are involved in conformational stability of RBD, NTD-binding antibody might affect RBD through interacting glycans. In this study, we performed MD simulations of complex systems consisting spike and Fv fragment of NTD-binding antibody, and investigated the effect of antibody binding on glycans.

1Pos040 Recombinant production, functional and structural analysis of antimicrobial peptides in mouse cryptdin family

Shaonan Yan, Yuchi Song, Yi Wang, Weiming Geng, Shinya Yoshino, Tomoyasu Aizawa (*Graduate School of Life Science, Hokkaido University*)

Cryptdins (Crps) are an α-defensin family from mouse containing Crp1-6 which have strong antimicrobial activity. Now, there are few published studies about other isoforms except Crp4. In this study, by using recombinant expression system in *E. coli* Origami B, the expression level of Crp family as inclusion body had been significantly improved. After overexpression, purification and refolding, large amount of recombinant Crp1, 2, 3, 4, 6 were successfully obtained and the production system established, including oxidized and reduced form peptides. From activity assay, all Crp isoforms were effective in killing both Gram-positive and Gram-negative bacteria, but showed different antibacterial spectra.

1Pos041 *Dictyostelium discoideum* の filopodia の cryo-EM 観察
Observation of filopodia in *Dictyostelium discoideum* by cryo-EM

Yuki Gomibuchi, Yukihisa Hayashida, Yusuke V. Morimoto, Takuo Yasunaga (*Grad. Sch Comp. Sci and Sys. Eng., KIT*)

Dictyostelium discoideum has been used to study cell motility as a model organism. *D. discoideum* cells form pseudopodia during cell migration and have been known to have actin filaments in the filopodia. This study observed the filopodia of Wild type and *mhcA*$^-$ cells by cryo-EM and reported new findings. The previous study reported the presence of short actin filaments in the filopodia. They proposed that it is due to the rapid elongation of the filopodia in *D. discoideum* cells. In contrast, our observations showed that both WT and *mhcA*$^-$ cells had long actin filaments in the filopodia, and they were arranged in parallel to bundles larger than 1 μm. We will discuss these differences.

1Pos042 Unraveling the coupling between conformational changes and ligand binding in ribose binding protein using MD simulations

Weitong Ren[1], Hisham Dokainish[1], Ai Shinobu[2], Hiraku Oshima[2], Yuji Sugita[1,2,3] ([1]*RIKEN Cluster for Pioneering Research*, [2]*RIKEN Center for Biosystems Dynamics Research*, [3]*RIKEN Center for Computational Science*)

We investigated the coupling between the conformational changes of ribose-binding protein (RBP) and ribose binding by combining coarse-grained MD, multiple atomistic cMD, and free-energy calculations together. It's found that the ribose binding is unstable in the open and open-like forms of RBP. In the contrast, the closed-like and closed states show high affinity for ribose. Importantly, we observed transitions from closed-like forms toward closed state in the presence of a bound ribose. On the basis of the computational results, we propose a molecular mechanism in which conformational selection and induced fit happen in the first and second halves of the open-to-closed transition of ribose-binding protein, respectively.

1Pos043 コーヒーポリフェノールと乳タンパク質の相互作用に関する分光学的研究
Spectroscopic study of the interaction between coffee polyphenols and milk proteins

Kazuki Horita[1,2], Hiroshi Suga[1], Atsushi Hirano[1,2] ([1]*Grad. Sch. Eng., Chiba Tec.*, [2]*NMRI, AIST*)

Coffee is rich in polyphenols. The interactions of coffee polyphenols with milk proteins lead to a decrease in their antioxidant activity. However, it is not clear which milk proteins interact primarily with coffee polyphenols. This study examined the interactions of coffee polyphenols with milk proteins using a fluorescence spectrophotometer. The proteins used were whey proteins, including α-lactalbumin and β-lactoglobulin, and caseins. The coffee polyphenol used was chlorogenic acid (CGA). Fluorescence intensity of CGA was increased by the addition of caseins, but was not significantly changed by the addition of the whey proteins. These results suggest that the caseins interact with CGA, whereas the whey proteins are unlikely to interact with it.

1Pos044 CD28 ペプチドとの相互作用に伴う PI3K nSH2 ドメインの構造動態変化
Changes in structural dynamics of PI3K nSH2 upon interaction with CD28 peptide

Yohei Miyanoiri[2], Suyong Re[3], Yuhi Hosoe[1], Yuya Asahina[2], Toru Kawakami[2], Masataka Kuroda[3,4], Kenji Mizuguchi[2,3], Masayuki Oda[1] ([1]*Grad. Sch. Life Environ. Sci., Kyoto Pref. Univ.*, [2]*Inst. Prot. Res., Osaka Univ.*, [3]*ArCHER, Natl. Inst. Biomed. Innov. Health Nutrition*, [4]*Discov. Tech. Lab., Mitsubishi Tanabe Pharma Corp.*)

Src homology 2 (SH2) domains are widely located in adapter proteins for signal transduction, and specifically bind to proteins at phosphorylated Tyr sites, following consensus residues. Here, we analyzed the interaction of the N-terminal SH2 (nSH2) of the regulatory p85 subunit of phosphoinositide 3-kinase (PI3K) with the cytoplasmic region of the T-cell co-receptor, CD28, using NMR spectroscopy and MD simulations. Chemical shift perturbation and NMR relaxation experiments revealed that nSH2 strongly bind to CD28 phosphopeptide via structural rearrangement. Moreover, our MD simulations detected major and minor conformations in nSH2-CD28 complex. In this meeting we will discuss about the correlation between the structural dynamics and biological functions of PI3K nSH2.

1Pos045 Acceleration of residue-level coarse-grained molecular dynamics by new development of parallelization

Jaewoon Jung[1,2], Cheng Tan[1], Chigusa Kobayashi[1], Diego Ugarte[1], Yuji Sugita[1,2,3] ([1]*RIKEN R-CCS*, [2]*RIKEN CPR*, [3]*RIKEN BDR*)

Residue-level coarse-grained (CG) models molecular dynamic is one of the most popular tools to investigate large-scale biological phenomena. Despite of its computational efficiency, it has not been tried for very huge-scale biomolecules because of difficulties in computational parallelization. To overcome it, we develop a new parallelization scheme of domain decomposition with good load balancing. The new scheme is implemented in GENESIS MD software and it speeds up 10~100 folds of the existing programs for a very huge system like chromatin.

1Pos046 新型コロナウイルスのスパイクタンパク質の動的残基相互作用ネットワーク分析
Dynamic Residue Interaction Network Analysis of the Spike Protein of SARS-CoV-2

Hirokazu Murata, Norifumi Yamamoto (*Chiba Tech*)

Since the end of 2019, SARS-CoV-2 is having a significant impact on our lives. Since the end of 2021, the Omicron variant of SARS-CoV-2 spread worldwide. As compared to wild-type, the Omicron variant has 30 mutations in SARS-CoV-2 Spike protein of which 15 mutations are present in the Receptor Binding Domain (RBD). Therefore, the changes in SARS-CoV-2 viral properties associated with the Omicron mutations are thought to be due to the changes in the intermolecular interaction between the SARS-CoV-2 Spike protein RBD and human ACE2 receptor in the host cell, but the details are not clear. In this study, we used dynamic residue interaction network (dRIN) analysis to clarify the changes in the intermolecular interaction between RBD and ACE2 due to Omicron mutations.

1Pos047 詳細反応モデリングとベイズパラメタ推定による KaiC の多量体構造の機能的役割の解明
Functional roles of the multimeric structure of KaiC revealed by detailed kinetic modeling and Bayesian parameter inference

Shin-ichi Koda[1,2], Shinji Saito[1,2] ([1]*Institute for Molecular Science*, [2]*SOKENDAI*)

The clock proteins of cyanobacteria, KaiA, KaiB, and KaiC, are known as a minimum circadian clock. The KaiB-KaiC complex is essential in determining the clock period due to its slowness. Significantly, the formation rate is elevated as KaiC is phosphorylated, implying a potential role in the period robustness. However, the molecular mechanism of this acceleration remains elusive. In the present study, we build mathematical kinetic models that can describe the acceleration. For quantitative analysis, we estimate the value of parameters under the framework of Bayesian inference. We then extract three requirements for the acceleration, indicating that the multimeric strucure of KaiC plays essential roles.

1Pos048 抗体の親和性成熟と安定性の変化；成熟した C6 とそのジャームライン型抗体
Antibody evolution for antigen binding and stability; maturated C6 and its germline-type antibodies

Saaya Yabuno[1], Takahiro Hayashi[2], Masayuki Oda[1,2] ([1]*Faculty Life. Environ. Sci., Kyoto Pref. Univ.*, [2]*Grad. Sch. Life. Environ. Sci., Kyoto Pref. Univ.*)

Somatic hypermutation is a process to produce an antibody (Ab) with higher affinity to an antigen, referred as affinity maturation, during the immune response. We studied the process in correlation with stability using single-chain Fv (scFv) Abs against anti-(4-hydroxy-3-nitrophenyl)acetyl (NP). In this study, we generated putative germline-type scFv Abs of C6, 9TG_R97K/Y98L, 9TG_L100Q, and 9TG_R97K/Y98L/L100Q, and analyzed the NP-binding affinities and thermal stabilities using surface plasmon resonance, isothermal titration calorimetry, circular dichroism, and differential scanning calorimetry, showing a trade-off between affinity and stability during affinity maturation of C6. We also discuss the structural basis of increased stability of 9TG_R97K/Y98L.

1Pos049 抗体の親和性成熟と安定性の変化；抗ニトロフェニル抗体の重鎖 58 番と 102 番残基の役割
Antibody evolution for antigen binding and stability; Role of residues at 58 and 102 of heavy chain of anti-nitrophenyl antibody

Mutsumi Yoshida[1], Yumi Kitagawa[2], Masayuki Oda[1,2] ([1]*Faculty Life. Environ. Sci., Kyoto Pref. Univ.*, [2]*Grad. Sch. Life. Environ. Sci., Kyoto Pref. Univ.*)

The process of affinity maturation has been studied using antibodies (Abs) against (4-hydroxy-3-nitrophenyl)acetyl (NP). In comparison of crystal structures of a germline-type Ab, N1G9, and a maturated Ab, C6, in complex with NP, the residues at 58 and 102 of heavy chain would be critical for maturation. In this study, we generated single-chain Fv (scFv) C6 and its mutant Abs, R58K and H102Y, mutating to the corresponding residues of N1G9, and analyzed the NP-binding affinities and thermal stabilities using surface plasmon resonance, isothermal titration calorimetry, circular dichroism, and differential scanning calorimetry. We also discuss trade-off phenomena between binding affinity and thermal stability during the course of affinity maturation.

1Pos050 Amyloid β aggregation and accumulation process under physiological conditions

Masahiro Kuragano, Shinya Yamanaka, Kiyotaka Tokuraku (*Grad. Sch. Eng., Muroran Inst. of Tech.*)

Abnormal aggregation of misfolded proteins is crucial process for the development of various amyloidosis. In this study, we clarified the aggregation and accumulation process of amyloid β (Aβ), which causes Alzheimer's disease (AD), under physiological conditions using quantum dots. 3D observations disclosed that Aβ aggregates size was significantly decreased in 40% glycerol exhibiting the human blood viscosity. Then, we revealed that these fibrils exhibited short and tangled morphology using transmission electron microscopy. Further, we demonstrated that several decades were required to develop the settling velocity and diameter of Aβ aggregates under physiological viscosity using numerical calculations, which is corresponded with real span of AD progression.

Poster

1Pos051 PSD95-PDZ3 の高温での可逆的なオリゴマー形成における速度論的効果の定量的な評価
The quantitative evaluation of kinetic effect on PSD95-PDZ3's reversible oligomerization at high temperature

Tomonori Saotome[1], Sawaros Onchaiya[2], Jose C Martinez[3], Yutaka Kuroda[2], Shun-ichi Kidokoro[1] ([1]*Dept. of Mate. Sci. and Bio., Nagaoka Univ. of Tech., Japan*, [2]*Dept. of Biotech. and Life Sci., Tokyo Univ. of Agric. and Tech., Japan*, [3]*Dept. of Phys. Chem., Univ. of Granada, Spain*)

The reversible oligomer (RO) formation at high temperature was found in various small globular proteins, and speculated that it would be the precursor of thermal aggregation of proteins such as amyloid fibrils. However, the kinetic effect of RO formation was not investigated, and the rate constant of RO formation was not known yet. Therefore, we performed DSC measurements using PSD95-PDZ3 and analyzed the kinetic effect on RO formation at high temperature. Furthermore, the effects of protein concentration were quantitatively investigated to determine the order of the reaction and the rate constant for RO formation and clarify the mechanism of the RO formation.

1Pos052 変性して小さくなる蛋白質
Antibody proteins can be smaller by denaturation

Hiroshi Imamura[1,2,3], Ayako Ooishi[3], Shinya Honda[3] ([1]*Dept. Bio-sci., Nagahama Inst. Bio-Sci. Tech.*, [2]*Coll. Life Sci., Ritsumeikan Univ.*, [3]*Biomed. Res. Inst., AIST*)

Canonical structures of proteins in their native states have been established using biophysical methods and sequence-structure prediction. In contrast, non-canonical structures of proteins in their denatured states remain under-reported in the literature. Although an intuitive understanding of the denatured structure suggests that denatured proteins are larger than the native protein, which is often illustrated in textbooks, our study challenges this understanding by reporting that antibodies can become smaller upon denaturation. We observed acid-induced compaction of immunoglobulin G antibody proteins using small-angle X-ray scattering. We hypothesize that intramolecular aggregation is widespread in multidomain proteins as non-canonical structures.

1Pos053 タンパク質表面電荷が溶解性に及ぼす影響の格子モデル解析
Lattice-model analysis of protein surface charge distribution on amorphous aggregation and condensation

Yutaka Kuroda, Yuki Matsuzawa, Shin Kohara (*Tokyo University of Agriculture and Technology (TUAT)*)

We describe a Monte Carlo simulation of a lattice model for analyzing the effect of protein surface charge distributions on solubility, amorphous aggregation, and condensation. Protein surface charges were modeled as a cubic particle with each face covered by four equal-area patches having "negative or positive charges". The particle net charge was nil. Inter-particle electrostatic-like interactions were defined between adjoining patches on adjacent particles. No hydrophobic nor Van der Waals-like interactions were included. We observed that the aggregation temperature depends on the surface charge distribution, and in a heterogeneous environment, the mixing of different types of particles affects the colloidal properties of the individual types.

1Pos054 (1SAA-8) GGGGCC-RNA は、TDP43 およびそのカルボキシ断片の凝集を抑制する
(1SAA-8) GGGGCC-RNA prevents aggregation of TDP43 and its carboxy terminal fragments

Ai Fujimoto[1], Masataka Kinjo[2], Akira Kitamura[2] ([1]*Grad. Sch. of Life Sci., Hokkaido. Univ*, [2]*Fac. Adv. Life Sci., Hokkaido. Univ*)

TDP-43 is an abnormally aggregation-prone protein associated with amyotrophic lateral sclerosis (ALS), and its 25 kDa carboxy-terminal fragments (CTFs), TDP25, are highly aggregation-prone. TDP25 aggregation is started by RNA elimination [Kitamura A. *et al.*, ***Sci. Rep.*** 6, 19230 (2016)]. We focus on the GGGGCC repeat sequence (rG4) as an RNA interacting with TDP25 and analyzed the interaction between them using fluorescence cross-correlation spectroscopy (FCCS). rG4 directly interacts with both TDP25 and TDP-43. Furthermore, rG4 expression in Neuro2a cells decreased the aggregates of both TDP25 and TDP-43. However, UG repeat RNA interaction with TDP43 did not inhibit aggregation. These results suggest that rG4 prevents the aggregate formation of ALS-associated TDP-43.

1Pos055 Difference between the Aβ40 and Aβ42 aggregation processes at the atomic level

Satoru G. Itoh[1,2,3], Maho Yagi-Utsumi[1,2,3,4], Koichi Kato[1,2,3,4], Hisashi Okumura[1,2,3] ([1]*IMS*, [2]*ExCELLS*, [3]*SOKENDAI*, [4]*Nagoya City Univ.*)

Amyloid-β peptides (Aβs) tend to form oligomers and amyloid fibrils, which are associated with the Alzheimer's disease. Aβ has two isoforms, Aβ40 and Aβ42, and the difference between these isoforms is only two additional C-terminal residues. However, Aβ42 rapidly forms aggregates. To investigate the difference in aggregation process between Aβ40 and Aβ42, we performed the Hamiltonian replica-permutation molecular dynamics simulations for these Aβs. Thioflavin T fluorescence experiments were also conducted to validate of the computational results. We will discuss the role of the two additional C-terminal residues in the aggregation process.

1Pos056 翻訳アレスト時のポリペプチド鎖を可視化する試み
Attempt to visualize the synthetic polypeptide during translational arrest

Takehito Tanzawa, Takayuki Kato (*IPR., Osaka Univ.*)

Protein synthesis on ribosome is very systematically controlled. Polypeptide chains synthesized at the peptidyl transferase center of the 50S ribosomal subunit during translation elongation passes through the ribosome exit tunnel. When the polypeptide chain is released from the tRNA after translation termination, it is precisely folded via chaperones and finally becomes a functional molecule “protein”. Recent studies have provided indirect experimental evidence suggesting that the polypeptide in the exit tunnel may take on some secondary structures rather than maintaining a complete primary structure. Here, we discuss the structure of polypeptide chain in the exit tunnel by using a translational arrest sequence that temporarily-paused elongation of the nascent chain.

1Pos057 Kinetic mechanisms of amyloid-β-(16–22) fibrillation

Keisuke Ikeda[1], Moe Yamazaki[1], Tomoshi Kameda[2], Hiroyuki Nakao[1], Minoru Nakano[1] ([1]*Fac. Pharm. Sci., Univ. Toyama*, [2]*AIST*)

The kinetic mechanism of amyloid fibril formation by a peptide fragment containing 7 residues of the amyloid-β protein, Aβ-(16–22), was investigated. The N- and C-terminal unprotected Aβ-(16–22), containing no aggregation nuclei, showed rapid fibrillation within seconds to minutes in a neutral aqueous buffer solution. The fibrillation kinetics were well described by the nucleation-elongation model, suggesting that primary nucleation was the rate-limiting step. The aggregated nucleus was estimated to be composed of 6–7 peptide molecules, wherein the two β-sheets were associated with their hydrophobic surfaces. After the formation of thin filaments, the lateral association of the fibers was observed.

1Pos058 アミロイド β ペプチドの凝集に対する NaCl 結晶の過渡的形成の影響
Effect of temporary NaCl crystal on the aggregation of amyloid β peptides

Masafumi Gushiken, Ikuo Kurisaki, Shigenori Tanaka (*Grad. Sch. system infomatics., Univ. Kobe*)

The amyloid β42 peptide (Aβ42) aggregates under certain conditions, and finally they assemble fibril structures. Dimeric to 20-mer aggregates (oligomers) generated during the Aβ42 aggregation process are thought to be the cause of Alzheimer's disease. However, the formation mechanism has been elusive at the molecular level. In this study, we focused on experimental observations that temporary sodium chloride (NaCl) crystal that repeated formation and dissolution locally promotes oligomeric aggregation of Aβ42. Using molecular dynamics simulations, we investigated the aggregation process of Aβ42 by analyzing free energy landscapes of dimer association. We discuss the effect of crystalized and dissolved NaCl on the Aβ42 aggregation in the aqueous system.

1Pos059 リン酸基で修飾したジルコニア粒子を用いた His タグタンパク質の精製
Purification of histidine-tagged proteins using phosphate-modified zirconia particles

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Histidine (His) tags are widely used to facilitate purification of proteins of interest. In this study, we developed a new purification method for His-tagged proteins using phosphate-modified zirconia particles, which have an affinity for His. We tested whether three His-tagged proteins can be purified using the zirconia particles by batch and chromatographic processes. It was found that the zirconia particles enable purification of these proteins under neutral pH conditions by changing the concentration of sodium phosphate in mobile phase. The method using the zirconia particles have the advantage of not requiring elution conditions of low pH or high imidazole concentration. This method will be more effective in purifying His-tagged proteins than conventional ones.

1Pos060 ヘモグロビンの S 字型酸素結合曲線によるカメレオンモデルの協同性の研究
Testing cooperativity of chameleon model by sigmoidal oxygen binding curve of hemoglobin

Itsuki Yoshida, Tomoki P. Terada (*Dept. Appl. Phys., Grad. Sch. Eng., Nagoya Univ.*)

Chameleon model is the coarse-grained model for description of two-state conformational transition of proteins. In the model, the interaction among residues changes depending on the similarity of the local environment around the interacting residues to that in the possible two states. We applied this model to hemoglobin which undergoes conformational transition between T state and R state. By gradually improving the functional form of the model interactions, we have succeeded in reproducing the two-state conformational transition with the strong correlation between the quarternary structure and the local environment around iron ion. We then move on to test whether this model can also reproduce the sigmoidal oxygen binding curve and we will discuss the result.

1Pos061 SARS-CoV-2 3CL プロテアーゼと基質ペプチドの結合解離過程の解析
Binding and unbinding kinetics of peptide substrate on SARS-CoV-2 3CL protease

Kei Moritsugu[1,2], Akinori Kidera[1] ([1]*Grad. Sch. Med. Life Sci., Yokohama City Univ.*, [2]*Grad. Sch. Sci., OMU*)

3C-like protease is one of the potential therapeutic candidates for SARS-CoV-2. Here, we challenged to obtain path ensembles for both the binding and unbinding processes of a flexible peptide substrate on the protease by use of weighted ensemble (WE) simulations. The WE simulations successfully sampled a bundle of bidirectional paths and yielded both the dissociation and association rate constants that were comparable with the experimental values for peptide-mimic compounds. Comprehensive path analyses clarified the atomic detail of the protein-peptide interaction process such as the sequence of the native HB formations and the P1_gln side chain packing that are modulated by the ordering of the peptide internal structure and the desolvation on the peptide interface.

1Pos062 クモ糸タンパク質フィブロインのナノファイバーの単位構造の解明
A Unit Structure of Nanofiber composed of Spider Silk Protein Fibroin

Rakuri Aiba[1], Kento Yonezawa[2], Yusuke Okamoto[1], Haruya Kajimoto[1], Takehiro Sato[3], Yoichi Yamazaki[1], Sachiko Toma-Fukai[1], Hironari Kamikubo[1,2] ([1]*MS.,NAIST*, [2]*CDG., NAIST*, [3]*Spiber Inc.*)

Fibroin protein that forms spider silk is composed of a repetitive region (poly-Ala region) and N- and C- terminal domains. We revealed that a precursor composed of three fibroin molecules forms nanofiber (NF) due to the self-assembly process. When gold nanoparticles (AuNPs) are added to NF composed of N-terminal His-tagged fibroin, the AuNPs are equally spaced on the NF surface. We performed the same analysis on fibroin with different amino acid sequences. It was found that the distance between AuNPs was almost the same in the case of the same molecular weight, even if the spacing of poly-Ala regions was different. These results suggest that fibroins on NF are aligned parallel to the fiber axis and repeatedly bound with a fixed period length.

1Pos063 フィブロインナノファイバーの違いによる延伸乾燥ハイドロゲルの特性の比較
Comparison of Properties of Stretch-Dried Hydrogels with Different Fibroin Nanofibers

Kenta Kimura[1], Kento Yonezawa[1,2], Yuki Nakatani[1], Satoru Onishi[1], Haruya Kajimoto[1], Takehiro Sato[3], Yoichi Yamazaki[1], Sachiko Toma-Fukai[1], Hironari Kamikubo[1,2] ([1]*NAIST ,MS*, [2]*NAIST, CDG*, [3]*Supiber inc*)

We had previously shown that fibroin in spider silk forms nanofibers in a self-assembling manner. Besides, we have shown that the nanofiber bundle structure of spider silk can be reproduced in a dried hydrogel obtained by fixing the ends of the hydrogel and stretching them while dehydrating. XRD analysis showed that Poly-Ala crystals and amyloid-like crystals coexist in the stretch-dried hydrogels. This study prepared stretch-dried fibroin hydrogels with different sequences and compared the structures. Although the nanofiber bundle structures were similar in different sequences, the ratio of those two types of crystals differed. The relation between amino acid sequence, structure, and mechanical properties will be discussed at the annual meeting.

1Pos064 Role of the si-face Tyr of *Bacillus subtilis* ferredoxin-NADPH oxidoreductase in the enzyme-substrate interactions

Daisuke Seo (*Grad. Sch. Nat. Sci. Tec., Kanazawa Univ.*)

In the crystal structure of ferredoxin-NADPH oxidoreductase (FNR) from *Bacillus subtilis*, Tyr50 stacks on the *si*-face of the isoalloxazine ring portion of FAD prosthetic group. To reveal the role of Tyr50 in the formation and redox equivalent transfer of the substrate-FNR complexes, spectroscopic and kinetic details of the Tyr50 variants were studied. Although mixing oxidized FNRs with NADPH resulted in similar properties to those of wild type, mixing reduced Y50G and Y50W FNRs with $NADP^+$ exhibited no significant absorption change, while Y50S provided a CT absorption band. The reduced three variants did not reduce $NADP^+$. Mixing with reduced ferredoxin promoted reduction of the oxidized three variants though the observed rates were differed among the three variants.

1Pos065 SOD1 への基質接近に対する静電ループと Arg143 の役割
Role of electrostatic loop and Arg143 on substrate approach to SOD1

Miu Nakamura[1], Yoshifumi Fukunishi[2], Juha Lintuluoto[3], Masami Lintuluoto[1] ([1]*Grad. Sch. Life and Environ. Sci., Kyoto Pref. Univ.*, [2]*AIST, CMB*, [3]*Grad. Sch. Eng., Kyoto univ.*)

Superoxide dismutase 1 (SOD1) catalyzes the dismutation of the superoxide anion (O_2^-) radical. The electrostatic loop (EL) located above the catalytic site and the Arg143 at the entrance of the catalytic site are supposed to provide electrostatic guidance for the negatively charged substrates. In our previous MD studies, the monomerization and the point mutations induced conformational change around the catalytic site including the EL. Furthermore, the conformational changes around the catalytic site of SOD1 mutants were found to lower the rate of substrate's approach to the catalytic site. In this study, we focused on the investigation of the roles of the EL and Arg143 for the approaching of O_2^- radical to the catalytic site by using MD simulations.

1Pos066 Truncated mutant of the hemolytic lectin CEL-III revealed the interaction between protomer in hemolytic oligomer

Shuichiro Goda[1,2], Keisuke Fukumoto[1], Yuta Yamawaki[1], Hideaki Unno[1], Tomomitsu Hatakeyama[1] ([1]*Grad. Sch. Of Eng., Nagasaki Univ.*, [2]*GaLSIC, Soka Univ.*)

The lectin CEL-III shows the hemolytic activity toward the rabbit red blood cell. This lectin forms heptameric pore on the cell membrane and disrupt it. It consists of three domains. Domains 1 and 2 are carbohydrate binding domain and domain 3 plays an important role in heptamerization. In this study, to elucidate the role of the domain 3 in oligomerization, some lengths of truncation mutants were made. Domain 3 truncated mutant or domain 1 and 2 of CEL-III existed as monomer. On the other hand, lack of transmembrane region of domain 3 showed heptameric form. This result showed that the domain 3 without the transmembrane region plays an important role in oligomerization.

1Pos067 Effect of microtubule-binding proteins on microtubule flexural rigidity

Takuto Nakamichi, Kosuke Matsumura, Keiya Shimamori, Kohei Nishida, Kiyotaka Tokuraku, Masahiro Kuragano (*Grad. Sch. Eng., Muroran Inst. of Tech*)

Microtubule-associated proteins (MAPs) bind to sides of microtubules and regulate microtubule polymerization and depolymerization. We recently have shown that only tau forms straight microtubules by expressing MAP2, MAP4, and tau, in cells. Here we evaluated flexural rigidity of MAP-bound microtubules by analyzing the shape of the teardrop pattern, to compare the effect of these three MAPs. The results showed that the radius of curvature of the teardrop pattern increased in the order of MAP2, MAP4, and tau. This result suggested that the flexural rigidity of tau-bound microtubules is significantly higher than that of MAP2- and MAP4-bound microtubules.

1Pos068 Characterization of fibrous condensations of CAHS proteins from an anhydrobiotic tardigrade

Seiji Nishimura[1], Maho Yagi-Utumi[1,2,3], Kazuhiro Aoki[2,4], Kazuharu Arakawa[2,5], Koichi Kato[1,2,3] ([1]*Graduate School of Pharmaceutical Sciences, Nagoya City University*, [2]*Exploratory Research Center on Life and Living Systems (ExCELLS), National Institutes of Natural Sciences*, [3]*Institute for Molecular Science (IMS), National Institutes of Natural Sciences*, [4]*National Institute for Basic Biology (NIBB), National Institutes of Natural Sciences*, [5]*Institute for Advanced Biosciences, Keio University*)

Tardigrades are unique microscopic animals that enter cryptobiotic states upon desiccation and thereby survive in extreme conditions. We have so far demonstrated that heat-soluble proteins abundant in tardigrade cytosols, called CAHS proteins, self-assemble into fibrous condensates under desiccation-mimicking conditions in a reversible manner. In this study, we characterized the cytosolic proteins that can be encapsulated in the CAHS condensates formed in mammalian cells as model systems and found that each CAHS isoform interacted with distinct proteins. Based on the results, we discuss the molecular strategies of tardigrades to adapt to extreme environments without water.

1Pos069 微小管切断酵素カタニンの活性評価と高速 AFM による可視化
Biochemical characterization and high-speed AFM visualization of AAA ATPase Katanin

Hayato Shibuya[1], Noriyuki Kodera[2], Ikuko Hayashi[1] ([1]*Grad. Sch. of Med. Lif. Sci., Yokohama City Univ.*, [2]*NanoLS., Kanazawa Univ.*)

Katanin is a AAA+ family ATPase that severs microtubules in an ATP-dependent manner. Katanin consists of two subunits: p60 which catalyzes the severing, and a regulatory subunit p80. p60 binds ATP, assembles into a hexamer and hydrolyzes ATP. p60 severs microtubules without p80; however, the molecular mechanism of Katanin's enzymatic activity has yet to be elucidated. In order to gain mechanistic understanding of Katanin, p60 alone or in complex with p80 were expressed in bacteria as an MBP-fusion form and purified to homogeneity. Expressed p60 had an ATPase in the presence of microtubules and its microtubule-severing activities was enhanced together with p80. We further performed high-speed AFM (HS-AFM) analysis to visualize the severing reaction by Katanin.

1Pos070 Target DNA binding dynamics of *Staphylococcus aureus* Cas9 as revealed by high-speed atomic force microscopy

Leonardo Puppulin[1,2], Junichiro Ishikawa[3], Hiroshi Nishimasu[3], Mikihiro Shibata[1,4] ([1]*Nano Life Science Institute (WPI-NanoLSI), Kanazawa University*, [2]*Kyoto Prefectural University of Medicine, Department of Pathology and Cell Regulation*, [3]*Structural Biology Division, Research Center for Advanced Science and Technology, The University of Tokyo*, [4]*Infinity for Frontier Science Initiative, Kanazawa University*)

Programmable DNA binding and cleavage by CRISPR-Cas9 has revolutionized life sciences. The endonuclease Cas9 in complex with an artificial single-guide RNA (Cas9/sgRNA) targets the desired complementary DNA sequence followed by the protospacer-adjacent motif (PAM) for double-stranded cleavage. According to present knowledge, the process of search and binding to target DNA is governed by 3D diffusion of Cas9/sgRNA, random collisions and presumably facilitated by 1D sliding. We show here observations by high-speed atomic force microscopy that reveal unexpected long-range attractive interaction between target DNA and *Staphylococcus aureus* Cas9/sgRNA, which leads to the formation of the ternary complex. The reaction is triggered by PAM proximity, up to a distance of 9 nm.

1Pos071 Analysis of amyloid β aggregation inhibitory activities and cytotoxicity suppressing activities of mushroom extracts from Hokkaido

Tuya Gegen[1], Rina Sasaki[1], Enkhmaa Enkhbat[2], Masahiro Kuragano[1], Keiya Shimamori[1], Yoshiko Suga[2], Yuta Murai[2], Masaki Anetai[2], Kenji Monde[2], Kiyokata Tokuraku[1] ([1]*Division of Sustainable and Environmental Engineering, Muroran Institute of Technology*, [2]*Frontier Research Center for Advanced Material and Life Science, Faculty of Advanced Life Science, Hokkaido University*)

The amyloid cascade hypothesis postulates that Alzheimer's disease (AD) is caused by abnormal accumulation of amyloid β (Aβ) proteins in various areas of the brain. Therefore, it is important to find inhibitors to prevent the aggregation of Aβ. In this study, we evaluated the Aβ aggregation inhibitory activity of 212 mushroom extracts by using a microliter-scale high-throughput screening (MSHTS) system. Then, we evaluated the cytotoxicity suppressing activities of 11 extracts, which showed Aβ aggregation inhibitory activity, by using MTT assay. To isolate the active compounds, highly active mushroom extracts were subjected to solvent partitioning and the Aβ aggregation inhibitory activity and cytotoxicity suppressing activities of each fraction were evaluated.

1Pos072 Escherichia coli inhibited amyloid β aggregation in a concentration-dependent manner

Sohta Katagiri, Na Zhu, Masahiro Kuragano, Kiyotaka Tokuraku (*Grad. Sch. Eng., Muroran Inst. of Tech.*)

Abnormal protein aggregation causes amyloidosis. Since amyloid β (Aβ) aggregation is involved in the development of Alzheimer's disease, it is important to clarify factors which promotes Aβ aggregation. Recently, it was reported that some bacteria promoted Aβ aggregation *in vivo* and *vitro*. Here, we investigated the effects of bacteria on Aβ aggregation using the Microliter-Scale High-Throughput Screening method (Ishigaki *et al*., 2013). Surprisingly, we found that Escherichia coli (E. coli) inhibited Aβ aggregation in a concentration-dependent manner. Further, transmission electron microscopy revealed that Aβ fibrils were localized around E. coli. These results implies that E. coli inhibits the growth of Aβ aggregates by trapping of Aβ fibrils to their surfaces.

1Pos073 機械学習を用いたペプチドの血圧降下活性の予測
Prediction of antihypertensive activity of peptides using machine learning

Kazushi Tamura, Yoshitaka Moriwaki, Tohru Terada, Kentaro Shimizu (*Grad. Sch. Agri. & Life Sci., Univ. Tokyo*)

Antihypertensive peptides (AHTP) are noted as a therapy of high blood pressure with less side effects or less excessive efficacy and have been studied and applied to products. Since it is time-consuming to analyze the effects of AHTPs in experiments, computational prediction methods with higher precision are demanded.
Our research aimed to predict the antihypertensive function of peptides from their amino acid sequences using machine learning methods.
In our research, I extracted some feature values reflecting its sequence pattern or physicochemical features from peptides, then machine learning models including random-forest are trained using the feature values. As a result, our model achieved prediction accuracy higher than the previous works.

1Pos074 回転拡散と並進拡散の解析による凝集性タンパク質の検出
Detection of protein aggregates using rotational and translational diffusion analysis

Riku Ando[1], Johtaro Yamamoto[2,3], Akira Kitamura[3], Nori Nakai[4], Sumio Terada[4], Masataka Kinjo[3] ([1]*Grad. Sch. Life Sci., Hokkaido Univ.*, [2]*Nat. Inst. Adv. Ind. Sci. & Tech.*, [3]*Fac. Adv. Life Sci., Hokkaido Univ.*, [4]*Grad. Sch. Med. & Dent. Sci., Tokyo Med. & Dent. Univ.*)

Toxic protein aggregates are formed in cells during neurodegeneration. However, no method has yet been existed to recognize and detect the initial state of this aggregation. The purpose of our research is to establish a method for analyzing the initial formation process of aggregation using polarization-dependent fluorescence correlation spectroscopy (Pol-FCS), which enables simultaneous measurement of rotational and translational diffusion of fluorescence molecules. To improve the stability of the system and the practicality of the analysis, we improved the detectors and reduced the number of pinholes, making the adjustment easier. The new instrument successfully detects the interaction between antibodies and a low aggregation-prone N-terminal fragment of Huntingtin.

1Pos075 非発光タンパク質の発光酵素反応
Enzymatic luminous reaction of non-bioluminescent proteins

Ryo Nishihara[1,2], Kazuki Niwa[1], Tatsunosuke Tomita[1], Ryoji Kurita[1] ([1]*National Institute of Advanced Industrial Science and Technology (AIST)*, [2]*Japan Science and Technology Agency (JST), PRESTO*)

We report the design, synthesis, and detailed characterization of an imidazopyrazinone-type luciferin, Human Luminophore**1** (HuLumino**1**), with the aim of unmasking the latent luciferase activity of non-luminous proteins. The investigation of reaction behavior of HuLumino**1** for the biological proteins revealed that only human serum albumin (HSA) led to a distinct luminescent enhancement, while other proteins resulted in no emission. HSA levels were quantified within 5% error margins of an enzyme-linked immunosorbent assay without the need for any sample pretreatments because of the high specificity of HuLumino**1**. These results indicate the advantages of the novel platform for protein analysis to detect non-labeled proteins, which generally do not function as enzymes.

1Pos076 (1SBA-4) 3D structural determination of proteins from fluctuation X-ray scattering data

Wenyang Zhao[1], Osamu Miyashita[1], Florence Tama[1,2] ([1]*Center for Computational Science, RIKEN*, [2]*Grad. Sch. Sci., Univ. Nagoya*)

Fluctuation X-ray scattering (FXS) can investigate the nanoscale structure of proteins in near-physiological conditions and consequently help understand protein dynamics. The technique measures thousands of 2D coherent diffraction images of multiple non-crystalized biological particles at random orientations using an X-ray free-electron laser (XFEL). Computation methods are required for reconstructing the 3D structure from the set of 2D images. The present research proposes an efficient reconstruction algorithm based on comparing the double, triple, and quadruple angular correlations of the 2D images. In this report, the computational pipeline is demonstrated and examples with simulated image data are given. Impacts of experimental parameters are also discussed.

1Pos077 残基特異的な熱力学・速度論解析が明らかにするスペクトリン SH3 ドメインの共同性の低いフォールディング
Reduced cooperativity of spectrin SH3 domain folding revealed by combined per-residue thermodynamic and kinetic analysis

Seiichiro Hayashi[1], Daisuke Fujinami[2], Daisuke Kohda[1] ([1]*Med. Inst. Bioreg., Kyushu Univ*, [2]*Grad. Sch. Integr. Pharm. Nutr. Sci., Univ. Shizuoka*)

In our previous NMR research, we found the dispersions of residue-specific equilibrium constants (K) and rate constants (k) of the two-state exchange of an antimicrobial peptide, nukacin ISK-1. This implies reduced cooperativity. Interestingly, we discovered a linear relationship in the log k vs. log K plots. We consider that the residue-based linear relationship is the physicochemical basis for the smooth conformational changes and provides useful insights into the transient states. However, some may argue that nukacin is a post-translationally modified polypeptide. We conducted the same experiments with an SH3 domain and found that the reduced cooperativity and the residue-based linear relationship were both valid in the case of a simple protein.

1Pos078 残基特異的 QFER（自由エネルギー 2 次関係）はスムーズな蛋白質折れ畳みを実現するコンシステンシー原理の数学的表現である
Residue-based Quadratic Free Energy Relationship is a Mathematical Formulation of the Consistency Principle of Protein Folding

Daisuke Kohda[1], Seiichiro Hayashi[1], Daisuke Fujinami[2] ([1]*Med. Inst. Bioreg., Kyushu Univ.*, [2]*Grad. Sch. Integr. Pharm. Nutr. Sci., Univ. Shizuoka*)

The consistency principle (Go model) represents a physicochemical condition requisite for ideal protein folding, but no experimental evidence has been presented. We used NMR to determine the residue-specific equilibrium constant K and rate constant k of the two-state exchange of a bioactive peptide and found a linear log k vs. log K relationship (J Phys Chem Lett 12:10551, 2021). We examined the theoretical framework under a basic equation, $\rho = 0.5(\phi+\phi')$, where ρ is the slope between two residues, and ϕ is the fraction of the native state in the transient state. We found that the alignment of data points on a parabolic curve is necessary and sufficient. The quadratic free energy relationship (QFER) enables us to devise a new ϕ analysis without mutations.

1Pos079 自由エネルギー摂動法を用いた VHH フレームワーク部位のアミノ酸配列最適化
In silico optimization of VHH framework sequence using free energy perturbation method

Kazuma Okada, Yasuhiro Matsunaga (*Grad. Sch. Sci. Eng., Saitama Univ.*)

Single domain antibodies, VHHs or nanobodies, are the smallest fragments that still have similar binding capacities to the conventional antibodies, attracting recent attention for new drug developments. For the use VHHs as drugs, it is crucial to design the structure of VHH stable even at relatively high temperatures. In this study, we apply the free energy perturbation method to examine the change in thermal stability of VHH structure caused by various mutations. By scanning the framework region of VHH by alanines and isoleucines, we have found several mutation candidates for stabilizing VHH structures. These mutations are further verified with long-time molecular dynamics simulations.

1Pos080 新型コロナウイルス並びにインフルエンザウイルス A 型を検出するチオ NAD サイクリング ELISA 法の開発
Development of Thio-NAD Cycling ELISA for Detection of SARS-CoV-2 and Influenza Virus Type A

Yuta Kyosei[1], Sou Yamura[1], Mayuri Namba[1], Etsuro Ito[1,2] ([1]*Department of Biology, Waseda University*, [2]*Waseda Research Institute for Science and Engineering, Waseda University*)

We developed a thio-NAD cycling ELISA for the detection of new type of coronavirus (SARS-CoV-2) and influenza virus type A (FluA). We noted proteins, but not nucleic acids, and attempted to measure the inactivated forms of viruses with ultra-sensitivity. The LOD of SARS-CoV-2 and that of FluA were 10^6 copies/100 µL and 3 pfu/mL, respectively, whose detection sensitivity competed with those of PCR.

1Pos081 gr Predictor：深層学習を活用したタンパク質水和分布の高速計算法
gr Predictor : An Efficient Method for Computing the Hydration Structure around Proteins using Deep Learning

Kosuke Kawama[1], Yusaku Fukushima[1], Mitsunori Ikeguchi[2,3], Masateru Ohta[3], **Takashi Yoshidome[1]** ([1]*Dep. of Appl. Phys., Tohoku Univ.*, [2]*Grad. Sch. of Med. Life Sci., Yokohama City Univ.*, [3]*RIKEN*)

Among the factors affecting biological processes such as protein folding and ligand binding, hydration, which is represented by a three-dimensional water-site-distribution-function around the protein, is crucial. However, the high computation costs of the typical methods to obtain the distribution functions, namely molecular dynamics simulations and 3D-RISM theory, hinder their applications to a large number of proteins. Here we propose a deep-learning model resolving this issue. Our model allows to successfully reproduce the hydration structures around proteins, and to reduce the computational time to a few tens of seconds. In the presentation, the performance of our program “gr Predictor” (https://github.com/YoshidomeGroup-Hydration/gr-predictor) is discussed.

1Pos082 タンパク質の局所構造の形状操作性に関するロボット工学的解析手法
Robotics-Based Method for Analyzing Shape Manipulability of Localized Protein Structures

Keisuke Arikawa (*Fcl. Eng., Kanagawa Inst. of Tech.*)

Deformations of localized protein structures are approximately determined by the changes in dihedral angles around the bond axes. By regarding the dihedral angles as joint angles of robotic mechanisms, we can assume that the structures can control their own shapes. Based on the manipulability analysis used to evaluate the controllability of robotic mechanisms, we have formulated a method to evaluate structural shape-changing ability (shape manipulability). Using the proposed method, we can obtain information about shapes that are easier or harder to realize based on the changes in dihedral angles. To understand the application of this method, we analyzed the shape manipulability of various types of localized protein structures using data from the Protein Data Bank.

1Pos083 マルチチェイン/マルチドメインタンパク質の構造変化の解析法について
A method for analyzing structural changes of protein with multi-chains/multi-domains

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Recent advances in the field of structural biology have revealed the structures of multi-domains and multi-chains proteins under various physiological conditions. In addition, advances in computer and algorithms, such as supercomputers, enable to perform simulations of such proteins over longer time. In analyzing such large data, it is still difficult to extract correlated motions of different domains. We propose an analysis method that uses the geometric average of domains to extract important structural changes. We apply this method to the cryo-EM structures of the S-protein of COVID-19 and those from gREST simulations to identify important structure changes.

1Pos084 Cryo-CLEM 法および Cryo-ET 法による糸状仮足先端の三次元構造観察
Observation of three dimensional structure of filopodial tips by Cryo-CLEM and Cryo-ET methods

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Cells move using filopodia as an antenna. We observed two types of the filopodial structure during cellar movement; one is a “Round structure” with a rounded tip, while the other is a “Sharp structure” formed up by F-actin bundles to the pointed end. We have investigated dynamical changes in conformation by Cryo-CLEM methods. Still, it is challenging to seemingly take photos of regions of interesting filopodial tips before photoing by Cryo-EM. We improved Cryo-CLEM and Cryo-ET observations using grids attaching two different sizes and fluorescent beads. We will present our trial observations and the problems that have emerged during their process.

1Pos085 タイムタグ光子測定方式によるナノ秒蛍光相関分光測定システムの開発
Development of the time-tag photon detection method of nanosecond fluorescence correlation spectroscopy

Yutaka Sano[1,2], Hiroyuki Oikawa[1,2], Satoshi Takahashi[1,2] ([1]*Institute of Multidisciplinary Research for Advanced Materials, Tohoku University*, [2]*Department of Chemistry, Graduate School of Science, Tohoku University*)

Nanosecond fluorescence correlation (ns-FCS) spectroscopy has been extensively used to detect ultrafast dynamics of proteins and other macromolecules labeled with donor and acceptor fluorophores, whose fluorescence intensities are modulated by the FRET mechanism. The conventional method of ns-FCS is based on the start-stop protocol and requires an extensive data accumulation time.
In this study, we used hybrid photodetector connected to highspeed digital counter, and detected all the donor and acceptor photons in the time-tag mode, enabling us to obtain fluorescence auto and cross-correlation curves in the time domain down to 50 ns simultaneously. The data accumulation time was reduced to about 1 hour.

1Pos086 生細胞中の細胞質タンパク質 CRAF の二量体化状態および構造状態遷移に関する詳細解析
Detailed analyses of dimerization state and conformational state transitions of cytoplasmic protein CRAF in live cells

Kenji Okamoto, Yasushi Sako (*RIKEN CPR*)

We have developed alternating laser excitation (ALEX) system to investigate behavior of cytosolic protein CRAF in live cells by detecting Förster resonance energy transfer (FRET) from single molecules, and found coexistence of two distinct closed conformations. But, fluorescence bursts, which are detected as signals in ALEX measurement, must contain richer information about the molecule state of the target protein. So, we introduced more detailed analyses to gain deeper insights into intracellular CRAFs. Dimerization state is analyzed based on the burst intensity distribution. Transitions between different structural states are detected by photon-by-photon hidden Markov model. The results suggest dynamic transitions between two closed conformations.

1Pos087 ラマン分光法を用いたタンパク質相分離液滴の濃度と熱力学的性質の検討
Investigation of concentration changes and thermodynamic properties of a single phase-separated protein droplet using Raman microscopy

Kohei Yokosawa[1], Shinji Kajimoto[1,2], Takakazu Nakabayashi[1] ([1]*Grad. Sch. Pharm. Sci., Tohoku Univ.*, [2]*JST PRESTO*)

Liquid-liquid phase separation (LLPS) of protein solutions has been widely studied in biology. LLPS results in the formation of small protein-rich droplets that are involved in many biological reactions. However, the properties of droplets formed via LLPS are still unclear. Thus both label-free and in situ techniques are needed to measure the droplets. We developed a label-free measurement method using Raman microscopy, and detected changes in protein concentration in a single droplet with varying parameters such as pH and temperature. We found that the concentration in the droplet decreased with solution conditions that were less prone to LLPS. We also analyzed the concentrations using Flory-Huggins theory to investigate the thermodynamic properties of the droplet.

1Pos088 Algorithm and Neural Network-Based Design, and Experimental Evaluations of Antimicrobial Peptides

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Antimicrobial peptides (AMPs) have drawn great attentions as candidates of novel antimicrobial agents. We applied an algorithmic data-mining method to extract common properties of broad-spectrum effective AMPs from peptide databases, and applied a neural network-based approach for AMP design. The designed AMPs were chemically solid-phase synthesized for experimental investigations. The peptide structures were validated with circular dichroism spectroscopy. The bactericidal effects, mammalian cell viability, and hemolysis of peptides were examined experimentally. Detailed bactericidal mechanism of peptides was analyzed with atomic force microscopy. With this platform, we have obtained several AMPs effective against both Gram-positive and -negative pathogenic bacteria.

1Pos089 Generation of microtubule superstructures by mimicking ciliary microtubule structures

Muneyoshi Ichikawa[1], Hiroshi Inaba[2], Yurina Sueki[2], Arif Md. Rashedul Kabir[3], Takashi Iwasaki[4], Hideki Shigematsu[5], Akira Kakugo[3], Kazuki Sada[3], Tomoya Tsukazaki[1], Kazunori Matsuura[2] ([1]*Div. of Biol. Sci., NAIST*, [2]*Grad. Sch. of Eng., Tottori Univ.*, [3]*Grad. Sch. of Chem. Sci. and Eng., Hokkaido Univ.*, [4]*Grad. Sch. of Agric. Sci., Tottori Univ.*, [5]*Struct. Biol. Div., Jap. Synchrot. Radiat. Res. Instit.*)

Microtubules are hollow cylinder-like cytoskeleton composed of tubulins. In vitro reconstituted microtubules are singlets which exhibit dynamic instability. In contrast, microtubules of cilia are stable and exhibit unique structures, such as doublets and branches. These features are mediated by microtubule inner proteins (MIPs). By mimicking the ciliary microtubule structure, stable microtubules or diverse microtubule structures should be formed. Here, we developed a method to encapsulate a tetrameric protein Azami-green (AG) inside the microtubules by adding Tau-peptide (TP) sequence. This TP-AG was shown to enhance microtubule polymerization, stabilize microtubule structures, and induce formation of microtubule superstructures, such as doublets and branches.

1Pos090 ウシ由来抗菌ペプチド BMAPs の大量発現系構築および機能・構造解析
Construction of an overexpression system and functional and structural analysis of bovine antimicrobial peptides BMAPs

Fumi Hirai[1], Mitsuki Shibagaki[2], Kotaro Tsukioka[1], Hao Gu[2], Tomoyasu Aizawa[1,2] ([1]*Sch. Sci., Hokkaido Univ.*, [2]*Grad. Sch. Life Sci., Hokkaido Univ.*)

While some mammals have only one type of cathelicidin, a member of the representative antimicrobial peptide (AMPs) family, bovines have seven. Bovine Myeloid Antimicrobial Peptides (BMAPs) are a family of bovine cathelicidin, and there are three types of BMAP-27, -28, and -34. BMAPs are known to have a broad antibacterial spectrum, but their detailed mechanisms of action are still unknown. To investigate the effect of structure on activity, it is important to elucidate the three-dimensional structure by NMR analysis. Recombinant expression is an effective method to obtain isotopically labeled peptides for NMR structural analysis. In this study, we constructed a novel fusion expression system using calmodulin as a carrier protein and overexpressed BMAPs.

1Pos091 ヘリックス–ループ–ヘリックスモチーフのヘリックス–ヘリックス角に着目したタンパク質複合体構造の計算機デザイン
Computational design of protein complexes focusing on the helix–helix angle of the helix-loop-helix motif

Marino Yamamoto, Naoya Kobayashi, Shun Hirota (*NAIST, Mat. Sci.*)

This study aimed to develop a simple method for constructing protein complexes with various association numbers from different monomeric proteins. The computational design of domain-swapped structures focusing on secondary structural motifs was performed. First, we roughly modeled designable oligomeric backbone placements based on the helix-helix angles of the helix-loop-helix motifs for all-α proteins, and de novo generated helical linkers linking between domains using Foldit Standalone. Next, we designed amino acid sequences to stabilize the modeled structures using Rosetta. The 3D structure prediction of the designed amino acid sequences using ColabFold showed desired structures.

1Pos092 機械学習を組み合わせたファージ提示法による抗体断片の指向性進化
Machine-learning application for in vitro selection of antibody fragments from a phage display library

Sakiya Kawada[1], Yoichi Kurumida[2], Tomoyuki Ito[1], Thuy Duong Nguyen[2], Hikaru Nakazawa[1], Hafumi Nishi[3,4,5], Yutaka Saito[2,6,7,8], Tomoshi Kameda[2,8], Koji Tsuda[7,8,9], Mitsuo Umetsu[1,8] ([1]*Grad. Sch. Eng., Tohoku Univ.*, [2]*AIRC, AIST*, [3]*Grad. Sch. Information Sci., Tohoku Univ.*, [4]*ToMMo, Tohoku Univ.*, [5]*Fac. Core Res., Ochanomizu Univ.*, [6]*CBBD-OIL, AIST-Waseda Univ.*, [7]*Grad. Sch. Frontier Sci., The Univ. of Tokyo*, [8]*Adv. Intell. Pro., RIKEN*, [9]*MaDIS, NIMS*)

Directed evolution has been utilized for improving or generating functional proteins. In the library approach of directed evolution, a variant library is prepared and desirable variants are selected from the library. However, in many cases, the number of the variants which theoretically appear in the designed library is much larger than that in the prepared library, and the size of screening is too small to analyze all the variants in the prepared library; so that functional variants are not always found in the screening process. In this study, we applied machine learning and next-generation sequencing technology to the library approach of directed evolution. We show the possibility that machine learning propose functional variants which are not experimentally found.

1Pos093 ファージ提示ライブラリーを用いた進化分子工学操作への機械学習利用による抗体様分子開発
Machine-learning-assisted molecular evolution with a phage display library of antibody mimetics

Tomoyuki Ito[1], Thuy Duong Nguyen[2], Yutaka Saito[2,3,4,5], Yoichi Kurumida[2], Hikaru Nakazawa[1], Sakiya Kawada[1], Hafumi Nishi[6,7,8], Koji Tsuda[4,5,9], Tomoshi Kameda[2,5], Mitsuo Umetsu[1,5] ([1]*Grad. Sch. Eng., Tohoku Univ.*, [2]*AIRC, AIST*, [3]*CBBD-OIL, AIST-Waseda Univ.*, [4]*Grad. Sch. Frontier Sci., The Univ. of Tokyo*, [5]*Adv. Intell. Pro., RIKEN*, [6]*Grad. Sch. Information Sci., Tohoku Univ.*, [7]*ToMMo, Tohoku Univ.*, [8]*Fac. Core Res., Ochanomizu Univ.*, [9]*MaDIS, NIMS*)

Molecular evolution with a variant library is used to obtain a molecular recognition protein. In the study on antibody mimetics, a scaffold protein is functionalized by means of molecular evolution. Recently, machine learning has been combined with directed molecular evolution to obtain variants with higher target-affinity than the experimentally selected variants. In this study, for the creation of antibody mimetics, we trained machine learning model with deep sequencing data, which supplies a large number of sequences with antigen-binding properties. Our machine learning approach led to the discovery of improved variants with target-specific affinity and showed its potential for designing a refined library with functional variants.

1Pos094 抗菌ペプチドαディフェンシンの高濃度変性剤存在下における野生型ジスルフィド結合形成機構の解析
Mechanism of correct disulfide bonds formation of α-defensins in the presence of high concentrations of denaturing agents

Shinya Yoshino, Hiromichi Taguchi, Yi Wang, Yuchi Song, Weiming Geng, Shaonan Yan, Tomoyasu Aizawa (*Grad. Sch. Life Sci., Hokkaido Univ.*)

In general, when proteins that form disulfide bonds are obtained in recombinant form, refolding operations are often required. The recombinant proteins and peptides obtained in inclusion bodies are considered to have random coils when solubilized with denaturing agents such as high concentrations of urea. However, cryptdin4 (crp4), a type of antimicrobial peptide, α-defensin from mouse, obtained in the inclusion body in recombinant expression in *E. coli* efficiently forms natural-type disulfide bonds under high urea concentration conditions. This phenomenon is very intriguing, and the detailed mechanism was unclear. Therefore, we investigated the mechanism by which disulfide bonds were formed when crp4 was refolded.

1Pos095 PD-1 アゴニスト開発に向けた PD-1 結合タンパク質の合理的設計
Rational design of PD-1 binding proteins to develop PD-1 agonists

Hirotaro Shimamura[1], Shunji Suetaka[2], Nao Sato[2], Yuuki Hayashi[2,3], Munehito Arai[1,2] ([1]*Dept. Phys., Univ. Tokyo*, [2]*Dept. Life Sci., Univ Tokyo*, [3]*Environmental Science Center, Univ. Tokyo*)

Programmed cell death protein 1 (PD-1) on the surface of T cells inhibits excessive T cell inflammatory activity by binding to programmed death ligand 1 (PD-L1) expressed on antigen-presenting cells. However, reduced PD-1 function can cause abnormally activated T cells to damage normal cells, leading to autoimmune disorders. To prevent the T-cell activation by turning on the immune checkpoint, we rationally designed PD-1 agonists that tightly bind the PD-L1 binding site of PD-1. We performed in silico saturation mutagenesis on the fragment of human PD-L1 and selected the mutants that are predicted to have high affinity with PD-1. Experimental verification showed that we have successfully designed the PD-1 binders with higher affinity than the wild-type PD-L1.

1Pos096 Analysis of receptor signaling using growth factor mutants designed by an in silico approach

Yuga Okada[1], Akihiro Eguchi[2], Daisuke Kuroda[3], Kohei Tsumoto[1], Ryosuke Ueki[1], Shinsuke Sando[1] ([1]*Grad. Sch. Eng., Univ. Tokyo*, [2]*Faculty of Health and Medical Sciences, University of Copenhagen.*, [3]*National Institute of Infectious Diseases, Ministry of Health, Labour, and Welfare.*)

Receptor tyrosine kinases (RTKs) are activated through the dimerization induced by growth factors (GFs) and mediate the signal transduction with multifaceted effects. The cell signaling has been attracting attention because of its implication in tumorigenesis and tissue regeneration. Thus, it is important to understand the molecular basis of the signaling mechanism behind RTK dimerization. Some GFs are known to activate their receptors with the help of heparan sulfate (HS). The role of HS in the receptor signaling has been investigated in several studies, but has not been fully understood. In this presentation, *in silico*-guided design of GF mutants with desired properties will be described. Also, the activity of these mutants on the receptor signaling will be discussed.

1Pos097 NMR 解析に向けたマウス由来抗菌ペプチド cathelicidin, CRAMP(cathelicidin related anti-microbial peptide)の大腸菌を用いた大量発現系構築
Construction of an overexpression system of mouse-derived antimicrobial peptide cathelicidin, CRAMP in *E. coli* for NMR analysis

Kotaro Tsukioka[1], Waka Ueda[1], Humi Hirai[1], Mitsuki Shibagaki[2], Hao Gu[2], Tomoyasu Aizawa[3] ([1]*Sch.Sci.,Hokkaido Univ.*, [2]*Grad. Sch. Life Sci., Hokkaido Univ.*, [3]*Fac. Adv. Life Sci., Hokkaido Univ.*)

Cathelicidin is a typical antimicrobial peptide, and mouse-derived cathelicidin CRAMP (cathelicidin related anti-microbial peptide) is known to exhibit a wide range of antimicrobial activity. Recent studies have suggested that CRAMP induces autoimmune diseases and activation of tumor cells, and its aspect as an immunomodulatory peptide has begun to attract attention. Although NMR analysis is useful for further understanding of the detailed molecular mechanisms of immunomodulation, NMR analysis using recombinant stable isotope-labeled peptides has not yet been reported. Therefore, in this study, we overexpressed CRAMP by both the calmodulin fusion expression system and the thioredoxin fusion expression system for NMR analysis.

1Pos098 ナノディスクに再構成した鉄還元膜タンパク質 CYB561D2 によって誘起される脂質過酸化の解析
Analysis of lipid peroxidation induced by iron-reducing membrane heme protein; CYB561D2 in nanodiscs

Aoi Yamaguchi, Motonari Tsubaki, Tetsunari Kimura (*Dept. of Chem., Grad Sch. of Sci., Kobe Univ.*)

CYB561D2 is a transmembrane reductase in ER membrane, which reduces the iron by the electron transfer (ET) from ascorbic acids (AAs). These reduced irons (Fe^{2+}) have been suggested to react with oxygen molecules, inducing the peroxidization of unsaturated fatty acids to trigger the cell death called "Ferroptosis." However, the experimental evidences that the Fe^{2+} produced by the ET from AAs through CYB561D2 causes lipid peroxidation, are limited. In this study, purified CYB561D2 were reconstituted into nanodiscs (CYB561D2-nd) containing unsaturated fatty acids. The iron reduction activity of reduced CYB561D2-nd was confirmed by the oxidation of heme and the formation of Fe^{2+}. The molecular mechanism of ferroptosis will be discussed based on mass spectrometry.

1Pos099 プロテオリポソーム中における Higd1A によるシトクロム *c* 酸化酵素の活性増強機構
The positive regulation mechanism of cytochrome *c* oxidase by Higd1A in proteoliposome

Wataru Sato[1], Sachiko Yanagisawa[1], Kyoko Shinzawa-Itoh[1], Yuya Nishida[2], Takemasa Nagao[2], Yasunori Shintani[2], Minoru Kubo[1] ([1]*Grad. Sch. Sci., Univ. Hyogo*, [2]*Mol. Pharmacol., NCVC*)

In respiratory chain, cytochrome *c* oxidase (C*c*O) performs proton pumping across the mitochondrial inner membrane through coupling with reduction of dioxygen to water. Recent studies have identified “Higd1A” as the positive regulator of C*c*O, but the physical mechanism how Higd1A contributes to the reactions, dioxygen reduction and proton pump, remains unclear. Here, we explored the effects of Higd1A on the multiple reactions in C*c*O by using liposome-reconstituted Higd1A-C*c*O complex. Various kinetic analyses suggested that Higd1A caused an increase in the proton pump rate, with the dioxygen reduction activity. In the presentation, the effects of Higd1A on the coupled reactions of C*c*O will be discussed in terms of the H^+/e^- ratio.

1Pos100 酸素バリア性フィルムを利用した嫌気下での構造解析の試み
Attempt to structural analysis under anaerobic condition using oxygen barrier film

Takehiko Tosha[1], Kanji Shimba[2], Hiroaki Matsuura[1], Kunio Hirata[1], Masaki Yamamoto[1], Yoshitsugu Shiro[2] ([1]*RIKEN SPring-8*, [2]*University of Hyogo*)

Membrane-integrated nitric oxide reductase (NOR) catalyzes the reduction of NO to nitrous oxide at a heme/non-heme iron binuclear center. The catalytic mechanism of NOR is still in debate due to the lack of the structural information on the reaction intermediates. Here, we aimed to develop the system for X-ray diffraction experiment under anaerobic condition, since anaerobic condition is required for the observation of the NOR reaction by time-resolved technique. Using an oxygen barrier film as a crystallization plate, we obtained the crystals of NOR. X-ray data collection with the film plate allowed us to determine the structure of NOR without its exposure to oxygen. Thus, this approach is promising for X-ray crystallography under anaerobic condition.

1Pos101 LoCoMock: Log*P* によって補正されたスコアによるタンパク質-リガンド-膜複合体のドッキングシミュレーション
LoCoMock: Log*P*-corrected Membrane Docking Score Screens Protein-Ligand-Membrane Complexes

Rikuri Morita, Yasuteru Shigeta, Ryuhei Harada (*CCS, Univ. Tsukuba*)

Membrane proteins have attracted attention as targets for drug discovery. To understand the function of membrane proteins, it is quite important to screen the binding modes between membrane proteins and amphiphilic molecules. Here, docking simulations screen protein-ligand complexes with low computational costs. However, it is generally difficult to find docking sites for a given ligand in a non-water environment such as a lipid bilayer. To screen for protein-ligand complexes embedded in the membrane, we proposed a new docking score called the log*P*-corrected membrane docking (LoCoMock) score and performed demonstrations using a variety of model ligands. Toward drug discovery, the LoCoMock score has the potential to propose reasonable protein-ligand-membrane complexes.

1Pos102 γ 切断酵素と APP/Notch のドッキング過程の粗視可モデルシミュレーション研究
Coarse-grained model Simulation study of the docking process of γ-secretase and APP/Notch

Chika Minami, Lisa Matsukura, Naoyuki Miyashita (*Grad. Sch. BOST, KINDAI Univ.*)

In the early stage of Alzheimer's disease, amyloid precursor protein (APP) is cleaved by β- and γ- secretases. γ-secretase also cleaved the signal transduction-mediating membrane protein Notch. If the differences between the cleavings of APP and Notch by γ-secretase, it is helpful to clarify the mechanism of the γ-secretase cleavage of the membrane proteins. To investigate the cleavage process, we performed coarse-grained molecular dynamics simulations of γ-secretase, γ-secretase and APP/Notch complex, and γ-secretase with APP/Notch. Our results suggested that the TM2 and TM3 helices help to bind the APP/Notch to the active site, and the cholesterols also support the γ-secretase and APP/Notch docking.

1Pos103 遺伝子変異が引き起こす EGFR 動態変化の 1 分子解析
Single-molecule analysis of mutation induced changes in EGF receptor behavior

Michio Hiroshima[1,2], Masahiro Ueda[1,3] ([1]*RIKEN BDR*, [2]*RIKEN CPR*, [3]*FBS, Osaka Univ.*)

Cell membrane receptors transduce signals from outside to inside cells, triggering cellular signaling to induce appropriate cell responses. During the process, epidermal growth factor receptor (EGFR) is phosphorylated in the dimer and activates downstream signaling through clustering, concurrent with changes in the receptor structure, mobility, and location. EGFR mutants relate serious diseases including cancers, however, it remains ambiguous how the EGFR behavior is affected by the mutations. By applying our developed methods, large-scale single-molecule imaging and machine learning-based molecular state analysis, specific characteristics in the EGFR behavior could be extracted for each structural/cancerous mutant and will contribute to EGFR targeted drug discovery.

1Pos104 1 分子イメージングを用いた薬剤スクリーニング
Drug screening platform using single molecule imaging

Daisuke Watanabe[1,2], Michio Hiroshima[2], Masahiro Ueda[1,2] ([1]*FBS Osaka Univ*, [2]*RIKEN BDR*)

Epidermal growth factor receptor (EGFR) plays an important role in cell responses such as proliferation and cell migration. Mutations in EGFR are known to cause various cancers (e.g. non-small cell lung cancer), and EGFR mutants with acquired drug resistance by secondary mutations are current targets for drug discovery. EGFR has been revealed to regulate cell signaling through changes in its mobility and multimer formation by single-molecule imaging, which enables direct visualization of molecules in living cells. A novel drug screening referring changes in the behavioral dynamics of molecules by applying single-molecule imaging was proposed but has not been demonstrated. In this study, we tried to validate the accuracy of the method and perform the screening.

1Pos105 計算科学的に明らかにするホモ二量体チロシル tRNA 合成酵素（TyrRS）のハーフサイト活性
A Computational Study on the Half-Site Activity Mechanism of Homodimeric Tyrosyl tRNA Synthetase（TyrRS）

Yoshino Okamoto[1], Takunori Yasuda[2], Rikuri Morita[3], Yasuteru Shigeta[3], Ryuhei Harada[3] ([1]*College of biological sciences, University of Tsukuba*, [2]*Doctoral program in biology, University of Tsukuba*, [3]*Center for computational Sciences*)

Aminoacyl-tRNA synthetase (aaRS) is an enzyme with an ability to discriminate both tRNA and amino acids, and it promotes the binding of amino acids to tRNA. As a typical aaRS, tyrosyl tRNA synthetase (TyrRS) acts as a homodimer with two binding sites for tyrosines. However, as a monomeric activity, biochemical experiments have reported that TyrRS promotes one of the tyrosines at their binding sites. Therefore, it remains unknown why the homodimeric TyrRS shows the half-site activity. To elucidate the mechanism of the monomeric activity, we performed molecular dynamics (MD) simulations on TyrRS under tyrosine-binding/unbinding conditions. By analyzing the MD trajectories, we discovered that the TyrRS dynamics were different depending on the binding conditions.

1Pos106 Elucidation of nucleosome sliding mechanism in all-atom detail via MD simulations

Syed Hashim Shah, Giovanni Bruno Brandani, Shoji Takada (*Department of Biophysics, Graduate school of science, Kyoto University, Kyoto*)

Nucleosome sliding is an important process for chromatin remodeling and essential to modulating gene expression. Twist defects have been proposed as a basic mechanism underlying spontaneous sliding and active remodeling based on theoretical and experimental evidence. However, the molecular mechanisms and energetics of twist defect formation and propagation are still unclear. In order to better understand this process, we employ the mean force string method to determine the most likely sliding pathway in all-atom detail and the free energy landscape of the process.

1Pos107 PPRP の RNA からの解離機構のシミュレーション研究
Simulation study of the dissociation mechanism of the PPRP with RNA

Sumile Tanaka[1], Lisa Matsukura[1], Masaki Ottawa[2], Naoyuki Miyashita[1] ([1]*Grad. Sch. BOST., KINDAI Univ.*, [2]*Sch. Phys. Sci., GUAS*)

Pentatricopeptide repeat protein (PPRP) is a nucleic acid-binding protein common in a chloroplast or mitochondria. The PPRP consists of PPR repeats, and each PPR repeat corresponds to the specific bases in RNA. Recently, it has been reported that the PPRP can be artificially modeled by the PPR repeat corresponding to each base. To find the specific binding site, the RPPR often binds to the mismatch sequence temporarily. However, it has not been known about the dissociation mechanism of PPRP with RNA. Thus, we performed the molecular dynamics simulations of Wild-type PPRP with RNA and two mutant PPRPs with RNA to clarify the mechanism. Our results show that the mismatch sequence decreases the interaction between phosphate in RNA and Lys13 in PPR repeat.

1Pos108 部分的にアンラップされたヌクレオソームからの、Nap1 による H2A/H2B 解離メカニズム
Nap1 dismantles a H2A/H2B dimer from a partially unwrapped nucleosome

Fritz Nagae, Shoji Takada, Tsuyoshi Terakawa (*Grad. Sch. Sci., Kyoto Univ.*)

On eukaryotic chromatin, RNA polymerases, replicative helicases, and exonucleases inevitably collide with nucleosomes. Previous studies have shown that histone chaperones play roles in nucleosome processing upon the collision. However, its molecular mechanism remains unclear. In this study, we performed in vitro transcription assays in the presence of a histone chaperone, Nap1, and molecular dynamics simulations, revealing that Nap1 binds to and dismantles an H2A/H2B dimer from a partially unwrapped nucleosome. These results showed that the highly acidic C-terminal flexible tails of Nap1 contribute to binding to an H2A/H2B dimer. This finding may improve the molecular understanding of DNA transactions on chromatin.

1Pos109 Simulation for the phase separation of DNA droplet with chemical reactions

Ryohei Furuichi[1], Tomoya Maruyama[2], Akihiro Yamamoto[1], Masahiro Takinoue[1,2] ([1]*School of Computing, Tokyo Institute of Technology*, [2]*School of Life Science and Technology, Tokyo Institute of Technology*)

The liquid-liquid phase separation phenomenon of DNA droplets has potential for use in artificial cells and droplet control. However, the phase separation phenomenon has not been well controlled. In this study, we developed a simulation focusing on the phase separation phenomena with chemical reactions.
Enzymatic reactions were simulated by implementing actual enzyme molecules or by introducing a method to cause reactions based on reaction rates.
This simulation was used to simulate the effect of the rate of the enzymatic reaction on the control of liquid-liquid phase separation. As a result, we found that when the reaction was divided into two stages, the time delay was effective in controlling the liquid-liquid phase separation.

1Pos110 ヌクレオソーム上を動く酵母 RNApolymerase Ⅱの粗子化 MD シミュレーション
Coarse-grained MD simulations of an elongation process of yeast RNA Pol2 moving toward a nucleosome

Takafumi Yamauchi, Genki Shino, Shoji Takada (*Kyoto University*)

In eukaryotes, nucleosomes play an important role in compactly storing DNA in the cell nucleus, but they also act as obstacles to proteins moving on DNA. Among such proteins, RNA polymerase, which transcribes mRNA, has been found to have the ability to overcome such obstacles. Recent cryo-EM studies elucidated several snapsots in that process. In this study, we perform coarse-grained MD simulations of an elongation process of yeast RNA Pol2 moving toward a nucleosome to investigate dynamic motions in the process. We setup simulations in which Pol2 moves along the DNA one by one base-pair invading into the nucleosome.

1Pos111 Mg イオンによるリボザイムのフォールディングとミスフォールディング機構
Mg-induced folding and misfolding of ribozymes

Naoto Hori[1], D Thirumalai[2] ([1]*School of Pharmacy, University of Nottingham*, [2]*Department of Chemistry, University of Texas at Austin*)

Functional RNA molecules need to be folded into specific tertiary structures, in which divalent cations play critical roles. We studied the effects of Mg^{2+} ions on RNA folding using coarse-grained simulations. From equilibrium simulations of the 16S rRNA central domain, we found that Mg^{2+} bindings to specific positions are coupled with folding of individual structural elements at distinct bulk [Mg^{2+}], although the global transition is cooperative. We also conducted ion-jump kinetics simulations of an intron ribozyme and obtained multi-step folding and misfolding trajectories. Our data shows how Mg^{2+} associations, conjugated with the counter-ion release, stimulate the secondary- and tertiary-structure formations, leading to diverse pathways of folding and misfolding.

1Pos112 線形および環状 DNA の交流電場応答の直接観測
Dynamics of circular and linear DNA under AC electric fields

Yunosuke Fuji, Shin Takano, Seiwa Yamagishi, Yuuta Moriyama, Toshiyuki Mitsui (*Dept. Phys. Sch. Sci. Aogaku Univ.*)

The difference between linear and circular polymers is the presence of free ends. However, the behavior of the topologically different polymers in saline is dissimilar. For example, self-entanglement, diffusion, and electromobility produce different values between circular and linear polymers, although the overall length is the same. Such experimental evidences attract a wide range of scientists. Recently, Doyle found that AC fields induce self-entanglement of circular 114.8 kbp DNA, and observed an anomalous slowing of relaxation. Inspired by this result, we tested circular DNA from 22.2 kbp to 162.8 kbp as well as linear DNA of 48.5 and 165.6 kbp under similar experimental conditions. In this presentation, we report DNA dynamics with length and topology dependence.

1Pos113 染色体レオロジー特性を介した核内ストレス顆粒のポジショニング機構
Mechanisms of nuclear stress granule positioning in the nucleus via rheological properties of chromatin

Takuya Nara, Haruko Takahashi, Yutaka Kikuchi (*Graduate School of Integrated Sciences for Life, Hiroshima University*)

Membrane-less organelles in the nucleus are known to be formed by liquid-liquid phase separation. It has been reported that nuclear stress granules, one of membrane-less organelles, are formed in stress conditions and localize in the vicinity of the human satellite III (HSAT III). However, little is known about the mechanisms of nuclear stress granule positioning. Recently, Polymer Dynamics Decoded from Hi-C data (PHIC2) was developed to capture dynamic viscoelastic properties (rheology) of chromatin. We found the chromatin region in the vicinity of HSAT III that undergoes stress-dependent rheological changes by using PHIC2. In our presentation, we will discuss the relation between the rheological changes of chromatin region and the location of nuclear stress granules.

1Pos114 高分子の表面吸着問題から理解する分裂酵母の構成的ヘテロクロマチン形成
Essence of assembly of constitutive heterochromatin in fission yeast lies in surface adhesion of polymers?

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Nascent RNA synthesized during transcription scaffolds RITS complexes that are necessary for the assembly of heterochromatin in fission yeast. Our recent experiments have shown that repeat sequences of transcription units become heterochromatin, analogous to the surface adhesion of polymers. Motivated by this result, we have constructed a model of the assembly of heterochromatin in fission yeast by taking into account the RNA interference pathway and H3K9 methylation of nucleosomes in an extension of the scaling theory of the surface adhesion of polymers. Our theory predicts the discontinuous change of the adhesion probability with increasing the transcription time if the number of repeats is larger than a critical value.

1Pos115 クロマチンのもつ液滴の性質
Intrinsic liquid droplet property of chromatin

Kazuhiro Maeshima[1], Sachiko Tamura[1], Tatsuya Fukuyama[2], Yusuke Maeda[2] ([1]*National Institute of Genetics & SOKENDAI*, [2]*Department of Physics, Kyushu University*)

Chromatin in eukaryotic cells is a negatively charged polymer of nucleosomes consisting of genomic DNA wrapped around the core histone proteins. Chromatin forms condensates with Mg2+. Although nucleosomes possess ten intrinsically disordered regions as histone tails, it remains unclear whether chromatin condensates are liquid droplets or not. To approach this issue, we investigated chromatin behavior under a temperature gradient built by infrared laser focusing. If the chromatin has a droplet surface, the surface tension caused by a temperature gradient moves it toward a higher temperature region (Marangoni effect). We demonstrated that the condensed chromatin was transferred toward the hot region, suggesting a liquid droplet property of the condensed chromatin.

1Pos116 修飾核酸特有の低質量プロダクトイオンによる定量を行うソフトウェア
Software for Quantification with Low-mass Product Ions peculiar to Modified Nucleic Acids

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Modified nucleic acids exhibit specific low-mass product ions in MS/MS. By focusing on the ions, it is possible to identify and quantify similar oligonucleotide therapeutic sequences.

We have now developed new functionality to support this method in "AQXeNA" for the identification and evaluation of nucleic acid sequences containing various modifications from LC-MS data. As a demonstration of the software, mixed samples of two oligonucleotide therapeutics were prepared and quantified.

Calibration curves were made with each oligonucleotide therapeutics using normalized peak area at ten points with different concentrations. Correlation coefficients curves were automatically obtained at 0.99 or higher, even though the samples involve another oligonucleotide therapeutic.

1Pos117 単分散 GUV を用いた濃度制御による DNA 凝集体の生成
GENERATION OF DNA CONDENSATES BY CONCENTRATION CONTROL IN MONODISPERSE GIANT UNILAMELLAR VESICLES

Ryotaro Yoneyama[1], Ryota Ushiyama[1], Tomoya Maruyama[2], Masahiro Takinoue[2,3], Hiroaki Suzuki[1] ([1]*Graduate School of Science and Engineering, Chuo University*, [2]*Life Science and Technology, Tokyo Institute of Technology*, [3]*Department of Computer Science, Tokyo Institute of Technology*)

We attempted to produce DNA gel condensates by encapsulating ssDNA, whose sequence was designed to form DNA gels, in monodisperse GUVs generated in microfluidic channels. Changes in DNA concentration and salt concentration were used to trigger condensation (network formation of DNA structures). The internal solution of the GUV was concentrated by using the osmotic difference across the lipid bilayer of the GUV. The effects of parameters such as DNA sequence, concentration, temperature, and salt concentration on DNA gel formation were investigated. DNA condensates were formed and observed to grow as the internal solution concentrated. Differences in the dynamics of condensate formation were discussed.

1Pos118 microRNA の機能発現を 1 細胞 1 分子レベルで可視化する新規技術の開発
In situ single-molecule imaging of microRNA function

Hotaka Kobayashi[1,2] ([1]*JST PRESTO*, [2]*IQB, The University of Tokyo*)

MicroRNAs are small non-coding RNAs, which control the expression of thousands of mRNAs; they are loaded into Argonaute proteins to form the functional RNP complex, and silence complementary mRNAs. Historically, microRNAs have been studied by “biochemical” methods, where a bulk collection of molecules is measured outside cells. Therefore, the behavior of individual molecules during gene silencing by microRNAs, as well as their spatiotemporal regulation inside cells, remains unknown. To address such “biophysical” and “cell biological” aspects of microRNAs, I have developed a novel method to image microRNA function with single-cell and single-molecule resolution. At the meeting, I will present the biophysical and cell biological findings revealed by this method.

1Pos119 *In silico* アプローチによるアプタマー-IgG 結合の熱力学的プロファイルの解析
In silico approach for identification of the thermodynamic profiles of aptamer-IgG binding

Ryoji Yamazaki[1], Azumi Ito[2], Tomoki Sakamoto[3,4], Masaki Komine[2], Takeshi Ishikawa[5], Masato Katahira[3,4], Takashi Nagata[3,4], Taiichi Sakamoto[2], Kenji Yamagishi[1] ([1]*Graduate School of Engineering Nihon University*, [2]*Faculty of Advanced Engineering Chiba Institute of Technology*, [3]*Graduate School of Energy Science Kyoto University*, [4]*Institute of Advanced Energy, Kyoto University*, [5]*Graduate School of Science and Engineering Kagoshima University*)

The ITC analysis demonstrated that the RNA-type and DNA/RNA-type aptamers have the same binding affinity to IgG, but the thermodynamic profiles of association of aptamers with IgG differ. The NMR analysis indicated the different behaviors of these aptamers.

In this study, we analyzed the conformational behaviors and dynamical features of aptamers using molecular dynamics simulations. We then analyzed the interaction energy and electrostatic complementarity between aptamer and IgG using IFIE analysis and VIINEC based on ab initio fragment molecular orbital calculations, respectively. Using *in silico* and *in vitro* approaches, we discuss the thermodynamic profile of aptamer–protein binding of these aptamers.

1Pos120 IgG に結合するアプタマーへの化学修飾の影響
Effect of chemical modification on the aptamer that binds to IgG

Azumi Ito[1], Yuuki Yatabe[1], Hisae Yoshida[2], Masahiro Sekiguchi[2], Kazumasa Akita[3], Yoshikazu Nakamura[3], Yusuke Nomura[4], Takeshi Ishikawa[5], Kenji Yamagishi[2], Taiichi Sakamoto[1] ([1]*Chiba Institute of Technology*, [2]*Nihon University*, [3]*Ribomic Inc.*, [4]*National Institute of Health Science*, [5]*Kagoshima University*)

Chemical modification of aptamers is essential to improve their biochemical stabilities and sometimes increases their binding activities to the targets. We are attempting to predict the effect of chemical modification of the aptamer that binds to IgG on the binding activity *in silico*. We have already reported that the binding activity is improved by introducing Locked Nucleic Acid (LNA) at the 18th position of the aptamer. In this study, we introduced 2'-O-methyl (OMe) and Bridged Nucleic Acid (BNA-NC(N-Me)) at the same position of the aptamer and found that the IgG binding of the aptamer was increased by OMe and decreased by BNA-NC(N-Me). We will discuss the effect of these modifications on the binding activity from the point of view of the aptamer’s structure.

1Pos121 (2SEP-2) 自由エネルギー地形から探る開始コドン認識機構
(2SEP-2) Computational Analysis of the Start Codon Recognition Mechanism Based on Free Energy Landscape

Takeru Kameda[1], Katsura Asano[2,3,4], Yuichi Togashi[1,5] ([1]*Coll. Life Sci., Ritsumeikan Univ.*, [2]*Div. Biol., Kansas State Univ.*, [3]*HiHA, Hiroshima Univ.*, [4]*Grad. Sch. Integ. Sci. Life, Hiroshima Univ.*, [5]*RIKEN BDR*)

Eukaryotic translation usually initiates at the AUG codon in mRNA. Alternatively, CUG is reported to play the role of start codons at a low frequency, and thus attention has been paid to the frequency and mechanism of translation initiation at non-AUG codons. Recently, we have studied start codon recognition mechanisms in eukaryotic ribosomes based on free-energy evaluation using computer simulations, and discussed them from the molecular dynamics viewpoint. We also reported the effects of chemically modified nucleotides (e.g. pseudouridine) on translation initiation. In this presentation, we will introduce these studies and discuss future directions of computational research on translation initiation.

1Pos122 ヌクレオソームから H2A-H2B2 量体が脱離する際の自由エネルギー曲線解析
Analysis of free energy curve of H2A-H2B dimer displacement from the nucleosome

Hisashi Ishida, Hidetoshi Kono (*Institute for Quantum Life Science, National Institutes for Quantum Science and Technology*)

Nucleosome reconstitution plays an important role in many cellular functions. As the initial step of the reconstitution, H2A-H2B dimer displacement (or eviction) should occur. To understand how the displacement occurs, we carried out all-atom molecular dynamics simulations of wrapped and unwrapped nucleosomes. The free energy curves showed that the H2A-H2B dimer displacement from unwrapped nucleosome is more likely to occur. We found that conformational disrupt at the interface between the docking domain of H2A and the adjacent H3-H4 dimer, and at the interface between H2B and H4 significantly contributed to the free energy. In addition, key residues are found to agree to mutations observed in cancer cells. This indicates the nucleosome instability in cancer cells.

1Pos123 細菌の翻訳開始前複合体における tRNA とリボソームタンパク質の相互作用に関する理論的考察
Theoretical investigation of the interactions between a tRNA and ribosomal proteins in bacterial translation pre-initiation complex

Yoshiharu Mori, Shigenori Tanaka (*Grad. Sch. Sys. Inf., Kobe Univ.*)

A ribosome is a protein-RNA complex that is responsible for protein synthesis in cells. During a translation initiation phase, a translation pre-initiation complex consisting of ribosomes and initiation-related proteins is formed to ensure the initiation of protein synthesis. This study aims to elucidate the roles of ribosomal proteins. We performed molecular dynamics simulations of the protein-RNA complex using a coarse-grained model to elucidate the roles of the ribosomal proteins. The free energy profile of tRNA dissociation from the complex was calculated. The interactions between the C-terminal region of the ribosomal proteins and tRNA can stabilize the ribosome and tRNA. This interaction could be necessary for accurately recognizing tRNA by the ribosome.

1Pos124 遠隔操作が可能な DNA 流体のマイクロ流制御
Microflow manipulation of DNA fluid with remote controllability

Hirotake Udono[1], Shin-ichiro Nomura M.[2], Masahiro Takinoue[1] ([1]*Sch. Comp., TiTech*, [2]*Grad. Sch. Eng., Tohoku Univ.*)

Remotely controlled microflow of DNA fluid, condensate of DNA motifs connected via sticky ends (SEs), is demonstrated by introducing azobenzene in the SE. Depending on wavelength, DNA fluid changes fluidity via photoinduced state transition. Compartmentalized DNA fluid creates interface-mediated flow, with reentrant-temperature dependence whose flow mode is adjustable with azobenzene arrangement in the SE. This non-monotonic temperature dependence results from competition between light- and temperature- controlled binding mechanisms of SEs. We relate this to photoinduced dynamic shift in binding enthalpy of SEs. Our remotely controlled DNA fluid will offer a facile mechanistic tool for intracellular microfluidic manipulation.

1Pos125 光ピンセットを用いたソレ効果による相分離ドロップレットの生成と DNA 濃縮 II
Generation of Phase Separated Droplet Induced by Soret Effect and DNA Enrichment by Optical Tweezers II

Mika Kobayashi, Yoshihiro Minagawa, Hiroyuki Noji (*Grad. Sch. of Eng., Univ. Tokyo*)

We demonstrate a generation of a phase separated droplet induced by Soret effect in a ternary mixture Dextran/PEG/water. We perform local heating in a sample at a single phase state by optical tweezers that brings system to a two phase region, resulting in phase separation. DNA is successfully enriched in the Dextran-rich droplet and this enrichment seems to be stable for surprisingly long time such as a few days. DNA enrichment can be also caused by high concentration of PEG without phase separation. However, the time evolution is clearly different from the case enriched in the droplet. We compare above two cases and discuss the mechanism behind the phenomena.

1Pos126 一定終状態光電子収量分光法を用いたタンパク質薄膜の電子構造観察
Application of Constant Final State Photoelectron Yield Spectroscopy to Protein Films to Elucidate Their Occupied Electronic Structure

Masaki Tomita[1], Bera Sudipta[4], Ryotaro Nakazawa[1], Rio Ushiroda[1], Ichiro Ide[1], Cahen David[4], Hisao Ishii[1,2,3] ([1]*GSSE Chiba Univ*, [2]*CFS Chiba Univ*, [3]*MCRC Chiba Univ*, [4]*Weizmann Inst*)

The electronic structure of biomolecules, including of HOMO, LUMO, and in-gap states is essential for understanding bio-related processes such as charge transfer through proteins. Photoelectron spectroscopy has been widely used to probe the electronic structure of materials. However, its application to proteins has been limited mainly due to sample charging effect. In this study, we have applied constant final state photoelectron yield spectroscopy (CFS-YS) to lysozyme and azurin films to elucidate the density-of-states (DOS) of the valence region as well as weak in-gap states without sample charging. The obtained DOS corresponded well with the result by MOPAC calculation, demonstrating the usefulness of CFS-YS in observing the electronic structure of proteins.

1Pos127 電子線回折を利用した構造解析における電子状態を考慮した構造精密化
Structural refinement considering the electron orbitals in structural analysis using electron diffraction

Yasuhisa Honda, Keigo Takahira, Takuo Yasunaga (*Dept of Computer Science and Engineering, Kyushu Institute of Technology*)

In electron diffraction analysis, molecular structures are often refined using software for X-ray crystallography.
In X-ray diffraction, the photons interact with the sample's electrons. Therefore, the analysis gives us the electron density map. In contrast, in electron diffraction, the electrons interact with the Coulomb force of the nucleus and electrons so that we can obtain the electrostatic potential map.
We propose a structural refinement method in electron diffraction, focusing on the difference: That is, by using an atomic model refined by an X-ray algorithm as an initial model, we calculated electron orbital states by quantum chemistry and repeatedly updated the model considering atomic charge and coordinates, in succuss of R-factor down.

1Pos128 酸化型[NiFe]ヒドロゲナーゼの生成経路と活性中心の電子・幾何構造についての理論的研究
Theoretical characterization of the active site and its formation pathway in oxidized [NiFe]-hydrogenase

Yuta Hori, Yasuteru Shigeta (*Center for Computational Sciences, Univ. Tsukuba*)

[NiFe]-hydrogenase has a binuclear Ni-Fe complex in the active site that reversibly catalyzes the oxidation of H_2. Recent studies have indicated that the aerobically isolated [NiFe]-hydrogenase contains an EPR-silent state (**Ni-SX**). However, their detailed geometrical and electronic structures have not been clarified.
In this study, DFT calculations were utilized to determine the geometrical and electronic structures in the **Ni-SX** form. The calculation results determined that the **Ni-SX** form has a Ni^{2+} atom in the low-spin state and a bridging monooxygen ligand. Furthermore, the reaction pathway of the oxidized states by oxygen was investigated using DFT calculations. The computed energy diagram shows that the Ni-SX form is generated under aerobic conditions.

1Pos129 Scala 言語を用いた生体高分子計算科学ツール STCSB への量子化学計算機能の追加
Further development of STCSB, Scala Tool for the Computational Science of Biomolecules, to add a quantum- chemistry calculation module

Ryoutarou Matsuda, Mika Mitsumatsu, Itaru Onishi, Masayuki Irisa (*Kyushu Inst. of tech*)

We have further developed STCSB, Scala Tool for the Computational Science of Biomolecules, to add a quantum-chemistry calculation module, DFTB3/3OB calculation. STCSB was made by our group and has been used for 3D-RISM calculations, molecular dynamics (MD) simulations, and QM/MM MD simulations. In this study, results of QM/MM dynamics simulations of an *Eco*RV–DNA complex, one of the type II restriction enzymes, are visualized as a 3D-graphics of electron-density distribution in an active site of *Eco*RV–DNA complex obtained from a MD trajectory where proton-transfers occurred for hydrolysis of DNA by *Eco*RV.

1Pos130 Continuum model for analyzing mechanical properties of *Dictyostelium* fruiting-body development

Seiya Nishikawa, Satoshi Kuwana, Hidenori Hashimura, Satoshi Sawai, Shuji Ishihara (*Grad. Sch. Arts & Sci., Univ. Tokyo*)

In starved *Dictyostelium discoideum*, more than 100,000 cells aggregate, and then form a three-dimensional tissue called “fruiting body”. Such 3D system exhibits complex structure and movement; thus, it is difficult to intuitively understand the mechanism of developmental process. In this study, we constructed a simple mathematical model to investigate how mechanical properties of the cells and cell migration determine the tissue shape. The model adopted a continuum description composed of velocity and phase fields for representing local tissue deformation and tissue shape, respectively. Effects of heterogeneous viscosity and the distribution of active stress exerted by cells on tissue morphology were analyzed using the model.

1Pos131 ゼブラフィッシュ自己組織化細胞塊における細胞挙動の解析
Characterization of cell dynamics in the process of self-organization in zebrafish explants

Momoka Tochizawa (*Dept. Phys. Sch. Sci. Aogaku Univ.*)

A fundamental future of biological system is a self-organizing process seen in collective cell mass. In embryonic development, cells exhibit self-organizing pattern and establish various organs. Thus far, we know a lot about gene expression patterns and its functions for the process of self-organization, but still we don’t know much about the dynamics of individual cells during the process. Here we investigated and characterized cell movements in the process of self-organization in zebrafish explants. Individual cells were traced over 4 hours. We present our current data and discuss how single/collective cell behaviour contribute self-organization.

1Pos132 線虫の初期胚発生における力学モデル
Mechanical Model in Early Embryogenesis of C. elegans

Takehiro Kurihara[1], Toshikaze Chiba[1], Naohito Urakami[2], Kazunori Yamamoto[3], Akatsuki Kimura[4] ([1]*Soft Matter and Biophysics Lab., Department of Physics, Faculty of Science, Tohoku University*, [2]*Graduate School of Sciences and Technology for Innovation, Yamaguchi University*, [3]*Department of Applied Bioscience, Faculty of Applied Bioscience, Kanagawa Institute of Technology*, [4]*Cell Architecture Laboratory, Department of Chromosome Science, National Institute of Genetics*)

Embryogenesis is the developmental process, where a fertilized egg repeats cleavage to be an adult. A unique feature of embryogenesis is that each species has its cleavage pattern even in the very early stage. Since the cleavage pattern is determined by the balance of mechanical forces regulated by various proteins, it is important to reveal the relationship between the pattern and mechanical parameters. So far, we have developed a mechanical model that described the morphology of vesicle assemblies. Using this model, we have succeeded in reproducing the cleavage patterns in the 1 - 3 cell stage of C. elegans. This analysis indicates that to complete the cleavage by a contractile ring, the bending rigidity of the membrane close to the ring must decrease significantly.

1Pos133 多細胞系の形態形成の近似モデルとしての細胞間相互作用の実効ポテンシャル
Effective mechanical potential of cell-cell interactions: approximated model for multicellular morphogenesis

Hiroshi Koyama, Toshihiko Fujimori (*Div. Embryology., Nat. Inst. Basic Biology*)

Mechanical forces of cell–cell interactions are critical for the emergence of diverse multicellular morphologies. However, live measurements of related parameters have been difficult due to technical limitations. Here, we propose a framework for inferring mechanical potentials of cell–cell interactions. By analogy to coarse-grained models in molecular and colloidal sciences, we approximated cells as spherical particles, where the mean potentials of pairwise cell–cell interactions were considered. This model was fitted to cell tracking data. We evaluated the applicability of our method to various cell types under various conditions, and conclude that the potential is a good approximation for describing 3D morphologies and mechanical properties of systems.

1Pos134 好熱菌 F_oF_1-ATPase のユニサイト触媒作用の構造的基盤
Structural basis of unisite catalysis of thermophilic F_oF_1-ATPase

Momoko Aoyama[1], Atsuki Nakano[1], Jun-ichi Kishikawa[2], Ken Yokoyama[1] ([1]*Department of Molecular Biosciences, Kyoto Sangyo Univ.*, [2]*IPR, Osaka Univ.*)

F_1 domain in FoF1 ATP synthase, can catalyze both the synthesis and hydrolysis of ATP with the rotation of the central γε rotor inside a cylinder made of $\alpha_3\beta_3$ in three different conformations. Here, we determined multiple cryo-electron microscopy structures of bacterial F_oF_1 exposed to different reaction conditions. The structure of F_oF_1 under conditions that permit only a single catalytic β subunit per enzyme to bind ATP is referred to as unisite catalysis and reveals that ATP hydrolysis unexpectedly occurs on β_{TP} instead of β_{DP}, where ATP hydrolysis proceeds in the steady-state catalysis of F_oF_1. This indicates that the unisite catalysis of bacterial F_oF_1 significantly differs from the kinetics of steady-state turnover with continuous rotation of the shaft.

1Pos135 祖先型 ATPase の作製と機能解析
Resurrection of the Ancestral ATPase

Aya Suzuki[1], Ryutaro Furukawa[1], Hiroshi Ueno[1], Satoshi Akanuma[2], Hiroyuki Noji[1] ([1]*Grad. Sch. Eng., Univ.Tokyo*, [2]*Fac. Human Sci., Waseda Univ*)

Rotary ATPases such as F-/V-ATPase are unique molecular motors which work as energy conversion machines. In F-/V-ATPase, alternately arranged two types of subunits (α and β for F-ATPase, and A and B for V-ATPase) form a hetero-hexameric stator ring. Subunits α, β, A, and B share high homology, and the ancestral ATPase is supposed to have homo-hexameric rings. On the other hand, type III secretion system (T3SS) ATPase has homo-hexameric stator rings such as $FliI_6$-rings. Here, the sequence of ancestral ATPases were predicted from 617 sequences of α, β, A, B, and FliI subunits from F, V- and T3SS ATPases. The ancestral ATPases of αβAB, αB, and βA were expressed. The sequence and the function of the ancestral and existing ATPases were compared and discussed.

1Pos136 Rotation dynamics and structure of F1-ATPase with all α-subunit-type P-loops

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F1-ATPase (F1) is one of the best characterized rotary molecular motor. However, its design principle, e.g., the origin of conformational change upon nucleotide binding, remains elusive. In this study, we focused on the P-loop of the α and β subunits, because the structures suggest the large conformational changes in the P-loop of the β subunit during catalysis. To elucidate the effect of P-loop on the conformational change in F1, we analyzed the engineered F1 having only P-loops of α subunit that shows no conformational change upon nucleotide binding. Interestingly, the engineered F1 showed extremely slow rotation, backsteps and lower torque. We will discuss these results based on the recently obtained cryo-EM structure of this F1.

1Pos137 (2SFA-5) Plus and minus ends of microtubules respond asymmetrically to kinesin binding by a long-range directionally driven allosteric mechanism

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Although it is known that the majority of kinesin motors walk predominantly toward the plus end of microtubules (MT) in a hand-over-hand manner, the structural origin of the stepping directionality is not understood. To resolve this issue, we modelled the structures of kinesin-1 (Kin1), MT, and the Kin1-MT complex using the elastic network model and calculated the residue-dependent responses to a local perturbation in the constructs. Kin1 binding elicits an asymmetric response, opening the clefts of multiple plus end tubulin heterodimers, creating binding-competent conformations which are required for processivity. Our findings explain the directionality of stepping and the long-range communication of kinesin.

1Pos138 Kinesin-1 および Kinesin-14 の In vitro 合成とデザイン
In vitro synthesis and design of kinesin-1 and kinesin-14

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The biomolecular motor system (microtubule; MTs-kinesin) is the main component of nanoscopic bio-actuators. Modification of kinesin, the core driving force part, provides advantages in biophysical assays and building nanodevices. However, the classical protein expression method is time-consuming to produce and design kinesins. Here, we demonstrated in vitro synthesis of two types of kinesins, *i.e.* kinesin 1 and 14, using a cell-free system that expresses proteins from DNA templates in coupled transcription and translation systems. Synthesized kinesins propelled MTs on a kinesin-coated substrate. We also successfully introduced SBP and Flag tags into kinesins using PCR fragments coding tag sequences. Our method will accelerate the study of biomolecular motor systems.

1Pos139 A novel photochromic regulator inhibits kinesin Eg5 at the ADP sate in the ATPase cycle

Md Alrazi Islam[1], Kozue Satoh[2], Shinsaku Maruta[1,2] ([1]*Grad. Sch. Sci & Eng., Soka Univ.*, [2]*Grad. Sch. Sci & Eng., Soka Univ.*)

Kinesin Eg5 is a member of the kinesin superfamily and has key physiological activities. It assists in the formation of a bipolar spindle during eukaryotic cell division. Eg5 has been reported to be overexpressed in cancer cells in order to trigger mitosis. Therefore, kinesin Eg5 is the cancer therapy's target. Previously we have demonstrated that Eg5 activity was controlled by spiropyan-azobenznen derivative (SPSAB) in three isomerization states such as SP-Trans (VIS), MC-Cis(UV), and MC- Trans (In the dark), respectively. In this study, we analyzed that SPSAB regulates which step in the Eg5 ATPase cycle by the mixed motor assay with conventional kinesin. The results suggested that SPSAB may inhibit the ADP state in the Eg5 ATPase.

1Pos140 野生型と疾患関連変異型で構成されるヘテロダイマー KIF1A(キネシン-3)の二足歩行運動モデル
A bipedal walking model for heterodimeric motors composed of wild-type KIF1A and disease-associated KIF1A

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KIF1A is a kinesin superfamily motor protein that transports synaptic vesicle precursors in axons. Mutations in human Kif1a lead to a group of neurodegenerative diseases called KIF1A- associated neuronal disorder (KAND). KAND mutations are mostly de novo and autosomal dominant; however, it is unknown how wild-type KIF1A motors is inhibited by heterodimerization with mutated KIF1A. Here, we established in vitro single-molecule assays to analyze the motility of heterodimeric motors and constructed a mathematical model to understand inhibition by heterodimerization with mutated KIF1A. Our model successfully describes the motility of heterodimeric motors by using the respective parameters of wild-type KIF1A and disease-associated KIF1A.

1Pos141 How does giraffe kinesin cope with the long distance axonal transport?

Taketoshi Kambara[1], Daisuke Taniguchi[2], Tomoya Mukai[3], Yasushi Okada[1,2,3,4,5] ([1]*BDR, RIKEN*, [2]*IRCN, Univ. Tokyo*, [3]*Grad. Sch. Sci., Univ. Tokyo*, [4]*Grad. Sch. Med., Univ. Tokyo*, [5]*UBI, Univ. Tokyo*)

Many neurodegenerative diseases are known to be caused by impaired axonal transport due to decreased velocity of kinesin. For example, point mutations of KIF5A is known to be causative for hereditary spastic paraplegia (HSP), which mainly affects the distal part of the long motor tracts in the spinal cord. The HSP mutations slightly decreased the velocity of KIF5A that would explain why neurons with longest axons are affected. If fast velocity is important for the survival of neurons with long axons, large animals with longer axons would require faster kinesin. Here, we asked if giraffe kinesin moves faster than small animals such as mice. Our data suggest that KIF5A of large animals with longer axons might have adapted for the longer axonal transport.

1Pos142 QCM 測定による周波数変化から測定したアクトミオシン滑り運動の機構
Sliding mechanism of actomyosin motility assay measured from frequency change by QCM

Honoka Kobayashi, Naoki Matsumoto, Taiki Nishimura, Yuki Sakurai, Kaho Yokomuro, Kazuya Soda, Ikuko Fujiwara, Hajime Honda (*Dept. of Matl. Sci. and Bioeng., Nagaoka Univ. of Tech*)

Myosin is a motor protein involved in intracellular motility by interacting with actin filaments.
The motor function of myosin causes the unidirectional sliding movement of actin filaments in the presence of ATP, which is called an in vitro motility assay.
Although the orientation and the ATPase cycle of myosin molecules along an actin filament should be random, the sliding of an actin filament is not inhibited in an apparent manner.
How they are organized is still not fully understood. Quartz crystal microbalances (QCM) is a tool to measure changes in the state of bound substances on surfaces.
We hypothesized that QCM could be used to measure actomyosin interactions.
We present quantitative data on frequency change during the motility assay monitored by QCM.

1Pos143 QCM 上でのアクトミオシンの滑走速度と周波数変化の関係
The relation between sliding velocities and frequency changes of actomyosin on the QCM

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The interaction of actomyosin plays a crucial role in living cells. In previous studies that used purified myosin and actin on the electrode of QCM, the frequency was increased unexpectedly with the addition of ATP. We hypothesized the positive frequency shifts are caused by (1) dissociation of F-actin from myosin that is tethered on the QCM, (2) detachment of both F-actin and myosin from QCM, or (3) changes in the interaction-manner between actin and myosin. In this study, we have constituted an in vitro motility assay on the QCM-electrode surface under a fluorescence microscope and simultaneously measured the sliding velocity. The quantitative relations among ATPase, sliding velocity, and frequency shifts of the actomyosin interaction will be discussed.

1Pos144 鞭毛内輸送を行うダイニンがどのように歩行する微小管を選択するのかに関する粗視化 MD 研究
Coarse-grained MD study on the function of dynein in selecting walking microtubules

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The microtubules (MTs) of eukaryotic cilia and flagella are doublet MTs composed of A- and B-tubules. It is known that dynein-2 and kinesin-2, responsible for the transportation in cilia, walk on A- and B-tubules, respectively. However, it is unknown how these motors select different tubules. Recent studies indicate that tubulin post-translational modifications (PTMs) are mostly enriched in the B-tubules. We hypothesized that the MT selection is based on the PTMs. In this study, we performed a molecular dynamics (MD) simulation to reveal how the movement of dynein-2 changes depending on the PTMs. For the effective sampling trajectories, we use a coarse-grained model for MD simulations. In the end, we found poly-glutamylation can inhibit dynein-2 walking on MTs.

1Pos145 Discovery of the fastest myosin, its amino acid sequence, and structural features

Takeshi Haraguchi[1], Masanori Tamanaha[1], Kano Suzuki[2], Kohei Yoshimura[1], Takuma Imi[1], Motoki Tominaga[3,4], Hidetoshi Sakayama[5], Tomoaki Nishiyama[6], Takeshi Murata[2], Kohji Ito[1] ([1]*Dept. of Bio. Sci., Grad. Sch. of Sci and Eng., Univ. of Chiba*, [2]*Dept. of Che. Sci., Grad. Sch. of Sci and Eng., Univ. of Chiba*, [3]*Grad. Sch. Adv. Sci. and Eng., Univ. Waseda*, [4]*Fac. Educ. Integrated Arts. Sci., Bio., Univ. Waseda*, [5]*Dept. of Bio. Sci., Grad. Sch. of Sci., Univ. of Kobe*, [6]*Adv. Sci. Res. Ctr., Univ. of Kanazawa*)

Cytoplasmic streaming with high velocity (~ 70 μm/s) occurs in cells of the *Chara braunii*. Because cytoplasmic streaming is driven by myosin XI, it has been suggested myosin XI with high velocity exists in *Chara* cells. In this study, we cloned four myosin XIs from *Chara braunii* (*Cb*XI-1, -2, -3, -4) and measured their velocities.
The velocities of *Cb*XI-3 and *Cb*XI-4 were about one-third of the velocity of cytoplasmic streaming in *Chara braunii*. While the velocities of *Cb*XI-1 and *Cb*XI-2 were almost the same as the velocity of cytoplasmic streaming in *Chara braunii*. These results suggest that *Cb*XI-1 and -2 are the main contributors to the cytoplasmic streaming in *Chara braunii* and that *Cb*XI-1 is the fastest myosin yet found.

1Pos146 バクテリアのべん毛モーターは減速機を持つか？
Does bacterial flagellar motor have a reduction drive?

Ryota Iino[1,2] ([1]*IMS, NINS*, [2]*SOKENDAI*)

The atomic structures of the stator MotAB complex of the bacterial flagellar motor were revealed in 2020, and a model in which the MotB dimer rotates within the MotA pentamer ring upon ion transport has been proposed. In this model, rotation of the rotor C-ring of the flagellar motor is driven by the rotation of the stator MotAB complex. From the viewpoint of the mechanics, this corresponds to a reduction drive, which is a combination of two gears with different numbers of teeth. The reduction drive is a mechanism that increases torque by reducing the rotational speed of the motor. Here I would like to discuss whether the bacterial flagellar motor really has a reduction drive and, if so, to what extent it can be explained by analogy with macroscopic machines.

1Pos147 高度好塩菌アーキアの回転モーターのステップ状回転の検出
Detection of stepwise rotation of the archaellar motor in *Haloferax volcanii*

Yoshiaki Kinosita, Jun Ando, Tastuya Iida, Rikiya Watanabe (*Molecular Physiology Lab, RIKEN*)

Archaea swim using the ATP-driven rotary motor, archaellum (archaeal flagellum). In a biophysical aspect, the significant question is how the chemical reaction couples to the motor works. To demand it, we performed the bead assay which enabled us to monitor the motor works, through the bead rotation attached to an archaellar filament. Furthermore, the permeabilized-ghost model allowed control of the rotary speed in ATPase by changing the [ATP] in the buffer. Combining these techniques, the 60°-steps could be detected. However, the bead movement between steps showed the creeping due to the viscous friction of bead size, inhibiting to characterize the dwell time. Now, we are performing the same assay using a gold nanoparticle to clarify the ATP-coupled motor works.

1Pos148 Cryo-EM structure analysis of the PomAB complex, a bacterial flagellar stator of sodium-driven motor in *Vibrio alginolyticus*

Tatsuro Nishikino[1], Norihiro Takekawa[2], Jun-ichi Kishikawa[1], Mika Hirose[1], Seiji Kojima[3], Michio Homma[3], Takayuki Kato[1], Katsumi Imada[2] ([1]*IPR., Osaka Univ.*, [2]*Dept. of Macromol. Sci., Grad. Sch. of Sci., Osaka Univ.*, [3]*Div. Biol. Sci. Grad. Sch. Sci., Nagoya Univ.*)

The bacterial flagellar motor consists of the rotor and stator, and their interaction is essential to generate torque. The stator is made up of two membrane proteins, PomA and PomB in marine *Vibrio*, and MotA and MotB in *E. coli* or *S. enterica*. The former functions as a sodium channel and the latter as a proton channel. The stator complex was thought to be composed of four MotA and two MotB molecules based on biochemical analyses. However, cryo-EM analysis revealed that the stator is composed of five MotA and two MotB molecules. In this study, we performed single particle cryo-EM analysis of purified PomAB complex and revealed that five PomA and two PomB molecules form the stator complex. We will discuss the difference between the sodium and proton driven stator.

1Pos149 バクテリアの膜電位揺らぎの解析手法の開発
Development of a method for analyzing membrane potential fluctuations in bacterial cells

Kenta Takemori, Yusuke V. Morimoto (*Fac, Comp. Sci. and Sys. Eng., Kyushu Inst. Tech*)

Bacterial cells utilize a proton motive force, the electrochemical gradient across the inner membrane, to synthesize ATP and drive flagella. The membrane potential fluctuates on a short-term basis, and it is not known how this fluctuation in membrane potential works within the cell. To study membrane potential fluctuations, we introduced and evaluated highly sensitive fluorescent probes that measure temporal changes in membrane potential and intracellular ion concentrations at the single-cell level. Membrane potentials of *E. coli* and *Salmonella* cells cultured under different conditions were measured. A new evaluation method for the obtained time series data of the fluctuations was investigated.

1Pos150 分子動力学シミュレーションによる SMC 蛋白質の DNA によって刺激される ATPase 活性の分子機構解明
Molecular Dynamics Simulations to Reveal Molecular Mechanism of DNA-Stimulated ATPase Activity of SMC Proteins

Masataka Yamauchi, Tsuyoshi Terakawa, Giovanni B. Brandani, Shoji Takada (*Dept. of Biophysics, Grad. of Sci., Kyoto Univ.*)

Structural maintenance of chromosomes (SMC) proteins, such as cohesin and condensin, are ATPases that play key roles in chromosome organization by DNA loop extrusion. ATPase activity of the SMC proteins is stimulated by DNA and this feature is highly conserved from prokaryotic to eukaryotic SMC proteins, implying the DNA-stimulated ATPase activity can be an important element for the DNA loop extrusion. To understand its molecular mechanism, we investigated the impact of DNA on the SMC proteins by all-atom molecular dynamics simulations. From the simulations, we found apparent differences in compactness of the SMC ATPase domains between w/ and w/o DNA, which results in changing coordination of amino acid residues to the ATP molecules.

1Pos151 除膜クラミドモナス細胞の巨大リポソームへの封入
Encapsulation of demembranated *Chlamydomonas* cell into giant liposomes

Koichiro Akiyama, Syunsuke Shiomi, Masahito Hayashi, Tomoyuki Kaneko (*Frontier Bioscience, Hosei Univ.*)

To create a self-propelling artificial cell, we use microorganisms as its engine. We have encapsulated a living *Chlamydomonas* cell into a giant liposome to find the liposome moved forward. As a next step, we encapsulated a demembranated *Chlamydomonas* cell, which is dead but swims in the presence of ATP, into a liposome to control its motion through the concentration of ATP. The demembranated *Chlamydomonas* cell was encapsulated in liposomes using the water-in-oil emulsion transfer method. We have highly efficient encapsulation of demembranated *Chlamydomonas* cells by making the lipid composition DOPC: DOPG = 4: 1. We will try to reactivate the demembranated *Chlamydomonas* cell in liposomes examining the condition such as centrifugal conditions and solution composition.

1Pos152 リゾチームアミロイド線維との接触に対する運動するアクチン線維の応答
Response of a moving actin filament to a contact with a lysozyme amyloid fibril

Kuniyuki Hatori, Ryusei Murata, Kazuto Mima (*Dep. Mech. Eng., Yamagata Univ.*)

Interactions between protein filaments are fundamental to the organization of cell architecture. Meanwhile, irregular assembly such as amyloids can induce cell disfunctions. To understand the interaction between distinct filaments, we directly observed contact events between single actin filaments and amyloid fibrils via fluorescence microscopy. Amyloid fibrils were prepared from AZDye647-labeled lysozyme under acidic conditions. The amyloid fibrils could attach to a HMM-coated collodion surface without any chemical treatment. TMR-phalloidin-actin filaments were loaded and the sliding movement was initiated by adding ATP. When an actin filament moved just across an amyloid fibril, the instantaneous speed decreased and the moving direction changed.

1Pos153 細胞配置換えの分子基盤の解明
Elucidating molecular basis of cell rearrangement

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Cell rearrangement, an elementary processes of morphogenesis, proceeds in three steps: 1) shrinkage of cell adhesion, 2) switching of cell adhesion at the four-way vertex, and 3) elongation of newly formed cell adhesion. It has been reported that force generation by myosin-II is responsible for both the shrinkage and elongation. However, the mechanisms that drive actin cytoskeletal regulation and cell adhesion switching have been unknown. Here, we discuss the mechanism by which actin cytoskeletal reorganization driven by cofilin and its cofactor AIP1 drives cell rearrangement, as well as a phenomenon discovered during this study in which actomyosin transiently detached from the AJs in the 4-way vertex regulates the switching of cell adhesion planes.

1Pos154 ウニ胚の細胞骨格分布極性に起因する外腸胚形成
Exogastrulation due to cytoskeletal polarity distribution in sea urchin embryo

Kaichi Watanabe[1], Yuhei Yasui[1], Yuta Kurose[2], Naoaki Sakamoto[1], Akinori Awazu[1] ([1]*Grad. Sch. Int., Univ. Hiroshima*, [2]*Grad. Sch. Sci., Univ. Hiroshima*)

Gastrulation is important and universal processes for morphogenesis. Sea urchin embryo was known to show typical and clear gastrulation. We found that the gastrulation of sea urchin embryo exhibited anomalous shape when H+/K+ pump activity was suppressed. Fluorescence observations and knockout experiments of related molecules and genes suggested H+/K+ pump regulates intracellular pH polarity, and pH polarity regulated the cytoskeleton polarity in each cell . We developed the mathematical model considering the change in whole embryonic cytoskeleton distribution based on the above observations to reproduce both normal and anomalous gastrulation. By these studies, we clarified the contributions of inter- and intracellular chemo-mechanical couplings to gastrulation.

1Pos155 アクチンとミオシン細胞骨格の組織化によって細胞質のカイラルな回転流が生まれる
Chiral cytoplasmic flow emerging from the spatial organization of actin and myosin cytoskeleton

Takaki Yamamoto, Tomoki Ishibashi, Sylvain Hiver, Mitsusuke Tarama, Yuko Mimori-Kiyosue, Masatoshi Takeichi, **Tatsuo Shibata** (*RIKEN BDR*)

Living organisms show left-right symmetry at the molecular, cellular, tissue and organismal levels. The chirality of organ and tissue is derived from the cellular chirality that compose of them, and the cellular chirality emerges from the molecular chirality within the cell. However, the principle of the emergence of cellular chirality is still unclear. To address this question, we experimentally study the dynamical chiral behaviors of epithelial cells and seek a theoretical understanding of how the chiral behaviors arise from the molecular-level chirality. Our experiment and theory suggest that the cell chirality emerges as a collective behavior of actin and myosin cytoskeleton even without macroscopic chiral orientational order of the cytoskeleton.

1Pos156 サルモネラ菌の感染時におけるアクチン細胞骨格動態の顕微力学解析
Micromechanical analysis of actin cytoskeleton dynamics during the *Salmonella* infection

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Force-dependent mechanisms of actin dynamics mediated by actin-binding proteins are meaningful in cells when Rho-family proteins are activated. To probe the practical contribution of force-dependent regulation, we employed *Salmonella* Typhimurium, one of bacterial pathogens invading gastrointestinal epithelial cells, to locally activate Rho-family proteins. Using optical tweezers, we manipulated the *S.* Typhimurium SL1344 individual and placed it on the MDCK cells. When the invasion of *S.* Typhimurium was initiated, membrane ruffling was clearly observed in phase-contrast images and actin cytoskeleton dynamics was fluorescently monitored. We are planning to investigate the mechanical response of actin cytoskeleton to force applied via invading *Salmonella*.

1Pos157 K^+-induced decrease in the matrix pH of mitochondria

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K^+ is a major ion in mammalian cells, and facilitate mitochondria to synthesize ATP and reduce the generation of reactive oxygen species (ROS). However, the mechanism of action of K^+ on mitochondria is not well understood. In this study, with fluorescence imaging, we examined the effects of K^+ on mitochondrial membrane potential, matrix pH, and ROS production, and found that K^+ entry into mitochondria decreased mitochondrial matrix pH and promoted ATP production and ROS reduction. Since an increase in H^+ concentration in the matrix can increase ATP production and decrease ROS generation, the decrease in the matrix pH appears to be an important factor affected by K^+ entry. The mechanism by which K^+ entry into mitochondria decreases the matrix pH is discussed.

1Pos158 RacGAP 因子 FilGAP は腎ポドサイトの細胞-基質接着と突起形成を制御する
FilGAP, a GAP for Rac1, controls cell-extracellular matrix adhesion and process formation of kidney podocytes

Koji Saito[1], Seiji Yokawa[1], Sari Mizuta[1], Kanae Tada[1], Moemi Oda[1], Hiroyasu Hatakeyama[2], Noriko Takahashi[2], Hidetake Kurihara[3], Yasutaka Ohta[1] ([1]*Division of Cell Biology, Department of Biosciences, School of Science, Kitasato University*, [2]*Department of Physiology, School of Medicine, Kitasato University*, [3]*Department of Physical Therapy, Faculty of Health Sciences, Aino University*)

The function of kidney podocytes is closely associated with actin cytoskeleton regulated by Rho small GTPases. Loss of actin-driven cell adhesions and processes in podocytes is connected to kidney diseases such as proteinuria. In this study, we addressed the function of FilGAP, a GTPase-activating protein (GAP) for Rho small GTPase Rac1, in podocytes *in vitro*. We found that depletion of FilGAP activates Rac1 and P21-activated kinase 1 (PAK1), a downstream effector of Rac1, and results in the impairment of cell-extracellular matrix (ECM) adhesion and process formation of cultured podocytes. We propose that FilGAP, as a RacGAP, contributes to both cell-ECM adhesion and process formation of podocytes by suppressing Rac1/PAK1 signaling.

1Pos159 パターン化モデル生体膜上でのアクチンのネットワーク形成
Actin network assembly on a patterned model membrane

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Near the plasma membrane, actin dynamically changes its network structure responding to external signals. This dynamic change is important for many cellular functions such as cell motility and morphogenesis. To study how the actin network assembly is controlled on the plasma membrane, we use a patterned array of square-shaped fluid lipid bilayers on a coverslip. This system allows us to localize actin nucleation promoting factors, such as N-WASP, on the patterned membrane. We show that actin networks grow like pillars from N-WASP-bound areas in the presence of Arp2/3, and its density and growth rate can be controlled. Moreover, the effects of the membrane fluidity on the network assembly can be investigated by our system. We will discuss advantages of our system.

1Pos160 細胞中のジュール熱産生
Joule heat production in cells

Tetsuichi Wazawa, Kai Lu, Takeharu Nagai (*SANKEN, Osaka Univ*)

Homeothermic animals maintain their body temperatures through the balance of producing and releasing heat. Although the shivering heat production is relatively well understood, the detail of the non-shivering heat production is still elusive. In this study, we investigated heat production involving ion transporters such as channel protein. Because the ion flow through a channel is driven by membrane potential, the channel is likely to encounter Joule heat production when it is open. We performed computer simulation to examine the possibility of the Joule heat involving channel protein as a mechanism of non-shivering heat production. Thereby, we demonstrate that in some situations the temperature distribution in a cell could be significantly affected by the Joule heat.

1Pos161 Highly conserved GYXLI motif of FlhA is directly involved in hierarchical flagellar protein export in *Salmonella*

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To construct the bacterial flagellum on the cell surface, flagellar building blocks are transported via the flagellar type III secretion system (fT3SS) from the cytoplasm to the distal end of the growing structure where their assembly occurs. FlhA is a transmembrane component of the fT3SS and not only acts as an ion-driven export engine but also coordinates flagellar protein export with assembly. The cytoplasmic portion of FlhA (FlhAc) undergoes cyclic open-close domain motions responsible for efficient flagellar protein export and assembly. Here, we provide direct evidence suggesting that a highly conserved GYXLI motif of FlhAc is directly involved in its dynamic domain motions responsible for hierarchical protein targeting and export during flagellar assembly.

1Pos162 Aberrant shape formation of fission yeast spheroplasts under microfluidic conditions

Hironori Sugiyama[1], Yuhei Goto[1,2,3], Kazuhiro Aoki[1,2,3] ([1]*ExCELLS, NINS*, [2]*NIBB, NINS*, [3]*Sch. Life Sci., SOKENDAI*)

The cell morphology of fission yeast is spatially regulated, as seen in the stably maintained cell dimensions during the cell cycle. We observed how cell-wall degraded fission yeast (spheroplasts) recover to the vegetative cell cycle, regaining spatial cues. Herein we report an aberrant shape formation of the initially round-shaped spheroplasts that were serendipitously observed during the recovery process in the microfluidic device. The spheroplasts continued the cell cycle with normal karyokinesis followed by incomplete cytokinesis. The cells were multinucleated and shaped far deviated from a spherical or rod shape with multiple nicks. Interestingly, a part of the whole cell regained a rod-like form gradually and returned to the normal vegetative cell cycle.

1Pos163 赤外線レーザー照射中の心筋細胞シートの伝導変化
Changes in conduction of cardiomyocyte sheet during infrared laser irradiation

Kentaro Kito, Masahito Hayashi, Tomoyuki Kaneko (*Frontier Bioscience, Grad. Sch. Sci. & Eng., Hosei Univ.*)

Cardiomyocytes exhibits various responses to external stimulation. It has been attempted to control the function of cardiomyocyte by noninvasive approach. In this study, a cardiomyocyte sheet was exposed to an infrared (IR) laser (λ = 1480 nm). The sheet was measured conduction direction and field potential duration (FPD) with multi-electrode array (MEA) system. As a result, the FPD was 0.20 s before IR laser irradiation and shortened to 0.15 s and 0.14 s by 0.5 W and 1.0 W IR laser irradiation, respectively. It was found that firing origin moved to the vicinity of the IR laser irradiation position. These results suggest that cardiomyocyte networks can controlled firing origins and conduction direction with IR laser irradiation.

1Pos164 好中球様細胞に分化させた HL-60 細胞のケモタキシスにおけるミトコンドリア関連タンパク質の役割
Roles of mitochondria associated protein in chemotaxis of neutrophil-like differentiated HL-60 cells

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During chemotaxis, neutrophils require energy supplied by mitochondria oxidative phosphorylation (OXPHOS), whereas neutrophils rely heavily on glycolysis under normal conditions. Previously, we found that mitochondrial morphology significantly changes after chemoattractant *f*MLP stimulation. The silencing of mitochondrial fusion protein *mitofusin 2* (*MFN2*) suppressed mitochondrial morphological changes, activity of OXPHOS and chemotaxis upon *f*MLP stimulation. In this study, we examined roles of mitochondria associated protein in chemotaxis of neutrophil-like differentiated HL-60 cells. The silencing of mitochondria associated protein suppresses mitochondrial morphological changes and chemotaxis upon *f*MLP stimulation. We will discuss in relation to MFN2.

1Pos165 Trans-dimer conformations of full-length ectodomains of Celsr cadherin in solution visualized using high-speed atomic force microscopy

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Celsr cadherin (Celsr) is an adhesion GPCR, whose extracellular domains (ectodomains) connect opposing cells and the binding is essential to planar cell polarity during tissue formation. The ectodomains of Celsr comprise nine extracellular cadherin domains (EC1–EC9) and other domains. However, the binding mechanism of Celsr has not been previously investigated. Here, we combined bead aggregation assay, high-speed atomic force microcopy (HS-AFM), and localization analysis of HS-AFM images to investigate the binding mechanism of Celsr. The analyses revealed that EC1–EC8 fully overlapped by twisting the ectodomains to form trans-dimer conformations, and EC1–EC5 were sufficient for the binding. This study provides important insights into the binding mechanism of Celsr.

1Pos166 アミロイドβ凝集体はヒト脳微小血管内皮細胞の異常なアクチンの組織化と細胞死を誘発する
Amyloid-β aggregates induce abnormal actin organization and death of human brain microvascular endothelial cell

Keiya Shimamori[1], Yushiro Take[2], Yusaku Chikai[1], Yukina Kuroraki[1], Masahiro Kuragano[1], Kiyotaka Tokuraku[1] ([1]*Grad. Sch. of Eng., Muroran Inst. of Tech.*, [2]*Ohkawara Neurosurgical Hospital*)

Cerebral amyloid angiopathy is a disease in which amyloid-β (Aβ) is deposited on the walls of cerebral blood vessels, causing hemorrhage. However, it's not well understood how Aβ destroys the walls of blood vessels. Here, we observed the effect of Aβ on human primary brain microvascular endothelial cells (hBMECs) in real-time. Visualization of Aβ aggregation using quantum dots revealed that aggregates firmly anchored the cells on the plate surface, eventually inhibited cell motility and caused cell death. Furthermore, we found that abnormal actin dots over 10 μm^2 were formed in Aβ treated cells. These results suggest that Aβ aggregates around hBMECs anchor them to the substrate, and induce abnormal actin organization, leading to cell death.

1Pos167 酸素消費を伴わないミトコンドリア電子伝達機構
Mitochondrial electron transfer mechanism without oxygen consumption

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Mitochondria obtain energy for ATP synthesis through electron transfer. Since electrons are finally passed to oxygen by cytochrome oxidase, mitochondrial electron transfer is measured by monitoring oxygen consumption. On the other hand, electron transfer is coupled with proton translocation to generate membrane potential. In this study, we measured electron transfer by monitoring membrane potential under conditions in which electrons were not transferred to oxygen. As a result, even when electrons were not transferred to oxygen in cytochrome oxidase, upon supply of electrons membrane potential was formed and ATP was synthesized, although only slightly. This mechanism may play some role in areas with low oxygen concentrations, such as obliteration.

1Pos168 局所加熱法を用いた表皮細胞内変異型ケラチンフィラメント熱ストレス応答の経時変化解析
Time-course analysis of mutant keratin filament dynamics in cultured epidermal cells under thermal stress using a local heating method

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Epidermolysis bullosa simplex, a form of skin blistrering disease, is caused by mutations in skin keratins KRT5 or KRT14. Disruption and aggregation of intracellular keratin filaments and increasing skin fragility are observed, and blisters appear after relativery minor mechanical stress. Previous reports have shown that various forms of stress cause aggregation of mutant keratin filaments in cells, particularly heat stress, but it is still unclear how keratin filaments aggregate over time. Here, we applied an optically controlled local heating method under the fluorescence microscope to quantitatively visualize the thermal response of intracellular keratin filaments.

1Pos169 シグナル伝達機構解明のための巨大細胞利用
Use of giant cells to study cell-cell signaling mechanisms

Yukihisa Hayashida, Yusuke Morimoto (*Kyushu Institute of Technology (Grad. Sch. Comp. Sci. and Sys. Eng., Kyushu Inst. Tech)*)

When considering relationships among multiple cells, each cell is assumed to be the same size, and the role and significance of cell size are unclear in many experimental systems. We used *Dictyostelium discoideum*, which has been used as a model organism for cell signaling and cell motility mechanisms. *D. discoideum* lives as a unicellular cell under nutritional conditions, but under starvation conditions, cAMP signaling causes aggregation of several hundred thousand cells. To clarify the relationship between the signaling mechanism and cell size, we analyzed changes in signaling when cell division was suppressed and cell size was increased.

1Pos170 べん毛のロッド-フック型タンパク質の輸送順序
Transport order of the flagellar rod-hook type proteins

Reika Igarashi, Norihiro Takekawa, Katsumi Imada (*Dept. Macromol. Sci., Grad. Sch. Sci., Osaka Univ.*)

The flagellar type III protein export apparatus (fT3SS) is used for construction of the flagellar axial structure, including the rod, the hook, and the filament. Previous studies have revealed that the rod-hook type proteins are transported prior to the filament type proteins. However, the order in transport of the rod-hook type proteins is still unknown. In this study, we analyzed the secretion of the rod-hook type proteins using inverted membrane vesicles (IMVs) and found a clear orderintransport of the rod proteins. The proximal rod component proteins are required for transport of distal rod component proteins. The hook type proteins also showed secretion order. We will discuss the molecular mechanism of the order in transport of the rod-hook type proteins.

1Pos171 無傷のミトコンドリアの単離・保存法の検討
Methods for isolating and preserving intact mitochondria

Asaka Ogihara, Arima Okutani, Wataru Uchiumi, Miki Kanatani, Yoshihiro Ohta (*Department of Biotechnology and Life Sciences, Graduate school of Engineering, Tokyo University of Agriculture and Technology*)

Intact isolated mitochondria have been desired for mitochondrial research and mitochondria administration therapy. However, most mitochondria are damaged during isolation because mitochondria are isolated by cell homogenization and detergent permeabilization of the cell membrane. Therefore, we developed a method for mitochondria isolation that does not involve permeabilization by homogenization or detergent. We also developed a method for freeze-thaw treatment of mitochondria that does not damage mitochondria. Mitochondria isolated with this method had intact outer membranes and were highly polarized. But mitochondria isolated with the conventional method did not and proteins in the intermembrane space were lost. Details are discussed.

1Pos172 アミロイドβの凝集が細胞の集合に与える影響の解析
Analysis of the effect of amyloid β aggregation on cell assembly

Ayaka Ota, Masahiro Kuragano, Kiyotaka Tokuraku (*Grad. Sch. Eng., Muroran Inst. of Tech.*)

Abnormal amyloid β (Aβ) aggregation in the brain tissue is thought to a cause of neuronal defects, resulting Alzheimer's disease. Therefore, new methods are needed to mimic structures in the brain and to quantitatively assess changes in the cell assembly by Aβ. Here, we succeeded in the spheroid formation of SH-SY5Y cells on poly-D-lysine coating and observed spheroids of about 500 μm^2. Further, we evaluated the effect of Aβ treatment in cell assembly by real-time imaging. We found that cell assembly was inhibited at 0.04 to 16 μM Aβ. Whereas, cell assembly was promoted at 0.0004 to 0.004 μM Aβ. We will clarify the physiological significance of effects of Aβ in the spheroid formation and to investigate effects of Aβ aggregation inhibitors on these phenomena.

1Pos173 Theoretical studies on macrophase separation in systems composed of two solutes and one solvent using a solvent-free coarse-grained model

Yuki Norizoe, Naoki Iso, Takahiro Sakaue (*Department of Physical Sciences, Aoyama Gakuin University*)

Macrophase separation observed in biological and cellular systems have been studied extensively in the past several years. Phase equilibria and binodal lines in systems composed of one solute and one solvent in particular were studied intensively in early works, whereas macrophase separation in systems consisting of more than one solute were reserved for future works. Here we cast light on this problem, and theoretically study the macrophase separation in systems composed of two solutes and one solvent using a solvent-free coarse-grained model. In this model, explicit solvent molecules are integrated out and replaced with implicit solvent, so that both theoretical consideration and the amount of computation in molecular simulation are relieved.

1Pos174 自発運動する細胞の興奮系 Ras を抑制する GAP の同定
Identification of GAP that suppresses the excitatory Ras in spontaneous cell motility

Guangyu Cheng[1], Satomi Matsuoka[1,2,3], Masahiro Ueda[1,2,3] ([1]*Grad. Sch. Sci., Osaka University*, [2]*Grad. Sch. of Front. Biosci., Osaka University*, [3]*BDR, RIKEN*)

Eukaryotic cells move without environmental spatial cues, called spontaneous cell motility, which arises due to an excitability of Ras that self-organizes an anterior-posterior polarity. It has been assumed that it depends on an activity of GTPase activating protein (GAP) inactivating Ras in a spatiotemporally coordinated manner, although it has not been identified so far. We have constructed a set of *Dictyostelium discoideum* cell strains over-expressing 14 GAPs in a GFP-tagged form, in which the excitable dynamics like traveling waves on the cell membrane was analyzed by imaging a fluorescent probe of activated Ras (RBD-RFP). We found several GAPs which over-expression caused a suppression of Ras excitability, suggesting potent components of the excitable system.

1Pos175 マイコプラズマ・モービレの滑走方向は細胞体の非対称な形状と相関がある
Gliding direction of *Mycoplasma mobile* correlates with asymmetric configuration of the cell body

Kana Suzuki[1], Daisuke Nakane[2], Azusa Kage[1], Takayuki Nishizaka[1] ([1]*Dept. Physics, Gakushuin Univ.*, [2]*Univ. of Electro-Communications*)

The bacterium *Mycoplasma mobile* has flask shape and glide on a solid surface with curved trajectories. We here hypothesize that the configuration of the cell guides the direction, keeping the balance between the gliding force and the friction. To test this idea, the intensity profile of the cell body was simultaneously fitted with the narrow and the wide two-dimensional gaussians as a single merged function, in which the center of the narrow one located on a longer axis of the wide one. The declination of the protruded part was then defined as the angle difference between the two longer axes of the gaussians. Notably, the declination showed strong positive correlation with the gliding direction (correlation coefficient 0.86; $n = 5$), which corroborates our hypothesis.

1Pos176 Direct observation of the functional dynamics by which CAP1 interacts with F-actin and cofilin by high-speed AFM

Phuong Doan N. Nguyen[1], Hiroshi Abe[2], Shoichiro Ono[3], Noriyuki Kodera[4] ([1]*Grad. Sch. NanoLS., Kanazawa Univ.*, [2]*Dept. Biol., Chiba Univ.*, [3]*Dept. Pathol. & Cell Biol., Emory Univ.*, [4]*WPI-NanoLSI, Kanazawa Univ.*)

Cyclase-associated protein 1 (CAP1) is one of the actin-binding proteins (ABPs) that is essential for the dynamic disassembly processes of F-actin. Here, we observed how individual XCAP1, CAP1 isolated from *Xenopus laevis oocytes*, interacts with actin filaments using high-speed AFM. We visualized that XCAP1 binds to the sides of actin filaments for ~0.7s in presence of ATP. Then, it impacts the structure of F-actin including height and helical pitch. Also, imaging data showed that cofilin dissociations occur extensively when XCAP1 is added to cofilin-saturated actin filaments. This result suggests that XCAP1 is responsible for making actin filaments susceptible to sever by cofilin, which well explains the function of CAP1 in increasing the actin turnover rate.

1Pos177 細胞の自発運動において Ras 興奮系のノイズ強度の最適化にスフィンゴミエリン代謝系が関与する
Noise generation by sphingomyelin metabolism optimizes Ras excitability for cell migration

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A small GTPase, Ras, constitutes an excitable system which works for a spontaneous generation of anterior-posterior polarity in eukaryotic motile cells. The mechanism how the excitability is regulated on the cell membrane has been unsolved. We have found that pharmacological inhibition of sphingomyelin metabolism suppressed the excitability and spontaneous cell motility, as well as chemotactic responses upon low concentration of chemoattractant. The mean and variance of the number density of Ras-GTP molecules on the membrane were reduced in these cells, revealed by super-resolution microscopy. The results suggest that the excitability is regulated by the noise generated by sphingomyelin metabolism in a manner similar to a stochastic resonance mechanism.

1Pos178 TIRF 観察によるアクチン線維に対するサイトカラシン D の作用理解
Inhibitory mechanism of cytochalasin D on actin by TIRF observations

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Cytochalasin D (CD) is the widely used inhibitor for actin polymerization for studying various functions in living cells. Most of the known functions were elucidated from spectroscopic measurements in the 1980s. Among them, the molecular mechanism of severing functions is still unclear. Because the barbed end of a severed actin filament is capped immediately after severing, both polymerization and depolymerization could not be detected. This makes it difficult to elucidate the inhibitory mechanism of CD on actin polymerization by solution assays. In this study, TIRF was used to observe the depolymerization of the single actin filament. We will analyze and detect the kinetical features of the interaction of CD to a single actin filament.

1Pos179 極性形成に関わる膜タンパク質 Frizzled の細胞間隙での蛍光 1 分子観察
Single molecule observation of polarity-related membrane proteins at the cell-cell interface; immobilization and accumulation of Frizzled

Rinshi Kasai[1], Yuri Nemoto[2] ([1]*iGCORE, Gifu Univ.*, [2]*OIST*)

Planar cell polarity is composed of various protein species. Adhesion GPCR (G-protein coupled receptor) forms a homophilic complex at the cell-cell interface, which provides an adhesion structure. Although Frizzled (FZD), one of the key proteins for polarity formation, is known to be accumulated at the interface, the regulation mechanism remains unclear. By observing FZD at the single molecule level in the plasma membrane where two cells were contacting via adhesion structures, we found that some of FZD proteins were immobilized at the interface, leading to an accumulation. Surprisingly, FZD without its carboxyl terminus was also found to be immobilized, suggesting that immobilization of FZD is synergistically regulated by multiple domains.

1Pos180 Bottom-up strategy による軸糸の屈曲波の再構築
Reconstitution of the axonemal beating by bottom-up strategy

Isabella Guido[1], Kenta Ishibashi[2], Hitoshi Sakakibara[2], Andrej Vilfan[3], Eberhard Bodenschatz[1], Ramin Golestanian[1], **Kazuhiro Oiwa[2,4]** ([1]*MPI. Dynamics Self-Organization*, [2]*Adv. ICT Res. Inst., NICT*, [3]*Jozef Stefan Inst.*, [4]*Grad. Sch. Sci., Univ. Hyogo*)

Full understanding of the propagating and switching mechanism of bend in eukaryotic cilia and flagella demands the precise knowledge of dynein activation and inhibition in the 3D lattice under strict structural constraints. Therefore, we constructed a 3D system with constant constraints that mimics an axoneme. The system, in which the microtubules with the same polarity were anchored at the basal end and the outer arm dynein were self-assembled along the microtubule, was found to repeatedly buckle in the presence of ATP. We call this system a "synthoneme" that mimics the repetitive dynamics of axonemes. The synthonemes have been used as a tool for study on the activation process of force generation and the suppression process of switching.

1Pos181 Anomalous dynamics of cardiomyocytes and fibroblasts on PDMS substrate

Arata Nagai, Kaito Kojima, Ryu Kidokoro, Shota Nozaki, Ayu Sasaki, Yuuta Moriyama, Toshiyuki Mitsui (*Dept. Phys. Sch. Sci. Aogaku Univ.*)

Cell migration on the substrate is a complex dynamic process. Although cell movement appears to be Brownian, the MSD is not linear. Co-cultures of cardiomyocytes and fibroblasts also show more complex dynamics to form cell aggregates that generate a beat, although cardiomyocytes are extremely immobile. Fibroblasts must play an important role in aggregate formation. Here we study these cell dynamics. The substrate is PDMS, which does not exert mechanical stress on the cells. We observed the cells every 15 minutes for more than 24 hours. We visualize the mobilities of individual cells. The cooperative diffusion of cardiomyocytes and fibroblasts to form aggregates will be presented. Finally, we discuss a way for cell-cell communication during their diffusion.

1Pos182 ミトコンドリア電子伝達系複合体の時間依存的酸化ダメージの検出
Detection of time-dependent oxidative damages of mitochondrial electron transfer complexes

Shizuku Saito, Yoshihiro Ohta (*Department of Biotechnology and Life Science, Graduate school of Engineering, Tokyo University of Agriculture and Technology*)

The mitochondrial electron transfer complexes are where reactive oxygen species（ROS) are generated and also where they are damaged by ROS. The damage of electron transfer complexes lead to further generation of ROS and reduces ATP synthesis. The purpose of this study is to detect in which order the five mitocondrial electron transfer complexes lose their activities when cells are incubated with hydrogen peroxide. The activity of the electron transfer complexes was examined by monitoring the mitochondrial membrane potential changes associated with proton translocation across the inner mitochondrial membrane. Our results showed that hydrogen peroxide first reduced the activity of complex I and then complexes IV and V. We would like to discuss the details.

1Pos183 回転方向に依存した大腸菌べん毛モーターの回転揺らぎの原因
Investigation for the cause of rotational fluctuations depending on the rotational direction of flagellar motor

Kazumi Akahoshi, Yumiko Uchida, Yong-Suk Che, Akihiko Ishijima, Hajime Fukuoka (*Grad. Sch. Frontier Biosci. Osaka Univ*)

Flagellar motor of *E. coli* rotates in clockwise (CW) and counterclockwise (CCW) directions. In this study, we investigated the rotational fluctuation depending on the rotational direction by measuring the rotation with high temporal resolution (12,500 fps). In wild-type cell, we found that CW rotation was stable, while CCW rotation was unstable and appeared to transiently shrink the rotational orbits. On the other hand, in mutant cell having straight hook, the transient shrink of rotational orbit during CCW rotation was not observed and both CCW and CW rotation were stable. These results indicate that the rotational fluctuation during CCW rotation is caused by the structure of the hook. We will discuss these results at annual meeting.

1Pos184 酵母ミトコンドリアの膜電位変動観察の試み
Observation of membrane potential fluctuations of yeast mitochondria

Sora Maekawa, Yoshihiro Ohta (*Department of Biotechnology and Life Sciences, Graduate school of Engineering, Tokyo University of Agriculture and Technology*)

Mitochondria are organelles involved in energy metabolisms and signal transductions. Since many of these are regulated by the membrane potential across the inner membrane, the membrane potential has been extensively measured in mammalian cells. In this study, we have tried the time-resolved measurement of mitochondrial membrane potential in yeast mitochondria by fluorescence imaging. To manipulate mitochondrial function, we aimed to measure mitochondria in semi-intact spheroplast or isolated mitochondria. In this presentation, we will report the results of our investigation on changes in the membrane potential upon addition of respiration substrates by fluorescence imaging with the membrane potential-sensitive fluorescent dye TMRE.

1Pos185 デスミンフィラメントとアクチンフィラメントとの相互作用の観察
Observation of the interaction between single desmin filaments and single actin filaments in a reconstituted motility system

Takumi Ishizaka, Kuniyuki Hatori (*Grad. Sch. Sci. Eng., Yamagata Univ.*)

Desmin is an intermediate filament (IF) protein expressed in muscle. Cross-talk between actin and desmin filaments may be involved in regulation of muscle architecture. To directly observe physical interactions between these filaments, we prepared the myosin-actin-desmin complexes on a collodion-coated slide glass. Actin and desmin were labeled with distinct fluorescent dyes. When adding ATP, moving actin filaments across desmin IFs were observed via fluorescence microscopy. Velocity analysis showed that the moving directions of actin filaments changed before and after contact with desmin IFs. The speed tended to decrease during the contact. This result suggests that a desmin IF has a potential ability to interact with an actin filament.

1Pos186 1 粒子観察による細胞外小胞の細胞選択的結合の分子機構解明
Molecular mechanisms of selective binding of small extracellular vesicles to recipient cells as revealed by single-particle imaging

Tatsuki Isogai[1], Koichiro M. Hirosawa[2], Miki Kanno[3], Ayano Syo[4], Yasuhiko Kizuka[2,5], Yasunari Yokota[6], Kenichi G. N. Suzuki[2,5] ([1]*UGSAS, Gifu Univ.*, [2]*iGCORE, Gifu Univ.*, [3]*Grad. Sch. Nat. Sci. Tech., Gifu Univ.*, [4]*Dept. App. Bio. Sci., Gifu Univ.*, [5]*CREST, JST*, [6]*Dept. Eng., Gifu Univ.*)

Small extracellular vesicles (sEVs) mediate cell-cell communication, and sEV studies may resolve issues of metastatic organotropism. Recent indirect experiments suggested that tumor-derived sEVs selectively bind to the recipient cells by integrin subunits. However, the molecular mechanisms are unknown. To solve this issue, we performed single-particle tracking, and found that several integrin subunits were responsible for binding of sEVs to extracellular matrix (ECM), which was regulated by N-glycans. Furthermore, we directly visualized the binding of sEVs with ECM on living cells by super-resolution microscopy. These results demonstrate that the selective binding of sEVs with the recipient cells is caused by specific binding of integrin in sEVs with ECM on the cells.

1Pos187 Morphology of Adhering Vesicles

Toshikaze Chiba[1], Hironori Sugiyama[2], Taro Toyota[3], Yuka Sakuma[1], Masayuki Imai[1], Primož Ziherl[4,5] ([1]*Department of Physics, Tohoku University*, [2]*ExCELLS, National Institutes of Natural Sciences*, [3]*Department of Basic Science, Graduate School of Arts and Sciences, The University of Tokyo*, [4]*Faculty of Mathematics and Physics, University of Ljubljana*, [5]*Jožef Stefan Institute*)

Multicellular organisms regulate their static morphology competing with passive forces in a single cell to tissue level. So far, morphologies of lipid vesicles are examined for understanding the deformation in plasma cell membrane, yet little is known for those of adhering vesicles. In this study, we examined the morphology of i) vesicle triplet and ii) vesicle planar assembly. We observed the two significant shapes: Floppy prolate and clumped sigmoidal contact those are supposed to be the weaker and stronger adhesion limits. We developed the microfluidics for assembling the iso-radius vesicle in a planar structure applying the fluid dynamic displacement. Our approaches pave the way to understanding the deflated membrane morphology such as organelle and tumorigenesis.

1Pos188 基板支持リン脂質積層膜の軟 X 線直線偏光による相状態解析
Soft X-ray polarization analysis of lipid order for phospholipid multilayers supported on hydrophilic surfaces

Shin-ichi Wada[1,2], Masataka Tabuse[1] ([1]*Grad. Sch. Adv. Sci. Eng., Hiroshima Univ.*, [2]*HiSOR, Hiroshima Univ.*)

Formation of quasi-biomembranes by immobilizing lipid films on surfaces is important as a fundamental process in nanotechnology applications such as biosensors and molecular electronic devices. We have found that substrate-supported phospholipid films prepared by a simple drop-drying method of lipid solution on a hydrophilic substrate maintain high orientation even for forming multilayers. In order to investigate the orientation information, lipid order, we measured the soft x-ray absorption of two kinds of phospholipid films, DPPC and DOPC. Polarization dependence of the absorption spectra allowed us to quantitatively analyze the two components: the orderly oriented carbon chains and the randomly ordered ones.

1Pos189 薬剤代謝におけるコレステロールの役割を探るためのモデル生体膜と薬剤の相互作用研究：リン脂質 POPE/コレステロール/クロルゾキサゾン系
A model biomembrane study on the role of cholesterol in cytochrome P450 drug metabolism: POPE/cholesterol/ chlorzoxazone systems

Shosei Kano, **Hiroshi Takahashi** (*Grad. Sch. Sci. Tech., Gunma Univ.*)

Many drugs are metabolized by cytochrome P450 (CYP) in the endoplasmic reticulum (ER) membrane. Here we studied the role of cholesterol in CYP-drug metabolism using model membrane systems comprising palmitoyl-oleoyl-phosphatidylethanolamine (POPE) and Chol [1]. Chlorzoxazone (CZX) was used as the CYP-substrate drug. Dialysis and X-ray structural analyses showed that Chol inhibited CZX entry into the bilayer with an increase in Chol concentration. The Chol concentration in the ER membrane is much lower than that in the plasma membrane. This fact may allow CYP-substrate drugs to enter the ER membrane more easily than other organelle membranes, yielding efficient drug metabolism.
[1] Kano & Takahashi, *BBA* (2022). doi:10.1016/j.bbamem.2022.183954.

1Pos190 薬物添加による血液脳関門モデル膜の膜厚変化に関する X 線回折研究：スフィンゴミエリンの役割
An X-ray diffraction study of changes in the blood-brain barrier model membrane thickness induced by adding drugs : role of sphingomyelin

Anna Ajima, Hiroshi Takahashi (*Grad. Sch. Sci. Tech., Gunma Univ.*)

The blood-brain barrier (BBB) regulates the exchange of substances between blood vessels and brain cells to protect the brain. The BBB membranes contain more sphingomyelin (SM) than other biomembranes. In this study, we aimed to clarify the importance of lipid composition in drug permeation of the BBB. We added various concentrations of drugs to model membranes with some lipid compositions and examined the changes in membrane thickness by X-ray diffraction measurements. We found that the model membranes without SM showed a more significant change in membrane thickness than those with SM, indicating that the drugs easily penetrated the membranes. This suggests that the inclusion of SM in model membranes is effective in mimicking the BBB.

1Pos191 パターン化人工膜へのエクソソーム導入技術の開発
Reconstitution of exosomes into a patterned model membrane

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Exosomes have important roles for intercellular communication and have potential as therapeutic and diagnostic tools. Exosome tropism and uptake should depend on their membranes, but the mechanisms are not well understood. We have been developing a new methodology for analyzing exosome membranes. We introduced exosomes having fluorescently labeled marker proteins into nanometric space between a silicone sheet and a patterned polymeric lipid bilayer on a substrate. Fluorescence microscopic observation showed lateral diffusion of the proteins in nanometric space, suggesting that exosomes formed a planar bilayer. Reconstitution of exosomes in a planar bilayer should provide new opportunities for characterizing the molecular properties of exosome membranes.

1Pos192 Laurdan の時間分解蛍光解析法からみる脂質膜水和状態
Lipid-Surrounding Hydration States Probed by Time-Resolved Emission Spectra of Laurdan

Nozomi Watanabe[1], Keishi Suga[2], J. Peter Slotte[3], Thomas K. M. Nyholm[3], Hiroshi Umakoshi[1] ([1]*Graduate School of Engineering Science, Osaka University*, [2]*Graduate School of Engineering, Tohoku University*, [3]*Faculty of Science and Engineering, Åbo Akademi University*)

The hydration properties of the lipid bilayer are essential for cell membrane activity. In this study, the hydration states of the interfacial region of lipid bilayers were investigated on the basis of the time-resolved emission spectra (TRES) analysis of Laurdan, a common fluorescence probe used to analyze membrane hydration. From the correlation of fluorescence lifetimes and spectra, the competition between the collisional quenching and the hydration effects of water molecules was indicated. Furthermore, based on the collisional quenching theory, the distribution of the water population per lipid was estimated. This approach provides novel insights for the analysis of molecular hydration states in dynamic lipid membrane using the fluorescence of Laurdan.

1Pos193 エクソソーム評価系としてのブラウン運動解析
Brownian motion analysis as an exosome evaluation system

Kei Takahashi, Yui Miyabayashi, Takuo Yamaki (*CellSource Co., Ltd.*)

Research on exosomes and their functions has broad implications ranging from physiological tissue regulation to pathogenic injury and organ remodeling. Exosomes are 100 nm scale extracellular vesicles, and the most conventional method for detecting them is based on Brownian motion analysis to obtain a particle size distribution. However, this method assumes that exosomes behave as Newtonian fluids and therefore is not suitable for distinguishing exosomes from other components. Here we focus on the viscoelasticity of exosomes as microrheology to find dynamic modes that are distinct from the motional behavior of Newtonian fluids. We apply our method to cell culture supernatants to confirm how many exosomes are present in samples of heterogeneous composition.

1Pos194 細胞質型ホスホリパーゼ A_2 活性化とセラミド 1-リン酸の膜動態の関連性
Relationship between the membrane dynamics of ceramide 1-phosphate domains and the activation of cytosolic phospholipase A_2

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Ceramide 1-phosphate (C1P) promotes the activity of cPLA$_2$α by specifically binding to the C2 domain of cPLA$_2$α. We hypothesized that the dynamic behavior of C1P in biomembranes was important for the molecular recognition of cPLA$_2$α. In this study, we evaluated the physical properties of C1P domains in model membranes by time-resolved fluorescence. The results indicated that the capacity of domain formation is dependent on the colipid compositions and hydrophilic structures of C1P. In addition, SPR measurements suggested that the membrane environment with higher domain forming ability has higher binding affinity to cPLA$_2$α. These findings will lead to a better understanding of the membrane dynamics that plays a key role in the biological function of lipid mediator.

1Pos195 浸透圧下の巨大リポソームでの抗菌ペプチド・マガイニン 2 のポア形成とその進化
Antimicrobial peptide magainin 2 (Mag)-induced pore formation and its evolution in single GUVs under osmotic pressure (Π)

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We examined the effect of membrane tension (σ) of GUVs under Π (1) on Mag-induced pore formation and its evolution (2). Under low Π, Mag induced nanopore formation. In contrast, Mag induced rupture of a subset of GUVs under higher Π. In the rupture, first a small micropore was formed, then its radius increased and concomitantly the fluorescence intensity of the membrane at the pore rim due to NBD-PE increased, and finally the GUV transformed into a membrane aggregate. Several results indicate that the GUV rupture is originated from Mag-induced pore formation. The rate constant of Mag-induced pore formation increased with σ in the inner leaflet. We discussed the effect of Π on Mag-induced pore formation. [1] J. Phys. Chem. B 124, 5588, 2020. [2] PCCP, 24, 6716,2022

1Pos196 酸性アミノ酸の側鎖長を調整することによる環状ペプチドの pH 依存性膜透過性の制御
Control of pH-dependent membrane permeation of cyclic peptides by adjusting side chain length of acidic amino acids

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For developing drug carriers targeted to cancer, we have attempted to control the pH-dependent membrane permeation of cyclic peptides. The liposomal membrane permeation of cyclic peptides was investigated at various pH using a fluorescence-based assay. The pK_a value of the membrane permeation was increased for cyclic peptides with longer acidic amino acid side chains. In particular, the cyclic peptide with 2-aminosuberic acid, which has a side chain carbon number of 6, permeated the liposomal membrane at pH 6.5, which corresponds to the typical pH of cancer tissue.

1Pos197 粗視化陰溶媒脂質力場、iSoLF、を用いて GENESIS による多成分脂質システムの分子動力学シミュレーション
Extension of the Implicit Solvent Lipid Force Field, iSoLF, for the simulation of large multi-component lipidic systems using GENESIS

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Molecular dynamics (**MD**) simulations of lipidic systems are of great interest due to the many biological phenomena taking place in biological membrane systems. By using coarse-grained (**CG**) models, which are simplified descriptions of the atomic models, the computational cost of MD simulations is greatly reduced, increasing the applicability in the temporal and spatial domain. In this work, we present a new iteration of the implicit solvent lipid force field, **iSoLF**, a CG model for lipid simulation. We have greatly increased the available parameters to more common lipids. Additionally, we have also included the treatment of electrostatic interactions. Finally, we demonstrate its application on large lipidic systems by implementing iSoLF in the **GENESIS** MD software.

1Pos198 一定張力による GUV 中のポア形成に対する脂質成分や分布の効果
Effect of lipid composition and distribution on constant tension-induced pore formation in GUVs

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The studies of constant tension-induced pore formation in GUVs can provide information on characteristics of lipidic pores and their line tension (1,2). Here we examined the effect of lipid composition and distribution on the rate constant of rupture (k_r) of GUVs. The values of k_r of DOPG/DOPE were smaller than those of DOPG/DOPC at the same tension. Its analysis indicates that the line tension of a lipidic pore in DOPG/DOPE is larger than that in DOPG/DOPC. The values of k_r of lyso PC/DOPG/DOPC were larger than those of DOPG/DOPC at the same tension. We also investigated the effect of asymmetric distribution (3) of lyso PC in GUV bilayer on the k_r.
[1] Phys. Rev. E, 92, 012708, 2015, [2] Biophys. J., 111,2190, 2016, [3] J. Phys. Chem. B, 123, 4645, 2019

1Pos199 Design and characterization of enzyme-responsive synthetic ion channels

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While passive synthetic ion channels have been studied extensively, stimuli-responsive control has been somewhat overlooked. Enzyme-responsiveness would provide a natural interface with biological targets utilizing enzyme-dependent signaling pathways. However, enzyme-responsiveness has not yet been demonstrated in synthetic ion channels. We designed an enzyme-responsive ion channel based on metal-organic polyhedra (MOP). A phosphorylatable peptide was conjugated to the MOP via coordination chemistry as an open-close control element. The effect of phosphorylation on channel function was studied with a microfabricated lipid bilayer model. With a view to applications in therapeutics, effects of channel activation on cell growth and viability were also studied.

1Pos200 膜水系における環状人工イオンチャネルの QM/MM シミュレーション
QM/MM simulations of cyclic artificial ion channel in membrane-water system

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The development of artificial molecular machines mimicking biomolecular functions has been advanced. Recently, a cyclic artificial ion channel $\mathbf{C_{FF}}$ has been developed by Kinbara et al. According to experimental results, $\mathbf{C_{FF}}$ transports cations across the membrane and has potassium selectivity. To assess channel structures of $\mathbf{C_{FF}}$ in the membrane-water system at atomic resolution, all-atom hybrid quantum-mechanical/molecular mechanical (QM/MM) simulations were performed. Specific interactions between the potassium ion in the pore center and the perfluorinated aromatic units were observed in QM/MM simulation. From the different interaction modes of the potassium and sodium ions, the mechanism underlying the ion selectivity could be understood.

1Pos201 CBB 法を用いた再構成膜でのアクアポリン 6 のイオン透過特性の解析
Ion conducting properties of Aquaporin 6 reconstituted in the contact bubble bilayer

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Aquaporin 6 (AQP6) is a unique AQP that allows ions as well as water to pass through, but its mechanism and physiological significance remain controversial. We aim to reveal the ion conducting properties of AQP6 electrophysiologically using the contact bubble bilayer (CBB). The purified human AQP6 was reconstituted into the CBB, and the ionic current was evaluated in the presence of symmetrical 100 mM NaCl. We successfully measured the single-AQP6 current at acidic pH where the ion-conducting pore was anion-selective, and the gate of the pore was constantly open at ±50 mV. AQP6 also exhibited ion conduction in the presence of Hg^{2+}, which has been reported to activate water permeation activity of AQP6.

1Pos202 アガロースゲルビーズを用いた人工膜チャネル電流測定
An artificial lipid bilayer ion-channel recording method using agarose gel beads

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The formation of rapid and stable lipid bilayers is key to improving the efficiency and accuracy of channel current recordings. By using agarose gel bead as support for lipid bilayers, we have succeeded in simplifying the lipid bilayer formation technique and dramatically shortening the time needed for the current measurement. Here, we show additional results of investigating the optimal conditions to simultaneously measure multiple channel currents. We measure to apply our technology to highly efficient drug screening devices.

1Pos203 リポソーム内タンパク質機能発現制御のための膜透過性ペプチドの利用
Use of Cell penetrating peptide for the regulation of protein functional expression in giant unilamellar vesicles

Akari Miwa, Koki Kamiya (*Grad. Sch. Sci. Tech., Gunma Univ.*)

Cell penetrating peptides (CPPs), which are conjugated with non-permeable molecules (proteins), can be transported across the membrane. The direct translocation is driven by the negative transmembrane potential generating the lipid bilayer. We investigated the translocation of CPPs-protein complexes into lipid membrane, and the enzyme reactions in GUVs. The complexes were interacted with asymmetric GUVs containing DOPG or DOPS in the inner leaflet. CPPs mediated translocation of DNase I into the GUVs was triggered by negatively charged lipid on the inner leaflet. Finally, we demonstrated the formation of cross-linked actin network into GUVs based on the translocation. This system has a potential to control the start of the protein reaction inside GUVs.

1Pos204 Development of DNA nanostructures that function as artificial channel/transducer on a giant vesicle membrane

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We designed an artificial channel based on DNA origami technology. The DNA origami channel has a pore of 10 nm in diameter. The larger pore can transport molecules that cannot be transported by natural membrane proteins. We confirmed the transport of ssDNA and dextran (MW≈40k) through the DNA origami channel on giant vesicle membranes.
We also designed a small DNA signal transducer. It consists of a six-helix bundle “body” and a movable dsDNA “shaft” located at the center of the body. The movement of the shaft transmits signals through lipid membranes. We confirmed the shaft movement using FRET technique. We also report the purification method of the DNA nanostructure with hydrophobic modifications.

1Pos205 Membrane Permeability of Mono-Amino Acids Estimated by Planar Lipid Bilayer System

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Understanding of membrane permeation of cell-penetrating peptides is essential for the application of cell modification and therapy. Although there are extensive efforts for revealing the mechanism of the permeation, it has still been argued. To understand the effect of the permeation at the mono-amino acid level, we evaluated the permeability of Arg, Lys, Asn, Tyr, Phe, Trp, Val, Leu, and Ile by planer lipid bilayer system which does not require the fluorescent label. We verified the system feasibility to determine the membrane permeability and found that the mono-amino acids (~20 mM) directly permeated the lipid membrane. We will discuss the relationship between the permeation efficiency and the chemical structure of amino acids.

1Pos206 分子動力学計算による CLC^F における F^-輸送機構の解析
F^- export mechanism in CLC^F using molecular dynamics simulations

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F^- ion can inhibit bacterial growth. However, many bacterial strains have evolved to be resistant to F^-, utilizing exporters situated in the bacterial cell membranes that quickly reduce the intracellular F^- concentration. Our goal is to unlock the molecular details of these F^- exporters. It has been hypothesized that the H^+ gate E118 in CLC^F-Eca undergoes rotation, carrying H^+ from the extracellular to intracellular solutions and propelling F^- through the pore. We also hypothesize that F^- passes more easily than Cl^- due to its smaller radius. Therefore, we investigate mechanism of F^- export in CLC^F by using molecular dynamics (MD) simulation, and analyzed the potential of mean force (PMF) of each ion transport in reactive coordinates of F^- .

1Pos207 筋小胞体 Ca ポンプのヘリックス M2 と M6 の Ca 輸送における役割
Role of M2 and M6 helices of sarcoplasmic reticulum Ca pump in Ca transport

Takashi Daiho (*Asahikawa Med. Univ. Biochemistry*)

Ca pump transport Ca coupled with ATP-hydrolysis. The catalytic site consists of the three cytoplasmic domains N, P, and A and the motion of A-domain functions in regulating Ca gating at transmembrane region (TM). The long M2 helix of TM linked with A-domain changes its structure during transport cycle. We have previously shown that Ala substitution of Gly105 at the border of transmembrane part (M2m) and cytoplasmic part (M2c) results in slow EP isomerization and uncoupling. Gly105 functions as a flexible hinge of M2m/M2c, which is critical for Ca transport. We have found that the defects of G105A could be restored by an additional mutation at M2m. In this study, we will report functional consequences of mutations on M2m and M6 residues.

1Pos208 PI3K シグナル伝達は S-G2 期の ERK の時間的調節において重要な役割を果たす
PI3K signaling plays a critical role in the temporal regulation of ERK in the S-G2 phase

Ryo Yoshizawa, Nobuhisa Umeki, Yasushi Sako (*Wako Inst., Riken*)

The growth factor-induced RTK signaling plays important roles in the regulation of cell cycle progression, especially from the G0/G1 phase. In this study, to investigate the relationship between RTK signaling and cell cycle progression, we observed the response dynamics of ERK to the EGF stimulation in A549 cells with the identification of the cell cycle phase. As a result, ERK showed a transient response in the G0/G1 phase but a sustained response in the S-G2 phase. A selective inhibitor analysis indicated that PI3K activity affects ERK dynamics in the S-G2 phase and arrested the cell cycle progression. These results suggest that PI3K is a key factor for the transition from the S-G2 phase, but not the G0/G1 phase, regulating the growth factor-induced RTK signaling.

1Pos209 ペプチドナノディスクを用いた光受容体ロドプシンのパターン化モデル生体膜への再構成
Reconstitution of photoreceptor rhodopsin into a patterned model membrane using peptide nanodisc

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Nanodisc from an amphiphilic α helical peptide (18A) is a novel tool for reconstituting membrane proteins into supported lipid bilayers (SLBs)[1]. By combining this technology and the scaffold of micropatterned polymeric membrane, we have successfully incorporated rhodopsin (Rh), a G-protein-coupled receptor, into SLBs. Here, we show that the density of incorporated rhodopsin in SLBs can be modulated by changing the Rh composition of peptide nanodisc. Thus, one can prepare SLBs containing a wide range of Rh densities used for single-particle tracking and massive quantitative analysis of the protein-protein and protein-lipid interactions.
1. Luchini et al. *Anal. Chem.* 2020, 92, 1, 1081–1088

1Pos210 色素再構成系を用いたシアノバクテリオクロム型光受容体の光変換機構の解析
Analysis of the photoconversion mechanism of cyanobacteriochrome-class photosensors using in vitro reconstitution approach

Takaaki Matsushita, Toshihiko Eki, Yuu Hirose (*Toyohashi Univ. of Tech*)

Cyanobacteriochromes are the bilin-binding photosensor proteins having diverse spectral sensitivity spanning near-UV to far-red regions. To investigate their spectral tuning mechanism, we utilized in vitro reconstitution approach of bilin chromophore with the apoprotein of cyanobacteriochromes. In this study, we focused phycoviolobilin (PVB) which has a disconnected conjugated system between the A- and B-rings of the bilin. PVB was purified PVB-bound photosynthetic antenna proteins using *E. coli* expression system. Then, PVB was cleaved from the protein using the pressurized liquid extraction method. The extracted PVB was reconstituted in vitro with the photoreceptor protein RcaE, and its effect on the photoconversion mechanism was investigated.

1Pos211 Thermodynamic and kinetic factors affecting the redox chemistry of a flavin cofactor in photolyases

Yuhei Hosokawa, Hiroyoshi Morita, Mai Nakamura, Shigenori Iwai, Junpei Yamamoto (*Grad. Sch. Eng. Sci., Osaka Univ.*)

Photolyases (PLs) have a catalytic flavin adenine dinucleotide (FAD) cofactor and use the energy of sunlight to convert carcinogenic UV-induced DNA lesions to the normal structure. Even though FAD can exist in several redox states in PLs, the two-electron reduced anion state ($FADH^-$) is the only form to catalyze the photorepair reaction.
This study focused on thermodynamic and kinetic factors stabilizing $FADH^-$ in various PLs. Our quantitative measurements of the redox reactions in PLs suggest that the thermodynamic and kinetic stability of $FADH^-$ should be affected by the FAD-binding pocket and distant residues, respectively. The oxidation mechanism of $FADH^-$ proposed by the study would help us understand how flavoproteins regulate their redox chemistry.

1Pos212 ロドプシンクラスター上における G 蛋白質トランスデューシンの高速 AFM による 1 分子動態観察
Single molecule observation of G protein transducin on rhodopsin cluster by high-speed AFM

Hayato Yamashita[1], Akihiro Tsuji[1], Fumio Hayashi[2], Kenichi Morigaki[3,4], Masashi Fujii[5,6], Akinori Awazu[5,6], Kazuhiko Hoshikaya[1], Masayuki Abe[1] ([1]*Grad. Sch. Eng. Sci., Osaka Univ.*, [2]*Grad. Sch. Sci., Kobe Univ.*, [3]*Grad. Sch. Agr. Sci., Kobe Univ.*, [4]*Biosignal Research Center, Kobe Univ.*, [5]*Grad. Sch. Sci., Hiroshima Univ.*, [6]*Grad. Sch. Int., Hiroshima Univ.*)

Photoreceptor rhodopsin (Rh) likely forms supramolecular structures such as dimers and dimer rows in retinal disc membrane. Single-molecule fluorescence imaging elucidated Rh dynamics in native discs[1] and molecular dynamics simulation study revealed the formation mechanism of Rh supramolecular structures[2]. In this study, we observed single molecule dynamics of G protein transducin (Gt) on Rh cluster by high-speed AFM. AFM movies showed that Gt molecules diffuses over Rh clusters consisting of dimer rows in the dark and then some of Gt molecules bind on Rh clusters after light illumination. The analyses of these Gt movements will elucidate the functional role of Rh dimer rows. [1] F. Hayashi et al, *Comm. Biol.* (2019), [2] Y. Kaneshige et al, *PLOS ONE* (2020)

1Pos213 繊毛型光受容細胞で機能するオプシンにおける収斂的な対イオン変位
Convergent evolutionary counterion displacement of ciliary opsins

Kazumi Sakai, Hiroki Ikeuchi, Chihiro Fujiyabu, Yasushi Imamoto, **Takahiro Yamashita** (*Grad. Sch. of Sci., Kyoto Univ.*)

The visible light sensitivity of animal photoreceptive protein opsins is attributed to a protonated Schiff base linkage to retinal, which is stabilized by a negatively charged counterion. Most opsins have the bistable photoreaction property and utilize Glu181 as a counterion, whereas vertebrate rhodopsin uniquely has the mono-stable photoreaction property and utilizes Glu113 as a counterion. Here, we show that an opsin group, which is phylogenetically distinct from vertebrate rhodopsin, has the bistable photoreaction property and displaces the counterion position from Glu181 to Glu113. We would like to discuss the convergent evolutionary acquisition of Glu113 as a counterion among opsins found in ciliary photoreceptor cells.

1Pos214 光サイクル型視覚ロドプシンを用いた細胞内 cAMP 濃度の一過的変化誘導
Transient induction of intracellular cAMP level changes using photocyclic visual rhodopsin

Kazumi Sakai, Shion Aoki, Takahiro Yamashita (*Grad. Sch. Sci., Kyoto Univ.*)

Opsins are photoreceptive proteins in animals and function as GPCRs, which change the intracellular second messenger levels by light to induce cellular responses. Vertebrate rhodopsin is known to decrease the intracellular cAMP level by activating Gi-type G protein. Thus, vertebrate rhodopsin has a potential as an optogenetic tool for regulating the cAMP level. However, vertebrate rhodopsin photo-converts to a metastable active state and cannot thermally recover to the dark state, which makes it difficult to induce repetitive responses. Recently, we successfully created a photocyclic rhodopsin mutant which self-regenerates to the dark state after photo-activation. Here, we would like to show the repetitive transient decrease of the cAMP level by photocyclic rhodopsin.

1Pos215 新奇微生物ロドプシン・ベストロドプシンのユニークな発色団レチナール異性化特性
Unique chromophore isomerization properties of a novel microbial rhodopsin bestrhodopsin

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Recently, a novel microbial rhodopsin subfamily, bestrhodopsins, was discovered from marine unicellular algae. Bestrhodopsins are composed of one or two rhodopsin domains having eight transmembrane helices and a C-terminally fused bestrophin channel. Their retinal-binding pockets are substantially different from that of other microbial rhodopsins, whereas their photochemical properties were unknown. In this study, we investigated chromophore isomerization of a bestrhodopsin by high-performance liquid chromatography and revealed unique isomerization properties. In addition to these results, we will report specific amino acid residues of bestrhodopsins that can confer a bestrhodopsin-like retinal isomerization property to another microbial rhodopsin.

1Pos216 新規微生物ロドプシン *Sm*ChR のイオン透過性
Ion permeability of the novel microbial rhodopsin *Sm*ChR

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Channelrhodopsins (ChRs) are light-gated ion channels intensively applied for optogenetics research. We report electrophysiological investigation of unique ion transport properties of SmChR, a newly identified ChR from a dinoflagellate *Symbiodinium microadriaticum*. Light-induced ionic current exhibited a transient peak component which is rapidly reduced into a lower steady state level. Although the steady state current is a passive transport, the transient peak showed inwardly-directed vectorial transport. We further report ion selectivity of the SmChR. Amino acid sequence of SmChR does not conserve characteristic residues in the ion permeation pathway in comparisons to that of channelrhodopsins. Light-gated ion transport mechanism of *Sm*ChR is presented in detail.

1Pos217 (2SCA-2) Conversion of light-driven outward proton pump rhodopsin into inward proton pump

Maria Del Carmen Marin Perez[1], Masae Konno[1,2], Himoru Yawo[1], Keiichi Inoue[1] ([1]*ISSP, Univ. Tokyo*, [2]*PRESTO, Japan Science and Technology Agency*)

Microbial rhodopsins are retinal-binding membrane proteins which function as ion-transporters, photo-sensors, and light-regulated enzymes. The most ubiquitous microbial rhodopsins are the outward-directed light-driven H^+ pumps. However, new sub-families of microbial rhodopsins exhibited an inwardly and unidirectionally H^+ transport. Although structural studies provide insight into their ion transporting mechanism, the key elements which determinate the direction of the H^+ transport pathway were not revealed. We report the H^+ transport activity of site-directed mutations of *Psp*R (outward H^+ pump) from *Pseudomonas putida*, to successfully convert *Psp*R into an inward H^+ pump by site-specific replacement of their amino acid residues involve in the H^+ transport pathway.

1Pos218 宿主由来のレチナールを利用する共生細菌 Saccharibacteria 由来 Type-1 ロドプシンの分子特性
Molecular properties of Type-1 rhodopsin from Saccharibacteria that may use host-derived all-*trans* retinal

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The Candidate Phyla Radiation (CPR) is a phylogenetically diverse group of putative episymbiotic bacteria, which have reduced metabolic pathways. Recently, metagenomic analyses have shown that some members of the CPR possess Type-1 rhodopsins, but their functions have not been clarified. In this study, we report the molecular characterization of the rhodopsin SacRs from Saccharibacteria, a lineage of CPRs, and show that SacRs function as light-driven outward H^+ pump. In addition, SacRs were able to rapidly capture exogenous all-*trans* retinal. These results suggest that Saccharibacteria, which lack enzyme genes essential for all-*trans* retinal synthesis, obtain all-*trans* retinal from their putative host, *Actinobacteria*, for phototrophic energy production.

1Pos219 高熱安定性光駆動型内向き H^+ポンプロドプシンにおける熱安定性要因の研究
Study on the factors contributing to the high thermal stability of thermostable light-driven inward H^+ pump rhodopsins

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Schizorhodopsin (SzR) is the subfamily of microbial rhodopsin which functions as light-driven inward H^+ pump. In 2021, we reported two thermostable SzRs (*Mt*SzR and *Ms*SzR) from archaea living in the high-temperature environments.

However, it is still unclear how *Mt*SzR and *Ms*SzR achieve their high thermal stability. To investigate the factors of the high thermal stability, amino acid sequences of *Mt*SzR and *Ms*SzR were compared with that of SzR1, a non-thermostable SzR, and characteristic amino acids in *Mt*SzR and *Ms*SzR were found. In this study, SzR1 mutants were constructed by introducing these characteristic amino acids and measured the thermal stability of the mutants to elucidate the mechanism of high thermal stability of *Mt*SzR and *Ms*SzR.

1Pos220 多様な温度環境に分布するプロトンポンプ型ロドプシンの熱力学的性質の網羅的解析
Comprehensive thermodynamic analysis for microbial proton pump rhodopsins identified in various temperature environments

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About 80% of the microbial photoreceptor protein rhodopsin functions as a proton pump and contributes to ATP production by making proton motive force across the cell membrane triggered by light. Genetic analysis has revealed that proton pump rhodopsin genes are distributed in diverse environments on earth. It is expected that functional optimization occurs at the molecular level according to the environment, but the fact and strategies for the optimization are not known. To clarify these, we performed transient absorption spectroscopy on proton pump rhodopsins distributed in low- (Antarctic red snow), medium- (ocean), and high-temperature (hot springs) environments, and compared thermodynamic parameters for intermediates responsible for the proton pump function.

1Pos221 光駆動 Na^+/H^+ハイブリッドポンプ型ロドプシン KR2 における N112 変異体のプロトン選択的ポンプ機構の研究
Study of proton-selective pumping mechanism of N112 mutants in light-driven Na^+/H^+ hybrid pump-type rhodopsin KR2

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KR2 is a microbial rhodopsin discovered in 2013 from a marine bacterium *Krokinobacter eikastus* and was characterized as the first light-driven Na^+/H^+ hybrid pump. KR2 constitutes a light-driven Na^+ pumping rhodopsin family (NaRs) that actively transports sodium and lithium ions in the presence of NaCl and LiCl, respectively, while it pumps protons in the other alkali metal cations such as KCl, RbCl and CsCl. NaR has a conserved NDQ (N112, D116, and Q123 in KR2) motif, and previous studies suggested an important role for N112 in the function of KR2. Here, I replaced N112 with 3 different amino acid residues (Ala, Cys, and Val), and studied the molecular properties of the mutants by using flash photolysis experiment and time-resolved infrared spectroscopy

1Pos222 Time-resolved cryo-Raman study of Na^+ uptake and release by a sodium pumping rhodopsin from *Indibacter alkaliphilus*

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Sodium pumping rhodopsins (NaRs) are membrane transporters that utilize light energy to pump Na^+ across the cellular membrane. Within the NaRs, the retinal Schiff base chromophore absorbs light and a photochemically produced transient state, referred to as O intermediate, performs both the uptake and release of Na^+. However, the structure of the O intermediate remains an open question. We used time-resolved cryo-Raman spectroscopy to study the structure of the O intermediate of an NaR from *Indibacter alkaliphilus*.

1Pos223 励起子電荷分離混成が酸素発生型光合成を駆動する
Exciton-charge transfer mixing drives oxygenic photosynthesis

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Photosystem II is crucial for life on Earth as it provides oxygen as a result of photoinduced electron transfer. The excited state dynamics of the photosystem II-reaction center (PSII-RC) has been a matter of vivid debate because the absorption spectra is highly congested and hence it is extremely difficult to distinguish transients. Here, we report the two-dimensional electronic-vibrational spectroscopic study of the PSII-RC. The simultaneous resolution along both the visible excitation and infrared detection axis is crucial in allowing for the character of the excitonic states and interplay between them to be clearly distinguished. In particular, this work demonstrates that the mixed exciton-charge transfer state is characterized by the $Chl_{D1}{}^+Phe^-$ radical pair.

1Pos224 遠赤色光に適応した光化学系 I の光捕集における Chlorophyll-*f* と Red-Chlorophyll の役割に関する理論的研究
Theoretical study on the role of Chlorophyll-*f* and Red-Chlorophyll in light-harvesting mechanism in far-red light adapted photosystem I

Yuka Nakamura, Mikihito Okochi, Shigeru Itoh, Akihiro Kimura (*Grad. Sch. Sci., Nagoya Univ.*)

Some cyanobacteria performs oxygen-evolving photosynthesis even under far-red light with the far-red light-adapted photosystem I (FR-PSI) using Chl-*a* and a small amount of Chl-*f* which absorbs far-red light.
We studied the mechanism of uphill excitation energy transfer (EET) from the long wavelength Chl-*f* absorption band to the short wavelength Chl-*a* absorption band during the light-harvesting process of FR-PSI theoretically using the structure-based simple exciton model.
The results suggest that the "Red-Chl-*a*" plays an important role on the uphill EET. We showed that the excited states of "Red-Chl-*a*" mediate the efficient uphill EET from the exciton bands of Chl-*f* to Chl-*a* and to the special pair (P700) of Chl-*a* by structure-based simple exciton theory.

1Pos225 Electrostatic charge controls spectral properties and thermal stabilities of LH1-RCs from triply extremophilic *Halorhodospira halochloris*

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Halorhodospira (*Hlr.*) *halochloris* exhibits the lowest light-harvesting 1 (LH1) Q_y transition energy among phototrophic organisms and is the only known triply extremophilic anoxygenic phototroph, displaying a thermophilic, halophilic, and alkaliphilic phenotype. Here, we examined the effects of salt and pH on the spectroscopic properties and thermal stability of LH1-RC complexes from *Hlr. halochloris* and compared with those from its mesophilic counterpart *Hlr. abdelmalekii.* Based on the present results and amino acid sequences of LH1 and reaction center (RC) proteins, we discuss the roles of electrostatic charges in the function and stabilization of the *Hlr. halochloris* LH1-RC complex to allow it to perform photosynthesis in its warm, hypersaline, and alkaline habitat.

1Pos226 フェムト秒ポンプ・プローブ分光法によるヘリオバクテリア反応中心におけるカロテノイドの励起エネルギー移動解析
Analysis of excitation energy transfer of carotenoids in the reaction center of heliobacteria with femto-second pump-probe spectroscopy

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Heliobacteria are obligatory anaerobic and anoxygenic photosynthetic bacteria. Their reaction center (hRC) is type 1 RC, which is the same as photosystem I (PSI) of higher plants and cyanobacteria, and has a homodimeric structure. Recently, the three-dimensional structure of hRC from *Heiobacterium. modesticaldum* has been reported (Gisriel et al., 2017), and excitation energy transfer among the pigments in hRC can be discussed. There are only two 4, 4'-diaponeurosporene molecules (Cars) in hRC complex, but its function is still unknown. In the present study, we measured absorption changes of the purified hRC with femtosecond pump-probe spectroscopy. As a result, a highly efficient excitation energy transfer from Cars to the antenna bacteriochlorophylls *g* is observed.

1Pos227 FTIR monitoring of photosynthetic quinone transport in the light-harvesting 1 reaction center complexes from purple bacteria

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Redox-active quinones play fundamental roles in efficient light energy conversion in the purple bacterial LH1-RC complexes. However, there is not concrete experimental evidences demonstrating the proposed quinone transfer mechanism. Here, we focused on several factors—PufX, Protein U, and phospholipids— for the regulation of the quinone transport, and examined the effects of these factors on the light-induced FTIR Q_B and Q_BH_2 signals using reconstituted photosynthetic membranes comprised of solubilized photocomplexes from *Tch. tepidum* and *Rba. sphaeroides*, phospholipids (CL, PG, PE, PC), and exogenous ubiquinone molecules. Based on the present results, the roles of PufX, Protein U, and phospholipids in the photosynthetic quinone transport are discussed.

1Pos228 Wavelength-Dependent Optical Response of Single Photosynthetic Antenna Complexes from Siphonous Macrogreen Alga *Codium fragile*

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A siphonous macrogreen alga *Codium fragile* has the siphonaxanthin-chlorophyll-protein (SCP) complex as a major light-harvesting complex. It is highly homologous to green plants LHCII. Interestingly, we find remarkable differences in the spectral response from individual SCP complexes when excited at 561 nm and at 639 nm. While excitation in the green spectral range reproduces the common LHCII-like emission features for most of the complexes, excitation in the red spectral range yields a red-shifted emission and a significant decrease of the fluorescence lifetime. We hypothesize that this can be associated with the adaption of the algae to their natural habitat under water, where excess light features a red-enhanced spectrum that comes at tidal timings.

Poster

1Pos229 クロロフィル *f* を含む光化学系 I の近赤外光による反応メカニズム解明を目指した蛍光バンドの帰属
Assignment of fluorescence bands of chlorophyll-f containing photosystem I to elucidate its reaction mechanism by near-infrared light

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While chlorophyll-*a* (Chl-*a*) is usually responsible for light absorption in photosynthesis, a cyanobacterium containing Chl-*f* with a red-shifted absorbance as photosynthetic pigment was discovered in 2011. A photoactive complex called photosystem I containing Chl-*f* (FR-PSI) performs photosynthesis with about 100 nm longer wavelength light. The structure of FR-PSI has been elucidated by the cryo-electron microscopy. However, the mechanism for the large red-shift has remained unclear. Assignment of each of 7 Chl-*f*s bound to FR-PSI to the three fluorescence peaks will provide a hint to resolve the puzzle. We aim to assign each fluorescence peak to Chl-*f* in the known structure by the measurement of fluorescent anisotropies of single-PSIs with an aid of clustering analysis.

1Pos230 緑色硫黄細菌の光合成反応中心複合体の表在性タンパク質の結合は PscB が足場となる
PscB is the scaffold for binding of other water-soluble subunits to the photosynthetic reaction center complex of green sulfur bacteria

Tomomi Inagaki, Kazuki Terauchi, Chihiro Azai (*Grad. Sch. Life Sci., Ritsumeikan Univ.*)

The photosynthetic reaction center complex of green sulfur bacteria (Gsb-RC) consists 5 proteins: PscA, B, C, D and FMO. The three of them (PscB, PscD, and FMO) are water-soluble peripheral subunits. Keeping the charge separation activity of Gsb-RC, we explored the biochemical treatment to strip them off from the membrane-spanning core complex. Increasing concentration of NaCl detached all of PscD and most of FMO, but few of PscB. However, as increasing pH, PscB was also detached. All the dissociation events were reversible and a fully-functional Gsb-RC was recovered by by desalting and pH neutralization. Negative electrostatic surface potential of PscB would be responsible for binding of the water-soluble subunits to the core complex.

1Pos231 極性カロテノイドの結合性向上を目指したシフォナス緑藻の光合成アンテナの in-vitro 再構成
Enhancement of polar-carotenoid binding in in-vitro reconstitution of a photosynthetic light-harvesting complex from siphonous green alga

Hikari Takakura[1], Naoko Norioka[2], Naohiro Oka[3], Soichiro Seki[1], Hideaki Tanaka[2,4], Genji Kurisu[2,4], Ritsuko Fujii[1,5] ([1]*Grad. Sch. Sci., Osaka City Univ.*, [2]*Inst. Protein Res., Osaka Univ.*, [3]*BRIC., Tokushima Univ.*, [4]*Grad. Sch. Sci., Osaka Univ.*, [5]*ReCAP., Osaka Metropolitan Univ.*)

Light-harvesting complex II (LHCII) absorbs the energy and transfers it to Photosystem II, where the photochemical reaction takes place. Compared to the well-studied plant LHCII, the LHCII from a siphonous green alga binds the unique polar carotenoid siphonaxanthin (Sx), allowing it to absorb green region of light. In-vitro reconstitution has been demonstrated for vascular plants using recombinant protein with natural pigments extracts. We have been applied this to siphonous LHCII, however the low binding affinity of Sx has been the issue when following the authorized protocol. It may be due to high polarity of the Sx. In this study, we focused on the improvement of Sx binding by modifying major parameters in the protocol.

1Pos232 Ras photocontrol by regulatory factor GAP modified with azobenzene derivative.

Rajib Ahmed, Nobuyuki Nishibe, Natsuki Yamamura, Kazunori Kondo, Shinsaku Maruta (*Department of Biosciences, Graduate School of Science and Engineering Soka University, Hachioji, Tokyo.*)

The small GTPase Ras is a central regulator of cellular signal transduction, growth, and migration among others, it also functions as a molecular switch. GEF and GAP are two types of Ras regulatory factors. GAP participates in the downstream effector system of the ras signaling pathway. In this study, functional sites of GAP with an innovative GAP modification with the photochromic molecule of monofunctional azobenzene derivatives control GTP-GAP exchange of Ras photo-reversibly. We have designed the sites in Ras to be modified by azobenzene and expressed the Ras mutant by the E.coli expression system. The mutant S1233C was prepared. Azobenzene derivative N-(4-phenylazophenyl) maleimide (PAM) was stoichiometrically incorporated into the cysteine of the mutant.

1Pos233 藍色光を吸収するチャネルロドプシン KnChR のイオン選択性と光遺伝学
Ion selectivity and optogenetics application of a deep blue absorbing channelrhodopsin

Satoshi Tsunoda[1,2], Rintaro Tashiro[1], Shoko Hososhima[1,2], Hideki Kandori[1,2] ([1]*Nagoya Institute of Technology, Department of Life Science and Applied Chemistry*, [2]*Nagoya Institute of Technology, OptoBioTechnology Research Center*)

Channelrhodopsins (ChRs) are light-gated ion channels extensively applied as optogenetics tools for manipulating neuronal excitability. We previously reported high Ca^{2+} permeability in KnChR, which could be further improved up to 100 times by an amino acid substitution. We here evaluate ion selectivity of the mutant KnChR and discuss its cation permeation mechanism. Maximal sensitivity was exhibited at 430 nm and 460 nm, the former making KnChR one of the most blue-shifted ChRs characterized thus far, serving as a novel prototype for studying the molecular mechanism of color tuning of the ChRs. We further demonstrate optical neuronal stimulation by using KnChR to test its applicability for optogenetics for short-wavelength excitation.

1Pos234 G タンパク質 βγ サブユニット依存的イオンチャネル応答を選択的に駆動する無脊椎動物オプシン
An invertebrate opsin functionally biased for Gβγ-dependent ion channel responses

Hisao Tsukamoto[1], Yoshihiro Kubo[2] ([1]*Department of Biology, Kobe University*, [2]*Department of Molecular Physiology, National Institute for Physiological Sciences*)

Animal opsins have been utilized for optogenetic tools to control G protein-dependent signaling pathways. Since opsins can drive multiple signaling pathways, some optical control tools functionally biased for specific pathways would be useful. We previously reported that an invertebrate opsin, *Platynereis* c-opsin1, transiently activates G proteins upon UV illumination. We expect the transient activation preferably drives kinetically fast Gβγ-dependent ion channel responses rather than Gα-dependent slow enzymatic responses. Here, we quantified the c-opsin1-induced ion channel and enzymatic responses. As expected, the c-opsin1 can drive preferably the fast ion channel-mediated responses, and thus the opsin could be a selective optical control tool.

1Pos235 微生物型ロドプシンの吸収波長とプロトン移動の制御機構
Regulation of absorption wavelength and proton transfer in microbial rhodopsins

Masaki Tsujimura[1], Hiroshi Ishikita[1,2] ([1]*Grad. Sch. Eng., Univ. Tokyo*, [2]*RCAST., Univ. Tokyo*)

Microbial rhodopsins are membrane proteins that have a retinal Schiff base as a chromophore and are involved in light-dependent biological functions in microorganisms. Ion-transporting rhodopsins are utilized as tools for controlling the neural activity (optogenetics). The functions of microbial rhodopsins are often triggered by proton transfer inside the protein. In this study, the regulation mechanisms of (i) the absorption wavelength of the retinal chromophore and (ii) the proton transfer inside the protein are investigated using a quantum mechanical/molecular mechanical approach and molecular dynamics simulations. (iii) The relationship between the proton transfer from/toward the chromophore and the absorption wavelength of the chromophore is also analyzed.

1Pos236 Photocontrol of chromatin remodelers Snf2 and BRG1 as an ATP driven molecular motor by photoresponsive protein Dronpa

Choi Eunji[1], Ziyun Zhang[1], Shinya Watanabe[2], Kazunori Kondo[1], Shinsaku Maruta[1] ([1]*Grad. Sch. Sci., Univ. Soka*, [2]*Med. Sch., Univ. Massachusetts*)

Snf2 and Brg1 are SWI/SNF chromatin remodeling complex which are involved in regulation of chromatin structure and transcription mechanically using ATP. Dronpa shows on and off fluorescent switching by 400 nm and 500 nm light irradiation. Dronpa variant 145K and 145N forms dimer upon 400 nm light and turn on. It becomes monomer upon 500 nm light and turned off. Therefore, it is expected that regulation of function is possible if Dronpa 145K-145N utilized as photoswitching molecule device for chromatin remodeler. In this study, we prepared novel photochromic Snf2 and BRG1 fused with Dronpa variants. We observed high DNA dependent ATPase activity of Dronpa-Snf2 under the off state and lower activity upon on state. Photoregulation of Dronpa-BRG1 was also examined.

1Pos237 QM/MM 分子シミュレーションによる光活性化酵素 OaPAC の研究
Study on photoactivated enzyme OaPAC by QM/MM molecular simulation

Masahiko Taguchi, Shun Sakuraba, Justin Chan, Hidetoshi Kono (*Inst. Quant. Life Sci., QST*)

Blue light activates the enzymatic reaction of PAC protein. The molecular structure of PAC is known at an atomic level, however, the photoisomerization reaction and the crosstalk mechanism between the photoreceptor domain and the enzymatic domain remain to be solved. Here, we performed QM/MM molecular simulation to address these problems. In the photoactivated state, we observed a distinct flip of Trp90 near the C-terminal helix that connects the two domains. This flip seems to trigger a subsequent change in the helix orientation to propagate a signal toward the AC domain. We discuss the crosstalk mechanism in the meeting.

1Pos238 Cationic Polyester Microdroplets as RNA-containing Protocells

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Polyester microdroplets generated from dehydration synthesis of various α-hydroxy acids (αHA) were suggested as potential primitive compartments that can compartmentalize primitive bio molecules. Here, we increased the chemical diversity of polyester microdroplet systems by combinatorially adding an αHA monomer with a basic side chain, 4-amino-2-hydroxybutyric acid (4a2h), to form combinatorial heteropolyesters via dehydration synthesis. Incorporation of 4a2h resulted in the assembly of some polyester microdroplets able to segregate fluorescent RNA, suggesting that minor modifications of polyester composition can significantly impact the functional properties of primitive compartments.

1Pos239 DNA 相互作用を用いたコアセルベート間でのタンパク質輸送
DNA-Mediated Protein Shuttling between Coacervate-Based Artificial Cells

Tsuyoshi Mashima[1], Jan van Hest[2], Luc Brunsveld[2] ([1]*NAIST*, [2]*Eindhoven Univ. Tech.*)

The regulation of protein uptake and secretion is crucial for cellular signaling. For mimicking these molecular events on engineering synthetic cellular systems, control over the uptake and release of proteins from synthetic cells is essential. Herein, we have developed an artificial cell that sequesters and releases proteins upon addition of single-stranded DNA as an external trigger. The molecular coded signal allows for regulation of the amount and rate of protein release, the sequential release of different proteins and transfer of a protein between two artificial cell populations. The system provides novel directions for engineering lifelike communication pathways in cellular structures.

1Pos240 ベシクルの自己生産: 人工ミニマルセルのボトムアップなデザイン
Reproduction of Vesicles: The Bottom-up Design for Synthetic Minimal Cell

Minoru Kurisu[1], Peter Walde[2], Yuka Sakuma[1], Masayuki Imai[1] ([1]*Dept. Physics, Grad. Sch. Sci., Tohoku Univ.*, [2]*ETH Zurich*)

Life is the system that reproduces itself, maintained by complex chemical reaction networks. To elucidate the physics describing the emergence of living systems from simple molecular assemblies, one of the promising approaches is to actually construct simple vesicle reproduction systems. Recently, we have developed the recursive vesicle reproduction cycle, *i.e.* membrane growth → deformation → vesicle division → volume growth, and have given their physical descriptions from the viewpoint of soft matter physics and membrane elasticity theory. In our poster, we will summarise the essence of each reproduction process and show their experimental realisation with AOT vesicles coupled with their surface confined-polymerization of aniline.

1Pos241 配列情報と連携したベシクル膜の成長：進化可能なミニマルセルを目指して
Vesicle membrane growth coupled with sequence information: toward evolvable minimal cell

Ryosuke Katayama, Minoru Kurisu, Yuka Sakuma, Masayuki Imai (*Grad. Sch. Sci., Tohoku Univ.*)

Life is a unique system that shows not only self-reproduction coupled with complex chemical reaction networks, but also evolution toward better fitness. The life system is conducted by the sequence information transfer from DNA to protein, which governs reproductive success. Recently we have succeeded in generating a synthetic minimal cell, where the success of AOT vesicle reproduction is determined by the sequence of information polymer, polyaniline. In this study we modify sequence of polyaniline segments using template effect of various membrane molecules and examine relationship between the sequence of segments and growth rate of the vesicle. We believe this study opens the pathway toward the evolvable minimal cell.

1Pos242 Formation of self-growing artificial cell droplets in aqueous two-phase separation system by internal amplification of nucleic acids

Yoshihiro Minagawa, Moe Yabuta, Hiroyuki Noji (*Department of Applied Chemistry, Graduate School of Engineering, The University of Tokyo.*)

The bottom-up reconstitution of self-proliferation protocells is an important milestone toward the construction of artificial cellular systems with autonomy. However, it remains challenging to construct a protocell model of autonomous growth of cellular reactors with internal replication of genetic polymers. We found that DNA can be stabilized in a two-phase system (ATPS) of dextran (DEX) and polyethylene glycol (PEG), which concentrates DNA in DEX-rich phase. When DNA was amplified in DEX/PEG below the critical concentration for phase separation, numerous DEX-rich droplets emerged and actively increased the droplet volume via coalescence and self-growth. Our findings pave the development of self-growing and self-replicating artificial cell models.

1Pos243 細胞モデル進化における表現型拘束に起因した交差耐性
Cross-resistance induced by phenotypic constraint in a cell model evolution

Takuya Sato[1], Kunihiko Kaneko[2] ([1]*RIKEN, BDR*, [2]*Niels Bohr Institute*)

Cells can adapt through adaptive evolution to various environmental stresses. It is often the case that adaptive evolution to one environment makes it easier or harder to adapt to another environment. This is called cross-resistance.
In the study (Horinouchi et. al. 2017 Scientific. Research.), it is suggested that a low-dimensional linear model that explains cross-resistance well can be constructed by using transcriptome changes in adaptive evolution.
In this presentation, we will suggest the relationship between cross-resistance and the high-dimensional data of the cellular state such as a transcriptome using evolutionary simulations of cellular models. In particular, a concept called phenotypic constraints will play an important role here.

1Pos244 Coarse-grained modeling of Nanog gene locus: Towards understanding enhancer-promoter communication

Soundhara Rajan Gopi[1], Giovanni Brandani[1], Cheng Tan[2], Jaewoon Jung[2,3], Chenyang Gu[1], Azuki Mizutani[1], Chigusa Kobayashi[2], Hiroshi Ochiai[4,5], Yuji Sugita[2,3,6], Shoji Takada[1] ([1]*Department of Biophysics, Graduate School of Science, Kyoto University, Kyoto 606-8502, Japan*, [2]*Computational Biophysics Research Team, Riken Center for Computational Science, Kobe 650-0047, Japan*, [3]*Theoretical Molecular Science Laboratory, RIKEN cluster for Pioneering Research, Saitama 351-0198, Japan*, [4]*Program of Mathematical and Life Sciences, Graduate School of Integrated Sciences for Life, Hiroshima University, Higashi-Hiroshima, Hiroshima 739-8511, Japan*, [5]*Genome Editing Innovation Center, Hiroshima University, Higashi-Hiroshima, Hiroshima 739-8511, Japan*, [6]*Laboratory for Biomolecular Function Simulation, RIKEN center for Biosystems Dynamics Research, Kobe 650-0047, Japan*)

Enhancers (E) influence the transcription of genes via interaction with promoters (P). However, the molecular mechanisms underlying such communication remain poorly understood, with various suggested models based on stable E-P loops, transcriptional condensates, and 3D diffusion of transcription factors (TFs) between E and P. To better understand the details of E-P communication, we built a comprehensive near-atomistic model of the Nanog gene locus (200kb) comprising of nucleosomes, TFs, co-activators and RNA polymerase complexes. Our model is tuned to reproduce the organization of chromatin and the condensation of TFs. The long time-scale simulations performed using the Fugaku supercomputer provide a molecular-level view to study and evaluate E-P communication models.

1Pos245 Biochemical fractionation separating open and compact chromatin based on local assembly of adjacent nucleosomes

Satoru Ishihara (*Fujita Health Univ. Sch. Med.*)

Events on the genome are controlled by chromatin structure, which is converted between open and compact states. To unveil the mechanism of this conversion, we established a method fractionating open and compact chromatin using sedimentation velocity centrifugation; open chromatin is retained in upper fractions as dispersed nucleosomes, while compact chromatin is sedimented into lower fractions as assembled nucleosomes. Blotting for fractions showed the distribution of histone H1 in lower fractions. Because H1 was found to self-associate and interacted with histone H3 in compact chromatin, H1 is likely to link adjacent nucleosomes. Genome-wide analyses revealed that compaction degree at transcription start sites was inversely correlated to transcription levels.

1Pos246 1 分子イメージングで迫るヒト染色体の凝縮機構
Single molecule imaging unveils human chromosome condensation

Kayo Hibino[1,2,3], Yuji Sakai[4], Masato Kanemaki[1,2], Kazuhiro Maeshima[1,2] ([1]*NIG*, [2]*SOKENDAI*, [3]*JST, PRESTO*, [4]*Inst. LiMe, Kyoto Univ.*)

The mitotic chromosome condensation during cell division is an extraordinary self-organizing process that converts the long thin genome chromatin polymers (several centimeters) into compact short chromosomes (several micrometers). Although ATP-driven DNA motors called condensins and topoisomerase IIα (TopoIIα), which untangles two sister chromatids, are essential for chromosome condensation, the basic principles of condensation are not known. Here, we analyzed the local motion of nucleosomes in the mitotic chromosomes during condensation by using intracellular single-molecule imaging techniques. Combining with simulations, we discuss how condensin, TopoIIα, and epigenetic modification involve the condensation process of the chromosomes from the physical aspect.

1Pos247 HDV ゲノムの分子進化における二次構造の制約の解析
Constraint of Base Pairing on HDV Genome Evolution

Saki Nagata, Ryoji Kiyohara, Hiroyuki Toh (*Grad. Sch. of Sci. Tech., KGU*)

The hepatitis delta virus (HDV) is a satellite virus of hepatitis B virus, which causes hepatitis D, a human liver disease. It has a single-stranded circular RNA genome consisting of about 1,700 nucleotides. The genome has high self-complementarity to generate a long rod-like secondary structure. Most of the tools for sequence alignment and phylogenetic tree construction assume the independence of the bases. To develop tools which take the secondary structure into account, HDV genome would provide a good material to examine the performance. In this study, we examined whether the secondary structure function as constraint for the HDV genome evolution. In this presentation, we will report how the base-pairings reduce the substitution rate of the HDV genome.

1Pos248 GPCR 間相互作用ペア予測手法の改善
Improvement of a method to predict interacting GPCR-GPCR pairs

Aoi Fukushima[1], Hiroaki Teruse[2], Sakie Shimamura[1], Hiroyuki Toh[2], Wataru Nemoto[1] ([1]*Dept. Sch. & Tech., Tokyo Denki Univ.*, [2]*Dept. of Sci. & Tech., Kwanseigakuin Univ.*)

G Protein-Coupled Receptor (GPCR) oligomer functions are different from those of monomers. Interactions between GPCRs are potential therapeutic targets for diseases. If we suppose that there are 871 GPCR genes in the human genome, then the number of all possible hetero GPCR pairs from the 871 GPCRs is 378,885. Systematic experimental studies of oligomerization would be time-consuming and costly. Accurate predictions could reduce the costs and accelerate such studies. We previously developed a method to predict GPCR-GPCR interaction pairs using support vector machine, the GPCR-GPCR interaction pair predictor (GGIP) [Nemoto et al. Proteins. 2016]. In this study, we tried to improve prediction accuracy by considering features derived from sequence and structure data.

1Pos249 Chiral selectivity mechanism on aminoacylation of an RNA minihelix studied by quantum mechanics/molecular mechanics simulations

Tadashi Ando (*Dep. of Appl. Elec., Tokyo Univ. of Sci.*)

The origin of homochirality in L-amino acid in proteins is one of the mysteries of the evolution of life. Experiments show that a non-enzymatic aminoacylation reaction of an RNA minihelix by aminoacyl phosphate oligonucleotides has a clear chiral preference for L-amino acids over D-amino acids. In this study, by employing quantum mechanics/molecular mechanics/molecular dynamics simulations combined with an umbrella sampling method, we examined free energy profiles along a reaction coordinate for the aminoacylation of L- and D-Ala in a modeled RNA minihelix. Free energy barrier for the reaction with L-Ala were lower than that with D-Ala, which is consistent with experiment. We will discuss the chiral selectivity mechanism based on the simulation results in the meeting.

1Pos250 光ピンセットを用いた fL リアクタ回収技術の開発
Development of new DNA recovery technology from fL droplet array using optical tweezers

Tetsuya Ohashi, Hiroshi Ueno, Yoshihiro Minagawa, Hiroyuki Noji (*Department of Applied Chemistry, Univ. Tokyo*)

As a high-throughput screening technology for directed evolution, we have recently developed artificial cell reactor technology based on digital protein synthesis in a femtoliter (fL) droplet array. However, microcapillaries, which have been currently used for DNA recovery from the droplets, have long recovery time (several minutes/droplet) and the problem of DNA adsorption to capillaries. Here, to solve this problem, we developed new DNA recovery technology from fL droplet array using optical tweezers. By the local heating and the manipulation with the laser beam of optical tweezers, we succeeded in detaching the fL droplets from the device within one minute. We optimized the device design and finally succeeded in detaching 83% of the droplets by the laser irradiation.

1Pos251 深層生成モデル CM-VAE を用いた RNA ファミリー人工配列生成
CM-VAE: a generative model for designing artificial members of RNA family

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Biomedical applications of RNA engineering often require the design of RNA sequences with desired functions. In recent years, sequence design methods based on deep learning have been actively developed. However, there have been no methods aimed at generating sequences for specific RNA families. Here, we propose a deep generation model CM-VAE that can efficiently design artificial sequences belonging to a specific RNA family, and the generation capability of CM-VAE is the highest compared to benchmark models. As a proof-of-concept, CM-VAE was trained with the self-cleavable RNA enzyme GlmS ribozyme and it was shown that the designed sequences actually have self-cleavage activity in vitro. These results suggest that CM-VAE can be a novel tool in RNA engineering.

1Pos252 人工的微生物複合系において観察された機能的安定性と不安定性
Functional stability and instability observed in engineered microbial complex systems

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To understand how the functional stability of a whole system is maintained, two engineered microbial complex cultures were enriched under a chemostat condition supplied with phenol as sole carbon and energy source and a forest soil as an inoculum. Phenol was hardly accumulated in a reactor I (R-I) but did in a reactor II (R-II). Affinities for phenol of R-I and R-II exhibited wide range and low values, respectively. Non-phenol utilizing bacteria were isolated in R-I but not in R-II. Amplicon sequence analyses targeting 16S rRNA gene revealed that bacterial community succession in R-I was gentle but was drastic in R-II. These results suggested that metabolic network would allow microbial complex systems to be stable, whereas a strong competition would cause unstable.

1Pos253 Diversity of swimming endurance and foraging strategy in marine bacteria

Kyosuke Takabe[1], Yiyun Zhang[2], Katsuki Hara[2], Tomohiro Hirayama[2], Yutaka Yawata[1,3] ([1]*Faculty of Life and Environmental Sciences, University of Tsukuba*, [2]*Master's Program in Agro-Bioresources Science and Technology, University of Tsukuba*, [3]*Microbiology Research Center for Sustainability, University of Tsukuba*)

Marine bacteria, e.g., Vibrio sp., swim and forage by using flagella in seawater and have known to be a main decomposer of the dissolved organic matter, indicating that the marine bacterial foraging is crucial for the ocean carbon cycle. Furthermore, marine bacteria are inferred to swim for long periods to encounter discretely distributed nutrients. However, it remains unclear how long bacteria keep on swimming in a starvation condition and whether the survival strategy varies among species. Here, we quantitatively analyzed the swimming behavior of three vibrio strains in artificial seawater. Our results showed the diversity of swimming stamina not only among strains but also among the clonal population and the diversity of vibrio foraging strategy.

1Pos254 北海道南部産ダルス内の PE 量に光が与える影響
Effect of light on the amount of PE in dulse from southern Hokkaido

Yukiko Sawayama, Yuzuka Takahashi, Rio Fukuda, Hibiki Nakamura (*HAKURYO High School attached to Hakodate University*)

Dulse is a type of seaweed that is used for food. This study investigated the amount of phycoerythrin (PE), a health functional ingredient, in dulse from southern Hokkaido at two different water depths, about 0.2, 1.2 m.
After collecting PE using our original protocol utilizing solvolytic precipitation, the amount of PE in both was measured. As a result, it was found that dulse with the shallower habitat contained more PE, 1.8 times more than that with the deeper habitat.
Furthermore, from the relationship between the results and the light intensity estimated from the depth of the sea near Usujiri by applying Lambert-Beer's law, it is suggested that the stronger light intensity, the more suitable for the growth of dulse and the larger amount of PE.

1Pos255 3 次元形態形成を表す隣接細胞間ネットワークモデル
Simulating Three-Dimensional Epithelial Morphogenesis: A Network Model Based on the Interactions Between Adjacent Cells

Tomohiro Mimura, Yasuhiro Inoue (*Grad. Sch. Eng.,Univ. Kyoto*)

Cell dynamics regulate the overall 3D morphogenesis of tissues and organs in living organisms. Various mathematical modeling and simulation studies have been conducted. One of the promising approaches is 3D vertex modeling, in which each cell is represented as a polyhedron. However, determining the geometric locations of the polyhedral vertices from experimental data is difficult. This disadvantage limits the application of 3D vertex models to predicting or estimating the biological parameters.
In the present study, we developed a mathematical model that is expected to be applicable to data assimilation with the location of trackers such as cell nuclei. This model was used to simulate the effects of cell division and apical constriction on 3D epithelial morphogenesis.

1Pos256 空間的局所相互作用を伴う動的可塑的ネットワーク系の自発的構造形成
Spontaneous Network Organizations of Dynamic-Plastic Network System with Spatial Local Interactions

Taito Nakanishi (*Grad. Sch. Int., Univ. Hiroshima*)

Living systems contain various self-organized networks. Neural networks in the brain and human networks on social networking sites are typical ones to spontaneously form their structures through global and local interactions among their components. However, recent studies on such structure formations focused only on the effects of global interactions. On the other hand, the involvement of glial cells in information processing in the brain and the existence of communities in SNS suggest that also local interactions provide dominant contributions to structural changes in networks. To reveal the influences of such contributions on network formations, we simulated a plastically all-to-all coupled dynamical system with local connections.

1Pos257 乳がんの転移に関連するオントロジーグループに基づいた遺伝子相関ネットワーク解析による予後予測
Prognosis prediction of breast cancer by gene correlation network analysis based on Gene Ontology terms involved in metastasis

Ayaka Yakushi[1], Masahiro Sugimoto[2], Takanori Sasaki[1] ([1]*Fac. Adv. Math. Sci., Meiji Univ.*, [2]*Tokyo Med. Univ*)

Prognostic prediction helps the decision-making of breast cancer (BC) treatment. This study employed weighted gene correlation network analysis (WGCNA) to analyze the relationship between gene expression profile and BC prognosis. Among the 366 microarray data collected from the patients with BC, 490 genes showing large variance were included in six gene ontologies (GOs) involved in BC metastasis. WGCNA identified nine gene modules, and one module including 61 genes showed a high predictive accuracy ($p = 5.0\times10^{-5}$). The WGCNA-based analysis successfully explored the gene modules for prognostic prediction. In addition, this result indicates specific high expressed genes in metastasis-related GOs correlates with the prognosis.

1Pos258 種内多型から テントウムシの模様形成メカニズムを予測する
Prediction of the pattern formation mechanism in ladybirds from polymorphism

Ryo Takeda (*Grad.sch.Sci.,Univ.Osaka*)

The ladybird polymorphism is an interesting model case for pattern formation. Several genotypes and genes have been identified for the ladybird ladybird polymorphism. However, it is difficult to reveal when and where all the genes are at work in order to reveal the mechanism of pattern formation. Therefore, in this study, we searched for the mechanism of pattern formation that produces polymorphisms by analyzing spot placement and using mathematical models. As a result, we predicted that two pattern-formation systems produce the polymorphic patterns in ladybirds. Furthermore, these two pattern-formation systems can also explain the non-polymorphic ladybird pattern. These results predict that the ladybird pattern is produced by two pattern-formation systems.

1Pos259 大腸菌走化性応答における細胞内シグナル伝達のデータ駆動によるモデル構築
Data-driven model construction of intracellular signal transduction in E. coli chemotaxis response

Hiroto Tanaka, Yasuaki Kazuta, Hiroaki Kojima (*Frontier Research Lab, Adv ICT Res Inst, NICT*)

Cells of E. coli exhibit chemotactic response (CR) to chemical stimuli. Although several mathematical models (MM) of intracellular signal transduction in CR have been proposed, they have not yet comprehensively explained observed responses.
We have combined tethered assays, microchannels, and self-made rotational analysis programs to build techniques for quantifying CRs at high throughput. This technique has realized data acquisition under various conditions (chemical type, stimulus intensity, ambient temperature, etc.) by simplifying measurement of CR.
Based on MMs proposed previously, we have constructed a data-driven MM using CR data under various conditions. At meeting, we would like to discuss our MM, intracellular signal transduction, and cellular responses.

1Pos260 混雑下での分子の構造変化を考慮した反応拡散モデル
A reaction-diffusion model considering the conformational change of molecules and crowded states

Masaki Okada[1], Yuichi Togashi[2,3] ([1]*Grad. Sch. of Integr. Sci. for Life, Hiroshima Univ.*, [2]*Coll. Life Sci., Ritsumeikan Univ.*, [3]*Riken BDR*)

When we consider the macroscopic behavior of chemical reactions, we implicitly assume that molecules are so small that they can freely diffuse. However, molecules have finite sizes and different shapes, which affect the behavior of chemical reactions. In the cell, we also need to consider situations crowded with macromolecules. This study aims at a (continuum) reaction-diffusion model that reproduces the behavior considering the situation, which would easily visualize complicated phenomena. First, we constructed a particle-based model where one molecule consists of a few particles and executed Brownian dynamics simulations. In this presentation, we discuss the model behavior compared with that of ordinary reaction-diffusion models.

1Pos261 細胞の遺伝子発現制御における学習過程
Learning processes in gene-expression regulation

Tomoyuki Yamaguchi (*Research Institute, Nozaki Tokushukai Hospital*)

The mechanism how to achieve the accurate expression of many genes is remains unclear. Here, I modeled the whole gene regulation by considering a cell as a learning machine. In the model, thousands of genes are regulated in a hierarchical-pair architecture, in which the activation degrees competitively amplify with a small addition noise term, while transducing the activation signal, and decay at four different probabilities depending on the difference between the current and target ratios in each pair. The simulation results well reproduced the changes in whole gene expression during human early embryogenesis and hematopoiesis. I propose the law of biological inertia as a principle for the regulation of multiple factors. This study was published in *Scientific Reports*.

1Pos262 細胞集団運動における界面張力の効果
Interface Tension Effect on Collective Cell Migration

Katsuyoshi Matsushita, Taiko Arakaki, Naoya Kamamoto, Maki Sudo, Koichi Fujimoto (*Dep. Bio. Sci., Osaka Univ.*)

Collective cell migration occurs to convey the cells to the proper places in the biological systems. In this migration, cell-cell adhesion serves to stabilize cell-cell contact or guide the migration. The physical origin of this function is that the cell-cell adhesion regulates the surface tension of the cells with various biological materials. One of the essential tensions which affect the collective migration is the interface tension between cells and medium. We theoretically investigate the effect of the interface tension in the collective migration of a cell cluster. We use the Cellular Potts model and show that the migration mode changes from the translational to rotational motions as the interface tension increases.

1Pos263 筋芽細胞集団が示す位相欠陥と収縮性流れの幾何的制御
Geometric control of topological defects and contractile flow in confined myoblast cell populations

Ryo Ienaga[1], Yusuke Maeda[1], Kazusa Beppu[2] ([1]*Grad. Sch. Sci.Phys., Univ. Kyushu*, [2]*Applied Phys., Univ. Aalto*)

Morphogenesis of eukaryotic systems exhibits ordered collective motion through the orientation alignment at high density, as seen in myoblast cells. One promising approach to understanding such collective motion is controlling the organized dynamics by confining the cell population in a designed geometry. In this study, we examined collective motion of C2C12 myoblast cells under a confined space defined by the geometry of overlapped two circles. We found C2C12 cell population organized its heading orientation parallel to the major axis under any geometric conditions. Moreover, confined cell population exhibits inward contractile flow along the major axis, which implies the interplay between the contractile flow and topological defects in active nematics.

1Pos264 ヒト iPS 細胞由来ニューロンの神経突起伸長過程における形態変化の数理解析とタンパク質凝集体発現の観察
Analysis of morphological change and observation of protein aggregations in the developmental process of neurites of iPSC-derived neurons

Narumi Maeda[1], Rio Hine[1], Yudai Kitayama[2], Yusuke Shibasaki[1], Yuka Shirakawa[3], Minoru Saito[1,2,3] ([1]*Grad. Sch. of Integ. Bas. Sci., Nihon Univ.*, [2]*Coll. Hum. Sci., Nihon Univ.*, [3]*Nat. Inst., Coll. Hum. Sci., Nihon Univ.*)

We analyzed the morphological change in the developmental process of neurites of cultured human iPSC-derived neurons. From microscopic images at each developmental stage, driving forces were calculated by a mathematical method (Loewner equation), and detrended fluctuation analysis (DFA) was performed for them. The day *in vitro* (DIV)-dependent behaviors of the fluctuation characteristics showed the differences between healthy and Alzheimer's disease (AD) neurites from the early stage. Immunofluorescence-staining results showed that these differences precede significant expressions of β-amyloid and phosphorylated tau aggregations, which are biological factors causing AD. We are also performing other similar analyses, that is, real-time analyses using time-lapse images.

1Pos265 解糖系の振動現象に及ぼす飢餓処理の影響
Effect of starvation on the glycolytic oscillation in yeast cells

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The living system drives metabolic reaction networks by taking nutrients from the external environment. If the supply of nutrients is stopped, the system will reach an equilibrium state, i.e., death. It is interesting to note that yeast cells in the starved state exhibit oscillation of metabolites in the glycolytic pathway. This glycolytic oscillation might play a role in delaying to reach the equilibrium state. In this context, we have investigated the concentration of metabolites in a yeast cell as a function of culture time and starvation time using a micro-Raman technique. This analysis indicates that intracellular glucose concentration is one of the key parameters. We will discuss the effect of the glucose concentration on the oscillation based on a kinetic model.

1Pos266 Neuro2a 細胞の神経突起伸長過程における形態変化のリアルタイム数理解析
Real-time mathematical analysis of morphological change in the developmental process of neurites of Neuro2a cells

Rio Hine[1], Narumi Maeda[1], Yudai Kitayama[2], Yusuke Shibasaki[3], Yuka Shirakawa[3], Minoru Saito[1,2,3] ([1]*Grad. Sch. of Integ. Bas. Sci., Nihon Univ.*, [2]*Coll. Hum. Sci., Nihon Univ.*, [3]*Nat. Inst., Coll. Hum. Sci., Nihon Univ.*)

The neurite morphologies are very diverse and inherently constitute ambiguous messages in their forms. In this study, we observed the morphological change in the developmental process of neurites of cultured neuroblastoma (Neuro2a) cells, and mathematically analyzed it in real time. For this purpose, we obtained the time-lapse images by a microscope (BZ-X800, KEYENCE), and the traces of neurites were automatically obtained by the attached application. Using the obtained traces, we mathematically quantified the neurite morphologies with some physical quantities, e.g. fractal dimension, winding angle and so on, in real time. The results showed some characteristics of the morphological change in the developmental process.

1Pos267 結合 BZ 反応の系の光応答性とその同期現象
Photoresponsivity and synchronization of coupled BZ reaction systems

Ryota Yamazaki[1], Sigeru Sakurazawa[2] ([1]*Grad. Sch., Future Univ. Hakodate, Systems Information Science*, [2]*Future Univ. Hakodate, School of systems information science, Department of complex and intelligent systems*)

When plasmodia of the true slime mold Physarum were periodically stimulated with light, they spontaneously reduced their locomotive speed at the time when the next stimulus would have occurred. This phenomenon is called SPS(spontaneous in-phased slowdown). SPS is realized by coupled with a lot of non-liner chemical reactions which have different periods in their cells. BZ reaction also has non-linearity and shows periodical oscillation. This study aims to realize SPS like phenomenon with BZ oscillators. When two BZ oscillators which had different frequencies were connected by Pt wire, they were synchronized after three consecutive light stimuli in spite of they didn't synchronize before the stimuli. And similar results were shown in numeric simulation with Oregonator.

1Pos268 上皮細胞の集団運動とペアリング秩序転移
Collective motion and pairing order transition of confined epithelial cells

Kazuyuki Shigeta[1], Kazusa Beppu[1], Aya Tanaka[2], Yusuke Maeda[1] ([1]*Dept. Phys. Kyushu Univ.*, [2]*NTT BRL, BMC*)

Active matter, a group of elements that move autonomously, such as epithelial cells, exhibits ordered collective motion due to their orientation interactions as their density increases. Recent studies have shown that the vortex pairing of active turbulence can rule the geometric nature of collective motion. To further extend this finding to the epithelial cell monolayer, this study examined confined MDCK epithelial cells within single and doublet circular boundaries defined by the center-to-center distance Δ and the radius size R to reveal the geometric rule of epithelial collective motion. Furthermore, we found the geometry-dependent vortex formation by analyzing the alignment at the intersect of the doublet boundary. The observed geometric rule will be discussed.

1Pos269 補償光学系と機械学習を用いて 1 分子輝点の 3 次元座標を精度良く計測する方法のシミュレーション研究
A simulation study to measure precisely three-dimensional coordinates of single molecule images using adaptive optics and machine learning

Xiang Zhou, Yuma Ito, **Makio Tokunaga** (*Sch. Life Sci. Tech., Tokyo Tech*)

Methods of three-dimensional single-molecule tracking (SPT) in living cells have been developed to overcome the limitation of tracking ability in the optical axis direction. However, poor signal-to-noise ratios of out-focus-images largely inhibit improving three-dimensional localization precision. Using a simulation framework to evaluate point-spread-function (PSF) engineering with adaptive optics, we achieved an improved localization method of single-molecule images acquired with EMCCD cameras in three-dimensional, especially in the optical axis direction. Image processing using machine learning also contributed largely to the accuracy. It was shown that adaptive optics-based microscopy is useful for three-dimensional single-molecule tracking.

1Pos270 細胞内ナノドメインにおける分子ダイナミクスの精密な測定を可能にする一粒子追跡手法の開発
A novel single-particle tracking system for precise measurement of molecular dynamics in intracellular nanodomains

Shinkuro Kobayashi, Shigeyuki Namiki, Daisuke Asanuma, Kenzo Hirose (*Grad. Sch. Med., Univ. Tokyo*)

Regulation of protein localization and dynamics is a key element in regulating cellular function. Since many proteins localize to nanometer-sized domains within the cell, analysis of protein dynamics at sub-micrometer spatial resolution is essential. We developed a nanometer-scale means of measuring molecular dynamics by combining single particle tracking (SPT) with regenerative protein fluorescence labeling methods, enabling the acquisition of molecular trajectories at high densities. We demonstrated the analysis of dynamics of synaptic protein (TARPg-8) within PSD95 clusters using our technique. These results suggest that our technique contributes to understanding the significance of protein dynamics in intracellular nanodomains based on molecular dynamics in cells.

1Pos271 Live prediction with image-based deep learning accesses temporal variability of single-cell transcriptomic states

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Transcriptomics has been immensely valuable for understanding biological phenomena. The increase in resolution by single-cell RNA (scRNA) sequencing has been key to unveil cell heterogeneity, and recently spatial methods have provided insights into cell location variability. However, RNA expression also varies over time, for example during cell development and plastic cell state transitions. Yet there is no method that measures real-time whole single cell transcriptome changes. We produce image-coupled scRNA data and leverage deep learning to predict transcriptome states from cell images. The resulting model enable continuous evaluation of transcriptomic states during state transitions, resolving the temporal variation of transcriptome states at single cell resolution.

1Pos272 聴覚の末梢器官である内耳蝸牛の感覚上皮振動に含まれる直流動作の検出と分析
Analyses of the sound-evoked nanoscale offset motion in the cochlea of the inner ear

Takeru Ota[1], Hiroshi Hibino[1,2] ([1]*Grad. Sch. Med., Univ. Osaka*, [2]*AMED-CREST, AMED*`)

Hearing is triggered by sound-evoked nano-vibrations in the sensory epithelium inside the cochlea of the inner ear. The epithelium contains hair cells that have mechanosensory ion channels at the top. The epithelial vibrations are modulated by cation-induced elastic motions in the cell bodies. Here we optimized a laser interferometry. When a live guinea pig sensory epithelium was exposed to acoustic stimuli, the interferometer recorded the vibration amplitude as described elsewhere. Additionally, an baseline shift of several nanometers was detected. This motion was negligible when the animal was dead or under pharmacological perturbation of cell body motions. A theoretical approach suggested that the shift protects the epithelium from injury induced by strong stimuli.

1Pos273 気液界面を用いた細胞メカニクス解析技術の開発
Development of gas-liquid interface-based cell mechanics analysis technology

Masaki Moriyama[1], Naoya Ishizawa[1], Ryo Kobayashi[1], Seri Hayashi[1], Makiko Takubo[1], Kaede Yokoyama[1], Masataka Murakami[1], Tetsuro Hoshino[1], Akio Iwasa[1], Masafumi Mimura[1], Hirohide Murai[2], Taichi Nakamura[2], Kiyoshi Nozaki[1], Shuhei Tanaka[1] ([1]*Nikon Corporation*, [2]*Nikon Systems Inc.*)

Cell mechanics analysis tools have been actively developed for the mechanobiology field. The gas-liquid (G/L) interface has the specific properties which are pressing an object with the interface and observing a 3D shape of the object by the interference fringes from the interface reflecting lights. A device having an air bubble at a tip of nozzle pressed a HELA cell with the G/L interface. These surface stress onto the cell and deformation of the cell were observed from a gas pressure and the interference fringes, respectively. The static and dynamic moduli of the cell were able to calculate from these stress and strain values. These results show that the G/L interface-based cell mechanics analysis technology may be useful in the mechanobiology field.

1Pos274 ラマンイメージングによる老化細胞のラベルフリー検出
Label-free detection of senescent cells by Raman imaging

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Senescent cells irreversibly cease to proliferate through repeated division and accumulate with age, contributing to various diseases. Senescent cells have various characteristics, but there are no specific and clear indicators for their detection. In this study, we obtained Raman imaging of NIH3T3 cells treated with hydrogen peroxide, a reactive oxygen species involved in cellular senescence, to investigate the label-free detection of senescent cells using Raman imaging. We compared Raman spectral changes between aged cells and cells exposed to different oxidative stresses and found the Raman bands specific to aged cells such as the decrease in the intensity of the Raman band at 1157 cm-1 in passaging cells.

1Pos275 多様体学習と機械学習の外力下での細胞運動ダイナミクスへの適用
Manifold and machine learning techniques applied to cell movement dynamics under external forces

Hiroshi Fujisaki[1], Kenta Odagiri[2], Hiromichi Suetani[3], Hiroya Takada[1], Rei Ogawa[1] ([1]*Nippon Medical School*, [2]*Senshu Univ.*, [3]*Oita Univ.*)

Although various imaging techniques now make it possible to experimentally acquire movies of multicellular dynamics, their interpretation is still difficult. In particular, since multicells are in collective motion but not a homogeneous system, it is safe to say that there is no systematic way to extract their collective nature. Therefore, here we use diffusion maps, a type of manifold learning, and time-delayed autoencoders to extract multiple collective coordinates from movies of cell dynamics under force (mechanobiological situation) and explore their biological meaning.

1Pos276 ソリッドステートナノポアによる H2A.B ヌクレオソームの構造安定性に関する研究
A study on the structural dynamics of the nucleosome containing H2A.B using solid-state nanopores

Hikaru Nozawa[1], Hirohito Yamazaki[1], Ryo Iizuka[1], Rina Hirano[1,2], Tomoya Kujirai[2,3], Hitoshi Kurumizaka[1,2], Sotaro Uemura[1] ([1]*Department of Biological Sciences, Graduate School of Science, The University of Tokyo*, [2]*Institute for Quantitative Biosciences, The University of Tokyo*, [3]*RIKEN Center for Biosystems Dynamics Research.*)

Eukaryotic genomic DNA is wrapped with the histone proteins H2A, H2B, H3, and H4 to form the nucleosome, the basic chromatin unit. H2A.B, the most divergent histone variant of H2A, is enriched in actively transcribed genes and is suggested to modulate nucleosome and chromatin structures. Here, we employed solid-state nanopores to probe the structural dynamics of the nucleosomes containing H2A and H2A.B. A narrow pore (2.4 nm in diameter) induced faster dissociation of the nucleosomes containing H2A.B. In addition, with a wide pore (4.4 nm in diameter), the different translocation dynamics of the nucleosomes containing H2A and H2A.B were observed. These results reflect the structural differences in the nucleosomes.

1Pos277 ナノポア計測による CALHM2 チャネルダイナミクスの解明
Investigation of CALHM2 Channel Dynamics using Nanopore measurement

Sotaro Nakamura, Hirohito Yamazaki, Wataru Shihoya, Osamu Nureki, Sotaro Uemura (*Department of Biological Sciences, The University of Tokyo*)

Calcium homeostasis modulator protein 2 (CALHM2) is identified as an ATP release channel expressed in a variety of tissues, but the underlying mechanism is still unclear. In this study, we performed nanopore measurements to investigate the mechanism of CALHM2. We found that the conductance of CALHM2 varied from approximately 1 to 48 nS. The conductance variation did not change in the presence of calcium ion, an inhibitor of CALHM2 previous patch clamp experiments showed. Our data suggested that calcium ion may not act directly on the CALHM2 dynamics. The deletion mutant of the N-terminal helix (NTH) showed less variation and did not have a large conductance, suggesting that the NTH regulates the opening and closing of CALHM2.

1Pos278 赤外超解像顕微鏡による爪ケラチンタンパク質の分布・配向観察
IR super-resolution imaging of keratin proteins in human nails based on non-linear optical process

Hirona Takahashi, Tetsuya Ida, Kohei Katayama, Makoto Sakai (*Faculty of Sci., Okayama Univ. of Sci.*)

It has been reported that human nails are layered and stacked with keratin proteins, with a mixture of α-helix, β-sheet, and random coil structures. On the other hand, the spatial inhomogeneity of keratin proteins, such as the distribution and orientation, could not be disclosed. In this study, we applied an IR super-resolution micro-spectroscopy based on the vibrational sum-frequency generation (VSFG) to human nail. VSFG is proportional to the second-order susceptibility and allows us to selectively detect only molecules located on the interfaces. It was found that only β-sheet structure is aligned at the interface between the layers. In the presentation, the spatial inhomogeneity of keratin proteins will be discussed in detail.

1Pos279 近赤外光検出が可能な微弱光検出器の現状
Current status of low-light photodetectors capable of detecting near-infrared light

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There are few options for low-light detectors capable of detecting near-infrared light (>900 nm). Such photodetectors have attracted attention in the vehicle-mounted LIDAR market. This wavelength band is also known as the optical window with low scattering and absorption by living organisms. The band thus is expected to be applied to high-sensitivity detection with high temporal resolution in biological measurements. In this presentation, we will report on the current status of low-light photodetectors capable of detecting near-infrared light and our efforts to extend the sensitivity of hybrid photodetectors (HPD) to longer wavelengths.

1Pos280 表面増強ラマン分光を用いたジペプチド繰り返し配列を有するペプチドの液-液相分離液滴の計測
Surface Enhanced Raman Spectroscopy of liquid-liquid phase separation droplets consisting of dipeptide repeats

Yui Yamazaki[1], Masayuki Fujiwara[2], Ryo Kato[2], Kohsuke Kanekura[3], Taka-aki Yano[2], Yuhei Hayamizu[1] ([1]*Dept. of Mat. Sci. and Eng., Tokyo Tech*, [2]*pLED, Tokushima Univ.*, [3]*Dept. of Molecular pathology, Tokyo Medical Univ.*)

The phenomenon of protein-RNA phase separation, which is associated with neurological diseases, has attracted much attention. To understand this phenomenon at the molecular level, it is crucial to establish a method. Raman spectroscopy, which allows direct observation of molecular vibrations, is an effective tool. However, existing methods have difficulty in obtaining sufficient signals in a short time. In this work, we aimed to efficiently obtain Raman spectra related to molecular interactions inside a droplet by plasmon resonance using metal nanoparticles to enhance the Raman signal. We mixed metal nanoparticles into a phase-separated solution consisting of dipeptide-repeats and RNA, and succeeded in the enhancement of the Raman signals.

1Pos281 CRISPR-Cas13 を用いたデュアルプローブシステムおよび液液相分離濃縮による RNA の高感度 1 分子計測
Sensitive CRISPR-Cas13 mediated digital bioassay of RNA with dual probe system and enrichment by liquid-liquid phase separation

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CRISPR-Cas13 mediated digital bioassay method, which uses target-programmable RNA recognizing enzyme Cas13 and encapsulating technology into ultra-small volumes enabled to detect low concentration RNA targets in minutes without time-consuming nucleic acid amplification process. Still, there are large demands for improved detection sensitivity to realize more accurate detection method. To meet such needs, it is required to reduce false positive signals and increase available reaction volume. Here, we show two approaches to achieve these requirements: distinguishing and removing signals by RNase which is considered to be the main cause of false positives with dual-probe system, and introducing an RNA/protein enrichment method utilizing liquid-liquid phase separation.

1Pos282 高速原子間力顕微鏡で観察されたミオシン V の歩行運動の隠れマルコフモデル解析
Hidden Markov model analysis of myosin V walking observed by high-speed atomic force microscopy

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High-speed atomic force microscopy (HS-AFM) is a powerful technique to observe the structural dynamics of a single biomolecule at work in real time and with nanometer resolution. However, its spatiotemporal resolution is not sufficient to reveal the atomic-level details. In the present study, we focus on myosin V walking along actin filament and aim to provide detailed dynamics information using HS-AFM data. We first performed coarse-grained molecular dynamics simulation of modeled myosin V in four different conformational states many times. Using obtained trajectories, we then constructed a Markov state model (MSM) of the walking dynamics. Finally, we performed a hidden Markov model analysis using HS-AFM data and MSM to reveal the conformational dynamics of myosin V.

1Pos283 (1SEP-6) Centromere-kinetochore structures revealed by 12x modified expansion microscopy

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The kinetochore is essential for faithful chromosome segregation during mitosis and is assembled on centromeres through dynamic processes involving numerous kinetochore proteins. However, the orientation of the kinetochore proteins remains elusive because of the limitation of fluorescence microscopy resolution despite super-resolution microscopies enabling us to resolve 50-100 nm structure. In this study, we applied 12x modified expansion microscopy (mExM) and obtained a diffraction-limited resolution in the expanded sample that corresponds to ~30 nm resolution in the original sample under conventional microscopy. By using the mExM, we found that constitutive centromere-association network proteins, CENP-T and CENP-C, formed a different structure in the kinetochore.

1Pos284 Fluorescence polarization light-sheet microscopy for studying 3D molecular architectures *in vivo*

Tomomi Tani (*Biomedical Research Institute, National Institute of Adavnced Industrial Science and Technology*)

Light sheet microscope uses a thin sheet of laser that excites only fluorophores within the focal volume, providing an excellent optical sectioning, low phototoxicity and fast image acquisition for thick live specimens. We have developed a new light sheet microscope that reports the molecular orientation of fluorophores in 3D space, allowing the analysis of 3D molecular architectures within developing spheroids, organoids, and embryos. The microscope has an illumination system that creates polarization neutral light sheet illumination and a polarization detection system that reports the fluorescence polarization orientations in the focus plane. A proof of concept imaging of 3D cytoskeletal architectures within spheroids of epithelial cells will be presented.

1Pos285 細胞分化に伴うクロマチン構造における状態特異的なヒストン動態の１分子イメージング
Single-molecule analysis of state-specific histone mobility in chromatin subcompartments during cellular differentiation

Masanori Hirose, Yuma Ito, Makio Tokunaga (*Sch. Life Sci. Tech., Tokyo Tech*)

Molecular mobility in the nucleus is closely related to the regulation of gene expression and to cellular differentiation. However, the relationship between them remains unsolved. We performed live-cell single-molecule imaging using C2C12 cells co-expressing HaloTag fused-histone H4 and mCherry-heterochromatin protein 1α. Quantification of the dynamics of histone H4 molecules before and after differentiation revealed that the variances of the anomalous exponent and the effective spring coefficient increased after differentiation. It suggests that differentiation promotes diversity in molecule mobility. We further examined single-molecular mobility in heterochromatin before and after differentiation, and we would like to discuss dynamics specific to chromatin states.

1Pos286 Alphafold2 による遺伝子にコードされた FRET 型カルシウム指示薬の設計
Alphafold2-assisted design of a genetically-encoded FRET-based calcium indicator

Shinya Sakai[1], Kei-ichi Okazaki[2], Tomoki Matsuda[3], Takeharu Nagai[3] ([1]*Graduate School of Frontier Biosciences, Osaka University, Japan,*, [2]*Research Center for Computational Science, Institute for Molecular Science, Japan*, [3]*SANKEN, Osaka University, Japan*)

FRET-based probes have been developed to investigate the physiological phenomena. However, the design and construction require repeated trial and error. Here, we present a method of semi-rational design of the probes based on the structural prediction by AlphaFold2, thereby we successfully developed a Ca^{2+} indicator with green- and red-fluorescent proteins(FPs). We predicted the probe structure that maximizes FRET efficiency by optimizing the distance and relative angles between the chromophores. The designed probe showed 1.5-fold higher dynamic range *in vitro* than the original one and clearly reported Ca^{2+} dynamics in live cells. This method would be applicable to design probes based on another principle such as single circularly-permuted FP-based probes.

1Pos287 細胞性粘菌における **c-di-GMP** シグナルの解析
Fluorescence imaging of cyclic di-GMP signal in *Dictyostelium discoideum*

Hayato Ide, Yusuke Morimoto (*Grad. Sch. Comp. Sci. and Sys. Eng., Kyushu Inst. Tech.*)

Cyclic di-GMP is known as a second messenger that works mainly in prokaryotes. In eukaryotes, only *Dictyostelium discoideum* uses c-di-GMP as a signaling molecule. Although the activity of c-di-GMP synthase and the induction of differentiation by c-di-GMP during the multicellular stages have been shown to be mediated by cAMP, there is no observation of c-di-GMP in the living cells using fluorescent probes. This study introduced fluorescent probes utilized in bacterial cells into *D. discoideum* cells to visualize intracellular c-di-GMP signals.

1Pos288 (3SAA-6) Size determination of cytoplasmic condensates of optineurin using spatial image correlation spectroscopy (SICS)

Yuta Hamada[1], Masataka Kinjo[2], Akira Kitamura[2] ([1]*Grad. Sch. Sci. of Life Sci., Hokkaido Univ.*, [2]*Fac. of Adv. Life Sci., Hokkaido Univ*)

Optineurin (OPTN) regulates many cellular processes and plays a neuroprotective role. Neurodegenerative diseases-associated mutations in OPTN make its cytoplasmic condensates to various sizes. However, since a standard procedure to quantify the sizes of the protein condensates has not been established, we establish an integrated analysis procedure using spatial image correlation spectroscopy (SICS), which determines the average sizes of foci from a single fluorescence microscopic image. The larger foci of E50K mutant of OPTN than its wild type were successfully determined in a single processing from the original microscopic fluorescence images. Our established procedure would contribute to standardize to determine other intracellular condensates.

1Pos289 (3SAA-4) Morphological Analysis of Hydrogel Induced Cancer Stem Cells in Synovial Sarcoma Model Cells

Zannatul Ferdous[1], Masumi Tsuda[1,3,4], Jean-Emmanuel Clément[3], Jian Ping Gong[1,3,6], Shinya Tanaka[3,4,6], Tamiki Komatsuzaki[2,3,5], Koji Tabata[2] ([1]*Graduate School of Life Science, Hokkaido University*, [2]*Research Center of Mathematics for Social Creativity, Research Institute for Electronic Science, Hokkaido University, Sapporo, Japan*, [3]*Institute for Chemical Reaction Design and Discovery (WPI-ICReDD), Hokkaido University, Sapporo, Japan*, [4]*Department of Cancer Pathology, Hokkaido University Faculty of Medicine, Sapporo*, [5]*Graduate School of Chemical Sciences and Engineering, Hokkaido University, Sapporo, Japan*, [6]*Global Station for Soft Matter, Global Institution for Collaborative Research and Education (GI-CoRE), Hokkaido University, Sapporo, Japan*)

Cancer tissues are composed of the heterogenous population composed of small numbers of cancer stem cells (CSCs), progenitor cells, and differentiated non-CSCs. CSCs cause therapy-resistance and recurrence, thus CSCs should be a therapeutic target for eradicating cancer. However, The identification of CSCs is extremely difficult because of the quite small number and only few markers. In this study, we studied the of morphological changes of the cancer cells on hydrogels in terms of stemness marker elevation. In this study, we studied the of morphological changes of the cancer cells on hydrogels in terms of stemness marker elevation.

1Pos290 細胞内ストレス顆粒の近赤外蛍光・ラマンイメージング：細胞固定化の相分離液滴への影響
Near-infrared fluorescence and Raman imaging of intracellular stress granules: Effects of cell fixation on droplets formed by LLPS

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We have studied stress granules, which are intracellular membrane-less organelles formed by liquid-liquid phase separation (LLPS) under environmental stresses, using Raman imaging. In this study, we performed near-infrared (NIR) fluorescence and Raman imaging of stress granules by expressing scaffold proteins, G3BP1, labeled with NIR fluorescent proteins. We obtained Raman images of stress granules in fixed cells, and revealed differences in components inside and outside of stress granules. In addition, we obtained NIR fluorescence and Raman images of stress granules in living cells. Based on the difference in Raman spectra between fixed and living cells, we discuss effects of fixation on stress granules and in the cytoplasmic components.

1Pos291 情報理論を使ったラマン画像に含まれる化学情報と形態情報の関係性の定量
Quantification of the relationship between chemical and spatial information in Raman images using information theory

Ryoya Kondo[1], James Nicholas Taylor[2], Yuta Mizuno[1,2,3], Jean-Emmanuel Clement[2,3], Katsumasa Fujita[4], Yoshinori Harada[5], Tamiki Komatsuzaki[1,2,3] ([1]*Grad. Chem. Sci. Eng., Hokkaido Univ.*, [2]*Res. Inst. Electr. Sci., Hokkaido Univ.*, [3]*WPI-ICReDD, Hokkaido Univ.*, [4]*Grad. Eng., Osaka Univ.*, [5]*Kyoto Pref. Univ. Med.*)

Raman spectroscopy provides information about spatial distributed molecules in cells or tissues. Our previous research extracted chemical features by classification of the spectra and sorted more detailed pathology than previous research. However, information on where each spectrum in the images is measured was not considered. On the other hands, on morphological analysis of bright field images, most chemical information is overlooked because pathologists observe spatial distribution of specific chemical species. We unified chemical information and morphological that in a clustering and evaluate relation between them. Here we quantify the two information and discuss probability that the separation suggests a new pathology or a new diagnosis criterion.

1Pos292 シグナル伝達反応進行過程における細胞膜上受容体動態の変化
Oligomerization and dynamics of receptor molecules during the signaling process

Hideaki Yoshimura, Takeaki Ozawa (*Sch. Sci., Univ. Tokyo*)

Singnal transduction processes on the plasma membran, which start from ligand sensing by receptors and induce the information to donwstream molecules, takes several minutes. To understand the mechanisms of the signal transduction, long time single receptor tracking of receptors and downstream molecules are ideal approach. In this study, we used extremely stable fluorescence dye to track motility of platelet derived growth factor receptor (PDGFR) and Akt for consecutive several minutes under low oxygen concentration atmosphere based on the method reported by Tsunoyama et al. Based on the results, we discuss the signal transduction mechanism of the Akt signaling system.

1Pos293 デュアルコム干渉計を用いた細胞膜電位のラベルフリー検出
Label-free detection of membrane potential using dual-comb interferometry

Satoshi Araoka[1,3], Yusuke Takashima[2], Yoshiki Naoi[2,3], Akira Emoto[3], Kazumichi Yoshii[3], Masatake Akutagawa[2], Hiroki Takanari[3] ([1]*Graduate School of Sciences and Technology for Innovation, Tokushima University*, [2]*Graduate School of Technology, Industrial and Social Science, University of Tokushima*, [3]*Institute of Post-LED Photonics, University of Tokushima*)

We propose a new method for a label-free for the detection of cell membrane potential using dual-comb interferometry. In this study, a thin film of Indium Tin Oxide (ITO, 200 Å thick) was deposited on both sides of a cover glass (0.25 mm thick) that could be regarded as a transparent parallel plate capacitor, and used as a simple model to mimic a cell membrane. A signal comb was transmitted through ITO glass and interferograms were acquired by interfering with a local comb that was phase-locked to the signal comb. When a voltage of 3 V was applied to the ITO glass, the phase of the interferogram changed significantly. The results indicated that the potential applied to thin films such as cell membranes could cause changes in the phase of the light.

1Pos294 脂質、ヌクレオチド依存的 Prx 高分子量複合体形成メカニズムの解明
Study on the formation mechanism of peroxiredoxin high molecular weight complex with lipid and nucleotide

Ryusei Yamada[1], Hiroki Konno[2] ([1]*Grad. Sch. of Nat. Sci. & Technol., Kanazawa University*, [2]*WPI Nano Life Sci. Inst. (WPI-NanoLSI), Kanazawa Univ*)

Peroxiredoxin (Prx) contributes to cell protection through the removal of various reactive oxygen species such as hydrogen peroxide in cells. On the other hand, when Prx associate with each other to form a complex, Prx loses the degradative activity of H2O2 and instead functions as a molecular chaperone that prevents the aggregation of denatured proteins. Furthermore, our laboratory recentry discovered that Prx associates with negatively charged phospholipids and nucleotide to form vesicles with a diameter of 30~80 nm. In this study, i conduct experiments using a high-speed AFM to investigate the formation mechanism of spherical high molecular weight complexes of Prx and report the results.

1Pos295 イメージプロセッシングによる細胞内小胞輸送の 3 次元トラッキングデータ解析の自動化に関する研究
An automatic detection and tracking method for the 3D reconstruction of vesicle movement in a living cell

Seohyun Lee[1], Hyuno Kim[2], Hideo Higuchi[3] ([1]*Institute for quantitative biosciences, The University of Tokyo*, [2]*Institute of Industrial Science, The University of Tokyo*, [3]*Graduate School of Science, The University of Tokyo*)

Analysis of the three-dimensional movement of vesicles in a living cell is one of the important tasks in biology, to understand how biological information can be delivered in a cytoplasmic area. Dual-focus optics, which calculates the 3D coordinates of a vesicle using the intensity of point spread function on two different focal planes, is one of the widely applicable methods to track a vesicle for fluorescence microscopy. In this presentation, we explain a linear transformation-based image processing method for the accurate detecting and 3D tracking of a vesicle the image of which is produced by dual-focus optics.

1Pos296 機械学習を駆使して高速 AFM 画像から細胞骨格ネットワーク構造の再構成
Machine learning-guided reconstruction of cytoskeleton network from Live-cell AFM Images

Kanaki Kiku[1], Shigehiro Yoshimura[1], Skibbe Henrik[2], Naoki Honda[3] ([1]*Graduate School of Biostudies, Kyoto University, Japan*, [2]*Brain Image Analysis Unit, RIKEN Center for Brain Science, Wako, Japan*, [3]*Graduate School of Integrated Sciences for Life, Hiroshima University, Japan*)

Actin cytoskeleton is of importance in a large range of cellular processes. Recently, a new high-speed atomic force microscopy (HS-AFM) was developed to visualize the structural dynamics of the cortical actin network. However, HS-AFM image has low resolution, and it is difficult for the human eye to recognize the actin network. In this study, we developed a new machine learning method to recognize F-actin networks from the low-resolution HS-AFM images in the level of individual filaments. This method can quantitatively recognize F-actin and then extract its topology from the low- resolution HS-AFM images. We successfully modeled the actin network from the HS-AFM images and then quantified some statistics such as angular distribution and length of the actin network.

1Pos297 ランダムドメイン挿入法を用いた FRET 型植物ホルモンセンサーのスクリーニング
Screening of FRET-type plant hormone sensor using Random domain insertion method

Ami Nakano (*Grad. Sch. Sci. Eng., Saitama Univ.*)

Genetically-encoded biosensors are powerful tools to monitor the spatiotemporal dynamics of signaling molecules. However, their development requires large amounts of time and effort due to difficulties in optimizing the sensor construction e.g., linker length and position of the fluorescent proteins. Here, we combined a random domain insertion (RDI) method and an in vitro cell-free protein synthesis (CFPS) and created a high-throughput screening system for FRET-based plant hormone sensors. This protocol provided 90 to 150 individual constructs, consisting of GFP and RFP sequences randomly inserted into the plant hormone-binding protein simultaneously, indicating that the RDI/CFPS method is a novel technique to quickly build large libraries of FRET biosensor constructs.

1Pos298 寒天培地上での海洋微生物の構造色の出現と発達のタイムラプス観察
Timelapse observation of the emergence and development of structural color of a marine bacterium on agar plates

Mikiko Tsudome, Shigeru Deguchi (*JAMSTEC*)

When cultured on agar plates, a marine bacterium, *Cellulophaga lytica*, exhibits the gliding motility and spreads across the agar surface, forming colonies that exhibit structural color. The structural color changes with the incubation time as the cell density within the colony increases. In this study, we developed a new time-lapse observation method and successfully captured the emergence and development of structural color with a stereomicroscope under transverse epi-illumination using a twin-arm LED illuminator.

1Pos299 生体内高感度シングルショット 3D 温度イメージング技術の開発
Sensitive single-shot 3D temperature imaging *in vivo*

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How does the high temperature of cells such as cancer cells affect normal surrounding cells? To address this question, we develop a method for high-sensitive single-shot 3D temperature imaging of multiple cells *in vivo*. We first established a system for tracking a freely moving *C. elegans* because body constraint acts as stimuli enhancing autofluorescence. Using fluorescent nanodiamonds (FNDs) for thermometry, we then built a novel electron spin resonance system, in which our high-resolution light-field microscopy (HR-LFM) allows for single-shot 3D extraction of fluorescent signals of multiple FNDs among fluorescent beads and autofluorescence with a high signal-to-background (S/B) ratio. We are now performing multiple cell thermometry in a freely moving worm.

1Pos300 Kilohertz imaging of intracellular heat diffusion with a genetically encoded temperature indicator

Kai Lu[1], Tetsuichi Wazawa[1], Joe Sakamoto[3], Cong Quang Vu[1,2], Masahiro Nakano[1], Yasuhiro Kamei[3], Takeharu Nagai[1,2] ([1]*SANKEN, Osaka Univ.*, [2]*Graduate School of Frontier Biosciences, Osaka Univ.*, [3]*NIBB*)

We developed B-gTEMP, a genetically encoded temperature indicator specializes in high-speed thermometry owing to its fast response kinetics and high signal-to-noise ratio. Using this indicator, we performed kilohertz temperature imaging and visualized heat diffusion inside live mammalian cells in real time. By comparing the *in cellulo* and *in silico* temperature dynamics during heat transfer, we managed to estimate the thermal diffusivity in the cell. This new method of thermometry combines sub-millisecond temporal resolution and subcellular spatial resolution, thus opens the p ossibility of investigating thermal properties in microscopic scale and in organelles.

1Pos301 従来の超解像用、生理機能用蛍光指示薬による生理機能超解像イメージング法
Functional super-resolution (fSR) imaging with conventional SR and functional fluorescent indicators

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Functional super-resolution (fSR) imaging is a technique to visualize intracellular physiological functions at high spatial resolution. However, fSR imaging developed so far has not been versatile, because the used indicators were too specifically designed to be applied to a wide variety of functions. Here we show a fSR method which can extend various types of functional and SR indicator and appropriate SR technique to the fSR imaging in principle. We demonstrated that we successfully observed Ca^{2+} around F-actin in living HeLa cell with conventional SR and Ca^{2+} probes and SPoD-OnSPAN, a SR technique, at a spatial resolution better than conventional fluorescence microscopy. Importantly, the present method can be applied to imaging of various physiological functions.

1Pos302 長期間ライブイメージングを可能にする光損傷を軽減する撮影条件の最適化
Optimization of image acquisition methods to reduce photodamage for long-term live-imaging

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To investigate the correlations between embryonic morphogenesis and cell dynamics, live-imaging experiments of a whole embryo with the single-cell resolution are indispensable. However, photodamage is a big issue in the experiments. In this study, we developed an evaluation system for photodamage. To reduce photodamage as much as possible, we investigated which parameter of light illumination was effective on photodamage. Then, we found that there is a tendency that higher scanning speed shows lower photodamage and that around 5min interval condition can reduce photodamage. Finally, we succeeded in taking live images of an entire E5.5 mouse embryo with the single-cell resolution for 16 hr. We found some characteristic phenomena by trans-scale analyses.

1Pos303 1 分子動態と局在による機能的クロマチン-RNA polymerase II 相互作用の統合解析
An integrated analysis of functional chromatin-RNA polymerase II interaction using single-molecule dynamics and localization

Yuma Ito, Makio Tokunaga (*Sch. Life Sci. Tech., Tokyo Tech*)

Live-cell single-molecule imaging has provided direct evidence of dynamics involved in the biological mechanism. However, the highly heterogeneous distribution and mobility of individual molecules make it difficult to identify functional dynamics. Here, we developed integrated spatial correlation analysis with machine-learning-based trajectory classification. We applied this method to RNA polymerase II (Pol II) dynamics and chromatin distribution. We have succeeded in identifying distinct Pol II mobility correlated with transcription states and surrounding chromatin nanostructures, suggesting epigenetically controlled Pol II-chromatin interaction. The present method provides a powerful approach to understanding protein functions by dynamics and localization.

1Pos304 クライオ電子線トモグラフィー法による糸状仮足中のアクチン繊維上ファシンのサブトモグラム平均化
Subtomogram Averaging of Fascin on Actin Filaments in Filopodia by Cryo-Electron Tomography

Kaoru Mitsuoka[1], Naoko Kajimura[1], Takuo Yasunaga[2] ([1]*Research Center for Ultra-High Voltage EM, Osaka Univ.*, [2]*Grad. Sch. Comp. Sci. Syst. Eng., KIT*)

Cryo-electron tomography (cryo-ET) could visualize the structures of macromolecular complexes in cells. In addition, high-resolution structures of the complexes could be obtained by the subtomogram averaging. Thus, we used it to get the structural information of actin bundles in neuronal model cells (NG108-15). In the filopodia of the model cells, fascin stabilized actin filaments in the bundles and so we focused on the complexes of fascin and actin filaments for the subtomogram averaging. We used the emClarity software for the calculation and also developed a visualizing program to select the appropriate regions for averaging. As a result, we could obtain a better three-dimensional structure of the complex than the one we calculated previously only using emClarity.

1Pos305 *Gloeobacter violaceus* の顕微分光イメージング
Microimaging of *Gloeobacter violaceus*

Kento Hashimoto[1], Reo Minami[1], Akio Murakami[2], Mamoru Nango[3], Mitsuru Sugisaki[3,4] ([1]*Grad. Sch. Sci., Osaka City University*, [2]*Grad. Sch. Sci., Kobe University*, [3]*Grad. Sch. Sci., Osaka Metropolitan University*, [4]*NITEP, Osaka Metropolitan University*)

Photosynthetic pigments in native pigment-protein complexes express their physiological functions when embedded in protein environment. To understand these functions, it is necessary to observe the spatial distribution and optical response of pigment-protein complexes simultaneously. In this study, we have developed a microscopic system that enables to simultaneously observe the fluorescence spectrum at each focal point. Furthermore, we introduced spectral deconvolution using Bayesian inference (Bayesian spectroscopy) and reconstructed fluorescence microscopic images of each type of pigment-protein complex. We discuss the spatial distribution of photosynthetic pigment-protein complexes in *Gloeobacter violaceus*.

1Pos306 骨格アニメーション法を活用したタンパク質構造変化の検証法
Utilizing skeletal animation for understanding structural change of proteins

Yutaka Ueno (*Artificial Intelligence Research Center, AIST*)

For studies of conformational changes of proteins utilizing general purpose 3D computer graphics (3DCG) software, the skeletal animation method became a useful tool. In addition to a previous report (Ueno *et al.* 2020, *J. integr. bioinform.*) that utilizes skeletal animation of protein in ribbon models, the method was also extended to be applied for the atomic models using Blender, a 3DCG software. The conformational change data of protein backbone was described in the skeletal animation file in BVH format, widely used in 3DCG field, and applied to a polygon mesh model of protein made by UCSF chimera. The technical details of available samples on https://github.com/uenoyt/skelmol will be discussed.

1Pos307 CRISPR 関連タンパク質によるプログラム可能な哺乳類細胞翻訳調節器
Programmable mammalian translational modulators by CRISPR-associated proteins

Shunsuke Kawasaki, Takeru Kuwabara, Hirohide Saito (*Center for iPS Cell Research and Application, Kyoto University*)

Precise control of gene expression in mammalian cells by using synthetic gene circuits is important for cell engineering and medical applications. In particular, the circuits based on translational modulators can function with various vectors such as synthetic RNAs and replicons which are regarded as the low genomic harm. However, the variety of translational modulators that can be implemented in complex circuits has been limited yet.
Here we show that Cas proteins can be repurposed as translational modulators. We designed over 50 different modulators and built over 60 synthetic circuits. These translational modulators have the potential to provide "biological Integrated-Circuits" which facilitate the development of biocomputers.

1Pos308 カップ型微小電極を用いた非接着細胞表面分子計測技術の開発
Development of a technology to detect surface molecules on non-adherent cells by using Cup-shaped microelectrodes

Taro Sasaki[1,2], Kohki Uchiyama[1,2], Tomoyuki Kamata[3], Dai Kato[3], Naoshi Kojima[3], Shohei Yamamura[3], Hyonchol Kim[1,2] ([1]*Cell. Mol. Biotechnol. Res. Inst., AIST*, [2]*Grad. Sch. Eng., Tokyo Univ. Agric. Technol*, [3]*Health Med. Res. Inst., AIST*)

Sensitive detection of surface molecules on non-adherent cells derives reliable blood diagnosis. Detection based on electrochemiluminescence (ECL) is one useful way. In the method, light emission is triggered by oxidization of both Ruthenium complex (Ru) and tripropylamine (TPA) near the electrode surface. In this study, we fabricated cup-shaped electrodes with similar diameter as cells to apply ECL for the detection. First, a solvent containing Ru and TPA was dropped for testing the electrodes, then observed ECL intensities were dependent on the concentration of Ru. Next, Ru-labeled cells were captured to the electrodes, then ECL irradiations were observed. These results indicate ECL detection can be applicable for evaluation of non-adherent cells by using our method.

1Pos309 3D DNA nanostructure-based assembled structures toward a construction of chromatin-like heterogeneous system

Hong Xuan Chai[1], Masahiro Takinoue[2] ([1]*Department of Life Science and Technology, School of Life Science and Technology, Tokyo Institute of Technology*, [2]*Department of Computer Science, School of Computing, Tokyo Institute of Technology*)

The transition between heterochromatin and euchromatin is important for gene expression. To better understand the process, we are creating chromatin-like heterogeneous system exhibiting both gel and liquid properties analogous to the heterochromatin and euchromatin respectively. DNA tetrahedral nanostructure with stability-differentiated sticky ends, one at each vertex, is used as the monomer to construct a string structure. We believe that the heterogeneous system with hierarchical characteristic can be controlled by controlling the connection along and between the string structure. Until now, we had successfully improved the DNA tetrahedral nanostructure assembly process and early result in controlling inter-nanostructure connection is promising.

1Pos310 DNA 増幅を動力源とするナノモーターの設計と評価
Design and evaluation of nanomotors powered by DNA amplification

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Nanomotors are micron scale devices that can “swim” by surface localized chemical reactions. Such devices have attracted particular attention in recent years as they may provide new therapeutic methods at the cellular level. Current nanomotors have low biocompatibility, severely limiting their use. In this study, we aimed to design and evaluate DNA amplification-powered nanomotors that show enhanced motion by biocompatible enzymatic activity at physiological temperatures. Micron-sized particles with surface attached DNA were synthesized and their motion was observed (with and without enzymatic solutions) and assessed by computer-aided particle tracking of recorded videos.

1Pos311 DNA を用いたシグナル伝達のための核酸生成回路の検証
Characterization of Nucleic Acid Generation Circuits for DNA-based Signal Transduction

Ken Komiya, Chizuru Noda (*X-star, JAMSTEC*)

We had previously developed various DNA generation circuits, that generate single-stranded DNA molecules as signals, for nucleic acid testing and synthetic signal transduction systems [1-3]. Their modular architecture allows modulation of signal generation performance via design and combination of template DNA strands. In the present study, we experimentally modified and investigated the signal generation circuits in terms of input and output forms and amplification performance for achieving versatile functions of DNA-based artificial molecular systems.

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1Pos312 リン脂質-タンパク質非対称膜小胞を用いた小胞分裂モデルの構築
Construction of vesicle fission model using asymmetric phospholipid-protein vesicles

Masato Suzuki (*Facut. Sci. Tech., Gunma. Univ*)

Lipid vesicles have been used to understand cellular functions, including membrane protein functions and membrane growth and fission. Recently, vesicles formed by amphiphilic proteins and polypeptides have been reported. Nano-sized protein vesicles have been realized as vesicle growth model by encapsulating a cell-free synthesis system. However, an observation of membrane protein function on the protein vesicle membranes are difficult. In this study, we generated cell-sized asymmetric lipid-protein vesicles which composed of lipids on the outer leaflet and protein on the inner leaflet. We demonstrated the observation of the membrane protein functions and construction of growth and fission model using the asymmetric lipid-protein vesicles.

1Pos313 原子間力顕微鏡液中測定によるパパイン分子と DNA で被覆された単層カーボンナノチューブ との相互作用の pH の影響の研究
Effects of pH on interaction of papain and DNA wrapped single walled carbon nanotubes studied by atomic force microscopy in fluid

Masaki Kitamura, Kazuo Umemura (*Physics. Science. Tokyo university of science/ Japanese*)

DNA wrapped single-walled carbon nanotubes (DNA-SWNTs) are one of the potential candidates to detect enzyme reactions instead of the use of fluorescent labelled substrates. However, aggregates of papain and DNA-SWNTs were appeared when the two compounds were mixed. In this study, we investigated the effects of pH on the interaction of papain and DNA-SWNTs by atomic force microscopy in fluid. Mixtures of papain and DNA-SWNTs were observed under two different pHs. Isoelectric point of papain molecules is 8.6. As a result, thick conjugates (almost 7.3 nm in diameters) were observed at pH 3.0 although it was around 4.6 nm at pH 10.5. It suggests that electrostatic interactions play an important role to decorate DNA-SWNTs with papain molecules.

1Pos314 フェリチンに内包されたマグネタイトナノ粒子の高周波磁場による加熱
Heat production by magnetite nanoparticles encapsulated in ferritin under alternating magnetic field

Kanamaru Tomoko[1], Yuta Hayashi[1], Hiroto Goshima[1], Toshiki Higuchi[1], Arun Kasimchetty[1], Shuji Kanamaru[2], **Hideyuki Yoshimura[1]** ([1]*Meiji Univ.*, [2]*Tokyo Institute of Techinology*)

Induction cooking utilize heat generation of ferromagnetic materials in alternating magnetic field due to eddy current. In contrast to this effect, nano-size ferromagnetic particles can be heated by magnetic energy dissipation during magnetic dipole relaxation. Apoferritin is known to produce magnetite nanoparticle in its cavity. We amid to utilize this magnetite nanoparticles for hyperthermia therapy. Magnetite nanoparticles were synthesized using several kinds of apoferritin, homo L-subunit apoferritin and H-subunit containing apoferritin. We succeeded to increase temperature of 100 μL solution with 30mg/mL homo L-ferritin up to 15 °C from room temperature in magnetic field of 2.3 MHz (1 mT). The effect of crystallinity of magnetite nanoparticles will be reported.

1Pos315 Inhibitory effect of nucleotides on acetylcholinesterase activity and its microflow based actuation in human plasma

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The inhibiting trend of phosphoesters with Acetylcholinesterase(AcHE) is studied in solution also with enzyme powered micropump (enzyme is immobilised with the help of layer by layer assembly. This makes enzyme micropump more useful in order to detect minimal amount of analyte in short duration.This lab-on-chip (LOC) is the device for forthcoming generation where one can monitor the changes in the system without help of any external sources. Also, herein we have immobilized human Plasma i.e., biological fluid which is more complex system. This nucleotide responsive AChE actuated fluid flow from human plasma can pave the way for designing future lab-on-a-chip devices in complex biological environments with potential clinical applications.

1Pos316 無細胞合成を用いたタンパク質結晶化と構造解析
Protein crystallization and structure analaysis using cell-free protein synthesis

Satoshi Abe, Junko Tanaka, Mariko Kojima, Takafumi Ueno (*Sch. Life Sci. Tech., Tokyo Tech.*)

In-cell protein crystallization has attracted attention as a structural biology tool because it does not require purification processes and large-scale crystallization screenings. However, significant issues remain to be solved to obtain various protein crystals in sufficient amounts and quality for structure determination. Here, we report the development of cell-free protein crystallization, a direct protein crystallization technique that uses cell-free protein synthesis. We have succeeded in crystallization and structure determination of polyhedra and CipA using cell-free protein synthesis. This technology significantly expands the tools available for high throughput protein structure determination of unstable, low-yield, or substrate-binding proteins.

1Pos317 細胞内タンパク質結晶を用いた天然変性タンパク質の網羅的構造解析
Comprehensive structure analysis of intrinsically disordered protein using in-cell protein crystal

Mariko Kojima, Satoshi Abe, Takafumi Ueno (*Sch. Life Sci. & Tech., Tokyo Tech*)

Protein crystals serve as porous scaffolds that capture foreign molecules. Especially, immobilization of target proteins into the scaffold crystals can be applied for the X-ray structure analysis. Protein engineering, which tunes the internal environment of scaffold crystal allows target proteins to form the structure that is not observed in an isolated state, applying to investigate the physical property of molecules that depend on their interactions with the surrounding surface. However, the synthesis of protein crystals has been limited because the design of screening scaffolds has difficulty capturing the targets and forming the crystals. In this study, we have developed a high-throughput screening system for structure analysis of intrinsically disordered peptides.

1Pos318 大気圧温度制御プラズマによる植物細胞への直接タンパク質導入法の開発及び導入機構解明
Direct protein introduction into plant cells by a temperature controllable atmospheric-pressure plasma and elucidation of the mechanism

Yuki Yanagawa[1,2], Yusuke Iijima[3], Toshiki Aizawa[3], Yuma Suenaga[3], Akitoshi Okino[3], Ichiro Mitsuhara[4] ([1]*Grad. Sch. Hortic., Chiba Univ.*, [2]*CSRS, RIKEN*, [3]*FIRST, Tokyo Inst. Tech.*, [4]*NIAS, NARO*)

Atmospheric-pressure plasmas are useful for various fields in not only basic research but also industrial uses. In this study, we developed a technique to introduce protein directly into the cells of intact plant tissues by the irradiation of plasmas generated from CO_2 or N_2 gas source. Using this technique, we indicated that sGFP fusion protein was introduced into the cells of tobacco and Arabidopsis leaves and rice roots. Next, we examined the mechanism underlying the protein uptake in tobacco leaf cells. Results showed that protein uptake potential was retained for at least 3h. Inhibitor experiments revealed that plasma treatment induced protein transportation across the plasma membrane via clathrin-mediated endocytosis in plants.

1Pos319 新規カロテノプロテインの分離と構造解析—青色にもピンク色にもなるアスタキサンチン
Isolation and structure analysis of a novel marine sponge carotenoprotein

Momoko Ishida, Momose Kuroda, Suzuho Iseya, Yui Fujita, Satoko Matsunaga (*N.I.T., Hakodate Col.*)

Carotenoprotein is a carotenoid-protein complexes, the famous of which are “crustacyanin” obtained from lobster carapace and “ovorubin”, a pink-colored carotenoprotein from the egg of apple snail. Although carotenoproteins are expected to have industrial applications because of their water-soluble behaver and wide range of color variations, there are only few studies of the protein structures despite that it is important to these applications. Therefore, we isolated and purified a novel blue carotenoprotein from a sponge and analyzed the amino acid sequence. This blue carotenoprotein, as well as “ovorubin”, possesses astaxanthin as a chromophore. We thus compared the sequences and the biochemical property of two carotenoproteins.

1Pos320 Construction of novel lipidomics platform combined of targeted and non-targeted analysis

Hideaki Kasahara, Yasuto Yokoi, Hideya Kuwabara, Tadahiro Hoshino (*MITSUI KNOWLEDGE INDUSTORY CO., LTD.*)

Targeted lipidomics (TL) using selected ion monitoring (SRM) enable high sensitive quantitative analysis for certain lipids in biological sample. However overlapped chromatographic peaks from isomer and fluctuations in retention time of chromatograms cause miss alignment among samples. Here we developed novel lipidomics platform named MetaboAlign which solve these issues combining TL with Non-targeted lipidomics on data dependent acquisition (DDA).
MetaboAlign consisted of peak detection module, alignment module, and viewer was written in Java. The software implements an RT-correction algorithm that enables highly accurate alignment of the large number of peaks in each sample.
Rapid and accurate quantitative analysis of large sample sets was achieved using the software.

1Pos321 ヒト角栓内部における脂質の不均一分布
Heterogeneous spatial distribution of lipid components in a follicular cast

Hitomi Matsushita[1], Hiromitsu Nakazawa[1], Noboru Ohta[2], Taro Moriwaki[2], Satoru Kato[1] ([1]*Grad. Sch. SciTech., Kwansei Gakuin Univ.*, [2]*JASRI/SPring-8*)

We examined the spatial distribution of triglycerides (TG) and free fatty acids (FFA), which are affected by Propionibacterium acnes lipase in a follicular cast (FC), to understand the FC formation mechanism and the development of acne vulgaris. We tried to reveal the localization of ordered structures and molecular species by microbeam X-ray diffraction (SPring-8, BL03XU) and synchrotron FTIR micro-spectroscopy (BL43IR), respectively. As a result, it is suggested that at least a part of TG, one of the major components of sebum, exist as randomly oriented microcrystals. Furthermore, we found that the distribution of TG and FFA on a cross-section of FC can be resolved by the FTIR method. This is the first report on heterogeneous distribution of lipid components in an FC.

1Pos322 変分オートエンコーダを用いた下顎骨形態の定量化
A method for morphological feature extraction based on variational auto-encoder: an application to mandible shape

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Shape analysis of biological data is crucial for investigating morphological variations. However, conventional approaches are difficult as exemplified by the ambiguity in the landmark-based method. In this study, we propose a morphological regulated variational autoencoder (Morpho-VAE) that conducts image-based shape analysis using imaging processing through a deep-learning framework. By applying Morpho-VAE to primate mandible data, we successfully extracted and visualized morphological features which allow us to distinguish different groups. In addition, Morpho-VAE can reconstruct a missing image segment based on the remaining structure. Therefore, Mopho-VAE is applicable to the shape analysis of various organisms, even those with a missing segment.

1Pos323 Evaluation of the Potent SARS-CoV-2 Main Protease Inhibitors using LB-PaCS-MD/FMO Technique

Kowit Hengphasatporn, Ryuhei Harada, Yasuteru Shigeta (*Center for Computational Sciences, Univ. Tsukuba*)

The application of the LB-PaCS-MD method combined with the FMO calculation was reported here for the first time. In this study, the LB-PaCS-MD/FMO is applied to understand how the inhibitor interacts with SAR-CoV-2 M^{pro}. The interaction binding energy of the potent complex is further identified using FMO-RIMP2/PCM. Simultaneously, the allosteric inhibition is elucidated using blind-docking and clustering techniques (BDK). The interaction profile, key binding residue, and the significant interaction of rubraxanthone binding to both sites of M^{pro} are clarified. The integrated LB-PaCS-MD/FMO method can provide a more reasonable complex structure for the ligand-binding at the active site, which is vital for antiviral drug discovery and design.

1Pos324 Flory-Huggins 理論を用いた 3 成分系における相分離挙動の解析
Analysis of phase separation behavior in three-component systems based on the Flory-Huggins theory

Naoki Iso, Takahiro Sakaue, Yuki Norizoe (*Aoyama Gakuin University*)

Liqud-liquid phase separation in cells occurs in a variety of situations, including the formation of membrane-less organelles and changes in genome structure caused by chromatin phase separation.
In this study, based on the Flory-Huggins theory, we consider the phase separation in three-component systems containing two solutes and one solvent, which shows richer behaviors compared to that in two-component systems, thus may be more relevant to the cellular phase separation.

1Pos325 多孔質ハイドロゲル固体試料中における紫膜積層に適した孔サイズ分布
Pore size distributions related to spontaneous purple membrane stacking in porous hydrogels

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We have developed purple membrane (PM) immobilized samples for future optoelectric devices. We have found out that PM stacking, which is advantageous for applications, occurred spontaneously in porous hydrogels. Pore size distributions in hydrogels immobilizing PM are elucidated by focusing on a relationship with PM stacking since it is recently suggested that porous gel network generations are essential for PM stacking. Here, to clarify a relationship with pore size, optical microscopic observations for hydrogels immobilizing PM were carried out. The results showed that PM stacking occurred at porous gels with a larger pore size than PM long axis length, while it did not occur in the smaller pores. These strongly suggest the appropriate pore size for PM stacking.

2Pos001* クライオ電子顕微鏡によるヒト LPA1 受容体の構造解析
Cryo-EM structure of Human Lysophosphatidic Acid Receptor 1

Hiroaki Akasaka, Tatsuki Tanaka, Fumiya Sano, Wataru Shihoya, Osamu Nureki (*Grad. Sch. Sci., The Univ. of Tokyo*)

Lysophosphatidic acid receptor 1 (LPA_1) is one of the six G protein-coupled receptors activated by the bioactive lipid, lysophosphatidic acid (LPA). LPA_1 is a drug target for various diseases, including cancer, inflammation, and neuropathic pain. Here, we report the cryo-electron microscopy structure of the active human LPA_1-Gi complex bound to the newly developed LPA analog ONO-0740556. Our structure elucidated the details of the agonist binding mode, lipid preference, and receptor activation mechanism. Moreover, we characterized the structural polymorphisms at the receptor-G-protein interface, which potentially reflect the G-protein dissociation process. Taken together, our study contributes to the design of drug-like agonists targeting LPA_1.

2Pos002* クライオ電子顕微鏡を用いたコレラ菌 Na^+輸送性 NADH-ユビキノン酸化還元酵素の構造解明
Cryo-EM structures of Na^+-pumping NADH-ubiquinone oxidoreductase from *Vibrio cholerae*

Moe Ishikawa[1], Jun-ichi Kishikawa[2], Takahiro Masuya[1], Masatoshi Murai[1], Yuki Kitazumi[1], L. Nicole Butler[3], Takayuki Kato[2], Blanca Barquera[3,4], Hideto Miyoshi[1] ([1]*Grad. Sch. Agri., Kyoto Univ./ Japanese*, [2]*Inst. Prot. Res., Osaka Univ./ Japanese*, [3]*Bio. Sci., RPI/ USA*, [4]*CBIS, RIP/ USA*)

The Na^+-pumping NADH-ubiquinone (UQ) oxidoreductase (Na^+-NQR) couples electron transfer from NADH to UQ with Na^+-pumping. Since Na^+-NQR is exclusively found in prokaryotes and is structurally unrelated to mitochondrial H^+-pumping NADH-UQ oxidoreductase (respiratory complex I), it is a promising target for highly selective antibiotics. However the molecular mechanism of inhibition is not well-understood for lack of the inhibitor-bound structure.
Here, we present high-resolution structures of *V. cholerae* Na^+-NQR with or without bound inhibitors by single-particle cryo-EM. We revealed the induced-fit binding of inhibitors, the complete arrangement of all six redox cofactors, and the flexibility of NqrF responsible for electron transfer.

2Pos003* (3SFA-3) クライオ電子顕微鏡による高分解能解析によって明らかになってきた二成分毒素の膜透過機構
(3SFA-3) High-resolution Cryo-EM analysis reveals the mechanism of binary toxin translocation

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Binary toxin is bacterial protein toxin which is composed of enzymatic A-component, and B-component which forms membrane spanning pore to translocate A-component into the cell. To study the translocation mechanism, we tried reconstituting *C. perfringens* iota toxin Ib-pore into liposome to mimic in vivo environment. However, the product was not proteo-liposomes, but clusters which are formed by radially assembled Ib-pores in lipid micelle (Ib-rosette). Surprisingly, single particle analysis of Ib-rosette produced Ib-pore map at 2.38Å resolution, revealing whole structure of membrane spanning β-barrel. This map exhibited hydrated water on the β-barrel, and clearly revealed the structures of the constriction-site which are located on A-component translocation pathway.

2Pos004 タンパク質間相互作用阻害を機序とする抗新型コロナウイルス薬の創出
Screening for new types of coronavirus inhibitors that block protein-protein interaction

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The SARS-CoV-2 envelope protein (SCV2-E) has a PDZ domain binding motif (PBM) at the C-terminus. Compounds that inhibit the interaction between SCV2-E PBM and intracellular proteins have the potential to be anti-coronavirus drugs. In this study, we searched for small compounds that inhibit above interactions. First, new compounds were searched by NMR screening used a compound library for PDZ domains and in silico screening. As a result, we identified some compounds with the anti-SCV2 activity by both screenings. These compounds interacted with the binding pocket of the PDZ domain as well as SCV2-E, and had a common backbone but differed in anti-SCV2 activity. We now analyze molecular details of the anti-SCV2 activity by using some kinetic analyses.

2Pos005* クライオ電子顕微鏡によるヒト由来メラトニン受容体シグナル伝達複合体の立体構造解析
Cryo-EM structure of the human MT_1–G_i signaling complex

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We report the cryo-EM structure of the MT_1-G_i signaling complex at 3.3 Å resolution, revealing the activation mechanism of MT_1, in which the ligand-induced conformational changes are propagated to the G-protein coupling interface. MT_1 exhibits a larger outward movement of TM6 than other G_i-coupled receptors, which is considered to be a specific feature of G_s-coupled receptors. The structural comparison among the G_i- and G_s-complexes demonstrated the conformational diversity of the C-terminal entry of the G_i protein, suggesting the loose and variable interactions at the helix end. These notions, together with our biochemical and computational analyses, highlight the different binding modes of $G\alpha_i$ and provide the basis for the selectivity of G-protein signaling.

2Pos006* FlhAc の高速原子間力顕微鏡画像の解析
Analysis of High Speed Atomic Force Microscopy Image of FlhAc

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High-speed atomic force microscopy (HS-AFM) has been attracting attention as an effective tool for observing of protein behavior in physiological conditions. However, HS-AFM only provides information on the molecular surface, and the horizontal resolution is less than 1 nm. Therefore, extracting useful information for analysis from HS-AFM movies is an issue. To solve this problem, we utilize MD simulation to determine the molecular structure corresponding to AFM image at atomic level. We generated many pseudo-AFM images by rotating MD simulation data using home build program and calculate correlation score between pseudo images and experiment images. We utilize FlhAc because a wide variety of structures is obtained by all-atom MD simulation and we verify above method.

2Pos007 デングウイルス由来 RNA 依存性 RNA ポリメラーゼと天然物ライブラリーから得られたその阻害剤との複合体の立体構造解析
Structure analysis of the dengue viral RNA-dependent RNA polymerase in complex with its inhibitor obtained from marine natural products

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RNA-dependent RNA polymerase (RdRp) is one of the potent targets for drug discovery against positive RNA viruses. In the present study, we focused on RdRp from dengue virus (DENV). Previous study identified several compounds possessing inhibitory activity from natural product libraries. Our study aims to reveal manner of action of these hit compounds from structural viewpoint. DENV-RdRp was expressed in *E. coli*, purified as soluble protein, and crystallized. Crystal structure of the apo form DENV-RdRp was determined at 2.0 Å resolution. Then, we prepared crystals of DENV-RdRp in complex with its inhibitor by soaking, and determined its structure at 2.6 Å resolution. Structure comparison revealed several structural differences between apo form and inhibitor-complex.

2Pos008* フェレドキシン-NADP⁺還元酵素の中性子結晶構造解析
Neutron crystallographic analysis of ferredoxin-NADP⁺ reductase

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Ferredoxin NADP⁺ reductase (FNR) catalyzes the redox reaction between ferredoxin (Fd) and NADP⁺ in plant plastids. Although it is known that chemical differences in FAD due to redox state cause conformational changes in the enzyme and are important for efficient redox reactions of FNR, detailed conformational changes upon redox of FNR, such as rearrangement of the hydrogen bond network, have not yet been elucidated. Therefore, we performed neutron crystallography to determine the hydrogen atom coordinates of FNR. We have established a crystal evaluation method using X-ray diffraction experiments and succeeded in obtaining large, high-quality crystals suitable for neutron crystal structure analysis. In this meeting we will discuss the structure of oxidized FNR.

2Pos009* クライオ電子顕微鏡を用いたビタミン C トランスポーター SVCT1 の構造解析
Cryo-EM structures of vitamin C transporter SVCT1

Takaaki Kobayashi, Hiroto Shimada, Fumiya Sano, Tsukasa Kusakizako, Osamu Nureki (*Dept. Biol. Sci., Grad. Sch. Sci., Univ. Tokyo*)

Vitamin C plays important roles as an antioxidant against oxidative stress and a cofactor for a variety of enzymatic reactions. Whole-body homeostasis of this vitamin is regulated by sodium-dependent vitamin C transporter 1 (SVCT1). Because of its physiological and clinical significance, numerous studies have focused on this transporter. However, the molecular mechanisms of substrate recognition and transport remain unclear due to the lack of detailed structural information. In this research, we present the first cryo-EM structures of SVCT1 in multiple conformations. Based on structural comparison and analysis of the substrate binding pocket, our results provide insight into the mechanisms of vitamin C specific recognition and sodium-dependent transport by SLC23 family.

2Pos010 赤色蛍光タンパク質の単一復帰変異による赤色蛍光消失の構造基盤
Structural basis of the loss of red fluorescence by single back mutation of an artificial red fluorescent protein

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Long-wavelength fluorescent proteins are suitable for deep tissue imaging of living organisms, but existing ones are rather dark. Recently, we created new bright red fluorescent protein, AzamiRed 1.0, by introducing 29 amino acid mutations into a coral-derived GFP, AzamiGreen. To analyze the contribution of each mutated residue to redification, we introduced single back mutation at the residues interacting with the red chromophore and found some single mutant proteins that lost the red fluorescence. We determined the crystal structures of these proteins and found that they contain immature chromophores. The structure of the immature chromophore depends on the mutation site. We will discuss the role of these residues in the maturation of the red chromophore.

2Pos011 MD シミュレーションによる LIM2 ドメインの構造解析
Structural analysis of Lim2 domain by MD simulation

Motokuni Nakajima[1], Yoh Noguchi[1,3], Hironao Yamada[2,3], Ryota Morikawa[1], Masako Takasu[1], Yukiko K. Hayashi[4] ([1]*Sch. of Life Sci., Tokyo Univ. of Pharm. and Life Sci.*, [2]*Sch. of Pharm., Tokyo Univ. of Pharm. and Life Sci.*, [3]*The Inst.of Statist. Math.*, [4]*Tokyo Med. Univ.*)

The FHL1 protein has been reported to be mutated in some patients with inherited muscle diseases. This protein consists of a LIM domain with a zinc finger, and in many of the mutations reported in hereditary muscle diseases, a coordinating residue in the LIM2 domain is mutated. However, the structural changes in the LIM2 domain caused by these mutations are not clear. Therefore, in this study, we performed two MD simulations for mutations (C104Y, H123Y, C126Y, C150Y, and C153Y) in which the wild-type coordinating residue in the LIM2 domain of FHL1 was changed to tyrosine. As a result, large structural changes were observed, especially in the H123Y and C150Y mutant models, in which severe cases have been reported.

2Pos012 尿素とトリエチルアミン N-オキシドが KaiC の ATPase 活性に及ぼす影響
Effects of urea and trimethylamine N-oxide on the ATPase activity of KaiC

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The cyanobacterial circadian clocks is composed of three proteins, KaiA, KaiB, KaiC, and ATP. The ATPase activity of KaiC is thought to be a determinant of the KaiC phosphorylation cycle, but the underlying tuning mechanism is still unknown. To understand the tuning mechanism, we examined the effects of urea (a protein desrabilizer) and trimrthylamine N-oxide (TMAO, a protein stabilizer) on the phosphorylation cycle was extended with increasing urea concentration, but shortened with increasing TMAO concentration. In addition, urea attenuated the ATPase activity of KaiC, whereas TMAO enhanced it. These opposite effects on enzymatic activities could produce a period length offset.

2Pos013 原子分解能でみた概日時計の朝夕昼夜
Visualizing a Day of Circadian Clock at Atomic Resolution

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KaiC is a core clock protein in cyanobacteria. In C-terminal domain of KaiC, cyclic phosphorylation and dephosphorylation proceed in a circadian manner (Phospho-cycle). We have captured KaiC in “four” distinct phosphorylation states covering Phospho-cycle by X-ray crystallography. The phospho-switch region (PSw) identified in the structures adopted “two” conformations depending on the phospho-states of S431. The PSw conformations were allosterically correlated with the intra- and intermolecular events such as ATP hydrolysis in N-terminal domain, dynamics of assembly with other clock proteins called KaiA and KaiB, and activity regulation to compensate for temperature influences. This is the first study tracking a circadian oscillator at atomic resolutions.

2Pos014 分子動力学シミュレーションを活用した VHH-抗原複合体のアンサンブルドッキング
Ensemble Docking of VHH-Antigen Complexes using Molecular Dynamics Simulations

Kohei Yamaguchi, Ren Higashida, Yasuhiro Matsunaga (*Grad. Sch. Sci. Eng., Saitama Univ.*)

VHH is a single-chain antibody that has attracted attention in terms of materials and medical applications. Although VHH has a rather long CDR-H3 loop compared with conventional antibodies, the influence of the flexibility of long loop on binding affinity is unknown. In this study, we perform ensemble docking using molecular dynamics simulations combined with rigid-body docking to investigate the relationship between the flexibility of loop and binding affinity. We sampled conformational ensemble of CDR-H3 loop with an enhanced samplined method (gREST) implemented in GENESIS. Then, conducted rigid-body docking with ZDOCK and HADDOCK. We compare the results of the ensemble docking with conventinal rigid-body docking, and discuss the influence of the loop flexibility.

2Pos015 Structure and stability analysis of Cry j 7, an antimicrobial peptide from Japanese cedar that causes the pollen-food allergic syndrome

Jingkang Zheng, Tomona Iizuka, Hiroyuki Kumeta, Yasuhiro Kumaki, Ami Hanaoka, Ichiho Yoshikawa, Yurie Nakajima, Soma Ishihara, Tomoyasu Aizawa (*Grad. Sch. Life Sci., Hokkaido Univ.*)

Cry j 7 is a small cysteine-rich gibberellin regulatory protein (GRP) with 6 disulfide bonds, which was isolated from Japanese cedar as the pollen allergen to make cross-reactivity with food allergens cause pollen-food allergy syndrome (PFAS). In our study, the recombinant Cry j 7 and other allergenic GRPs were overexpressed by *Pichia pastoris* for structural characterization analysis. The NMR results provided important data of the three-dimensional structure of Cry j 7. In addition, the structural stability and other properties that may be involved in allergenicity were examined.

2Pos016 細菌由来グルカンスクラーゼのアクセプター特異性に関連するループ構造
The loop structure responsible to the acceptor specificity of bacterial glucansucrase

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Two bacterial glucansucrases *Streptococcus* GTF-I and *Leuconostoc*/*Lactobacillus* GTF-A are thought to be derived from a common ancestor. They catalyze glucosyltransfer reactions using sucrose as a donor to produce glycosides. Our previous study of acceptor-specificity of GTF-I and GTF-A suggests that GTF-I activity for acceptors with molecular weight higher than176 is lower than GTF-A. The comparison of 3D-structures and sequences of bacterial glucansucrese found a *Streptococcus* GTF-I-specific loop structure around the active-site, and the loop structure may be responsible to the acceptor-specificity for high molecular weight acceptors. To examine the role of loop structure, we are engineering a loop-deleting mutant of GTF-I and will analyze its acceptor-specificity.

2Pos017 構造解析に向けたヒト免疫不全ウイルス２（HIV-2）エンベロープ糖タンパク質の調製
Preparation of human immunodeficiency virus type-2 (HIV-2) envelope glycoprotein for structure analysis

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Human immunodeficiency virus (HIV) is composed of HIV-1 and HIV-2. Of note, HIV-2 infected patients produce higher titers of neutralizing antibodies that target envelope protein (Env) trimer than HIV-1 infected patients. To investigate this unique antigenicity, we are trying to prepare the HIV-2 Env trimer for structure analysis.
It is well known that recombinant HIV-1 Env trimer tends to dissociate to be a monomer during purification. To overcome this, some mutations were incorporated into HIV-2 Env constructs and their oligomeric states were evaluated. Finally, we succeeded in preparing a contrast that retains the trimer state and does not impair binding to neutralizing antibodies.

2Pos018 粗視化モデルによる微小管の安定性の理論的研究
Theoretical study of stability of microtubules by a coarse-grained model

Ayasa Kurahashi, Hiro Takeda, Kazutomo Kawaguchi, Hidemi Nagao (*Grad. Sch. Nat. Sci. Tech., Kanazawa Univ.*)

Microtubules (MTs) are one of cytoskeleton elements and formed by dimers consisting of alpha- and beta-tubulin. MTs stably expand when GTP cap exist, whereas they shorten in the absence of it. It is confirmed that protofilaments (PTs) are curled outward when MTs shrink. In the previous research by Monte Carlo simulation, it turned out that thermal fluctuation had important role in peeling off. However, changes in the conformational stability over time wasn't considered. Therefore, we study the behavior of MT using molecular dynamics simulation and demonstrate needed factors for its stability. A coarse-grained model is applied, and we calculate with Langevin equation. A parameter representing how open the tip of MT is defined and its transition over time are clarified.

2Pos019 X 線小角散乱測定を用いたクラミドモナス由来クリプトクロムの溶液構造解析
Structural analyses of the animal-like cryptochrome from *Chlamydomonas reinhardtii* by small angle X-ray scattering

Soma Matsuda, Satoshi Nagao, Daichi Yamada, Minoru Kubo (*Grad. Sch. Sci., Univ. Hyogo*)

The animal-like cryptochrome from *Chlamydomonas reinhardtii* (CraCRY) is a flavoprotein with bi-function of DNA repairing as well as gene expression controls. CraCRY has a photolyase homology region and an intrinsically disordered region. Although the bifunctionality of CraCRY is believed to be regulated through dynamic structural changes of the disordered region in response to light, its mechanism is still unclear. We expect that small angle X-ray scattering (SAXS) analyses can reveal the role of the disordered region in CraCRY. Here we have shown that the oxidized state of CraCRY, as-prepared from *E. coli* cells, exists as a monomer. Additionally, we suggest that the disordered region of CraCRY has a relatively compact conformation by structural modeling with SAXS.

2Pos020 蛋白質天然変性領域を模倣する生理活性化合物の探索
Search of bioactive compounds that imitate intrinsically disordered regions of proteins

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Ets1 has Ser282 and Ser285 residues in the intrinsically disordered regions (IDRs) and the phosphorylation of these residues inhibits the DNA-binding because the phosphorylated residues bind to Arg residues in the DNA-binding helix. In this study, we searched the ligands that bind to the DNA-binding helix from Namiki database and selected negatively charged 20 ligands in the order of high structure similarity to IDRs. Then, we screened only two ligands that have high binding similarity to the IDRs based on the 20 Ets1-ligand docking structures predicted by AutoDock. To improve prediction accuracy of docking software, we developed a new method to verify docking structure based on statistic of PDB and detected interaction hot spots of Ets1 surface.

2Pos021 Effect of a narrowest clamp of binary toxin on cell toxicity

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Binary toxin consists of two components, an enzymatic A component and B component as protein membrane-transport machine. As binary toxin, Clostridium perfringens Iota toxin and CPILE were known. The latter was identified as a causative toxin of food poisoning. There are different narrowest clamp sites in the center pore, which were formed by Phe in iota and Ser in CPILE. However, there is open question of whether these differences cause toxicity. In this study, I mainly conducted cell experiment trans-epithelial electrical resistance (TEER) measurement with Caco-2 cells using the wt and clamp mutants toxins. I also performed the structure analysis of clamp mutants of Ib by cryo-EM. Finally, I will discuss the role of the narrowest clamp of binary toxin.

2Pos022 β シートにおける隣接ストランド間でのペア特異的 Cα 距離の解析
Pair-specific analysis of Cα distances between adjacent strands in β-sheets

Hiromi Suzuki (*Sch. Agri., Meiji Univ.*)

We selected 21,312 protein chains from PDB and analyzed Cα distances located on the adjacent strands in β-sheets. Among non-hydrogen bond (nHB) pairs of anti-parallel strands, Leu and Gly recorded 18 times as the longest and shortest partners, respectively. Among hydrogen bond (HB) pairs, Leu was recorded 12 times as the shortest partner, while Cys was selected 6 times as the longest partner. For parallel pairs, Leu and Asp were recorded 10 and 5 times, respectively, as the longest partners of nHB residues, while Gly, Ala and Thr were recorded 7, 6 and 4 times, respectively, as the shortest partners. When nHB residue was fixed, Thr was recorded 6 times as the longest partner, but there was not precise tendency between Cα distances and HB residues.

2Pos023 分子動力学シミュレーションによる凝集性を有するペプチドの密度依存性に着目した構造分布解析
Distribution and structure analysis of fibril-forming peptides focusing on concentration dependency by molecular dynamics simulation

Yoshitake Sakae[1,2], Takeshi Kawasaki[2], Yuko Okamoto[3] ([1]*RIST*, [2]*Dep. Phys., Nagoya Univ.*, [3]*Info. and Comm., Naogya Univ.*)

We focus on the concentration dependency of fibril-forming peptides, which have the potential of aggregation by themselves. In this study, we performed replica-exchange molecular dynamics simulations of Lys-Phe-Phe-Glu (KFFE) fragments, which are known to form fibrils in experiments under different concentration environments. According to the analysis by static structure factor, the density fluctuation of the KFFE fragments becomes large as the concentration increases. In addition, the number of β-structures and oligomers also increase under the high concentration environment. Hence, high concentration environment of fibril-forming peptides is likely to cause the protein aggregation.
Ref: Y. Sakae, T. Kawasaki, Y. Okamoto, ACS Omega 2022, 7, 12, 10012-10021.

2Pos024 An extended bound-water network and hydrophobic hydration determine the activity of microbial antifreeze protein

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Antifreeze protein (AFP) binds to an ice crystal to inhibit its growth. AFPs from various microorganisms share a close similarity in 3D structures, while they exhibit diverse antifreeze activity. The bound-water molecules in the ice-binding site (IBS) of AFP are thought to connect AFP and ice crystal. Less is known, however, about the key determinants for the antifreeze activity of microbial AFPs.
In our poster presentation, we report crystal structures of three AFP isoforms from a snow mold fungus, *Typhula ishikariensis* (*Tis*AFP6, 7, and 8). The bound-water network was most extended for hyperactive isoform *Tis*AFP8 whereas less extensive for the moderately active *Tis*AFP6. An additional ring-like network was observed around the Phe residue in the IBS of *Tis*AFP7.

2Pos025 Gly-kink 導入 β バレルナノポアを用いた単一分子検出
Single-molecule detection using β-barrel nanopore with Gly-kink

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Nanopore sensing is a rapid and label-free method for detecting a single molecule. It is necessary to use nanopores suitable for target size, but the size variation of nanopores is insufficient; therefore, constructing a size controllable nanopore is required. We previously reported β-hairpin peptide (SV28), which formed a multidisperse-size β-barrel nanopore in a lipid membrane. To construct a monodisperse-size nanopore, we focused on Gly-kink which is reported to stabilize a β-barrel structure, and we introduce Gly-kink into SV28, named SVG28. The pore-forming ability was evaluated by channel current measurement. Resulting, SVG28 nanopore converged relatively monodisperse-size. Towards nanopore amino acid sequencing, we are trying to detect polypeptides using it.

2Pos026* (2SDP-5) Structural basis of the significant metal-histidine coordination in *E. coli* RNase HI

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RNase HI is an endonuclease that cleaves the RNA strand of a DNA/RNA hybrid by a canonical metal cation catalytic mechanism. Its activity is the highest in the presence of Mg^{2+}, while it is limited in the presence of other metal cations such as Mn^{2+} and Zn^{2+}. Biophysical experiments have shown that the carboxyl groups of the conserved DEDD motif creates a delicate field at the active center. Moreover, an adjacent His may also be one piece of the puzzle yet not well-defined. Our crystallographic analyses of *E. coli* RNase HI-Mg^{2+} showed two Mg^{2+} binding in the absence of substrate. The structural features of the imidazole ring of His124, along with the RNase HI-Zn^{2+} structures, provided significant insights into the pivotal metal dependent enzymatic mechanism.

2Pos027* *De novo* ペプチドナノポアの無細胞合成へのアプローチ
Approaches to cell-free synthesis of *de novo* peptide nanopores

Shoko Fujita, Miyu Fukuda, Ikuro Mizoguchi, Ryuji Kawano (*Department of Biotechnology and Life Science, Tokyo University of Agriculture and Technology*)

Single-molecule sensing technology using nanopore has been applied to DNA sequencing. For the detection and identification of a wider range of molecules, we previously designed a *de novo* nanopore using a β-hairpin peptide, SVG28. It has hydrophobic sequences to be embedded in lipid membranes, which makes its chemical synthesis difficult and is a barrier to further functionalization. In this study, we focus on cell-free synthesis that should be able to express peptides more rapidly than solid-phase synthesis. For cell-free synthesis, we designed SVG28 variants in terms of hydrophobicity. The variants were successfully synthesized and their pore-forming ability was confirmed, showing the potential to accelerate design and evaluation process for the modification of SVG28.

2Pos028* K48 結合型環状ユビキチン鎖の物性解析
Physical property analysis of cyclic K48-linked ubiquitin chains

Tomoki Sorada[1], Daichi Morimoto[1], Erik Walinda[2], Kenji Sugase[3] ([1]*Grad. Sch. Eng., Univ. Kyoto*, [2]*Grad. Sch. Med., Univ. Kyoto*, [3]*Grad. Sch. Agr., Univ. Kyoto*)

Ubiquitin chains are known to regulate a wide range of intracellular reactions depending on their characteristic chain forms: linear, branched, and cyclic chains. Cyclic K48-linked ubiquitin chains are the only ubiquitin chains that exist in cells as a cyclic form. Although the synthesize mechanism and quantities of cyclic K48-linked ubiquitin chains are studied, their intracellular functions still remain unclear.

We find that cyclic ubiquitin chains show high thermal stability and cleavage resistance due to conformational stabilization. In addition, our NMR analysis shows that the intrinsic open-closed motion of ubiquitin chains is drastically repressed for cyclic ubiquitin chains and cyclic ubiquitin chains strongly interact with a ubiquitin binding protein.

2Pos029 アミノ酸生産菌の呼吸鎖の拡張型超複合体の電子顕微鏡による観察と解析
Electron microscopic observation and analysis of extended supercomplexes of the respiratory chain of amino acid-producing bacteria

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Corynebacterium glutamicum is an aerobic gram-positive bacterium with high GC content. In the respiratory chain of these bacteria, two cytochrome *bcc* complexes and two aa_3 oxidases form a supercomplex. To elucidate the structure of the supercomplex of *C. glutamicum*, we washed it with MEGA (9+10), extracted it with LMNG, and purified it by column chromatography. SDS-PAGE of the purified fractions showed around 50 kDa corresponding to NDH-II, with NDH activity. We suggested the presence of NDH-II in the supercomplex. We named this complex, including NDH-II, the extended supercomplex (ESC). We solved the ESC structure using Cryo-EM and single-particle analysis. Our results showed no obvious NDH-II but an unknown helix. We will present the present work of the complexes.

2Pos030 グルタミン酸脱水素酵素における補酵素結合経路のクライオ電子顕微鏡観察
Cofactor binding pathway in glutamate dehydrogenase studied using cryoTEM

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Crystal structures of enzyme-ligand complexes help understand the interaction modes and for developing novel inhibitor molecules. However, the structures provide little information on the binding process of ligands to enzymes. Therefore, it is unclear whether substrates directly associate with the binding sites of enzymes similar to those in the final bound state or through meta-stable sites depending on the conformations of enzymes. To clarify this, we applied cryoTEM for glutamate dehydrogenase in the presence of a cofactor. The classification of images revealed several binding sites of cofactor molecules on the active-site cleft. Accordingly, we speculated the binding pathway of the cofactor correlating with the domain motion of the enzyme.

2Pos031* *In silico* design of cross-reactive antibodies binding to SARS-CoV and SARS-CoV-2 spike RBDs

Yoshiki Yasuda[1], Daisuke Kuroda[2], Jiei Sasaki[3], Makoto Nakakido[1], Ryo Matsunaga[1], Hashiguchi Takao[3], Kouhei Tsumoto[1] ([1]*Grad. Sch. Eng., The University of Tokyo*, [2]*Research Center for Drug and Vaccine development, National Institute of Infectious Diseases*, [3]*Laboratory of Medical Virology, Institute for Life and Medical Sciences, Kyoto University*)

Antibodies play a crucial role in the immune system in vertebrate against pathogens and can be used as therapeutics. There are high expectations for computational methods to efficiently create antibodies toward arbitrary pathogens. In this study, we attempted to generate antibodies that can neutralize SARS-CoV-2 through redesign of an anti-SARS-CoV-1 RBD antibody. Our computational prediction based on multiple crystal structures of the template antibody-antigen complexes and the subsequent physicochemical measurements suggested some mutations that generate a μM binding toward SARS-CoV-2 and an improvement in binding affinity (pM) toward SARS-CoV-1. We also confirmed their improved neutralizing activities. We will discuss success and failure of our computational design.

2Pos032 動的・静的構造解析による南極産好冷細菌由来グルコキナーゼの低温適応・高熱安定性機構の解明
X-ray crystallography and spin-labeling ESR reveal cold adaptation and high thermal stability mechanism of cold-adapted glucokinase

Akane Yato[1], Rio Asaka[2], Hiroshi Sugimoto[3], Keiichi Watanabe[2], Masaki Horitani[2] ([1]*United Grad. Sch. Agri. Sci., Kagoshima Univ.*, [2]*Agri., Saga Univ.*, [3]*SPring-8, RIKEN*)

Generally, the cold-adapted enzyme has high flexible structure, so that it can maintain enzyme activity in low temperatures and its thermal stability is decreased. However, our previous studies revealed that glucokinase (GK) derived from psychrophile, *Pseudoalteromonas* sp. AS-131 (PsGK) has high thermal stability in spite of cold-adapted enzymes, compared to GK derived from mesophile, *E. coli* (EcGK). In this study, we used site-directed spin-labeling ESR and X-ray crystallography to clarify this unique mechanisms of PsGK at the molecular level. As a result, it was revealed that PsGK has duality, “rigid and flexible” structure and “connection” of the N- and C-terminus with S-S bond, thus we conclude that they affect the unique functions of PsGK.

2Pos033 EPR 法による中温菌、好冷細菌由来複核 Mn 酵素の活性中心における微細構造変化の検出
EPR Spectroscopy Reveals the Differences of Active Site Structures for Di-Mn Enzymes from Mesophilic and Psychrophilic Bacteria

Masaki Horitani[1,2], Yuri Kasu[1] ([1]*Fac. Agric., Saga Univ.*, [2]*Unit. Grad. Sch. Agric. Sci., Kagoshima Univ.*)

Inorganic pyrophosphatase (PPase) has di-Mn^{2+} center in the active site and catalyzes the hydrolysis reaction of inorganic pyrophosphate to inorganic phosphates. We previously established overexpression and purification system for PPase from mesophilic bacteria (*Bacillus subtilis*: Bs-PPase) and psychrophilic bacteria (*Shwanella* sp. AS-11: Sh-PPase). Interestingly, Sh-PPase showed characteristic biochemical properties for cold adaptation. To elucidate the mechanism of cold adaptation for Sh-PPase, we have performed EPR measurements for both PPases. Our results showed that considerably weak coupling for only Sh-PPase. Thus, we concluded that unique active site for Sh-PPase contribute to the cold adaptation.

2Pos034* FixL 二量体感覚領域のリガンド認識機構
Computational Study on the Ligand Discrimination of Dimeric Sensory Domain of FixL Protein

Tingting Wang, Takahisa Yamato (*Graduate School of Science, Nagoya University*)

The ligand discrimination mechanism in oxygen sensor protein, *Bj*FixLH, was investigated by molecular dynamics simulation and vibrational energy transfer model. Based on vibrational energy transfer pathways, we found the allosteric effect upon imidazole binding, starts from the FG loop, through an internal hydrophobic G/H/I β strands bridge and coiled-coil linker region, to the kinase domain. Although a small structural difference between two forms, ligand binding caused considerable reorganization of the energy exchange network and weakened inter-residue interactions across dimer interface. The signaling in FixLH is not localized around heme, but propagated to downstream area by a network constructed by multiple conserved residues.

2Pos035 QM/MM 法による *C*-メチル基転移酵素 Fur6 の反応機構解析
QM/MM study on the catalytic mechanism of the *C*-methyltransferase Fur6

Fan Zhao[1], Tomohiro Noguchi[1], Yoshitaka Moriwaki[1], Tohru Terada[1], Tomohisa Kuzuyama[1,2], Kentaro Shimizu[1] ([1]*Grad. Sch. of Agri. and Life Sci., Univ. of Tokyo*, [2]*CRIIM, Univ. of Tokyo*)

Actinomycetes bacteria have attracted great attention for their ability to produce various secondary metabolites with complex molecular scaffolds. Among them, the *Streptomyces* sp. strain KO-3988 produces furaquinocin D, a polyketide-isoprenoid hybrid that exhibits antitumor and cytotoxicity activities. In its biosynthetic process, a methyltransferase, Fur6 catalyzes the methylation of the C3 of 1,2,4,5,7-pentahydroxynaphthalene (PHN). However, the reaction mechanism has not been clarified due to the O_2 lability of the substrate PHN. In this study, a structural model of Fur6 in the complex with PHN and the cofactor *S*-adenosylmethionine was constructed by molecular docking and MD simulations. The QM/MM study demonstrated the whole reaction mechanism of Fur6.

2Pos036 CD28 結合と構造安定性に寄与する Grb2 のドメイン間相互作用
Interdomain interactions in Grb2 contribute to the conformational stability and CD28 binding

Saki Ochi, Momoka Iiyama, Masayuki Oda (*Grad. Sch. Life Environ. Sci., Kyoto Pref. Univ.*)

An adaptor protein, growth-factor receptor-bound protein 2 (Grb2), contains three domains, nSH3-SH2-cSH3, and binds to the cytoplasmic region of CD28 receptor. Grb2 SH2 binds to the motif, pYXNX, of CD28, and SH3 binds to the motif, PXXP. To clarify the contribution of respective SH3 domains, we analyzed CD28 binding of Grb2 and its SH3-deletion mutants as the monomer state using isothermal titration calorimetry and surface plasmon resonance. We also analyzed their thermal stabilities using circular dichroism and differential scanning calorimetry, showing that SH3 domains, particularly nSH3, contribute to stabilizing the structure of Grb2. The effects of the interdomain interaction on the stability would also contribute to the stable complex formation with CD28.

2Pos037* リョビュウイルスの核蛋白質 -RNA 複合体のクライオ電子顕微鏡構造
Cryo-EM structure of the nucleoprotein-RNA complex of a novel filovirus, Lloviu virus

Shang fan Hu[1,2,3], Yoko Fujita-Fujiharu[1,2,3], Yukihiko Sugita[1,2,4], Lisa Wendt[5], Yukiko Muramoto[1,2,3], Masahiro Nakano[1,2,3], Thomas Hoenen[5], Takeshi Noda[1,2,3] ([1]*Laboratory of Ultrastructural Virology, Institute for Life and Medical Sciences, Kyoto University*, [2]*Laboratory of Ultrastructural Virology, Graduate School of Biostudies, Kyoto University*, [3]*CREST, Japan Science and Technology Agency*, [4]*Hakubi Center for Advanced Research, Kyoto University*, [5]*Laboratory for Integrative Cell and Infection Biology, Institute of Molecular Virology and Cell Biology, Friedrich-Loeffler-Institut*)

Lloviu virus (LLOV), classified in the family *Filoviridae* together with the Ebola and Marburg virus, is a newly identified virus in bats in Europe. Viral nucleoprotein (NP) binds to the viral genomic RNA to form a helical NP-RNA complex, acting as a scaffold for nucleocapsid formation and RNA synthesis. However, the structural basis for the helical assembly remains unknown. Here, we solved the three-dimensional structures of the LLOV NP-RNA complexes by cryo-EM. The structure-based mutational analysis determined the residues involved in helical assembly and viral RNA synthesis. Our results advance our understanding of the filovirus nucleocapsid formation and can be useful for designing broad-spectrum anti-filoviral drugs.

2Pos038 シトクロム P450 によるメチレンジオキシブリッジ形成の反応機構
Reaction mechanism of methylenedioxybridge formation by cytochrome P450

Kenshin Kondoh, Ryo Yonezawa, Eiichi Mizohata (*Grad.Sch.Eng., Osaka Univ.*)

Methylenedioxybridge (MDB) is a widely distributed structure in natural products, and lignans with MDB structure exist as secondary metabolites in various plants. Cytochrome P450 enzymes have attracted attention as a useful tool in industrial applications because they synthesize substances with complex chiral centers using water as a solvent that does not adversely affect the human body. Here we report the X-ray crystallographic analysis of cytochrome P450 that catalyzes the MDB formation reaction using pinoresinol as a substrate. The multi-species method targeting14 orthologs from different plants was applied to crystallize the proteins. Finally, the structures of two orthologs were successfully determined. We propose the reaction mechanism for MDB formation.

2Pos039* ヒト stomatin SPFH ドメインのリン酸イオンに依存した線維状構造
The SPFH domain of human stomatin forms fibril-like assembly at high concentrations, whose formation is promoted by phosphate ions

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Stomatin (STOM) is a monotopic membrane protein whose detailed molecular function remains unclear. STOM is a member of the stomatin-prohibitin-flotillin-HflC/K (SPFH) domain-containing protein family. We focused on the SPFH domain to elucidate the molecular function of STOM. We first determined the solution structure of the SPFH domain of human STOM (SPFH) and found the structure of SPFH has a small hydrophilic pockets that may interact with phosphate ions by NMR analysis. In addition, electron microscopy revealed that lyophilized SPFH with phosphate formed fibril-like assembly when dissolved water. We hypothesize that STOM forms fibril-like assembly by interacting with phosphate ions and contributes to membrane stability and stiffness as a membrane skeleton.

2Pos040* 天然変性タンパク質が引き起こす滑膜肉腫発生の新規メカニズム
A Novel Mechanism of Synovial Sarcoma Induced by Intrinsic Disordered Proteins

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Synovial Sarcoma (SS) is an extremely rare malignancy that occurs primarily in young adults. In all cases the pathogenic fusion protein SS18-SSX is produced, suggesting that when it binds to the chromatin remodeling complex BAF, it causes abnormal gene expression. This event is believed to be a trigger for the development of SS. However, the structure and biochemical characteristics of SS18-SSX remain largely unknown. In this study, we are focusing on the SSX region, which is the culprit domain. We found that SSX binds specifically to the linker DNA segments of nucleosomes as well as free DNA and acidic patches of nucleosomes. Combining these results with those of structural studies, we present a novel mechanism for the development of SS.

2Pos041 HSP40 結合による HSP70 の安定性への影響
HSP40 binding affects the stability of HSP70

Lisa Matsukura, Naoyuki Miyashita (*Grad. Sch. BOST, KINDAI Univ.*)

Heat Shock Protein (HSP) 70 is known as one of the chaperone proteins. In the chaperone cycle, HSP40 bind to the HSP70 and deliver the unfolded protein to HSP70. Then, the HSP70 folds the client protein using ATP hydrolysis. Previous studies have shown the J-domain in HSP40 binds to the HSP70, and the crystal structure of the J-domain and HSP70 complex is determined. HSP40 binding would be essential to the HSP70 cycle. Therefore, we performed the molecular dynamics simulations of the HSP70 with the J-domain of the HSP40 complex and HSP70 to examine the affection of the HSP40 binding. As a result, we found that the binding of the J-domain of HSP40 induces the fluctuations around the ATP binding site and the unfolded protein binding site.

2Pos042* 緑藻クラミドモナス由来シトクロム b_6f 複合体のクライオ電子顕微鏡構造が示す Rieske 鉄硫黄蛋白質の機能的構造変化
Cryo-EM structure of cytochrome b_6f complex from *Chlamydomonas reinhardtii* reveals the functional domain movement of Rieske ISP

Hatsuki Tanabe[1,2], Shinichiro Ozawa[3], Akihiro Kawamoto[1,2], Hideaki Tanaka[1,2], Yuichiro Takahashi[4], Genji Kurisu[1,2] ([1]*IPR., Osaka Univ.*, [2]*Grad. Sch. Eng., Osaka Univ.*, [3]*IPSR., Okayama Univ.*, [4]*RIIS., Okayama Univ.*)

In the photosynthetic electron transport chain, cytochrome b_6f complex (Cyt b_6f) connects the electron relay between Photosystem II and I, and is pumping protons across the thylakoid membrane. In this study, we aim to understand the structural basis of the electron shuttle between the Rieske iron-sulfur protein (ISP) and the cytochrome *f* which are physically separated more than 29 Å. The strategy was to determine the cryo-EM structure of the Cyt b_6f at high resolution, which can resolve the multiple conformations of Rieske ISP using multi-state single-particle analysis. We have successfully prepared highly homogeneous samples and analyzed the structure of the Cyt b_6f at 2.7 Å resolution. In this poster, we will discuss the functional domain movement of Rieske ISP.

2Pos043 疾患関連変異のタンパク質構造上の三次元分布に基づく新規機能部位の探索
Search for undiscovered protein functional sites based on the spatial distribution of disease-associated missense variants

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Effective utilization of large number of disease-associated variants (DAVs) revealed through sequencing projects is one of the major challenges in medical and pharmaceutical field. DAVs tend to gather around functional sites such as ligand binding sites and PPI interfaces. In this study, we comprehensively defined 3D variant clusters by clustering of the spatially-distributed DAVs on structure-known human proteins. The 3D variant clusters not related to known functional sites would indicate undiscovered functional sites such as cryptic sites. We will report annotations of the 3D variant clusters and then exploration of novel functional sites based on the functional-unknown 3D variant clusters using mixed solvent molecular dynamics simulation.

2Pos044 拡張アンサンブル法を用いた 3 次元ドメインスワッピング(3D-DS)の研究
3 Dimensional Domain Swapping (3D-DS) Studied by Advanced Molecular Dynamics Simulation

Hiromitsu Shimoyama, Yasuteru Shigeta (*CCS, Tsukuba Univ.*)

The 3-dimensional domain swapping (3D-DS) is a phenomenon by which multiple proteins form complexes. 3D-DS is characteristic in the point that the formed complex can be expected to be a stable complex because the inter-protein interactions are the same as the inter-domain interactions that stabilize their monomer structure. Then, 3D-DS is possibly utilized to make an artificial complex to regulate, combine, encourage or discourage their functions. In this study, 3D-DS for the cytochrome *c* complex formation was studied by molecular dynamics simulations with a coarse-grained model and the smoothed Wang-Landau method. The results of a free-energy analysis will be explained in the presentation.

2Pos045 構造に基づくキラターゼ CfbA のポルフィリン型基質選択性の理解
Structural insights into porphyrinoid substrate selectivity of chelatase CfbA

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CfbA is a chelatase which catalyzes Ni^{2+} insertion into sirohydrochlorin (SHC), yielding Ni^{2+}-SHC, via a Ni^{2+}-$(His)_2$-SHC intermediate with a carboxy ligand of SHC. Meanwhile, CfbA can also use SHC-like compounds, such as uroporphyrin III (UPIII) and uroporphyrin I (UPI) as substrates with low activities. To understand substrate selectivity of CfbA, we performed X-ray crystallographic analysis of UPIII- and UPI-bound CfbA. As a result, the substrate selectivity of CfbA was subject to the number of interaction between porphyrinoid substrates and amino acids at the active site. In addition, it is proposed the formation of the Ni^{2+}-$(His)_2$-SHC intermediate could be critical for the high turnover rate, based on the structural comparison of SHC-, UPIII- and UPI-bound CfbA.

2Pos046 Structure-function relationship of Zn finger domain in Heliorhodopsin

Manish Singh[1], Kota Katayama[1], Yuji Furutani[1], Oded Béjà[2], Rohit Ghai[3], Hideki Kandori[1] ([1]*Nagoya Institute of Technology (Japan)*, [2]*Technion –Israel Institute of Technology (Israel)*, [3]*Department of Aquatic Microbial Ecology (Czech Republic)*)

A new family of microbial rhodopsins (heliorhodopsins; HeR) in contrast to known rhodopsins, having inverted membrane topology and but retain similarities in structure and light response. While no transport activity has been demonstrated and fundamental questions regarding their cellular and ecological function or even their taxonomic distribution remain unresolved. Previously, we reported significant matches in a set of six (originating from Thermoplasmatales archaea) to zinc ribbon proteins at the N terminus of heliorhodopsins. This common stretch of CxxC-17x-CxxC can be putative ion binding pocket for metal ions (e.g. zinc or iron). Here, we elucidate role of extra longer N-terminal extensions compare to previous reported heliorhodopsin by spectroscopic techniques.

2Pos047 Torque transmission of the F_1-ATPase with an inelastic driveshaft

Shou Furuike, Yasushi Maki, Hideji Yoshida (*Dept. of Phys. Osaka Med. Pharm. Univ.*)

F_1-ATPase ($\alpha_3\beta_3\gamma$) is an ATP-driven rotary molecular motor. The axle of the γ-rotor, formed by an antiparallel α-helical coiled coil of the N-ter and C-ter of the γ, is set in the central cavity of the cylinder-like stator ($\alpha_3\beta_3$-ring). The axle has two portions in contact with the upside and the bottom of the ring. The other portion would work as simply a driveshaft because of no interaction with the ring. We constructed the mutant A having an inelastic driveshaft, and the mutant B lacking bottom side of the axle. Rotation rates without drag of mutant A and B were ~1/3 and ~1/40 of wild type, respectively. And, the rates with drag of mutant A were also ~1/3 of wild type. Rotary torque might be transmitted via not only the driveshaft but the stator.

2Pos048 環境変化によるタンパク質の構造変化を取り込んだ粗視化タンパク質モデル
An improved coarse grained protein model to include an environment-driven conformational change

Teppei Yamada[1], Wataru Shinoda[2] ([1]*Graduate School of Natural Science, Okayama University*, [2]*Research Institute for Interdisciplinary Science, Okayama University*)

We have successfully incorporated a Gō-like coarse-grained (CG) model into the SPICA force field, which are useful for a simulation of protein/membrane complex systems. Previously, an elastic network model was used in SPICA, which limited a possible large conformational change of protein even when expected. Our new model provides a better description of protein conformational changes in response to the environment change. A simple application study of the present model showed that an unfolded magainin peptide in aqueous solution, folded into an expected alpha-helical structure on the adsorption to a model lipid membrane. We are now working on the free energy evaluation of peptide membrane binding including the energy cost due to the conformational changes.

2Pos049* 表面電荷改変抗体のコロイド安定性・結合親和性とその溶媒依存性の解析
Analysis of buffer-dependent colloidal stability and binding affinity of supercharged antibodies

Keisuke Kasahara[1], Daisuke Kuroda[2], Satoru Nagatoishi[3], Kouhei Tsumoto[1,3] ([1]*Dept. Bioeng., Grad. Sch. Eng., Univ. Tokyo*, [2]*Res. Ctr. Drug Vaccine Dev., NIID*, [3]*Inst. Med. Sci., Univ. Tokyo*)

Surface mutations with charged amino acids, called **supercharging**, could potentially control antibodies' physicochemical properties. We computationally designed supercharged Fabs with the net charge of +10 (pos10) and –10 (neg10) compared to –4 of the wild-type (WT) Fab.
pos10 and neg10 showed improved colloidal stability in acidic and basic conditions, respectively. Interestingly, pos10 showed its positive surface charge in acetate buffer but did not in phosphate buffer. Furthermore, only in the presence of phosphate ions, all the Fabs was able to bind the antigen with almost the same binding parameters. In the other conditions, electrostatic interactions were prominent, which caused the difference in the surface characteristics and binding parameters of antibodies.

2Pos050* (1SBA-3) タンパク質ケージ内における芳香環相互作用ネットワークの熱力学・分子動力学的解析
(1SBA-3) Thermodynamic and Molecular Dynamic Analysis of Aromatic Interaction Networks in Protein Cages

Yuki Hishikawa[1], Noya Hiroki[1], Asuka Asanuma[1], Basudev Maity[1], Satoru Nagatoishi[2], Kouhei Tsumoto[2,3], Satoshi Abe[1], Takafumi Ueno[1] ([1]*Sch. Life Sci. Technol., Tokyo Inst. Technol.*, [2]*Inst. Med. Sci., Univ. Tokyo*, [3]*Sch. Eng., Univ. Tokyo*)

Non-covalent interactions involving aromatic amino acids are ubiquitous in nature and play essential roles in biological systems. Multiple aromatic residues assemble to form higher ordered structures – aromatic clusters or aromatic interaction networks, which govern protein folding, thermal stability and molecular recognition. The current challenge is to assess thermophysical and dynamic properties of aromatic interaction networks and relevance to their structural correlation at the atomic level. To address these issues, we constructed Phe/Tyr/Trp residue clusters using protein cages and examined their thermodynamic features and dynamic behaviors by circular dichroism (CD) spectroscopy, differential scanning calorimetry (DSC) and molecular dynamics (MD) simulations.

2Pos051 (1SAA-7) 蝶々型金ナノデバイスが可能にするタンパク質液液相分離過程の制御
(1SAA-7) Control of protein condensation by butterfly-shaped gold nanodevices

Tomohiro Nobeyama[1], Koji Takata[2], Tatsuya Murakami[2], Kentaro Shiraki[1,2] ([1]*Pure and Appli.Sci., Univ.Tsukuba*, [2]*Grad. Sch. Sci. Toyama Pref. Univ*)

Protein droplets caused by liquid-liquid phase separation（LLPS) are a key concept to comprehending dynamic phenomenon in cells. The droplets would form and change their shape through interactions with other molecules. We hypothesize that the butterfly-shaped gold nanomaterial (GNB) works as a controller of protein droplets due to the concave curved shape. We investigated the droplet formation of ATP and poly-Lysine, which is a model of protein droplets, in high concentrations with gold nanomaterials (GNs). GNBs induced large droplets. The comparative analysis of GNB and ball and rod shapes of GNs imply that the shape of GNs is critical to form the droplets. Details of the mechanism will be discussed at this meeting.

2Pos052 6 M 塩化グアニジニウム中でアンフォールドした 3 ヘリックス・バンドル蛋白質の残存構造の H/D 交換 2 次元 NMR による研究
Residual structures in the unfolded state in a three-helix-bundle protein in 6 M guanidinium chloride studied by H/D-exchange 2D NMR

Kunihiro Kuwajima[1], Saeko Yanaka[2], Maho Yagi-Utsumi[2], Koichi Kato[2] ([1]*Grad. Sch. Sci., Univ. Tokyo*, [2]*ExCELLS & IMS, NINS*)

The characterization of residual structures persistent in unfolded proteins in concentrated denaturant is an important issue in studies of protein folding. Here, we studied the hydrogen/deuterium (H/D)-exchange behavior of the B-domain of protein A (BDPA), a typical three-helix-bundle protein of 62 residues, in 6 M guanidinium chloride by the dimethylsulfoxide-quenched H/D-exchange 2D NMR method with the use of spin desalting columns. We successfully monitored the H/D-exchange kinetics of 29 peptide NH protons out of 55 NH groups. The NH protons in the 3rd helix was most strongly protected with protection factors as high as 5.2, whereas the 1st and 2nd helices were less protected. The relevance of the observations to the folding mechanism of BDPA will be discussed.

2Pos053 Isolation and characterization of a 200kDa fibroin precursor

Kok Sim Chan[1], Kento Yonezawa[2], Haruya Kajimoto[1], Takehiro Sato[3], Yoichi Yamazaki[1], Sachiko Toma-Fukai[1], Hironari Kamikubo[1,2] ([1]*1Division of Materials Science, Graduate School of Science and Technology, Nara Institute of Science and Technology*, [2]*Center for Digital Green-innovation, Nara Institute of Science and Technology*, [3]*Spiber Inc.*)

Fibroin is a protein that is involved in the formation of spider silk. Our lab discovered the 50kDa fibroin would assemble and form into a trimeric structure. This trimeric structure acts as a precursor to elongate into nanofibers. However, we are not sure if fibroin with higher molecular weight would form this trimeric structure and be assembled into nanofibers. In this study, we aim to isolate the 200kDa fibroin precursor and investigate its characteristics. By using the isolation method for 50kDa fibroin precursor, 200kDa fibroin formed a white-snowball-like aggregate under high centrifugation force. In this presentation, we will discuss the characteristics of 200kDa fibroin precursor and its ability to elongate into nanofibers.

2Pos054 スタフィロコッカル・ヌクレアーゼにおける、自発的フォールディングからリガンド誘導フォールディングへの機構転移
How to shift the mechanisms from spontaneous folding to ligand-induced folding of staphylococcal nuclease?

Yujiro Mori[1], Issei Suzuki[2], Shingo Fukazawa[2], Kosuke Maki[1] ([1]*Grad. Sch. Sci., Nagoya Univ.*, [2]*Sch. Sci., Nagoya Univ.*)

Although many proteins spontaneously fold into the native state, some proteins are folded coupled with binding to partner proteins or ligands even under physiological conditions. Staphylococcal nuclease (SNase), a model protein, has been shown to undergo a shift in the mechanisms from spontaneous folding to ligand-induced folding depending on denaturant and ligand concentrations. It remains to be understood, however, whether the spontaneous and ligand-induced folding of a single protein occurs with a common mechanism or not. To address this issue, we characterized the difference and similarity in the two types of folding of SNase. On the basis of the results obtained, we will discuss the physical-chemical mechanisms of the folding/binding behavior.

2Pos055 液-液相分離により形成されるドロップレット内部でのタンパク質及び RNA の分子ダイナミクス
Molecular dynamics of proteins and RNA within droplets formed by liquid-liquid phase separation

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The membraneless organelles, such as stress granules and Cajal bodies, are liquid droplets formed by liquid-liquid phase separation (LLPS). The LLPS driven under certain conditions in the cell is a significant process that controls the spatial and temporal organization of many cellular components. Since the multivalent interaction of LLPS-relevant molecules, such as proteins and RNA, is a key factor in forming and maintaining the droplet, revealing the effect of the multivalent interaction on LLPS is important. In this study, using coarse-grained molecular dynamics simulations, we investigate the interaction of proteins and RNA and how the interaction affects their dynamics in the complex droplet.

2Pos056 剪断応力がフィブロインナノファイバーに及ぼす影響
Effect of shear stress on fibroin nanofibers

Keita Iwasaki[1], Kento Yonezawa[1,2], Satoru Onishi[1], Muneya Daidai[1], Haruya Kajimoto[1], Takehiro Sato[3], Yoichi Yamazaki[1], Sachiko Toma-Fukai[1], Hironari Kamikubo[1,2] ([1]*NAIST, MS*, [2]*NAIST, CDG*, [3]*Spiber Inc*)

Fibroin is a structural protein composing spider silk. We found that the formation of trimeric precursors is essential for the self-assembling nanofibers(NFs) formation of fibroin. Usually, the precursor is prepared by kinetic trap procedure. But we showed that mechanical processing could also prepare the precursors. On the other hand, continuous mechanical treatment during the elongation reaction process yields aggregates of short NFs instead of long NFs. This fact suggests that mechanical energy prevent the NF elongation reaction. This study applied mechanical energy to the pre-fabricated NFs to verify the fracturing effect. It was observed that the mechanical energy fragmented the nanofibers and broke them down to particles of size similar to the precursor.

2Pos057* 神経変性疾患関連タンパク質 Ataxin-3 の液-液相分離と凝集ダイナミクスのポリ Q 鎖長依存性
PolyQ chain length dependence of liquid-liquid phase separation and aggregation dynamics of a neurodegeneration-related protein ataxin-3

Uchu Matsuura[1], Shinya Tahara[1], Shinji Kajimoto[1,2], Takakazu Nakabayashi[1] ([1]*Graduate School of Pharmaceutical Sciences, Tohoku University*, [2]*JST PRESTO, Japan.*)

Ataxin-3 (AT-3) is a neurodegeneration-related protein having glutamine repeat (polyQ) and becomes pathogenic when polyQ is abnormally elongated. We previously showed AT-3 undergoes liquid-liquid phase separation (LLPS). In this study, we investigated LLPS and subsequent dynamics of AT-3 proteins with 28- and 64-reisdues polyQ (Q28 and Q64) by tryptophan fluorescence lifetime and Raman spectroscopy. We found that solvent environments within droplets of Q28 and Q64 are different from each other. Both proteins showed unfolding and aggregation in droplets, but Q64 exhibited slower unfolding and aggregation than Q28. In addition, changes in the Raman bands were observed only for Q64 droplet. We concluded that the polyQ elongation affects the aggregation dynamics via LLPS.

2Pos058 疾病関連 α-シヌクレイン変異体の構造およびダイナミクス特性
Structural and dynamical properties of the disease-related mutants of α-synuclein

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Formation of amyloid fibrils of α-synuclein (αSyn) is closely related to the pathogenesis of Parkinson's disease (PD). Characterization of the behavior of αSyn is important to elucidate the mechanism of fibril formation. Among various mutants of the αSyn related to familial PD, the mutants A30P, A53T, and G51D are known to show different propensities for fibril formation. Characterization of the physicochemical properties of these mutants should thus provide clues to specify the key behavior for fibril formation. Here, by using small-angle X-ray scattering and quasielastic neutron scattering, the structural and dynamical properties of these mutants are characterized. The relationship between the structural and dynamical properties is discussed.

2Pos059 統計力学モデルによるアポミオグロビンのフォールディング反応機構の予測
Folding mechanisms of apomyoglobin predicted by an extended statistical mechanical model

Koji Ooka[1], Munehito Arai[2,3] ([1]*Col. Arts & Sci., Univ. Tokyo*, [2]*Dept. Life Sci., Univ. Tokyo*, [3]*Dept. Phys., Univ. Tokyo*)

Wako-Saitô-Muñoz-Eaton (WSME) model is a structure-based statistical mechanical model of proteins and can calculate folding free energy landscapes. However, the WSME model is unsuitable for prediction of folding reactions of large proteins. To overcome this limitation, we extended the WSME model by introducing virtual linkers. We applied our model to apomyoglobin and successfully predicted the free energy landscapes consistent with experimentally observed folding pathways. Moreover, we also succeeded in obtaining residue-specific structure formation of apomyoglobin, consistent with the experimental results. Therefore, the extended model can pave the way for predicting the folding mechanisms of various proteins without the limitations of protein size and shape.

2Pos060 コンタクト計算を厳密化した改良型統計力学モデルによるタンパク質フォールディング経路の予測
Predicting protein folding pathways using the statistical mechanical model modified with accurate contact calculation

Runjing Liu[1], Koji Ooka[2], Munehito Arai[1,3] ([1]*Dept. Life Sci., Univ. Tokyo*, [2]*Col. Arts & Sci., Univ. Tokyo*, [3]*Dept. Phys., Univ. Tokyo*)

Many proteins drive biological phenomena after folding into native specific structures. Therefore, elucidating protein folding mechanism is an important issue in life science. A statistical mechanical model, Wako-Saitô-Muñoz-Eaton model, is promising for predicting folding processes of small globular proteins with low computational complexity. We previously introduced accurate contact calculations to this model and successfully reproduced the folding pathway of a small all-α protein over a wide temperature range. Here, to examine whether our modified WSME model generally improves folding predictions of various small proteins, we applied it to other protein with different structure, including α/β protein. The results suggest the versatility and utility of our model.

2Pos061 AlphaFold は条件付きでフォールドする天然変性タンパク質・天然変性領域（ProS）の構造をどのように予測したか
How AlphaFold predicts conditionally-foldable segments in intrinsically disordered proteins

Koya Sakuma[1], Hiroto Anbo[2], Satoshi Fukuchi[2], Motonori Ota[1] ([1]*Grad. Sch. Informatics, Nagoya Univ.*, [2]*Faculty of Engineering, Maebashi Inst. of Technology*)

Some regions of intrinsically disordered proteins undergo disorder-to-order transition upon binding and are observed as folded segments in experimental structures, which we previously named as protean segments (ProSs). As ProSs can be taken as both structured and unstructured regions, it remains unclear whether their conformations can be predicted by structure prediction methods such as AlphaFold. To clarify whether AlphaFold can predict ProS structures, we composed a set of new-ProS candidates and performed “blind” structure prediction. We performed monomer and multimer predictions to compare their predicted conformations with/without the binding partners. We also analyzed the binding pose. Some lessons on applying the structure predictor to ProSs will be discussed.

2Pos062 Liquid-liquid phase separation and amyloid formation of Sup35 from four different yeast species

Yumiko Ohhashi[1], Suguru Nishinami[2], Kentaro Shiraki[2], Eri Chatani[1] ([1]*Grad. Sch of Sci., Kobe Univ.*, [2]*Inst. Appl. Phys., Univ. of Tsukuba*)

When different proteins are mixed, high sequence homology is required to coexist in amyloid fibril. While coexistence in phase-separated droplets does not require high sequence homology and requires similar amino acid content. This means that it is possible to design proteins that can coexist in phase-separated droplets but cannot coexist in amyloid fibrils.
In recent years, it has become clear that many of the causative proteins of neurodegenerative diseases progress to amyloid via LLPS. The above-mentioned designed proteins may be able to suppress amyloid formation induced by LLPS.
In this study, we used Sup35 derived from four different yeast strains to investigate the coexistence in droplets and its effect on amyloid formation.

2Pos063 トランスサイレチン断片のアミロイド線維形成
Amyloid fibril formation of transthyretin fragments

Keisuke Yuzu[1], Misato Matsumura[1], Naoki Yamamoto[2], Masatomo So[3], Keiichi Yamaguchi[4], Yuji Goto[4], Eri Chatani[1] ([1]*Grad. Sch. Sci., Kobe Univ.*, [2]*Fac. Med., Jichi Med. Univ.*, [3]*Inst. Protein Res., Osaka Univ.*, [4]*Grad. Sch. Eng., Osaka Univ.*)

Transthyretin (TTR) is a tetrameric plasma protein that functions as a transporter of thyroxin and retinol. TTR is also known as an amyloidogenic protein and amyloid deposition of TTR is associated with the onset of serious amyloidoses such as familial amyloid polyneuropathy. Nevertheless, much remains unclear about the fibrillation mechanism of TTR. Recently, fibrillation of a TTR49-127 fragment, which is a N-terminal truncated TTR, has been suggested. Here, we investigated the fibrillation of several TTR fragments excised from full-length TTR. We identified that not only TTR49-127 but also TTR16-36 and TTR81-127 form amyloid fibrils. Based on further analyses, the formation mechanism of TTR amyloid fibrils induced by fragmentation will be discussed.

2Pos064* β アレスチンの新規 PIP2 結合サイトとその機能
Novel PIP2 binding site of βarrestin and its function

Ritsuki Kuramoto, Tatsuya Ikuta, Koki Kawakami, Asuka Inoue (*Graduate School of Pharmaceutical Sciences, Tohoku University*)

Phosphatidylinositol 4,5-bisphosphate (PIP2) is a phospholipid present in the inner leaflet of the plasma membrane bilayer. Recent study showed that PIP2 can be an activation factor of β-arrstin (β-arr) .

To understand how PIP2 affects β-arr in the complex, we performed molecular dynamics simulations. In the simulations, we observed that PIP2 interacted with β-arr at two sites (termed here canonical and non-canonical sites). While the canonical site is comparable to the GPCR-β-arr complex, the non-canonical site is at the edge of β-arr.

Next, we measured recruitment of PIP2-binding-deficient mutants in HEK293A cells. A non-canonical site mutant reduced GPCR-stimulated recruitment to the plasma membrane as well as the canonical site mutant does.

2Pos065 クチナーゼ様酵素 Cut190 による微粉化 PET 分解
Degradation of homogenized PET with cutinase-like enzyme Cut190 form *Saccharomonospora viridis* AHK190

Fumiya Kondo[1], Miho Emori[2], Masayuki Oda[1,2] ([1]*Faculty Life. Environ. Sci., Kyoto Pref. Univ.*, [2]*Grad. Sch. Life. Environ. Sci., Kyoto Pref. Univ.*)

Cutinase-like enzyme Cut190, from *Saccharomonospora viridis* AHK190 has an ability to depolymerize polyethylene terephthalate (PET). This enzyme could hydrolyze ester bonds of PET in the presence of Ca^{2+}, degrading it to the monomer level. Disulfide-bond introduced mutants of Cut190, Cut190**_SS series, showed increased thermostability with keeping the catalytic activity, and could depolymerize PET at 70ºC, the glass transition temperature of PET. The degradation experiments were performed on the Cut190**_SS series for homogenized PET as substrate and the degradation products were analyzed by reversed-phase HPLC, quantitatively. We also discuss the structure-activity relationship of Cut190**_SS series on the crystal structures.

2Pos066 不凍タンパク質と粘性物質を組み合わせた培養細胞の新規凍結保護剤
Novel cryoprotectants consist of antifreeze protein and viscous additive for cryopreservation of cultured cells

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Antifreeze protein (AFP) is expressed in various organisms including polar fish, insects, and microbes. AFPs exhibit thermal hysteresis, ice recrystallization inhibition, and stabilization of cell membrane to avoid cold and freezing injury. Ice recrystallization is one of the main factors that damage cells during the freezing process and frozen storage. In many cases, DMSO is used as a cryoprotectant for freezing cell lines while it is toxic to the cells. In the present study, we employ AFP to prepare the cell preservation solution combined with less toxic compounds such as glycerol. The survival rate of the cells after 24 hours at -80°C was increased when AFP was added to the preservation solution, indicating AFP can reduce freezing-induced damage.

2Pos067 オオクワガタ由来不凍タンパク質の特性評価
Characteri zation of antifreeze protein from a stag beetle *Dorcus hopei binodulosus*

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Some species adapted to cold temperatures produce antifreeze protein (AFP), which binds to ice crystals and lowers the freezing point of the fluid to protect cells and the body from the freezing injury. Our previous research found that a stag beetle *Dorcus hopei binodulosus* produces AFP (*Dhb*AFP). *Dhb*AFP has 6 isoforms that show close similarity in amino acid sequences with hyperactive AFP from mealworm *Tenebrio molitor* (*Tm*AFP). However, less is known about the 3D structure and the detailed antifreeze activities of *Dhb*AFP isoforms. In the present study, we prepared a fusion protein of a *Dhb*AFP isoform tagged with thioredoxin using the *Escherichia coli* expression system to analyze its structure and antifreeze activity.

2Pos068 氷結晶結合蛋白質の非凍結細胞保護機能の分子メカニズム解明
Elucidating the molecular mechanism of cell protective function of ice-binding proteins at non-freezing temperature

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Ice-binding proteins (IBPs) adsorb not only onto ice-crystal to inhibit its growth but also onto cellar surface to protect the cell from hypothermic damage. However, the molecular mechanism of the latter function is not understood well. Since the cellular death at non-freezing hypothermic temperature is mainly due to cell swelling, we hypothesized that IBPs have an ability to maintain the water and ion balance of cells. Here we demonstrated that IBP avoided cellar swelling in a hypotonic solution, suggesting that IBP binds to and inhibits water channels. Furthermore, we further showed that IBP inhibited Ca^{2+} influx through a calcium channel. From these results, we concluded that the cell protective function of IBP is ascribed to its binding to water and ion channels.

2Pos069* アミロイドβと細胞骨格蛋白質のアクチンおよびチューブリンの間の相互作用は、それらの重合状態に依存する
The interaction between amyloid β and cytoskeletal proteins, actin and tubulin, depends on their polymerization state

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Amyloid β (Aβ) aggregation induces neurite degeneration, but the mechanism remains unclear. Since various proteins coexist with Aβ in the body, in this study, we first evaluated the effects of various proteins for Aβ aggregation using the quantum dot imaging we previously reported. The result revealed monomeric actin has the highest inhibitory activity for Aβ aggregation among tested proteins, followed by tubulin. Interestingly, the polymerization of actin and tubulin reduced Aβ aggregation inhibitory activity. We also found that Aβ induced the formation of abnormal aggregates of actin. These results suggest that the interaction between Aβ and actin or tubulin are involved in neurite degeneration.

2Pos070 ヒト血清のアミロイドβ凝集阻害活性の評価
Evaluation of Amyloid β aggregation inhibitory activity of human serum

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Alzheimer's disease is currently a serious problem worldwide. The most promising mechanism for the onset of the disease is the Amyloid cascade hypothesis, in which amyloid-β protein (Aβ) aggregates and accumulates in the brain. Our laboratory evaluated the Aβ aggregation inhibitory activity of mouse serum and found that mouse serum itself has an inhibitory effect on Aβ aggregation. In this study, we evaluated 130 human sera and revealed that the activity decreased with increasing age and that there were differences in Aβ aggregation inhibitory activity effects among individuals. We believe that if we can understand this amyloid aggregation inhibitory activity inherent in blood, we can realize a society of healthy longevity and create a new healthcare market.

2Pos071 セリンプロテアーゼ Neuropsin の基質特異性の決定因子に関する MD 研究
MD simulation study on determinant factors for substrate specificity of serine protease neuropsin

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Neuropsin, which is a serine protease expressed in the central nerve system, cleaves at the specific sites of substrates including neuregulin-1 (NRG-1). The specific cleavage of NRG-1 by neuropsin has been suggested to regulate the signaling system including GABA release. We investigated the catalytic activity and the substrate specificity of neuropsin by using MD simulations. The substrate specificity and catalytic activity were found to depend on multiple factors. Enough strong substrate binding induced local conformational change around the substrate pocket to form the proper alignment in the catalytic triad. In addition, the formation of the oxyanion hole and the appropriate orientation of the cleavage site were found essential for the reaction progress.

2Pos072* 改良型 Raichu を用いた静水圧印加時の Ras 活性測定
Ras activity measurement under hydrostatic pressure using improved Raichu

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Ras is activated by hydrostatic pressure (HP) in cultured mouse chondrocytes. Thus, Ras itself, Ras regulators (GAP, GEF), the upstream receptor and/or interactions between them should have the HP sensitivity. To identify which factor(s) has the HP sensitivity, we are constructing an *in vitro* system to measure Ras activity responding to HP using a FRET-based probe Raichu (Mochizuki et al. 2005). We found interaction between fluorescent proteins in Raichu generates false signal and resolved this problem by mutating these proteins. Using this improved system, HP showed no significant effect on Ras activity either in the presence or absence of a regulator. We are currently assaying in the presence of both regulators, mimicking the cellular condition.

2Pos073 *Eco*RV による DNA 加水分解におけるプロトン移動の量子化学計算による観察
Proton-transfer in hydrolysis of DNA by EcoRV calculated by quantum-chemical metadynamics

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Restriction enzyme, *Eco*RV, recognizes a specific DNA sequence and selectively cuts double-stranded DNA. *Eco*RV, is a homo dimer and requires Mg^{2+} for its function. In our previous studies, a QM/MM metadynamics simulation of *Eco*RV–DNA complex structure was performed. The Potential of Mean Force surface obtained from the QM/MM metadynamics simulations shows two pathways, dissociative reaction path and associative reaction path, for DNA hydrolysis by *Eco*RV. In this study, we made video movies to investigate proton-transfers in DNA hydrolysis by *Eco*RV along the two pathways. Observation of the movies shows us a sequence of proton-transfers to proceed hydrolysis.

2Pos074* Molecular structure dynamics identification method development based on High speed AFM imaging data

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HS-AFM is a powerful tool that can reveal the relationship between the global dynamics of proteins and their functions in liquid solution. Pseudo-AFM images reconstructed based on collision simulations using rigid sphere models are often used to clarify the correspondence between the structure obtained by HS-AFM and known static 3D structures, but the parameters of the simulations are visually adjusted based on experience and lack reliability and quantitativeness. In this presentation, we will discuss a method to quantitatively optimize the parameters of simulations of pseudo-AFM images in order to identify the dynamics structure based on HS-AFM data.

2Pos075* ブリルアン・ラマン同時イメージングによる液-液相分離によるタンパク質液滴の変化の観測
Observation of the change in physical condition of a liquid droplet formed by liquid-liquid phase separation using Brillouin-Raman imaging

Daiki Shibata[1], Shinji Kajimoto[1,2], Takakazu Nakabayashi[1] ([1]*Grad. Sch. Sci., Tohoku Univ.*, [2]*JST PRESTO*)

Liquid-liquid phase separation (LLPS) is a crucial phenomenon in cellular biology. The liquid droplet, that is the dense phase, which is formed via LLPS of certain proteins, have vital roles such as enzymatic reactions. Moreover, it is proposed that liquid droplets formed by proteins causing neurodegenerative diseases are precursor of the fibrils. In this study, we quantitatively examined a single liquid droplet using Raman-Brillouin hybrid imaging system. Raman imaging provides information on protein concentration and secondary structure, and Brillouin imaging provides information on viscosity and elasticity, both of which can be obtained simultaneously. We measured the time course of a single droplet of ataxin-3, a protein associated with Machado-Joseph disease.

2Pos076 タンパク質モーフィング手法と半自動簡略化経路探索法の膜タンパク質二量体のダイナミクスへの適用
Application of the Protein Morphing Method and the Semi-automatic Simplified Path Exploration to the Membrane Protein Dimers Dynamics

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The protein morphing technique usually gives us essential information about the protein structure changes. If we can obtain a more realistic and smooth motion in the morphing, we can clarify the dynamics of the protein in more detail, and it supports the investigation of the protein function. In this study, we developed a protein morphing method using MD simulations and deep learning. It realizes the protein structure changes to morph in arbitrary reaction pathways. We also developed the semi-automatic pathfinding methods for the protein structure changes, using the Nudged Elastic Band method with Markov Chain Monte Carlo simulation. In this presentation, we will introduce the application of these methods to the dynamics of the membrane protein dimer.

2Pos077* 蛍光寿命を用いた LLPS によって生じた FUSLC 液滴の時間変化ダイナミクスの定量解析
Quantitative analysis of time-dependent dynamics of FUS LC droplets formed by LLPS using fluorescence lifetime

Kaichi Nagai[1], Shinya Tahara[2], Uchuu Matusura[2], Mizuki Sugimoto[3], Eita Sasaki[4], Shinji Kajimoto[2,5], Kenjiro Hanaoka[4], Takakazu Nakabayashi[2] ([1]*Faculty of Pharmaceutical Sciences, Tohoku University*, [2]*Graduate school of Pharmaceutical Sciences, Tohoku University*, [3]*Faculty of Pharmacy, Keio University*, [4]*Graduate School of Pharmaceutical Sciences, Keio University*, [5]*JST PRESTO*)

Liquid-Liquid Phase Separation (LLPS) is the phenomenon in which two or more different mixtures are separated into multiple liquid phases. LLPS forms Droplets that are highly concentrated and fluid aggregates of proteins. Droplets undergo a phase transition to gel and fibril that contributes to neurodegenerative diseases. Suppression of droplet formation and gelation can inhibit pathogenesis of diseases, butthere is no quantitative parameter of the three protein states. In this study, we applied fluorescence lifetime technics to perform quantitative evaluation of proteins forming LLPS. Autofluorescence lifetime was used for detecting structural changes in protein, and the change in the viscosity forming droplets was evaluated using a fluorescent probe.

2Pos078 スプリット Akaluc を用いた個体深部における GPCR/β-アレスチン相互作用と細胞融合の検出法
Split Akaluc reconstitution methods for detecting GPCR/β-arrestin interaction and cell fusion event in deep tissues

Yiling Li, Genki Kawamura, Qiaojing Li, Takeaki Ozawa (*Department of Chemistry, School of Science, The University of Tokyo*)

Akaluc is an artificial mutant of firefly luciferase that can emit near-infrared light. This study aimed to use the split Akaluc fragments to detect GPCR/β-arrestin interaction and cell fusion event in deep tissues.
The split Akaluc fragments were used to sense the ligand-induced GPCR/β-arrestin interaction. The luminescence increase due to the GPCR/β-arrestin interaction was confirmed using a stable cell line expressed GPCR-AkalucC and AkalucN-β-arrestin. The cell fusion event upon myogenesis was detected via the protein splicing-based split Akaluc complementation. The luminescence intensity increased with the progression of cell fusion. In conclusion, split Akaluc reconstitution provides a useful method to detect GPCR/β-arrestin interaction and cell fusion event.

2Pos079 **X 線 1 分子追跡法によるイベルメクチン存在下での nAChR α7 の逆回転運動の測定**
The Opposite Twisting Motions of Ivermectin-nAChR α7 Monitored by Diffracted X-ray Tracking

Yue Yang[1], Tatsuya Arai[1,2], Daisuke Sasaki[1], Masahiro Kuramochi[1,3], Hiroshi Sekiguchi[4], Kazuhiro Mio[2], Tai Kubo[5], Yuji C. Sasaki[1,2,4] ([1]*Grad Sch. of Fron. Sci., Univ. Tokyo*, [2]*AIST-UTokyo*, [3]*Grad Sch. of Sci. and Eng., Univ. Ibaraki*, [4]*JASRI/ SPring-8*, [5]*GlyTech Inc.*)

Diffracted X-ray Tracking (DXT) is a method to monitor the rotational motions of a single protein in real time and real space. A ligand-gated ion channel, neuronal nicotinic acetylcholine receptor (nAChR) α7 consists of five α7 subunits symmetrically arranged around a central pore, which is activated by Acetylcholine (ACh). The detailed molecular dynamics of the ligand-bound states of nAChR α7 have not been exhaustively studied. In this study, we applied DXT to nAChR α7 with or without ACh or a type I Positive Allosteric Modulator, Ivermectin (IVM), in BL40XU at SPring8. We found nAChR α7 twist in counterclockwise order when the channel opening by ACh; however, nAChR α7 twist in clockwise order without the channel opening in the presence of only IVM.

2Pos080* 凝集体形成機構解明に向けた電場存在下におけるタンパク質の動的構造解析基盤の確立
Development of a platform for dynamic structural analysis of proteins in electric fields to elucidate the mechanism of aggregate formation

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The electric field is thought to affect biomolecules. α-synuclein, associated with the onset of Parkinson's disease, has been reported to be oligomerized in vitro by electric fields. However, studies on the mechanism of α-synuclein oligomer formation in electric fields have not yet been achieved at the atomic level. In this study, to clarify this mechanism, we developed the electric field NMR system (E-NMR) and electric field MD (E-MD) simulation. Our results suggest that the electric field may respond not only to proteins but also to the surrounding water molecules, resulting in unusual conformational changes in proteins. Since electric fields are also used in the fields of food and medicine, our study is expected to contribute to the development of these fields.

2Pos081 糊化デンプンを使用したマイクロプレートへの MBP 融合タンパク質固定化法の開発及びタンパク質間相互作用解析への応用
An immobilization method of MBP-fusion proteins using a gelatinized starch-agarose mixture and its application for PPI analysis

Ryoya Katayama[1], Yuri Emoto[2], Reiji Hijikata[3], Emi Hibino[2], Natsuko Goda[2], Takeshi Tenno[2], Hidekazu Hiroaki[2], Akihiro Narita[1] ([1]*Graduate School of Science, Nagoya University*, [2]*Graduated School of Pharmaceutical Sciences, Nagoya University*, [3]*School of Science, Nagoya University*)

Detection and quantitative analysis of protein–protein interaction (PPI) is a key technique that typically uses recombinant proteins prepared using fusion-protein tags, such as maltose binding protein (MBP) and glutathione-S-transferase (GST). Here, we adopted the gelatinized starch, which has muddled and sticky properties by adding agarose. The gelatinized starch/agarose (GSA) mixture easily coated over the bottom of a microtiter plate. MBP-tagged proteins were efficiently immobilized onto GSA-coated plates for biochemical assays, such as indirect ELISA-like PPI assays. We successfully determined dissociation constants of MBP-tagged proteins and GST-tagged proteins on the GSA plates and detected binding partners using enzymatic activity of GST as an indicator.

2Pos082* インタクトなミトコンドリアにおける電子伝達複合体活性計測
Measurements of electron transfer complex activities in intact mitochondria

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The mitochondrial electron transfer complexes are key proteins in ATP synthesis. Some of these complex mutations cause severe disease, but it is unclear which mutations and how they reduce the activity of the complex. In this study, we placed mitochondria in several different environments to determine when a mutation decrease the complex activity. The activity of each complex was examined by measuring the polarization of mitochondria with fluorescence imaging. The mutations examined were complex I (3 types), complex III (1 type) complex IV (3 types), and complex V (2 types). Some of the complex I and IV mutations showed a decrease in activity under normal conditions, while others showed a decrease in activity in the presence of hydrogen peroxide.

2Pos083 ペプチドの伸長に伴うエネルギー準位統計の分化と分子進化
Evolution of Energy Level Statistics and Molecular Evolution with Peptide Elongation

Masanori Yamanaka (*CST, Nihon Univ.*)

Based on the energy level statistics of amino acids, dipeptides, and tripeptides, the molecular evolution of proteins was discussed. The energy levels of these peptides were calculated numerically using ab initio methods, and the statistical distributions of the energy level statistics were calculated according to the energy level analysis method in random matrix theory. Specifically, molecular orbitals were calculated by ab initio methods and Kohn-Sham orbitals were calculated by density functional theory. To improve the statistical accuracy, a large number of conformations of the same molecular species were sampled at room temperature using molecular dynamics. The energy level statistics for most molecules were found to be critical statistics.

2Pos084 ポリアミノ酸検出のためのナノポア阻害電流解析法の開発
Developing Current Analyses for Nanopore Detection of Poly(amino acid)s

Misa Yamaji, Ryuji Kawano (*Department of Biotechnology and Life Science, Tokyo University of Agriculture and Technology*)

Nanopore measurement is a powerful tool for detecting a single molecule. We have recently reported the *de novo* design of pore-forming peptide SVG28, whose signal-to-noise ratio was much better than nanopore proteins, and it can detect polypeptides. However, the close distributions of blocking current and dwell time made it difficult to identify polypeptides because of the similar structure. This study tried to classify the small peptide (MW<1,500) by combining the SVG28 nanopore and machine learning. Our previous study suggested the detection signals had the peptide-specific patterns reflecting the interaction between the nanopore and the peptide. Learning these patterns may classify the small peptide.

2Pos085* 生体用ナノポア用いた α-helix 及び β-hairpin ペプチドのアンフォールディング挙動観察
Observation of unfolding behavior of peptides with a-helix and b-hairpin through a biological nanopore

Miyu Fukuda, Ryuji Kawano (*Department of Biotechnology and Life Science, Tokyo University of Agriculture and Technology.*)

Nanopore is a useful tool for the rapid detection of analytes at the single-molecule level. Since this technology allows high sensitivity detection based on ion currents, it is expected to be applied to protein sequencing and folding analysis of proteins. To apply the nanopores in protein folding analysis, it is necessary to clarify the compatibility between the protein structures and the obtained signals. Here, we attempted to elucidate the association between the blocking levels of the ion currents and unfolding of peptides with α-helix, and β-hairpin structures that translocate through the nanopore. Based on this analysis, we will establish the method for identifying the protein structures by the ion current of the nanopore measurements.

2Pos086* 合理的設計手法による SARS-CoV-2 変異体に対する中和抗体の開発
Development of neutralizing antibodies against SARS-CoV-2 variants by rational design

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Infection with the novel coronavirus (SARS-CoV-2) is caused by the binding of the receptor binding domain (RBD) of the spike protein on the viral envelope to the ACE2 receptor on human cell membrane. Neutralizing antibodies that bind the RBD are thus used as therapeutic agents to inhibit the binding of RBD to ACE2. However, mutations in the RBD can result in loss of efficacy of therapeutic antibodies. Here, we aim to develop antibodies that are effective for the E484K mutant of RBD. We theoretically designed antibodies using the Rosetta software and experimentally validated the affinity of the designed antibodies with the RBD mutant by surface plasmon resonance. The results indicate that we have successfully obtained antibodies that can bind tightly to the RBD mutant.

2Pos087* Reverse Engineering Analysis of the High-Temperature Reversible Oligomerization and Amyloidogenicity of PSD95-PDZ3

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PSD95-PDZ3 in the intermediate state (I) undergoes reversible oligomerization (RO). We previously reported a point mutation (F340A) that inhibits both ROs and amyloidogenesis. Here, we "reverse engineered" PDZ3-F340A for inducing high-temperature RO and amyloidogenesis. We produced three variants (R309L, E310L, and N326L). Differential scanning calorimetry (DSC) indicated that only PDZ3-F340A/N326L denatured according to a three-state model and produced high-temperature ROs. Furthermore, the correlation between T_m and T_{mid} at $N \leftrightarrow I_n + D$ suggests that the intermediate state of PDZ3-F340A/N326L and PDZ3-wt is unfolded. Thus, these results demonstrate that a single amino acid mutation can trigger the formation of high-temperature RO and be a precursor of amyloidogenesis.

Poster

2Pos088 アレルギー疾患を阻害しうるタンパク質の合理的設計
Rational design of proteins that can inhibit allergic diseases

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Formation of a ternary complex by interleukin 33 (IL-33), its receptor ST2, and IL-1 receptor accessory protein (IL-1RAcP) is known to induce allergic diseases, and inhibition of the complex formation has been a target for drug discovery. Here, we theoretically designed small proteins using IL-33 as a template to develop inhibitors of allergic diseases, which tightly bind ST2 and inhibit interaction with IL-1RAcP. First, we calculated the ST2 binding energies of various IL-33 mutants and selected those predicted to enhance binding. Then, we measured the binding affinity of the designed mutants to ST2 and successfully obtained the mutants that bind ST2 more tightly than the wild-type IL-33. Designing the mutants that inhibit binding to IL-1RAcP is ongoing.

2Pos089* タンパク質間相互作用を阻害するヘリックス模倣化合物の探索
Search for helix-mimetic compounds that inhibit protein-protein interactions

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Protein-protein interactions (PPIs) are promising targets for drug discovery. Although small compounds are generally difficult to inhibit PPIs due to their wide and shallow interfaces, small-to-medium compounds that mimic α-helical structure of proteins are expected to serve as a novel modality to inhibit PPIs. Here, we designed the compounds mimicking the 1–1.5-turn of α-helices targeting the interactions between the KIX domain of the transcription coactivator CBP and the transcriptional activators involved in various diseases. We screened the designed compounds by fluorescence polarization assay and succeeded in obtaining the helix-mimetic compounds with PPI inhibitory activity. These results suggest that helix-mimetic compounds are promising as PPI inhibitors.

2Pos090* *Pichia pastoris* を用いた組換えタンパク質発現系におけるシステインに富んだタンパク質の折りたたみと収量に関わる因子の解明
Factors involved in the folding and yield of cysteine-rich proteins in recombinant expression system using *Pichia pastoris*.

Ami Hanaoka[1], Tomona Iizuka[1], Jingkang Zheng[1], Ichiho Yoshikawa[2], Wenqing Cai[1], Yurie Nakajima[1], Soma Ishihara[2], Tomoyasu Aizawa[1,2] ([1]*Grad. Sch. Life Sci., Hokkaido Univ.*, [2]*Sch. Sci., Hokkaido Univ.*)

Gibberellin Regulated Protein (GRP) is a small cysteine-rich peptide and widely conserved among plants. Recently, GRPs have gained attention as allergens responsible for Pollen-Food Associated Syndrome (PFAS). To reveal specific mechanisms involved in allergy induction, structural insights are important but still unresolved. For NMR analysis, our laboratory constructed an expression system using *Pichia pastoris*, which secretes correctly folding proteins. However, the product of the previous expression system contained miss folding GRPs, which have a different conformation from nature. The purpose of this study is to elucidate factors involved in the folding and yield. We evaluated the proportion of correctly folding GRP under various culture conditions.

2Pos091* 細胞内光遺伝学ツール Magnets 変異体の比較とさらなる改良
Comparison and further improvement of the intracellular optogenetic tool Magnets variants

Masataka Yoshimura[1], Yuki Aono[1], Yuuki Hayashi[1,2], Fuun Kawano[1], Moritoshi Sato[1], Munehito Arai[1,3] ([1]*Dept. Life Sci., Univ. Tokyo*, [2]*Env. Sci. Ctr., Univ. Tokyo*, [3]*Dept. Phys., Univ. Tokyo*)

Magnets (pMag/nMag) are optogenetic tools for manipulating intracellular protein-protein interactions (PPIs) in cell biology and medicine. The Magnets heterodimerize when exposed to blue light, thereby inducing interactions between proteins fused with them. However, to improve the efficiency of light-induced PPI formation, enhancement in mutual affinity of the Magnet components has been demanded. Since many Magnets variants have been reported to overcome these issues, here we compared the mutual affinity of the Magnets variants by computation and experiment. Moreover, we developed a method to predict the binding affinity and designed new Magnets variants with an improved mutual affinity. These variants may be useful for efficient light induction of intracellular PPIs.

2Pos092 ピキア酵母を用いたシステインリッチアレルゲン蛋白質の過剰発現系における非天然型ジスルフィド結合と修飾の検討
Investigation of non-native disulfide bonds and modification in the overexpression of cysteine-rich allergens by *Pichia pastoris*

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GRPs (Gibberellin-Regulated Proteins) are cysteine-rich proteins present in a wide range of plant species and are known as the allergen family responsible for PFAS (Pollen Food Allergy Syndrome). In terms of the IgE cross-reactivities among them and prevalence, a large amount of high-purity GRPs is necessary for structure analysis and cohort study. We have successfully overexpressed recombinant GRPs using the *Pichia pastoris* secretion system. However, in this process, molecules with disulfide bonds different from those in nature or molecules with modifications were also expressed, which may adversely affect the yield and purity. In this study, we examined these issues in detail using reversed-phase HPLC, MS, and NMR to enable the more efficient expression of GRPs.

2Pos093* LL-37 型 cathelicidin ファミリー抗菌ペプチドの組換え発現と NMR 解析による免疫進化研究
Immunological evolution studies combining NMR and recombinant overexpression of the LL-37-like cathelicidin family antimicrobial peptides

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LL-37, the human cathelicidin family antimicrobial peptide has attracted much attention as an alternative to antibiotics for their multiple immunomodulatory functions in addition to direct antimicrobial activity. The peptides in this family have rapidly evolved and diversified even in closely related species. Understanding the mechanisms of action of this family in nature is important for applications, but detailed structural insights are insufficient. To perform structure-function relationship analysis by NMR, isotope-labeled peptides produced by recombinant overexpression systems are useful. We have successfully produced target peptides using a novel calmodulin fusion expression system. The purified peptides were analyzed in a membrane mimicking environment.

2Pos094* 相分離タンパク質の天然変性領域の配列に基づく、相分離ペプチドの合理的設計
Rational design of phase-separating peptides based on natural phase-separating protein disordered sequence

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Phase-separating (PS) proteins form liquid condensates through multivalent interactions between long intrinsically disordered regions (IDRs) and provide continuous biochemical reaction field with guest molecules selectively incorporated into the condensates. In contrast, PS peptides are hardly known. In this study, we devised a rational design method of PS peptides based on the IDR sequences of natural PS protein. As a proof of concept, we designed three artificial peptides from p53 IDRs and found that they formed liquid-phase or solid-phase condensates. The liquid peptide condensates were electrostatically stabilized, similar with p53 condensates. They showed composition- and size-specific uptake of guest peptides and p53 mutants, different from p53 condensates.

2Pos095* シトクロム P450BM3 の非天然反応を誘起するペプチド性小分子の開発およびその作用の解明
Evolution of Dipeptidic Molecules for the Induction of the Non-native Catalysis of Cytochrome P450BM3 and the Analysis of the Mechanisms

Kai Yonemura[1], Shinya Ariyasu[1], Hiroshi Sugimoto[2], Shigeru Matsuoka[3], Osami Shoji[1] ([1]*Graduate School of Science, Nagoya University*, [2]*RIKEN/SPring-8*, [3]*Faculty of Medicine, Oita University*)

Cytochrome P450BM3 (P450BM3) is a heme enzyme which catalyzes hydroxylation of long chain fatty acids at an extremely high rate. While the enzyme does not hydroxylate non-native substrates such as benzene, benzene is hydroxylated by wild-type P450BM3 in the presence of some peptidic derivatives. We named such molecules “decoy molecules.” In this work, we screened decoy molecules to optimize the peptidic structure for benzene hydroxylation. The binding mode of the best decoy molecule was clarified by X-ray protein crystallography. Benzene molecule was also incorporated at the active site. The benzene molecule was fixed at the active site by π-π interaction. In addition, recognition mechanism of the decoy molecule was revealed by calorimetric analysis.

2Pos096 Direct Visualization of Hydrogen Atoms in the Haem-Acquisition Protein HasA Capturing a Synthetic Metal Complex by Protein Crystallography

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In the iron-devoid environment of their hosts, certain bacterial pathogens, such as *Pseudomonas aeruginosa* and *Serratia marcescens*, secrete the haem-acquisition protein HasA to pirate haem from hosts. Recently, we reported that HasA can bind a wide range of synthetic metal complexes, that, until then, could not be used in the field of protein science. Furthermore, these artificial-HasAs can be used as an antimicrobial agent attacking multiple strains of multidrug-resistant *P. aeruginosa*. Here we discover that a synthetic metal complex triggers the formation of high-quality crystals of HasA, enabling observation of H atoms in HasA by X-ray (0.68 Å) and neutron (1.58 Å) crystallography. This also unmasked hydrogen interactions surrounding the haem-binding site of HasA.

2Pos097 インドールアミン 2,3-ジオキシゲナーゼの電気化学的なレドックス制御と超速な阻害アッセイ
Redox control of human indoleamine 2,3-dioxygenase at nanostructured electrode surface and its inhibitor screening

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Human indoleamine 2,3-dioxygenase (hIDO) plays a key role in promoting tumoral immune escape. Hence, the accurate analysis of hIDO is vital for developing anti-cancer pharmaceuticals. However, the conventional assay of hIDO suffers from the interference with the reductant, which reduces the heme iron for hIDO to initiate its catalytic reaction. In the present study, we developed the electrochemical strategy to evaluate the hIDO catalysis. The nanostructurization of the conventional electrode surface enabled the electrochemically driven hIDO reactions to solve the aforementioned issue. With the aid of in silico study, we also found the strong inhibitor for hIDO reaction using the present simple assay system.

2Pos098 ミオグロビンへの協同的な配位子結合性付与に向けた二量体の合理的設計
Rational design of myoglobin dimers for ligand binding cooperativity

Satoshi Nagao[1], Chihiro Maruo[2], Masashi Yamada[2], Daichi Yamada[1], Minoru Kubo[1] ([1]*Grad. Sch. Sci., Univ. Hyogo*, [2]*Sch. Sci., Univ. Hyogo*)

Hemoproteins contain heme(s) as a functional center, where various ligands can bind to the heme iron. Tetrameric hemoglobin can cooperatively bind oxygen molecules by its quarterly structural change. However, such a ligand binding cooperativity cannot be created by simply connecting monomers; a specific mechanism to transmit structural changes caused by ligand binding between the hemes is essential. In this study, we have prepared mutant dimeric myoglobin (Mb) with long rigid helices connecting hemes and investigated its ligand binding properties. X-ray crystallographic analyses showed the mutant can change its quaternary structure by redox changes and oxygen binding. Additionally, spectroscopic analyses suggested that carbon monoxides cooperatively bind to the hemes.

2Pos099 シュウ酸トランスポーター OxlT の未解明構造の分子動力学的探索
Molecular dynamics search for the unknown structural state of oxalate transporter OxlT

Jun Ohnuki, Kei-ichi Okazaki (*Institute for Molecular Science*)

OxlT is an oxalate transporter in a bacterium in the gut, which plays a role to maintain oxalate homeostasis. It is suggested that OxlT uptakes oxalate by conformational transitions among the outward-facing, occluded, and inward-facing states. Although previous structural and computational studies clarified the structure of the former two states and its transition mechanism, the uptake process of oxalate by OxlT is still not fully understood due to the lack of the inward-facing structure that opens to the cytoplasm. Here, the unknown inward-facing state was explored by molecular dynamics simulation with the aid of enhanced sampling techniques. We will discuss roles of the intra-OxlT and the OxlT-oxalate interaction in transition to the inward-facing sate.

2Pos100 ヒトL型アミノ酸トランスポーター LAT1-CD98hc 複合体の基質輸送シミュレーション
Substrate transport simulations of human L-type amino acid transporter LAT1-CD98hc complex coupled with conformational changes

Natsumi Yoshida[1], Toru Ekimoto[1], Tsutomu Yamane[2], Mitsunori Ikeguchi[1,2] ([1]*Grad. Sch. Med. Life Sci., Yokohama City Univ.*, [2]*RIKEN R-CCS*)

Amino acid transporters supply essential amino acids to cells. The human L-type amino acid transporter 1 (LAT1) transports several large neutral amino acids and their analogues across the membrane. Because LAT1 is overexpressed in tumor cells, developments of LAT1 inhibitors are pharmaceutically demanded. Recently, multiple structures of LAT1-CD98hc complex have been solved in both outward-facing (OF) and inward-facing (IF) states using cryo-EM. However, the substrate transport mechanism coupled with the conformational changes between OF and IF states has not been well understood in dynamical points of view. To clarify the dynamic features underlying the conformational changes, the transport simulations were performed using all-atom molecular dynamics simulations.

2Pos101 病原菌ヘム ABC トランスポーターのクライオ電子顕微鏡解析
Cryo-EM analysis of bacterial heme ABC transporter

Machika Kataoka[1,2], Ayaho Abe[1,2], Gopalashingam Chai[2], Gerle Christoph[2], Yoshitsugu Shiro[1], Masaki Yamamoto[2], Hideki Shigematsu[3], Hiroshi Sugimoto[1,2] ([1]*Grad. Sch. Sci., Univ. Hyogo*, [2]*RIKEN SPring-8 Center*, [3]*JASRI*)

Pathogenic bacteria obtain heme or iron from their vertebrate hosts to survive. In Gram-negative pathogenic bacterial, a member of ATP-dependent transporter family is involved in the import of the heme from periplasm to cytoplasm across the inner membrane. Previous structural study revealed the crystal structure of heme importer from Burkholderia cenocepacia in post-translocation state. In this study, we attempted to analyze the structure in heme-bound state or nucleotide-bound state by cryo-electron microscopy to understand the molecular mechanism of the conformational change of importer for the ATP-hydrolysis and heme transport. Our analysis showed an asymmetric structure along the heme-translocation channel in the transmembrane subunit of transporter.

2Pos102 高速 AFM による ABC トランスポーター P-gp の動態観察
HS-AFM Observation of Conformational Dynamics of ABC transporter P-gp

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P-gp is one of the ABC transporters expressed on human cell membranes and exports a variety of substrates. Cryo Electron microscopic analysis has revealed that the two nucleotide-binding domains (NBDs) have open and closed states depending on the nucleotide states, but the conformation dynamics corresponding to each nucleotide state in the ATP hydrolysis cycle remains unclear. Thus, we applied high-speed atomic force microscopy to visualize conformational changes of P-gp embedded in nanodisk (ND) upon ATP hydrolysis. Two NBDs were clearly observed, and the distance between the two NBDs changed significantly compared to the cryo-EM analysis. In the presentation, the dynamics of opening and closing of NBDs and the effect of inhibitors will be discussed.

2Pos103* 局所熱パルス法を用いた 1 型リアノジン受容体の中間領域変異体の高熱感受性解析
Malignant hyperthermia-implicated heat hypersensitive mutations in the central region of RyR1 channel studied by a local heat pulse method

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Ca^{2+} release channel ryanodine-receptor-type-1 (RyR1) is located in sarcoplasmic reticulum of skeletal muscle. Some RyR1 mutants are implicated in malignant hyperthermia (MH), which is marked by uncontrollable Ca^{2+} release and malignant thermogenesis. We have recently found that heat induces Ca^{2+} release from RyR1. The heat-induced Ca^{2+} release (HICR) is potentially important in the progression of MH. However, it is still unknown how only single mutation changes the whole protein function. Here, using an optically controlled local heat pulse method and HEK293 cells overexpressing RyR1, HICR of RyR1 mutants in the central region is examined comprehensively to explore the molecular insights of the heat sensitivity.

2Pos104 ナノディスクに挿入したカリウムチャネル **KcsA** の構造
KcsA K+ Channel Structure Incorporated into Nanodisc

Hiroko Takazaki[1], Hirofumi Shimizu[2], Takuo Yasunaga[3] ([1]*IPR, Univ. Osaka*, [2]*Fac. Med. Sci., Univ. Fukui*, [3]*Grad. Sch. Comp. Sci. Syst. Eng., KIT*)

KcsA is a potassium channel with high ion selectivity. It is considered the smallest unit with channel function because of its small molecular weight, 70 kDa. We solubilized KcsA by amphipol and obtained 3D KcsA structures at sub-nanometer resolutions by cryo-EM and single-particle analysis (SPA). The results suggested conformational changes of its N-terminal M0-helix predicted to interact with the lipid bilayer. However, it might be an artefact caused by amphipol different from the lipid bilayer. This study aims to elucidate near-native structures of KcsA incorporated into nanodisc. We challenge to seek optimal conditions for cryo-EM SPA of KcsA using several kinds of MPSs and lipids. We will report their current process.

2Pos105 X 線 1 分子追跡法を用いた TRPV1 チャネルの細胞内ドメイン動態計測
Intramolecular dynamics of TRPV1 channel using Diffracted X-ray Tracking

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TRPV1 channel responds to various stimuli that include capsaicin, heat, and protons, and is particularly expressed in nervous systems and brain. Understanding molecular mechanisms of TRPV1 leads to develop analgesic agents. We analyzed intramolecular dynamics of TRPV1 using Diffracted X-ray Tracking (DXT). DXT can detect tilting and twisting motion of a protein by analyzing trajectories generated from gold-nanocrystals bound to the protein. DXT at 100 microsecond frame rate revealed the enhanced dynamics of N-terminus in both capsaicin and AMG9810 bound TRPV1. Life-time filtering analysis can extract domain rotation to classify the protein motion by the molecular velocity. The fast- and slow-lifetime TRPV1 molecules showed independent rotational motion against AMG9810.

2Pos106* EXP2 ナノポアとその変異体を用いたペプチドの 1 分子検出
Single-molecule detection of peptides using EXP2 nanopore and its variant

Mitsuki Miyagi, Sotaro Takiguchi, Kazuaki Hakamada, Masafumi Yohda, Ryuji Kawano (*Department of Biotechnology and Life Science, Tokyo University of Agriculture and Technology*)

Nanopore technology has attracted attention as a single-molecule analyzer. DNA sequencing using nanopore have been achieved and commercialized; the next step in advancing nanopore technology is towards peptide sequencing. Although many attempts have been reported for discriminating each amino acid using biological nanopores, it remains challenging. In this study, we focused on the translocon nanopore, EXP2 because a translocon intrinsically transports a polypeptide chain through the nanopore. Here, we conducted a single-molecule translocation of peptides using wild-type EXP2, and its variant (ΔD231-EXP2), which lacked the C-terminus region to decrease the current noise of EXP2. As a result, we succeeded in discriminating oligopeptides due to using ΔD231-EXP2 nanopore.

2Pos107 DNA 液滴内での DNA 結合タンパク質の標的 DNA 探索の単分子観察
Single-molecule characterization of target search of DNA-binding proteins inside liquid DNA droplets

Ryo Kusano[1,2], Trishit Banerjee[1,2], Saori Kambayashi[1], Kiyoto Kamagata[1] ([1]*IMRAM, Tohoku Univ.*, [2]*Department of Chemistry, Tohoku Univ.*)

DNA-binding proteins would have efficient mechanisms to search for their target sites on long genomic DNA. The target search dynamics have been characterized on DNA at very low concentration. Recently, it has been shown that liquid-liquid phase separation (LLPS) occurs in crowded DNA. In this study, we investigated the target search dynamics of DNA- binding proteins under LLPS condition using single-molecule fluorescence microscopy. To mimic a cellular LLPS condition, we prepared DNA droplets using PEG/Dextran mixture. We observed the movements of four DNA-binding proteins inside DNA droplets. Interestingly, we found very slow diffusion mode, suggesting that crowded DNAs under LLPS arrest DNA-binding proteins, focusing on the target search for DNAs located nearby.

2Pos108 Molecular dynamics study of the three prime repair exonuclease 1 and its mutants

Hiroki Otaki (*Grad. Sch. of Biomedical Sci., Nagasaki Univ.*)

The three prime repair exonuclease 1 (*TREX1*) gene encodes a nuclear protein (TREX1) with 3′ to 5′ DNA-specific exonuclease activity. Mutations in *TREX1* gene are associated with a wide spectrum of disorders, including systemic lupus erythematosus, Aicardi–Goutières syndrome, and familial chilblain lupus. In order to clarify the effect of mutations on the TREX1 system, we have modeled the complexes of TREX1 mutants with double-stranded DNA and conducted molecular dynamics simulations. By using a network graph to visualize interaction network, we have found the differences in the interaction around the active site between the mutants and wild type. This work was supported by GSK Japan Research Grant 2021 and JSPS KAKENHI Grant Number 19K16058.

2Pos109* (2SEP-3) RNase T2 のリボソームへの結合を介した翻訳阻害機構
(2SEP-3) Regulation mechanism of translation through the interaction of RNase T2 with ribosome

Atsushi Minami[1], Takehito Tanzawa[2], Zhuohao Yang[3], Takashi Funatsu[3], Takayuki Kato[2], Tomohisa Kuzuyama[1,4], Hideji Yoshida[5], Tetsuhiro Ogawa[1,4] ([1]*Grad. Sch. Agri. and Life Sci., Univ. Tokyo*, [2]*IPR, Osaka Univ.*, [3]*Grad. Sch. Pharm. Sci., Univ. Tokyo*, [4]*CRIIM, Univ. Tokyo*, [5]*Fac. Med., Osaka Med. Pharm. Univ.*)

RNase T2 is a conserved ribonuclease found in almost all organisms. Although the enzymatic activity is quite simple that it cleaves single-stranded RNA nonspecifically, it is involved in diverse and important biological events, e.g. tumor suppressor in mammals and biofilm formation in *Escherichia coli*.
It is known that *E. coli* RNase T2 interacts with ribosomes, but the physiological role remains elusive. During our analysis of the biofilm formation mechanism, we found that RNase T2 interacts with ribosomes that are not engaged in translation. Moreover, the ribosome bound to RNase T2 cannot initiate translation. Together with the Cryo-EM structure of RNase T2 complexed with ribosome, we will discuss the mechanism of translation impairment in this presentation.

2Pos110 ヌクレオリン核酸結合ドメインと 4 重鎖 DNA との結合過程
The binding process of quadruplex DNA to RNA/DNA binding domains of nucleolin

Masato Morikawa[1], Kota Yamaguchi[1], Kazuki Kawada[2], Koji Umezawa[1,2,3] ([1]*Grad. Sch. of Sci. & Tech., Shinshu Univ.*, [2]*Dept. Agri., Shinshu Univ.*, [3]*IBS., Shinshu Univ.*)

The quadruplex DNA, AT11, inhibits cancer cell growth by binding to the RNA/DNA binding domains (RBDs) of nucleolin. Nucleolin is a protein which has the four RBDs connected with flexible linker regions. It has not been clear the detailed process that AT11 binds to the RBDs. To investigate effects of RBDs on the binding process, molecular dynamics (MD) simulations were performed for the two systems: RBD1-2 and AT11, RBD1-2-3-4 and AT11. The results showed that the initial binding site was K427 of RBD2 in RBD1-2 and AT11 system while K521 of RBD3 was bound quickly in RBD1-2-3-4 and AT11 system. The intermolecular interaction could be modulated by internal domain motion, which was suggested by MD simulation with different ionic concentrations.

2Pos111 微小閉鎖空間がポリヌクレオソーム凝縮に与える影響の検討
Investigation of the effect of spherical (three-dimensional) confinement on the higher order structure of 12-mer nucleosome arrays

Masahiro Okabe (*Dept. Biol. Sci., Grad. Sch. Sci., The Univ. Tokyo*)

Polymers spontaneously form unique structures when the polymer molecules are assembled in confined spaces. In this study, we investigated the effect of spherical confinement on the higher-order structure of 12-mer nucleosome arrays. The nucleosome arrays were reconstituted with ATTO647-labeled histone octamers and encapsulated into water-in-oil (W/O) microdroplets with a diameter of 15−80 μm to observe under a fluorescence microscope. In the absence of salts, the nucleosome arrays were condensed in W/O microdroplets with a diameter of less than 30 μm, irrespective of the concentrations. On the other hand, the confinement effect was limited in the buffer used in liquid-liquid phase separation experiments. The details will be discussed.

2Pos112 一本鎖 DNA は核小体周囲に凝集体を形成する
Single-stranded DNA forms condensates surrounding nucleoli

Koichiro Maki[1,2], Jumpei Fukute[1,3], Taiji Adachi[1,2,3] ([1]*Inst. Life Med. Sci., Kyoto University*, [2]*Grad. Sch. Eng., Kyoto University*, [3]*Grad. Sch. Biostudies, Kyoto University*)

Nuclear chromatin is known to change the conformation depending on mechanical environment, resulting in altered gene transcription patterns. In this study, we focus on intranuclear single-stranded (ss) DNA, as its local accumulation inside the nucleus would be important in modulating specific gene transcription. We developed a novel imaging technique for ssDNA in the nucleus, using a fluorescent dye which binds to ssDNA. By utilizing this technique, we revealed that ssDNA forms condensates surrounding nucleoli, where ribosomal RNA is transcribed. In the future, we will aim to understand how ssDNA condensates are formed under mechanical environment and modulate gene transcription.

2Pos113* ヒト生細胞内環境における三重鎖 DNA 分子の構造及びダイナミクスの解析
Analysis of the structure and dynamics of triplex forming oligodeoxynucleotide in living human cells

Tomoki Sakamoto[1,2], Yudai Yamaoki[1,2], Takashi Nagata[1,2], Masato Katahira[1,2] ([1]*Inst. Adv. Energy, Kyoto Univ.*, [2]*Grad. Sch. Energy Sci., Kyoto Univ.*)

DNA triplex structures are reportedly involved in gene regulation. **We obtained the first direct evidence for an actual formation of the DNA triplex structures in living human cells by in-cell NMR technique [Sakamoto *et al.*, *Chem. Commun.*, 2021].** Then, to understand the intracellular properties of DNA triplex structures, the quantitative analyses on thermodynamics and kinetics under *in vitro* molecular crowding conditions that mimic intracellular environment were carried out. The imino proton-water proton exchange analysis gave invaluable kinetics parameters for each base pair. **Our study indicated differences of stabilities of the DNA triplex structures under two *in vitro* conditions, dilute and molecular crowded.** Our findings may be extrapolated to living cell conditions.

2Pos114 動的ループによる染色体コンパートメントの形成と変化
Dynamic loops shape and reshape chromosome compartments

Shin Fujishiro[1,2], Masaki Sasai[1,2] ([1]*Fukui Inst. Fund. Chem., Kyoto Univ.*, [2]*Dept. Complex Sys. Sci., Nagoya Univ.*)

Interphase chromosomes are segregated into euchromatin-like (type-A) and heterochromatin-like (type-B) regions. A popular hypothesis was that molecular droplets mediate this AB phase separation, but we showed *in silico* that locally heterogeneous chromatin compaction without droplets is sufficient as a separation driver (Fujishiro et al. *PNAS* 2022). This finding suggested the relationship between AB phase separation and transcription or replication. We show that the loop-reeling motion of cohesin compacts type-B chromatin, while complexes for transcription or replication block the cohesin motion, extending type-A chromatin, which leads to the AB phase separation. We show that perturbations to chromatin-bound complexes switch chromatin regions from A to B or vice versa.

2Pos115 FRET study of the sequence dependence of nucleosomal DNA unwrapping

Tomoko Sunami, Hidetoshi Kono (*QST, iQLS*)

We previously showed that AA/TT is enriched in the entry sites of +1 nucleosomes in the yeast genome and that those regions are easily cleaved with MNase. To further understand the mechanism of the AA/TT dependence of the stability of the nucleosome, we studied DNA unwrapping of nucleosomal DNA by PAGE and FRET measurements. We found that nucleosome with AA/TT is disrupted at a lower ethidium concentration than those without AA/TT. FRET analysis showed that the extent of unwrapping of AA/TT or TA sequence are similar to those of 601 sequence at low salt concentrations. With increasing the concentration, DNAs with AA/TT start to unwrap at a lower concentration than those with TA. In addition, we found that the unwrapping is dependent on the type of the cations.

2Pos116* (2SBA-4) 細胞核内における underwound DNA の蛍光イメージング
(2SBA-4) Fluorescence imaging of underwound DNA in the cell nucleus

Jumpei Fukute[1,2], Koichiro Maki[1,3], Taiji Adachi[1,2,3] ([1]*Inst. Life & Med. Sci., Kyoto Univ.*, [2]*Grad. Sch. Biostudies, Kyoto Univ.*, [3]*Grad. Sch. Eng., Kyoto Univ.*)

In the cell nucleus, underwound DNA is known to affect key biological processes such as gene transcription. In this study, we aimed to reveal the intranuclear distribution of underwound DNA by developing a fluorescence imaging method. We utilized biotinylated-psoralen (bio-psoralen), which binds to underwound DNA. Based on this new method, we found that underwound DNA was predominantly distributed in the nucleolus, where ribosomal RNA was transcribed by RNA polymerase I. Our novel imaging technique could be useful to explore DNA underwinding-mediated mechanisms.

2Pos117 ラマン顕微鏡を用いた生細胞内のクロモセンターのラベルフリー成分・構造解析
Label-free compositional and structural analysis of chromocenters in living cells using Raman microscopy

Masato Machida[1], Atsushi Shibata[2], Kentaro Hujii[3], Shinji Kajimoto[1,4], Takakazu Nakabayashi[1] ([1]*Grad. Sch. Pharm. Sci., Univ. Tohoku*, [2]*GIAR., Univ. Gunma*, [3]*QST.*, [4]*JST PRESTO.*)

Heterochromatin (Hch) is an important and complex structure that is involved in gene expression and cellular morphology. In NIH3T3 cells, Hch is aggregated and can be observed as spots called chromocenters. However, little is known about the structures and constituents of chromocenters and there are few studies in label-free manner. In this study, we obtained Raman images of living NIH3T3 cells and succeeded in distinguishing between nucleolus, nucleoplasm, and chromocenters. Different Raman bands were observed in these spectra, suggesting that chromocenters are enriched in nucleic acids and other substances such as lipids. The concentration of nucleic acids and lipids seemed to be reduced in Hch after the treatment of trichostatin A which loosens the chromocenters.

2Pos118* 高速原子間力顕微鏡による H2A.Z.1 ヌクレオソームの DNA 上での自発的スライディングの直接観察
Direct imaging of spontaneous sliding along DNA of H2A.Z.1 nucleosome by high-speed atomic force microscopy

Shin Morioka[1], Shoko Sato[2], Naoki Horikoshi[2], Tomoya Kujirai[2], Hitoshi Kurumizaka[2], Mikihiro Shibata[3,4] ([1]*Grad. Sch. Math. & Phys., Kanazawa Univ.*, [2]*Institute of Quantitative Biosciences, Tokyo Univ.*, [3]*WPI-NanoLSI, Kanazawa Univ.*,, [4]*InFiniti, Kanazawa Univ.*)

Nucleosomes are a basic unit of chromatin consisted of the complex of DNA and histone proteins and regulate gene expression. An H2A histone variant, H2A.Z.1, has been reported to involve in both transcription repression and activation, but its molecular mechanism is still unknown. Here, we visualized nano-dynamics of the canonical and H2A.Z.1 nucleosomes using high-speed atomic force microscopy. We found that the histone core of H2A.Z.1 nucleosome spontaneously slides along the DNA about 4 nm within 0.3 s, but not the canonical nucleosome. This result suggests that the histone core sliding along DNA may facilitate access of transcription factors to the unwrapping DNA and, conversely, prevent access to the newly wrapping DNA.

2Pos119* DNA ハイブリダイゼーションのカイネティックなエラー抑制
Kinetic error suppression of DNA hybridization

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Suppression of DNA hybridization error is significant in biotechnologies. For example, in PCR, the hybridization error results in various problems such as false-positive. Energetic approaches to suppress the error, including a careful primer sequence design, have an inherent limitation in terms of reaction efficiency. A kinetic approach that suppresses the hybridization error by building a barrier could be an alternative way. This study demonstrates that a blocker strand significantly suppressed the hybridization error in PCR. Our theoretical analysis revealed that this blocker method corresponds to the kinetic approach. The model provides the mathematical representation of the barrier height, which would enable a broad range of applications other than PCR.

2Pos120* (1SGA-2) 人工核酸 PNA を用いた DNA の液ー液相分離制御
(1SGA-2) Regulation of liquid-liquid phase separation of DNA using peptide nucleic acid (PNA)

Rikuto Soma, Yuichiro Aiba, Masanari Shibata, Shinya Ariyasu, Osami Shoji (*Graduate School of Science, Nagoya University.*)

The phenomenon of liquid-liquid phase separation (LLPS) in cells has attracted much attention, and it has become clear that nucleic acids also undergo LLPS. In this study, we developed a novel method to control the LLPS of DNA by using peptide nucleic acid (PNA), a type of artificial nucleic acid. PNA, which has a neutral peptide backbone, can form a stable duplex with complementary DNA, and its charge can be easily modulated by introducing amino acids into PNA. Therefore, PNA can potentially be applied to LLPS, where electrostatic interaction is one of the major driving forces. When PNA was mixed with target DNA, droplet formation was observed. Furthermore, we have succeeded in controlling the LLPS of DNA in a sequence-selective manner.

2Pos121* 非平衡ダイナミクスを示す酵素反応によって活性化された DNA 液滴
Enzymatically activated DNA-droplets exhibiting non-equilibrium dynamics

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Biomolecular condensates called membrane-less organelles (MLOs) formed by liquid-liquid phase separation are known to regulate biochemical reactions in living cells. Some of such condensates show dynamic behaviors realized by using chemical reactions dependent on chemical energy such as ATPs, but the behaviors and their mechanisms have not been understood so much. In this study, we report dynamic DNA droplets, which are synthetic condensates formed by the self-assembly of DNA nanostructures, showing dynamical behaviors by enzymatic reaction of helicase using ATP. We believe that this system will help to elucidate the dynamic nature of MLOs

2Pos122* 再構成転写翻訳系におけるトランスファー RNA の合成と共役した翻訳および DNA 複製システム
Transfer RNA synthesis-coupled translation and DNA replication in a reconstituted transcription/translation system

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Transfer RNAs (tRNA) are key molecules involved in translation. *In vitro* synthesis of tRNAs and their coupled translation are important challenges in the construction of a self-regenerative molecular system. Here, we first purified EF-Tu and ribosome components in a reconstituted translation system of *Escherichia coli* to remove residual tRNAs. Next, we expressed 15 types of tRNAs in the repurified translation system and performed translation of the reporter luciferase gene depending on the expression. Moreover, we demonstrated DNA replication through expression of a tRNA encoded by DNA, mimicking information processing within the cell. Our findings highlight the feasibility of an *in vitro* self-reproductive system in which tRNAs can be synthesized from replicating DNA.

2Pos123 MD シミュレーションによるタンパク質モデルペプチド周囲の水和ダイナミクスの解明
MD simulations reveals hydration dynamics around protein model peptides

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We focused on the secondary structure of proteins and theoretically elucidated the dynamics of hydrated water. Multiple peptides were selected as targets for the protein model. Specifically, we used polyglutamic acid, alanine-based peptides whose helix preservation is different depending on the sequence, and signoline composed of 10 amino acid residues having a beta structure. Using these peptides as protein models, we analyzed the dynamics of hydrated water in different structures. Unlike proteins,peptides do not have large and stable hydrophobic nuclei, and all atoms are exposed to a large amount of solvent, so they can be expected to be a useful model for clarifying the effects of water on the structure of proteins in detail.

2Pos124* Effect of local electric field on the rotational dynamics of water dipole in protein solutions

Kang Hu[1,2], Ryo Shirakashi[1] ([1]*IIS, Univ. Tokyo*, [2]*Grad. Sch. Eng., Univ. Tokyo*)

In the present molecular dynamics (MD) simulation study, we calculate the dipole moment and the local electric field of each water molecule in the aqueous lysozyme solutions. We find that water dipole rotation and local electric field reorientation have nearly identical relaxation times. This result suggests that water dipole synchronizes with the local electric field. By separating the local electric field according to its origins, *i.e.,* protein or solvent, we also find that the rotation of water staying only near the protein surface in the "*hydration layer*", is dominated by the protein tumbling through the electric field originating in the protein, while the tendency of water dipoles to align themselves with the electric field is an intrinsic property as pure water.

2Pos125 ニューラルネットワークと経験分布の融合的手法による膜蛋白質の水和構造予測
Prediction of hydration structures of membrane proteins using neural networks in combination with the empirical hydration distribution

Kochi Sato[1,2], Mao Oide[1,2], Masayoshi Nakasako[1,2] ([1]*Dept. Phys., Keio Univ.*, [2]*RSC, RIKEN*)

The hydration structures of proteins are indispensable for their folding, stability, and functions. However, complete visualizations of the hydration structure over the entire protein surfaces remain difficult. Accordingly, we constructed a prediction method based on a three-dimensional convolutional neural network to compensate for this incompleteness. Although the prediction approach accurately reproduces hydration probabilities over the hydrophilic and hydrophobic surfaces of water-soluble proteins, the transmembrane regions of membrane proteins could not be precisely predicted. Here, we developed the prediction method to deal with membrane proteins by the hybrid use of the neural network and a set of the empirical hydration distribution function around polar atoms.

2Pos126 Free energy analysis of the addition of small molecules with simple structures to elucidate co-solvent effects in insulin dissociation

Simon Hikiri, Nobuyuki Matubayasi (*Grad. Sch. Eng. Sci., Osaka Univ.*)

We analyze the co-solvent effect on insulin dissociation from the viewpoint of free energy. Treating insulin as an all-atom model, we combine molecular dynamics simulation and energy representation theory to analyze the free energy of the co-solvent effect. The solvation free energy changes of insulin from complex to monomer in pure water and in co-solvent solutions are calculated. We focus on the acquisition of co-solvent effects from a fundamental point of view, and dealt with co-solvent molecules with simple structures. Correlation analysis of the interacting components of the free energy are performed to identify the dominant components of the dissociation control.

2Pos127* 酸性タンパク質凝集解明のための分子シミュレーションによる電解質溶液中のアニオン間実効引力の研究
Molecular simulation study of effective attraction between anions in an electrolyte solution for elucidation of acidic protein aggregation

Michika Takeda[1], Ryo Akiyama[2] ([1]*Grad. Sch. Sci. Kyushu Univ.*, [2]*Inst. Sci. Kyushu Univ.*)

Acidic proteins, which are negatively charged particles, show an interesting condensation behavior in an electrolyte solution which has multivalent cations. As the electrolyte concentration increases, the state changes dispersion, and re-dispersion. So far, to explain this phenomenon, we calculated the effective interaction between anions by using the OZ-HNC theory. These results reproduced the above experimental results qualitatively. The confirmation using molecular simulations is important due to approximate of OZ-HNC theory. Thus, we calculate the effective interaction between anions by using the Monte Carlo simulation in the present study. We carried out the modeling using the results of the OZ-HNC theory to survey the reentrant behavior.

2Pos128 水と生体分子のシミュレーションにおける静電相互作用計算：オンサーガモデルによる理論的検証
Theoretical study on the electrostatic calculation in biomolecular simulation

Yoshiteru Yonetani (*QST*)

Accurate electrostatic calculation is essential for simulating water and biomolecules. Recently, real-space treatments have become an attractive choice; the development is now a challenging subject. In 1980, Neumann and Steinhauser employed the Onsager dielectric model to explain how simple real-space cutoff produces artificial dipolar orientation. Using this dielectric model, we here explored fundamental properties of the recent real-space treatments of shifting. The result of the Kirkwood function showed that the simple cutoff produces a well-known hole-shape artifact, whereas the shift treatments can remove it. Yet, the shift treatments are not sufficient. This implies that not only shifting but also damping is required, as Wolf treatment suggests.

2Pos129* 幹細胞分化のモデル系を模した人工遺伝子回路の生じる空間パターン
Spatial patterns formed by a synthetic genetic circuit mimicking the model of stem cell differentiation

Kei Ikemori, Yuichi Wakamoto (*Grad. Sch. of Art. & Sci., Univ. Tokyo*)

Coexistence of self-renewal and differentiation is an essential property of stem cell and lies at the core of the developmental process of multicellular organisms. It is theoretically predicted that the characteristics of stem cell can be realized by a simple genetic network with cell-cell interactions. We observed the dynamics of synthetic genetic circuits mimicking this "minimal model for stem cell" in E. coli using microfluidic devices. Characteristic spatial patterns were observed in the cell population, which depended on the shape of the culture chamber. This pattern formation may be caused by the spatially heterogeneous diffusivity of low-molecular compounds that mediates the cell-cell interaction. We tested this hypothesis experimentally and numerically.

2Pos130 Planar cell polarity–dependent asymmetric organization of microtubules for polarized positioning of the basal body in node cells

Xiao Rei Sai[1], Kastura Minegishi[2], Hiroshi Hamada[1] ([1]*Riken BDR*, [2]*National Center of Neurology and Psychiatry*)

The precise posterior positioning of ciliary basal bodies in mouse node is critical for ciliary function which is related to left-right (L/R) asymmetry establishment. Previously we have shown that noncanonical Wnt signaling and core PCP proteins, Pk and Vangl1, played essential roles in positioning of basal body to posterior side of the node cells. However, the detailed molecular mechanism remains unknown.
In this study we found Dchs is required to establish polarity of PCP proteins and actomyosin. Myosin II functions in the downstream of PCP proteins, perhaps directly regulates the orientation of basal body microtubule which is essential for producing mechanical force to drive basal body backward to posterior side of node cells for breaking of L/R symmetry.

2Pos131 マウスノード不動繊毛は変形の向きを感知して左右軸を決定する: 非対称性を生み出すメカニカルな機構
Mouse nodal immotile cilia sense bending direction for left-right determination: Mechanical regulation in initiation of symmetry breaking

Takanobu A Katoh[1], Toshihiro Omori[2], Katsutoshi Mizuno[3], Takeshi Itabashi[1], Atsuko H. Iwane[1], Takuji Ishikawa[2], Yasushi Okada[1,4], Takayuki Nishizaka[5], Hiroshi Hamada[1] ([1]*BDR, Riken*, [2]*Grad. Sch. Eng., Tohoku Univ.*, [3]*Fac. Med. Sci., Univ. of Fukui*, [4]*Grad. Sch. Med., Grad. Sch. Sci., UBI, WPI-IRCN, The Univ. of Tokyo*, [5]*Fac. Sci., Gakushuin Univ.*)

Immotile cilia at the node of mouse embryos are required for sensing of a leftward fluid flow that breaks L-R symmetry of the body. The flow-sensing mechanism has long remained elusive, however. Here we show that immotile cilia at the node undergo asymmetric deformation along the D-V axis in response to the flow. Application of mechanical stimuli to immotile cilia by optical tweezers induced Ca^{2+} transient and degradation of *Dand5* mRNA in the targeted cells. The *Pkd2* channel protein was preferentially localized to the dorsal side of immotile cilia, and Ca^{2+} transients were preferentially induced by mechanical stimuli directed toward the ventral side. Our results explain the biophysical mechanism as to how immotile cilia at the node sense the direction of fluid flow.

2Pos132* 物理的環境の非対称性が上皮折り畳みパターン選択に果たす役割
Role of asymmetry of physical environment in epithelial folding pattern selection

Kentaro Morikawa, Daich Kuroda, Yasuhiro Inoue (*Grad. Sch. Eng., Kyoto Univ.*)

The shape of the insect exoskeleton is formed as a complex folding structure of the epithelial sheet. The folding structure is developed in the larva as the epithelial tissue grows under physical constraints imposed by the surrounding environment (e.g., connective tissue and cuticle). To investigate the relationship between the asymmetry of the physical constraints on the apical and basal sides of the epithelium and the folding pattern, we obtained the Swift-Hohenberg-like equation as an overdamped equation that reduced the variation of the mechanical energy functional. Numerical integration of the equation showed that dot, labyrinth, and hole patterns are formed depending on the asymmetry of the environment.

2Pos133 微小管脱重合薬により骨格筋の粘弾性は変化する
The viscoelasticity of skeletal muscle is altered by microtubule destabilized agent

Takuya Kobayashi, Takashi Murayama, Nagomi Kurebayashi (*Dept. of Cellular and Molecular Pharmacology, Juntendo University*)

Microtubule (MT) plays important roles for cellular system. However, the role of MT is not well understood in skeletal muscles. We here examined the effect of microtubule stability on physical and contractile properties of skeletal muscle by measuring the tension of mouse EDL muscles in the absence or presence of colchicine. Colchicine treatment substantially reduced the muscle viscosity. Thus, MT is involved in intracellular viscosity of skeletal muscle. Whereas the twitch tension was not different between the two conditions, the tetanic tension of colchicine-treated muscles tended to be smaller than that of nontreated muscles. These results suggest that the intracellular viscosity is involved in the development of tetanic tension of skeletal muscles.

2Pos134 細菌アクチン MreB の繊維構造多型
Filament structural polymorphism of bacterial actin MreB

Daichi Takahashi[1], Ikuko Fujiwara[1,2,3], Akihiro Narita[4], Makoto Miyata[1,2] ([1]*Grad. Sch. Sci., Osaka Metropolitan Univ.*, [2]*OCARINA, Osaka Metropolitan Univ.*, [3]*Dept. Mater. Sci. Bioeng., Nagaoka Univ. Tech.*, [4]*Grad. Sch. Sci., Nagoya Univ.*)

Spiroplasma is a helical-shaped bacterium that shows unique swimming motility using five classes of bacterial actin proteins, MreB (MreB1-5). MreB5, which is one of the essential MreBs for the swimming, forms a sheet structure widely interacting with membrane and other protein filaments composing the swimming machinery. However, the underlying nature of the sheet has been unclear. To clarify it, we examined the structural polymorphism of MreB5 filaments. Our electron microscopy and light scattering assay showed that MreB5 was assembled into paracrystal structures followed by the sheet formation in neutral pH conditions. These results suggest that the MreB5 sheet possesses both positively and negatively charged regions to be attracted to form paracrystals.

2Pos135 Absolute Reward in Large Feature Space: Tracking by Linear Bandit

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Linear bandit can determine the arm having the highest expected reward by repeating the arm selection under the assumption that for the arm i, reward y_i is defined as $y\,i = x\,i\,,\ \theta * + \eta\,i\,$, where $x\,i$ is the feature and $\theta * \in R\,d$ is unknown parameter and $\eta\,i$ is random noise. This research, focused on the problem where not only the arm with the highest reward but also the arm with the lowest reward is important and proposed a linear bandit algorithm to identify the arm with the largest absolute value of the reward along with their features. Modified Optimistic in the Face of Uncertainty Linear (OFUL) bandit is developed, which can select the arm with the highest absolute value of upper and lower bound. Boruta, LASSO and PCA are used for feature reduction.

Poster

2Pos136 アクトミオシンの弱結合ー強結合転移におけるクーロン駆動機構
Coulombic drive for the weak-to-strong binding transition in actomyosin

Kyohei Shoji, Mitsunori Takano (*Dept. of Pure & Appl. Phys., Grad. Scl. Adv. Sci. & Eng., Waseda Univ.*)

Myosin undergoes the transition from the weak to the strong binding to actin in the course of force generation. While it is thought that the hydrophobic interaction is responsible for the strong binding, our previous molecular dynamics (MD) simulation showed that the Coulombic interaction plays a critical role in the strong binding as well. In this study, to clarify the role of the Coulomb interaction and the residues involved in the strong binding, we conducted all-atom MD simulation of the actin-myosin binding in explicit water, and analyzed the contribution of the Coulomb energies with careful treatment of the dielectric boundary. We found a large Coulombic drive for the strong binding and well-designed complementarity of charged residues between actin and myosin.

2Pos137 自由エネルギーランドスケープの切り替えとパワーストロークを考慮した筋収縮の 6 状態モデルの構築
Construction of six-state model of muscle contraction with switched free energy landscape and power stroke

Shunta Oda, Tomoki P. Terada (*Dept. Appl. Phys., Grad. Sch. Eng., Nagoya Univ.*)

Muscle contraction is caused by a shortening of the myofibrils, as the actin and myosin filaments slide to each other shortening the sarcomere. This sliding motion is caused by the interaction of the myosin head with the actin filament. The biochemical reaction cycle of myosin and actin filaments is composed of six states. In addition, there are two mechanical models of sliding motion, the lever arm model and the biased Brownian motion model, and it has also been suggested that the two models may coexist. We constructed a six-state model of muscle contraction that reflects the interaction and incorporates two mechanical models. Using this model, we performed calculations corresponding to the experiments and discuss the role of the biased Brownian motion.

2Pos138 F_oF_1-ATPase の非触媒部位の機能解明
Functional elucidation of the non-catalytic site of F_oF_1-ATPase

Ren Kobayashi, Atsuki Nakano, Ken Yokoyama (*Department of Molecular Biosciences,Kyoto Sangyo*)

The F_1 domain of ATP synthase F_oF_1 contains six nucleotide-binding sites. Three of them are called Non-Catalytic sites because the bound ATP is not hydrolyzed. The mutant F_oF1, which lacks the ATP binding ability to the noncatalytic site (ΔNC F_oF_1), exhibit loss of ATP hydrolysis activity, but the reason is still unclear.

In this study, we tried to determine the structure of ΔNC F_oF_1 under ATP saturated condition using cryo-electron microscopy. By comparing the structure of Wild type F_oF_1 during the reaction, the molecular basis for the loss of ATPase activity due to the deletion of ATP binding at non-catalytic sites will provide an insight on the role of the non-catalytic sites on the F_oF_1.

2Pos139* 無細胞タンパク質合成と 1 分子回転観察を組み合わせた F_1-ATPase の *in vitro* スクリーニング
In vitro screening of F_1-ATPase based on single molecule rotation assay coupled to cell-free protein synthesis

Mai Taguchi, Hiroshi Ueno, Hiroyuki Noji (*Grad. Sch. Eng., Univ. Tokyo*)

F_1-ATPase (F_1) is a rotary molecular motor driven by ATP hydrolysis. The rotation characteristics of F_1 have been well studied in single molecule experiments. However, the design principles of F_1 are still unknown and it is still difficult to create F_1 with the desired functions. Here, in order to create F_1 with the desired functions (e.g. faster F_1), we developed an *in vitro* screening system that integrates the cell-free synthesis of F_1 mutants and the single molecule rotation assay. By using the sequence of slow F_1 mutant (βE190D) as a template, the screening of faster F_1 was tested. As a result, we successfully identified faster wild-type F_1 from 8 single-site variants containing wild-type sequence in a single trial.

2Pos140 H⁺輸送律速における変異型 F_oF_1-ATPase の回転
ATP driven rotation of mutant F_oF_1 where H^+ translocation is rate-limiting

Kiyoto Yasuda[1], Daichi Ando[1], Ryohei Kobayashi[1,2], Hiroshi Ueno[1], Hiroyuki Noji[1] ([1]*Appl. Chem., Grad. Sch. Eng., Univ. Tokyo*, [2]*Inst. for Mol. Sci.*)

F_oF_1-ATP synthase (F_oF_1) is a reversible molecular motor that couples ATP hydrolysis/synthesis in F_1 with H^+ translocation in F_o via rotation. Despite extensive research on rotary catalysis of F_1, little is known about rotary dynamics of F_o during H^+ translocation. Here, to visualize the rotary dynamics of F_o during ATP-driven H^+ translocation, we conducted rotation assay of a F_oF_1 mutant (*c*E56D), where Glu-56 of F_o-*c* subunit essential for H^+ translocation was replaced with Asp. As a result, two distinct populations were found for the rotation rate of *c*E56D, one of which showed a one-fourth rate of WT, whereas the other showed almost the same rate as WT. Slow-rotating fraction might reflect H^+ translocation-coupled rotation, where H^+ translocation is rate-limiting.

2Pos141* Vo 部分での回転によるプロトン輸送機構の分子基盤
Structural basis on the rotary mechanism of Vo domain by proton translocation

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The rotary V-ATPase consists of a soluble V1 portion and a membrane-embedded Vo portion; V1 is driven by hydrolysis/synthesis and Vo by transmembrane flow of protons. Protons are transported through two aqueous half-channels at the interface between the C-ring and the a-subunit. However, the full extent of the proton transfer is not yet clear due to the lack of high-resolution information on the Vo domain. In addition, all the currently published structures of the Vo part reflect the structure when the rotation is stopped. Therefore, we attempt to determine the high-resolution structure of Vo by analyzing VoV1 in motion, and we propose a new mechanism for proton translocation, known as “Two-channels model”.

2Pos142 分子動力学計算による F_1-ATPase のリン酸放出経路の探索
Exploration of phosphate release pathway of F1-ATPase with molecular dynamics calculation

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F_1-ATPase (F_1) is a rotary molecular motor in which a central γ subunit rotates against hexagonally arranged subunits $\alpha_3\beta_3$. The single-molecule rotation assay shows that γ rotates 120° for each ATP hydrolyzed. It was also suggested P_i release is one of the triggers to rotate. Therefore, its timing and pathway are important to understand the rotational mechanism.
Recently, the structure of TF_1 was obtained by structural analysis using cryo-EM. It was pointed out P_i is released from back door similar to that of myosin.
We have conducted molecular dynamics (MD) calculation using enhanced sampling method in MD software GENESIS and supercomputer FUGAKU and HOKUSAI. By doing this, we strive to elucidate the rotational mechanism, especially P_i release timing and pathway.

2Pos143 Single molecule observation of kinesin-1 on collectively aligned microtubules

Tomoka Kashiwabara[1], Syeda Rubaiya Nasrin[2], Arif Md. Rashedul Kabir[2], Akira Kakugo[2], Yusuke T. Maeda[1] ([1]*Fac. Sci. Grad. Sch. Sci., Univ. Kyushu*, [2]*Fac. Science, Hokkaido University*)

Single molecule observation of kinesin motor protein in vitro has revealed the mechanism of chemical-mechanical energy conversion and its mechanical properties. Although conventional analysis has been done mainly with kinesin moving on a single microtubule, there are highly ordered structures of microtubules in living cells that are relevant to physiological function of diverse molecular motors. To better understand molecular motor action in highly ordered environments, we developed a method to utilize the collective motion of gliding microtubules for single molecule analysis in vitro. This presentation shows experimental details on the assembly and quenching of collectively gliding microtubules for future single molecule observation of kinesin-1.

2Pos144 Hybrid kinesin-1 dimer conjugated with synthetic PEG linker shows processive and fast motion with robust hand-over-hand mechanism

Jakia Jannat Keya[1], Akasit Visootsat[1], Kimitoshi Takeda[1], Akihiro Otomo[1], Wijak Yospanya[2], Sanghun Han[2], Kazushi Kinbara[2], Ryota Iino[1] ([1]*Institute for Molecular Science, National Institutes of Natural Sciences*, [2]*School of Life Science and Technology, Tokyo Institute of Technology*)

We engineered hybrid kinesin-1 dimers by conjugating motor domains with synthetic PEG linker through truncated neck-linkers (NL). Hybrid kinesins with long PEG_8 linker showed relatively stable velocity (337~442 nm/s at 1 mM ATP) and run length (>2500 nm) up to 4 amino acid (AA) NL deletions, suggesting flexibility of PEG contributes to the robustness. Furthermore, a hybrid kinesin with short PEG_2 linker and 1AA NL deletion showed fastest motion (736 nm/s) comparable to the wild-type (748 nm/s), although run length decreased to half. Importantly, most hybrid kinesins showed straight motions with 8 nm forward steps along single protofilament of the microtubule. Therefore, hand-over-hand mechanism is robust and natural peptide can be replaced with the synthetic linker.

2Pos145* The movement of kinesin with the neck linker hanging free in solution

Rieko Sumiyoshi, Masahiko Yamagishi, Mitsuhiro Sugawa, Junichiro Yajima (*Grad. Arts & Sci., Univ. Tokyo*)

Kinesin is a motor protein that take steps along microtubules. The structural change of neck linker has been proposed to generate force and to be essential for kinesin's motility, but its exact role in the motor mechanism remains undissolved. So far, there is no research that excludes the effect of the neck linker structural change to the force generation. In this study, we bound kinesin monomers to the substrate via their loops to observe kinesin's movement with neck linker in a free state. We found that kinesin moved under conditions in which structural changes of the neck linker were not involved in kinesin's force generation directly. We propose that neck linker controls the interaction between kinesin and microtubule.

2Pos146 架橋微小管-キネシンの *in vitro* 運動系でマクロに出力する微小管群の観察
Observation of cross-linked microtubules transmitting integrated forces of multiple kinesin motors *in vitro*

Ryuzo Kawamura[1], Naruaki Tsuji[1], Naritaka Kobayashi[2], Takahisa Matsuzaki[1,3], Hiroshi Y. Yoshikawa[1,3] ([1]*Grad. Sch. Sci. Eng., Saitama Univ.*, [2]*Sch. Eng., Univ. of Shiga Pref.*, [3]*Grad. Sch. Eng., Osaka Univ.*)

Motor proteins have potentials not only to show nanometric precise movements but also to generate integrated macroscopic forces, as seen in natural system. We have been trying to realize an integrated output force in an artificial system using purified motor proteins of kinesin and microtubules. Here, the microtubules were simply cross-linked by chemicals and driven by kinesins on a glass substrate with consumption of adenosine-triphosphate. While the network fluctuates with amplitudes up to several tens of micrometers, output force at nanonewton order was measured from bending of a glass microneedle placed on it, and even some oscillation was detected. For elucidation of the mechanism, distribution of the microtubules was observed under fluorescent microscopy.

2Pos147 タンパク質の 2D 投影像の深層学習によるミオシンの構造分類法の研究
Structure classification of myosin by deep learning of 2D projection images

Hitomi Wada[1], Hiroko Takazaki[2], Takuo Yasunaga[1] ([1]*Grad. Sch. Comp. Sci. Syst. Eng., KIT.*, [2]*IPR, Univ. Osaka*)

The lever arm theory focusing on the structural changes of myosin is essential for clarifying the muscle contraction mechanism. Moreover, in recent years, the progress of image analysis using Deep Leaning has been remarkable. So, we used unsupervised learning, in which learning is performed without a teacher label. This may apply to the classification by feature by mapping to the latent space.

This research analyzed 2D projection myosin images created from the protein databank (PDB) with a variable auto-encoder (VAE). As a result, we found a difference in distribution depending on the myosin heads' projection angle and neck angle. We will apply this model to the raw data of cryo-electron microscopy.

2Pos148* ミオシン 1c に駆動される F-アクチンのコークスクリュー運動
Corkscrew motion of F-actin driven by myosin-1c

Yusei Sato[1], Kohei Yoshimura[2], Kyohei Matsuda[1], Akisato Marumo[1], Takeshi Haraguchi[3], Masahiko Yamagishi[1], Mitsuhiro Sugawa[1], Kohji Ito[2,3], Junichiro Yajima[1] ([1]*Dep. of Life Sciences, Grad. School of Arts and Sciences, The University of Tokyo*, [2]*Dep. of Biology, Chiba Uni.*, [3]*Dep. of Biology, Chiba Uni.*)

Myosin-1c, a membrane-bound single-headed myosin, shows chiral motility in *in vitro* gliding assay. Myosin-1c is known to be participated in critical processes of the establishment of the left-right axis of animals, although the mechanism is not well understood. In this study, we evaluated the property of motility of *Drosophila melanogaster* myosin-1c by three-dimensional tracking of quantum dots bound to F-actin moving on a surface coated with myosin-1c molecules. Our technique showed that myosin-1c drove a left-handed corkscrew motion of F-actin in its longitudinal axis, and it was revealed that myosin-1c generates a torque component perpendicular to F-actin, as is known for dimeric myosin II, V, VI, and X.

2Pos149 軸糸ダイニンの協調性は外腕ダイニン中間鎖 2 によって制御される
Cooperative interactions between axonemal dyneins are regulated by the intermediate chain 2 of outer-arm dynein

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Ciliary motility is based on the microtubule sliding powered by outer and inner arm dyneins (OAD, IAD). We previously isolated a Chlamydomonas mutant with a point mutation in the intermediate chain 2 (IC2) of OAD, which swam 30% slower than wild type. Here we found that the mutant also displays abnormal photo-behavior. Previous studies showed that the behavior is controlled by regulating IAD activity. Thus, it is likely that the mutation affects IAD as well as OAD. One of newly isolated mutants which recovers low motility of the IC2 mutant had a mutation in OAD γ heavy chain (HC). Recent structural studies revealed that IC2 associates with γ HC of the adjacent OAD. These results suggest that IC2 regulates the cooperative actions of OAD-OAD and OAD-IAD molecules.

2Pos150 細菌べん毛モーター回転子ー固定子間相互作用のアミノ酸レベルでの解析
Analysis of the interaction interface between the rotor and stator of the bacterial flagellar motor at the amino acid residue level

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Most motile bacteria have a flagellar motor composed of a rotor and multiple stator complexes. The motor generates its rotational torque by the interaction between the stator protein MotA and the rotor protein FliG. In this study, we applied in vivo photo-crosslinking using pBPA, which forms covalent bonds with neighboring C-H upon UV irradiation, to detect FliG-MotA interactions. Furthermore, we constructed a new assay system by combining the in vivo photo-crosslinking method with rotation measurement. When pBPA locates where FliG and MotA are in direct contact, the motor rotation stops upon UV irradiation. By quantifying this stopping rate, we speculated the interaction interface between rotor and stator at the amino acid residue level.

2Pos151 真核生物鞭毛・繊毛軸糸構造の X 線回折トモグラフィー：クシクラゲ櫛板の利用
X-ray diffraction-based computed tomography of axonemal structure of eukaryotic flagella/cilia: Use of Ctenophore comb plates

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Diffraction-based X-ray computed tomography was achieved by using a comb plate of a Ctenophore, a motile organelle consisting of very regularly packed with motile cilia with rotationally well-aligned axonemes. Here we collected a series of diffraction patterns by rotating a quick-frozen comb plate with1° steps for a 180° range while it was kept frozen at ~100 K. The 3-D axonemal structure was restored by applying a 3-D extended version of a common phase-retrieval algorithm to the obtained 3-D diffraction pattern. The restored structure is a hollow tube with a ~200 nm diameter, covered with particles with an axial repeat of 96 nm, reminiscent of dynein arms. This is the first demonstration that the 3-D structure of a biological sample is restorable with this technique.

2Pos152 べん毛 III 型輸送 ATPase 複合体の構造変化と作動機構
Structural change of the ATPase ring complex of the flagellar Type III export apparatus

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The cytoplasmic ATPase ring complex of the flagellar Type III export apparatus (fT3-ATPase) is structurally similar to F/V-ATPase. The hydrolytic unit of fT3-ATPase is composed of FliI homohexamer, whereas that of F/V-ATPase is heterohexamer. Therefore, fT3-ATPase is believed to be an ancestral rotary motor of F/V-ATPase, but its rotation has not been proven. To elucidate the functional mechanism of fT3-ATPase, we purified a FliI mutant (FliI3A) that can form a stable homohexamer and observed it using Hi speed AFM and electron microscope. FliI3A forms a hexagonal ring structure with ADP-Mg AlF3 but a 3-fold symmetric clover-like structure with ADP AlF3. These observations suggest that the fT3-ATPase ring changes its conformation depending on the nucleotide binding.

2Pos153 Structural modeling of condensin by assimilating high-speed atomic force microscopy images

Hiroki Koide[1], Noriyuki Kodera[2], Mayu Terakawa[1], Shoji Takada[1], Tsuyoshi Terakawa[1] ([1]*Grad. Sch. Sci. Kyoto Univ.*, [2]*NanoLSI Kanazawa Univ.*)

Chromatin higher-order structure is maintained by a variety of proteins and is highly condensed during the mitotic phase of the cell cycle. One of the proteins responsible for this condensation is condensin. Previous studies have suggested that condensins cause chromatin condensation by so-called the DNA loop extrusion mechanism. However, its molecular basis remains unclear. In this study, we directly observed the structural dynamics of condensin by high-speed atomic force microscopy (AFM), constructed a structural model based on these AFM images, and performed coarse-grained molecular dynamics simulations. The results provided broad implications for the DNA loop extrusion mechanism.

2Pos154* べん毛 III 型分泌装置の ATPase FliI の HS-AFM 観察
Observation of flagellar type III secretion system ATPase FliI by HS-AFM

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FliI is an ATPase of flagellar type III secretion system. FliI forms a hexameric ring, and FliJ binds to its center pore. Because of the structural similarity to F_1-ATPase, a well-known as a rotary motor, FliI is assumed to be a rotary motor, but there has been no experimental evidence. Therefore, we tried to use HS-AFM to observe the conformational change of $FliI_6$ upon ATP hydrolysis. The observations revealed the stability of the ring varied depending on type of nucleotides. The $FliI_6$ bound by $ADPAlF_3$ has a 3-fold symmetric structure, and the addition of Mg^{2+} induced a 6-fold symmetric structure. In the absence of nucleotides, the three bright point structures are dominant. These suggest $FliI_6$ undergoes large conformational changes depending on its nucleotide states.

2Pos155* 蛍光色や偏光方向を選択可能な汎用的分子配向プローブ Nanobody-based POLArIS の開発
Nanobody-based POLArIS: a versatile molecular orientation probe with options of colors and fluorescence polarization orientations

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Fluorescence polarization microscopy (FPM) is a unique microscope that visualizes molecular orientations. To monitor the orientations, target molecules must be “rigidly” labeled with fluorophores so that the fluorophores do not freely rotate. The difficulty of this “rigid” labeling has limited the application of FPM to a few molecules such as actin. In this study, we have developed molecular orientation probes consisting of nanobodies and cyan/green/yellow/red fluorescent proteins (nanobody-based POLArIS). Furthermore, we made probes that have different dipole orientations, which enabled adjusting the polarization orientation. Nanobody-based POLArIS, which offers options of colors and polarization orientations, will support broader applications of FPM.

2Pos156 Understanding of robustness in cancer morphology in cold temperature

Yuta Sekiguchi, Hideo Higuchi, Motoshi Kaya (*Grad. Sch. Sci., Univ. Tokyo*)

Cancer cells are known to be highly robust against chemical changes. Meanwhile, the resistance for temperature changes have been investigated exclusively in higher temperature. Thus, our aim is to clarify the dynamics of morphological changes in cancer cells in response to low temperatures. When breast cancer cells were exposed to 4℃, depolymerization of cytoskeletal proteins was accelerated, resulting in losses of cell shapes and adhesions. When the temperature was returned to 37℃ from low temperatures, cytoskeletons were restructured rapidly and cell adhesions were restored completely. We will further perform quantitative evaluation of cytoskeletal structures and mechanical measurements of cell tractions using traction force microscopy in the future.

2Pos157* 酵母胞子の形成・復帰過程における分子混雑の可逆的な制御
Reversible regulation of molecular crowding in fission yeast during sporulation and germination

Keiichiro Sakai[1,2,3], Yuhei Goto[1,2,3], Yohei Kondo[1,2,3], Kazuhiro Aoki[1,2,3] ([1]*NIBB*, [2]*ExCELLS*, [3]*SOKENDAI*)

The cellular cytoplasm is a crowded environment by macromolecules, affecting biochemical reactions within a cell. The cytoplasmic crowding changes dramatically during sporulation and germination in fungal species, which are cell growth arrest and resumption, respectively. However, it remains unclear when and how molecular crowding reversibly changes during these processes. Here, we measured the diffusion of nanoparticles in yeast spores. The diffusion was substantially restricted in spores, but it rapidly increased after the germination induction. By gene knockout analysis, we found that trehalose degradation and nutrient sensing were required for the decrease in molecular crowding in spores, implicating a key mechanism for sporulation and germination.

2Pos158 光照射による多細胞システムの運動制御
Regulation of cell motility in a multicellular system by photodamage

Shinji Yokoyama (*grad. Sch Comp. Sci and Sys .Eng.,Kyushyu Inst. Tech*)

Dictyostelium discoideum has been used as a model organism for multicellular migration. The cell lives in a unicellular state, but the cells aggregate to form a multicellular body when starved. Although it is known that new migratory fronts are formed when the multicellular body is physically disconnected, the mechanism of how the location of new migratory fronts is determined has remained unclear. To clarify the decision-making process of the cells, we observed the behavior of motile cells when the multicellular body was exposed to light irradiation.

2Pos159 深層学習を用いた *D. discoideum* の 2 細胞型混合集団運動における運動規則の推定
Deep learning-based estimation of motion rules for 2-cell type mixed collective motion of *D. discoideum*

Masahito Uwamichi, Hidenori Hashimura, Tomoko Adachi, Sumie Eto, Satoshi Sawai (*Grad. Sch. Arts and Sci., The Univ. of Tokyo*)

The collective motion of *Dictyostelium discoideum* during slug formation, called the cell sorting process, is a phase-separation-like pattern formation of two cell types. In this process, differences in movement between cell types, specific tracking by intercellular adhesion, and chemotaxis to cAMP are essential for pattern formation. To construct a model that includes both mechanics and such biological states, it is necessary to understand the relationship between biological states and motion. Here, we numerically analyzed the relationship between cell motility and biological factors such as cell type, using deep learning. We will discuss the cell type-dependent kinetic rules of the cell sorting process obtained by interpreting the learned neural network.

2Pos160* ATP 産生阻害した細胞における細胞内流動性低下の定量的評価
Quantitative evaluation of the decrease in intracellular mobility of cells in which ATP synthesis is inhibited

Hideaki Ota, Hideo Higuchi (*Grad. Sch. Sci., Univ. Tokyo*)

Most of intracellular mobility is activated by the energy of ATP hydrolysis. The concentration of ATP will affect the mobility and the activity of cells. Here, we quantified intracellular mobility by measuring diffusion constants of vesicles and fluorescent protein in human cells in which ATP was depleted by the inhibitors of ATP synthesis. The diffusion constant of the vesicles decreased to 1/300 by ATP depletion, while that of fluorescent protein did not change significantly. The intracellular mobility was recovered partially by removing the inhibitors. Mechanisms of changing the mobility will be discussed at our poster.

2Pos161 プライマリー神経堤細胞の定量的運動解析
Quantitative characterization of random and persistent locomotion in neural crest cell primary cultures

Takehiro Nakamura, Satoshi Sawai (*Grad. Sch. Arts & Sci., Univ. Tokyo*)

Neural crest cells (NCCs) are a highly motile cell population that appears transiently during the development of vertebrates. Despite the importance of its ability to migrate to multiple specific locations in the embryo, the single-cell level migratory dynamics have not been well characterized in vitro. Here, we developed an assay system that employs zebrafish primary NCC cultures. Sox10+ cells from 10-somite stage embryos of Tg(sox10:EGFP) were isolated using FACS and cultured in modified culture conditions. We characterized its random movement on fibronectin-patterned surfaces. We will analyze the results based on a few basic parameters of a simple stochastic model and discuss how cells interact with the environment.

2Pos162* ケラトサイト細胞集団運動におけるアクトミオシンケーブルの切断と集団運動での役割
Breaking of actomyosin cables in keratocyte collectives and their role in the coordinated collective migration

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Fish epidermal keratocytes are motile cells responsible for wound repair. When a scale is taken from a fish skin and adhered to the coverslip, keratocyte collectives crawl out from the scale and spreads radially. All cells at the leading edge are connected to each other with actomyosin cables. At the same time, they expand lamellipodia and advance as leader cells to pull subsequent follower cells. It was a mystery how the leading edge, in which leader cells connected tightly by the actomyosin cable, can spread. We found that the cables between the leader cells were mechanically torn off by protruding lamellipodia of an interrupting follower cell. We will discuss the role of actomyosin cables in collective cell migration.

2Pos163 真核生物の走化性に焦点を当てた、細胞膜上での Gα2 の PALM イメージングと空間的解析
PALM imaging and spatial analysis of Gα2 across the cell membrane: exploring the meaning in eukaryotic chemotaxis

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Chemotaxis is one of the robust cell responses. The eukaryotic model organism *Dictyostelium discoideum* is able to respond to at least sub-nM of 3',5'-cyclic adenosine monophosphate (cAMP). Gradient sensing under such a low concentration is susceptible to the spatial distribution of the molecules on the cell membrane. Here, the distribution of heterotrimeric G protein α subunit (Gα2), coupled to a certain type of cAMP receptor, was examined at a nanoscale resolution by photoactivated localization microscopy (PALM) in the chemically fixed cells expressing exogenous mKikGR-tagged Gα2. Our results suggest that Gα2 is distributed in a clustered manner. Quantitative characteristics of the cluster and its role in the gradient sensing will be discussed.

2Pos164* GEFB と GEFX は細胞運動に重要な興奮系 Ras の自発的対称性の破れを制御する
GEFB and GEFX regulate spontaneous symmetry breaking of the excitable system Ras for cell motility

Koji Iwamoto[1], Satomi Matsuoka[1,2,3], Masahiro Ueda[1,2,3] ([1]*Grad. Sch. Sci. Bio, Univ. Osaka*, [2]*Grad. Sch. of Front. Biosci., Univ. Osaka*, [3]*BDR., Riken*)

An excitability provides an asymmetric localization of activated Ras on the plasma membrane in eukaryotic motile cells, although the molecular basis for spontaneous symmetry breaking remains unsolved. We constructed a set of *Dictyostelium discoideum* strains overexpressing 25 GEFs and performed an imaging analysis of the spontaneous dynamics of activated Ras. Hierarchical clustering to classify GEFs by similarity of impact on the dynamics suggested 5 clusters including the most influential one consisting of GEFB/M/X/U. Among them, GEFB and GEFX co-localized with activated Ras showing traveling waves, and cell motility was impaired by their genetic knockout. Our results suggest that the asymmetry of activated Ras arises at least due to GEFB and GEFX without spatial cues.

2Pos165 Loss of synchronous behavior in cardiomyocyte networks is independent of their spatial network patterns during hERG ion channel blocking

Kazufumi Sakamoto, Kenji Yasuda (*Dept. Pure & Appl. Phys., Grad. Sch. Adv. Sci. & Eng., Waseda Univ.*)

We have investigated the effect of community size and spatial arrangement of cardiomyocyte networks on their synchronization and stability against hERG ion channel blocker E4031. Five different formats of cell networks on the multielectrode array platform were prepared with agarose microfabrication technology to measure the field potential (FP) waveform change of component cells in each network. When a high dose of E4031 was applied, the FP duration (FPD) was prolonged up to 40% regardless of the difference in five network patterns and component cell numbers, indicating the effect of hERG blocking is independent of component cell number and network geometry. Therefore, the response of hERG blocking in single isolated cells is enough to predict that of heart tissues.

2Pos166* 電子線トモグラフィーによる *Mycoplasma mobile* 内部滑走装置の解析
Mycoplasma mobile internal gliding machinery analyzed by electron tomography

Minoru Fukushima[1], Takuma Toyonaga[1,2], Yuhei Oba Tahara[1], Daisuke Nakane[3], Makoto Miyata[1,2] ([1]*Grad. Sch. Sci., Osaka Metropolitan Univ. Osaka*, [2]*OCARINA, Osaka Metropolitan Univ.*, [3]*Grad. Sch. Info. Eng., Univ. Electro-Communication. Tokyo*)

Mycoplasma mobile has a unique gliding motility that is found only in four related species. The internal part of gliding machinery is jellyfish-like shaped, about half the size of the cell. The front part of the internal machinery is called “bell,” from which several “chains” of dimeric gliding motors, evolved from F-type ATPase/synthase extend toward the backside. In this study, we used electron tomography to clarify the structure of internal machinery. The bell was a bowl-shaped structure with a wall thickness of 20–30 nm. Wedge-like structures connect the end of the chains to the bell. The chains were connected with neighboring ones through multiple linkers and form a sheet. We discuss details and roles of individual structures.

2Pos167 ヒト原腸形成の自己組織化を模倣する：ヒト iPS 細胞のマイクロパターン培養
Mimicking the self-organization of human gastrulation: micro pattern culture of human iPS cells

Chihiro Takeuchi[1], Ryo Kobayashi[1], Kiyoshi Ohnuma[2] ([1]*Grad. Sch. Eng., Univ. Nagaoka Tech.*, [2]*Inn., Univ. Nagaoka Tech.*)

Human gastrulation starts from a single discoidal layer (sub-mm in diameter) of epiblast, which gives rise to discoidal three germ layers (mesoderm, endoderm, and ectoderm). However, little is known about gastrulation dynamics. Here, to mimic discoidal multi-layer formation during human gastrulation, mesoderm and epiblast-like cells derived from human iPS cells were cultured in a circular micro pattern. Our hypothesis is that multiple layer formation can be reproduced by mixing cells in a limited 2D pattern because the cells with more integrins adhere to the culture dish to form the basal layer and the weakly adherent cells form the upper layer. To investigate the dynamics of multiple layer formation, we changed the cell ratio and observed the behavior of the cells.

2Pos168 Real-Time Feedback 機構を用いた細胞集合体への機械刺激
Mechanical stimulus on cell aggregation with Real-Time Feedback control

Ayu Sasaki, Ryu Kidokoro, Shota Nozaki, Kaito Kojima, Arata Nagai, Yuuta Moriyama, Toshiyuki Mitsui (*Grad. Sch. Sci., Univ. Aogaku*)

Mechanical stress can lead to heart failure. Microscopically, fibroblasts, composition of the heart, differentiate into myofibroblasts under such stress. Recently, the presence of myofibroblasts has been implicated as a cause of heart disease. Now it is interesting to intentionally stimulate and stress cardiac cell aggregates. Since cardiac cells beat intrinsically, we have developed a real-time feedback control system to control the timing of stimulation relative to the beating cycle. Primary cultured cells from chick heart were used. We will report the short-term stimulus response and the long-term morphological changes of the aggregates induced by the phase-controlled stimulus. In addition, the differentiation into myofibroblasts by stimulus will be described.

2Pos169 ゆらぎの定理に基づく細胞張力ホメオスタシスに関する研究
Analyzing cellular tensional homeostasis from a physical point of view

Shinji Deguchi, Yuika Ueda (*Grad. Sch. Eng. Sci., Osaka Univ.*)

As the unit of life, individual cells are known to maintain their internal conditions even with time-varying intra/extracellular milieu, a feature known as homeostasis. Among them, we are particularly curious about the mechanism of “tensional homeostasis,” in which cells are allowed to keep a base level of intrinsic physical tension even upon mechanical stress that disturbs intracellular tensional balance. We have so far understood basic response of nonmuscle cells to mechanical stress, and are thus now in the position to tackle this challenging but exciting topic. Here, complex properties of actin stress fibers, critical to the emergence of tensional homeostasis, are analyzed from a physical point of view to finally provide new insights into the underlying mechanism.

2Pos170 制御理論に基づくアクチン細胞骨格の力学・生化学応答に関する理論解析
Modeling mechanochemical reaction of the actin cytoskeleton based on control theory

Eiji Matsumoto, Daiki Matsunaga, Shinji Deguchi (*Grad. Sch. Eng. Sci., Osaka Univ.*)

The actin cytoskeleton, a polymer of globular actin, is essential for cell functions such as cell motility and structural maintenance. Recent studies imply that the reaction rate of the cytoskeleton is modulated upon loading of mechanical forces to cause a specific change in the structure. The mechanical stress sustained in the cytoskeleton is consequently kept unchanged over time. The interactions between the biochemical and mechanical factors provide the mechanochemical reaction, but the mechanism remains unclear. Here we propose a theoretical model based on mechanics, control theory, and biochemistry to describe the underlying mechanism. We also derive time-associated parameters of the basic behavior and requirements for keeping the specific stress.

2Pos171* 脱水ストレス依存に細胞骨格様の線維やゲルを形成するクマムシタンパク質 CAHS による細胞の機械的強度の向上
Stress-dependent cell stiffening by tardigrade tolerance proteins CAHS reversibly forming cytoskeleton-like filament networks and gels

Akihiro Tanaka[1], Tomomi Nakano[1], Kento Watanabe[1], Kazutoshi Masuda[2,3], Gen Honda[2,3], Shuichi Kamata[1], Reitaro Yasui[1], Satoshi Sawai[1,3], Miho Yanagisawa[2,3], Takekazu Kunieda[1] ([1]*Dept. of Bio. Sci., Grad. Sch. of Sci., Univ. of Tokyo.*, [2]*Komaba Inst. for Sci., Grad. Sch. of Arts and Sci., Univ. of Tokyo.*, [3]*Dept. of Basic Sci., Grad. Sch. of Arts and Sci., Univ. of Tokyo*)

Tardigrades are able to tolerate almost complete dehydration. Although tardigrades abundantly produce tardigrade-unique protective proteins termed CAHS which are essential for their anhydrobiotic survival, their precise protective mechanisms are not fully understood. In the present study, we revealed that CAHS proteins reversibly form cytoskeleton-like filamentous networks in animal cells depending on hyperosmotic stress and undergo reversible gel-transition *in vitro*. CAHS filamentation increases cell stiffness to resist deformation and improves resistance to dehydration-like stress. On the basis of these results, we propose that CAHS proteins stabilize cell integrity against deformative forces during dehydration through on-demand filamentation or gelation.

2Pos172 Jasplakinolide または Phalloidin が結合したアクチンフィラメントのゆらぎの違いを FRET 解析により可視化した
Fluctuation difference in actin filaments bound Jasplakinolide or Phalloidin was visualized by using FRET

Ai Takahashi[1], Miku Nezasa[2], Kuruto Toda[2], Irfan Huzifah Ahmad[2], Ichiro Nishikata[4], Kenji Kamimura[3], Ikuko Fujiwara[1], Hajime Honda[1] ([1]*Dept. of Matl. Sci. and Bioeng., Nagaoka Univ. of Tech.*, [2]*Dept. Bioeng., Nagaoka Univ. of Tech.*, [3]*Dept. of Elect.Ctrl.Eng ., NIT. Nagaoka College*, [4]*ACEM., NIT. Nagaoka college*)

Actin can polymerize and form filaments. Jasplakinolide and phalloidin are widely used reagents to stabilize actin cytoskeleton. Recent cryo-EM observations by Sabrina Pospich et al. showed overlapping binding sites for both reagents on actin filaments. They have also reported that both reagents bind across several actin subunits within a filament. Interestingly, jasplakinolide stabilizes actin filaments as ADP-Pi bound form while phalloidin does not. Here, spatiotemporal dynamic changes of actin filaments covalently modified with two different fluorescent dyes are decorated with either jasplakinolide or phalloidin to visualize the structural changes of actin subunits by FRET.

2Pos173* 2 種の細菌アクチン MreB が駆動する最小の細胞運動システム
Minimal cell motility system driven by two bacterial actin MreB

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Spiroplasma is a helical-shaped bacterium that exhibits unique swimming motility using a ribbon-like structure along the entire cell axis. It contains five classes of bacterial actin MreB, which is not directly related to motility in other bacteria. We have succeeded in inducing helical cell morphology and swimming in a non-motile minimal bacterium JCVI-syn3.0B by inducing a gene cluster including five *mreB* genes of *Spiroplasma*. Here, we clarified that two different MreBs are sufficient to generate the cell helicity and swimming. To the best of our knowledge, this is the minimal cell motility system to date. We will discuss how *Spiroplasma* MreBs have acquired their function, based on the analyses of mutations causing non-motile cell phenotypes.

2Pos174 腫瘍微小環境におけるエクソソーム中 GRP78 タンパク質の増加が腫瘍進行を促進する
Increased GRP78 protein in exosomes in the tumor microenvironment promotes tumor progression

Kanako Iha, Etsuro Ito (*Department of Biology, Waseda University*)

Our research focuses on exosomes to understand the construction of the tumor microenvironment caused by cell-cell communication. We have developed a method that enables measurement of exosomes with 1/100 of the sample volume of conventional methods. Using the developed assay, we measured GRP78, an intracellular stress-related protein known to be associated with cancer progression. In gastric cancer cell lines placed under nutrient starvation and addition of anticancer drugs, we found a significant increase in exosome mediated GRP78 secretion. Furthermore, the experiments using exosomes secreted from GRP78 overexpressed or knockdown cells showed that GRP78 in exosomes has effects on vascular endothelial cells and cancer cells that may lead to tumor progression.

2Pos175* 細胞の生死の網羅的・定量的理解に向けた、機械学習による細胞の運命予測
Predicting cell fates by image-based machine learning for comprehensive and quantitative understanding of cell death and survival

Tomoaki Okaniwa[1,2], Katsuyuki Shiroguchi[1] ([1]*RIKEN BDR*, [2]*Grad. Sch. Frontier Biosciences, Osaka Univ.*)

“What is death?” is one of the most fundamental questions in biological science, but the point of no return to death is still unclear even at the cellular level. For example, it has recently been reported that cells can recover after the initiation of conventional death processes (anastasis). To investigate the point of no return, we quantify the gene expression differences between cells fated to die and survive after perturbations (e.g., heating) by transcriptome analysis. First, we make a machine learning model to predict the cell fates from the cell images that we obtained. Second, we perform single-cell RNA-seq of the fate-predicted cells using our developed robot, ALPS. Finally, we discuss what in transcriptome determines the point of no return to cell death.

2Pos176 Understanding the results of black box Convolution Neural Network to identify Follicular thyroid cancer

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A convolutional neural network (CNN) is a deep learning approach that has attained excellent performance in Raman spectra analysis. But CNN is treated as a backbox method due to the lack of model interpretability. In this work, we proposed a CNN model to interpret the results in terms of chemistry and biology. Our focus is on what type of information is learned by CNN. We performed the feature extraction by CNN and then calculate the score (weighted summation of feature extraction and weights). We found the high scores in the lipid regions for FTC (cancer) image, however for Nthy (noncancer) image, high scores are found in cytochrome regions mainly. Moreover, PCA projection of all train and test spectra after feature extraction by CNN shows excellent performance.

2Pos177 Elucidation of macrophage's spatial discrimination limit between target antigen and non-target objects

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We have examined macrophages' phagocytosis of clusters composed of opsonized and non-opsonized microbeads to understand their ability of spatial discrimination between target antigen and non-target objects. We prepared the clusters by aggregating IgG/BSA-opsonized polystyrene microbeads and non-opsonized ones, and contacted them to macrophages. Macrophages phagocyted various sizes and shapes of the clusters, not only the opsonized beads clusters but those mixtures of opsonized and non-opsonized ones, whereas the non-opsonized clusters were not engulfed. These results suggest the origin of incorrect antigen presentation by macrophages through their phagocytosis of non-target particles within the target mixture clusters due to their limit of discrimination in clusters.

2Pos178 細胞内のタンパク質動態の 3 次元の流れとその定量化に関する研究
Research on three-dimensional flow of protein dynamics in cells and its quantification

Yuya Enokida (*Grad. Sch. Comp. Sci. and Sys. Eng., Kyushu Inst. Tech*)

It is essential to understand movements and processes such as motor protein-based drives and diffusion by thermal fluctuations in living organisms. In addition, the evolution of microscopy has increased the importance of methods for analyzing three-dimensional time-series data. Therefore, we have developed a tool using an optical flow algorithm, which is often used for moving object detection. 3D time-lapse images of living organisms taken by microscopy appear as objects with relatively faint textural information and blurred images. We developed a 3D-OpticalFlow method to observe moving objects with various velocities and quantify the three-dimensional flow of protein dynamics in cells for EB-1 and actin.

2Pos179 海洋ビブリオ細胞分化におけるべん毛モーター回転制御因子 CheY の役割
Role of the flagellar motor-controlling factor CheY in cell differentiation of marine *Vibrio*

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Marine *Vibrio* undergoes cell differentiation: rod-shaped swimmer cells each with a single polar flagellum (Pof) and elongated multinucleate swarmer cells each with many lateral flagella (Laf). Rotation of the Pof and Laf motors are regulated by the same factor namely the response regulator CheY but in different manners: counterclockwise/clockwise or fast/slow, respectively. We found that deletion of *cheY* accelerates motility of cells on surfaces but does not allow net spreading over surfaces or surface-induced cell elongation. The *cheY* deletion had differential effects on the abundance of two differentiation marker proteins. These results suggest that the motor-regulating protein CheY is also involved in cell differentiation.

2Pos180 海洋性ビブリオ菌において細胞極局在膜タンパク質 HubP はべん毛本数制御因子 FlhG の ATPase 活性を上昇させる
The polar landmark protein HubP enhances the ATPase activity of the flagellar number regulator FlhG in *Vibrio alginolyticus*

Yuxi Hao[1], Norihiro Takekawa[2], Michio Homma[1], Seiji Kojima[1] ([1]*Div. Biol. Sci., Grad. Sch. Sci., Nagoya Univ.*, [2]*Dept. Macromol. Sci., Grad. Sch. Sci., Osaka Univ.*)

The marine bacterium *V. alginolyticus* has a single flagellum at the cell pole. FlhG, a MinD-type ATPase, negatively regulates the flagellar formation. This regulation requires the polar landmark protein HubP. In *V. cholerae,* it has been shown that FlhG localizes to the pole by interacting with the C-terminus of HubP. We made some HubP truncation mutants and purified HubP C-terminal fragments, and found that a HubP C-terminal fragment (1267-1393) enhanced FlhG ATPase activity. ATPase active FlhG D171A mutant is easy to aggregate, and the HubP fragment above suppressed this precipitation. These results suggests C-terminal of HubP interacts with FlhG to increase ATPase activity, which would be involved in negative regulation of flagellar formation in *V. alginolyticus*.

2Pos181 クラスリン軽鎖の細胞膜上での構造変化は被覆構造、そしてエンドサイトーシスを制御する
A conformational switch in clathrin light chain regulates lattice structure and endocytosis at the plasma membrane of mammalian cells

Kazuki Obashi, Kem Sochacki, Marie-Paule Strub, Justin Taraska (*National Heart, Lung, and Blood Institute, National Institutes of Health*)

Conformations of endocytic proteins are key regulators of clathrin-mediated endocytosis. Here, we develop a correlative fluorescence resonance energy transfer (FRET) and platinum replica electron microscopy method, named FRET-CLEM. With FRET-CLEM, we measure conformational changes in proteins at single clathrin lattice structure resolution at morphologically distinct stages of endocytosis at the plasma membrane. We identify a lattice-curvature-dependent structural switch in clathrin light chain. Preventing this conformational switch with acute chemical tools alters clathrin lattice structure and blocks endocytosis of cargo. Therefore, a specific conformational switch in clathrin light chain regulates lattice curvature and endocytosis in mammalian cells.

2Pos182 歯周病菌の Fim 線毛の先端タンパク質 FimC の構造
Structure of FimC, a tip protein of the Fim pilus in a gum disease bacterium *Porphyromonas gingivalis*

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Porphyromonas gingivalis has Fim pili, which are formed by five pilin proteins: anchor pilins (FimB), stalk pilins (FimA), and tip pilins (FimC, FimD, and FimE). Here we solved the crystal structure of FimC at 2.16 Å resolution. FimC consists of a core domain, whose structure is similar to FimA, and a C-terminal additional domain (named $FimC_C$). The $FimC_C$ domain might disturb polymerization of the pilins at the tip of the pilus by structural hindrance. The $FimC_C$ domain is structurally similar to the BACON domain, which binds to the mucin. The mucin is composed of glycoproteins secreted from animal epithelial cells, suggesting that FimC has a role in the binding to glycans on the host cell surface.

2Pos183 細胞外小胞が引き起こす標的細胞でのシグナル伝達機構の解明：超解像顕微鏡法と 1 粒子追跡による研究
Intracellular signaling triggered by small extracellular vesicles as revealed by super-resolution microscopy and single-particle tracking

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Small extracellular vesicles (sEVs) has drawn extensive attention as intercellular messengers. Recent studies suggest that sEVs play critical roles in tumor metastasis. However, the molecular mechanisms of the sEV binding to the target cell plasma membranes (PMs) are totally unknown. To solve this issue, we simultaneously performed single-particle tracking of sEVs and super-resolution imaging of membrane structures in living cell PMs. We found that a subtype of sEVs transiently recruited raftophilic molecules, proteins involved in cell adhesion such as integrin on the target cell PMs, and induced intracellular signaling right after the sEV binding. These results suggest that sEVs triggered intracellular signaling in cell PMs by forming rafts including integrin clusters.

2Pos184* アミノアシル tRNA 合成酵素 20 種の自己再生産と共役した DNA 複製系の構築
In vitro transcription/translation-coupled DNA replication through the regeneration of 20 aminoacyl-tRNA synthetases

Katsumi Hagino[1], Norikazu Ichihashi[1,2,3] ([1]*Department of Life Science, Graduate School of Arts and Science, The University of Tokyo.*, [2]*Komaba Institute for Science, The University of Tokyo.*, [3]*Research Center for Complex Systems Biology, Universal Biology Institute, The University of Tokyo.*)

Reconstruction of autonomous self-reproduce ability is one of the greatest functions required to completely construct an artificial cell in vitro. The construction of this system needs to combine the regeneration of enzymes required for gene expression with the replication of genetic information. However, such a self-reproduction system has not been achieved due to the low activity of the cell-free translation system and the complexity of the DNA replication system. In this study, we succeeded in the continuous replication of all 20 aaRS DNAs through the expression of aaRSs from themselves in the cell-free translation system that lacks aaRSs. In this poster, we will report on this system and discuss the next challenges for developing self-reproductive artificial cells.

2Pos185 1 細胞内での CheB 局在変化による忌避応答および適応
Repellent response and adaptation through the CheB-localization in single E. coli cell

Taiga Deguchi[1], Yumiko Uchida[1], Yong-Suk Che[1], Akihiko Ishijima[1], Tatsuki Hamamoto[2], Hajime Fukuoka[1] ([1]*Grad. Sch. Frontier Biosci. Osaka Univ.*, [2]*OIST. Grad. Univ.*)

Adaptation in chemotaxis of *E. coli* is achieved by CheR and CheB. To clarify the relation between intracellular dynamics of CheB and cellular behavior, we simultaneously observed CheB-localization and flagellar rotation in either strains expressing wild-type Tsr or Tsr mutant lacking binding target of CheB. In both strains, the CW bias and the CheB-localization increased immediately after adding repellent. In wild-type strain, the CW bias and the CheB-localization gradually returned to original levels, however, both persisted in mutant strain. Thus the CW bias and the CheB-localization are consistent indicating the CheB-localization reflects receptor's activity. We will discuss the quantification of response to repellent stimuli by CheB-localization at the meeting.

2Pos186* 膜融合性リポソーム膜のデザインのための系統的な膜特性解析
Systematic membrane characteristic analysis for the design of fusogenic liposome

Natsuumi Ito, Nozomi Watanabe, Yukihiro Okamoto, Hiroshi Umakoshi (*Bio-Inspired Chemical Engineering Laboratory / Division of Chemical Engineering / Graduate School of Engineering Science / Osaka University*)

Liposomes have been already used as drug carriers, and several formulations are currently marketed or in clinical trials. Membrane fusion pathways are very promising, since it leads to the release of the entrapped drug directly in the cytosol of the targeted cells. Membrane fusion mechanism of liposomes into the cell is favored by the presence of DOPE , a fusogenic lipid in the liposome membrane, as its conical geometry promotes the formation of inverted hexagonal intermediate structures that lead to the formation of fusion pores. However, systematic membrane analysis of DOPE miscibility in the carrier liposome membranes has not been done. In this study, the membrane properties of fusogenic liposomes were studied by comparing with presence and absence of DOPE.

2Pos187 A Liposome Prepared by Microfluidic Device Vomits the Inner Solution

Jiajue Ji, Kayano Izumi, Ryuji Kawano (*Department of Biotechnology and Life Science, University of Agriculture and Technology*)

Morphologic change of liposomes is different in response to various environments. Understanding the principle behind morphological changes is helpful for us to develop new potential applications in many fields such as drug delivery. Here, we prepared monodispersed and cell-sized liposomes with dextran/glucose solutions with different osmolarities by microfluidic technology. We observed two major responses of liposomes, 1) it was ruptured and then reconstituted simultaneously, 2) it was ruptured and did not recover. The results show that the vomiting frequently occurred at the condition of 20wt% dextran and 1000 mM glucose concentration. The principle and mechanism behind morphological change will be discussed in this presentation.

2Pos188* (3SGA-5) DNA ゲル骨格が決定する人工細胞の力学特性
(3SGA-5) Cytoskeletons of self-assembled DNA regulate the mechanical properties of artificial cells

Kazutoshi Masuda[1], Fuyu Ohno[2], Miho Yanagisawa[1,2] ([1]*College of Arts and Sciences, The University of Tokyo*, [2]*Graduate school of Arts and Sciences, The University of Tokyo*)

Artificial cells composed of lipid membranes are more fragile than living cells due to the lack of cytoskeletons, making their application problematic. We previously reported that self-assembled DNA networks under the membrane stabilize the artificial cells. However, it was unclear what kind of DNA structure would improve the mechanical properties of cells. Here, we tested the correlation between the viscoelasticity of cells and the structure of the DNA network by using two types of DNA nanostructures, Y- and X-shaped, with different lengths of the sticky-ends. Our results show Y-shaped DNA can stabilize membranes better than X-shaped DNA. The reasons based on the morphology of DNA networks and the potential applications of DNA-stabilized artificial cells are discussed.

2Pos189 両親媒性ブロックポリマーを用いたポリマー二分子膜の作製
Preparation of planar bilayer polymer membrane using amphiphilic di- and tri-block copolymers

Hiroaki Kihara, Harune Suzuki, Ryuji Kawano (*Department of Biotechnology and Life Science, Tokyo University of Agriculture and Technology*)

Nanopore sensing is a technique to detect and quantify at the single-molecule level using nanosized pores. In recent years, a nanopore DNA sequencer has been the practical application, which uses a synthetic bilayer membrane. Thus, it is necessary to understand the relationship between membrane structure, stability, and nanopore proteins. In this study, we used amphiphilic di- and tri-block copolymers as planar bilayer polymer membranes (pBPMs) to understand the difference in membrane properties in terms of the chemical structure of polymers. As the result of ion current measurement of the pBPMs, diblock polymers were higher stability against the applying voltages than the triblock polymers. Furthermore, nanopore protein was reconstituted in both polymer membranes.

2Pos190 海水中で長期間安定に存在し得るリポソームの調製
Preparation for long-term stable liposomes in seawater

Kayano Izumi[1], Keiichiro Koiwai[2], Ryuji Kawano[1] ([1]*Tokyo University of Agriculture and Technology*, [2]*Tokyo University of Marine science and Technology*)

Liposomes are lipid vesicles used as bodies in molecular robotics. The objective of molecular robotics is to develop robots which work in various situations. Liposomes are promising bodies for molecular robots due to their vesicle-structures and high biocompatibility. However, the robots are hardly implemented in actually due to the lack of stability. For an example of implementation, we considered that stable liposome robots work in seawater. To improve the stability, we used of polyethylene glycol (PEG) lipids; they are suggested to improve liposome stability. We hypothesized that the unique conformations of PEGs affect to liposome stability. In the presentation, we will discuss stabilities of liposomes based on the survival rate of the liposomes for two weeks.

2Pos191* 脂質二重膜へのエタノール分子の浸透に対する塩添加の影響：分子動力学法による検討
Effect of salt addition on the penetration of ethanol molecules into lipid bilayers: a molecular dynamics study

Haru Kitaoka, Naoya Nishi, Yuko Yokoyama, Tetsuo Sakka (*Graduate School of Engineering, Kyoto University*)

Yeasts cannot survive under high ethanol concentrations, which limits the efficiency of bioethanol production. Ethanol molecules interact with oxygen atoms in the ester and phosphate groups in the lipid molecules to severely disrupt the structure of yeast lipid membranes. Cations in water are also known to adsorb the same oxygen sites in the ester and phosphate groups, however, it has been unclear how cation adsorption affects ethanol penetration.
We present molecular dynamics simulations that investigate ethanol penetration under salt concentration in the range of 0 to 1000 mmol/dm^3. We found that the adsorptions of cations and ethanol molecules are competitive at low salt concentrations whereas they turned to be cooperative at high concentrations.

2Pos192 高分子液滴を用いた細胞サイズ依存的な相分離
Cell-size dependent phase separation in polymer droplet

Chiho Watanabe[1,2], Tomohiro Furuki[2], Yuki Kanakubo[2], Fumiya Kanie[2], Keisuke Koyanagi[3], Jun Takeshita[2], Miho Yanagisawa[2] ([1]*Hiroshima Univ.*, [2]*Univ. Tokyo*, [3]*Tokyo Univ. Agri. Tech.*)

Intracellular phase separation attracts attention as a novel mechanism to rule biochemical reactions and metabolism in cells. There have been reports that intracellular phase separation alters membrane structure in cells, but the inverse, whether the membrane confinement induces phase separation or not is still elusive. Here, using polymer droplets containing two polymers, dextran, and poly(ethylene glycol), we show that the membrane confinement induces phase separation in its size-dependent manner. In addition, the partitioning of the polymers is also size-dependent, detected by fluorescent analogs. We will discuss the mechanism of the phenomena by competitive membrane wetting of polymers.

2Pos193 マガイニン 2 の膜相互作用に対する膜相転移の効果
Contributions of Membrane Phase Transitions to Interaction of Magainin 2 with Membrane

Ryoga Tsuji[1], Munehiro Kumashiro[2], Koichi Matsuo[3] ([1]*Grad. Sch. Adv. Sci. Eng., Hiroshima Univ.*, [2]*Inst. Adv. Med. Sci., Tokushima Univ.*, [3]*HiSOR., Hiroshima Univ.*)

Membrane-bound conformations of magainin 2 (M2) in the presence of phosphatidylcholine membranes with different phase-transition temperature (T_m) were analyzed by synchrotron-radiation circular-dichroism spectroscopy. The formation of helix structure of M2 at 25°C depended on the types of membrane but the helix increased for the membrane with T_m less than 25°C as the temperature decreased. No structural change was observed for the membrane with T_m more than 25°C as the temperature increased but the temperature decrement from T_m enhanced the helical formation. Fluorescence anisotropy showed the intrinsic T_m of each membrane was kept under the experimental conditions, suggesting that the membrane-M2 interactions require the phase transition from liquid crystalline to gel.

2Pos194* 生体膜の不均一性が分子の拡散性に与える影響
Effect of biological membrane's heterogeneity on the diffusivity of molecules

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In the plasma membrane, nanoscale confinement of specific proteins is regulated by dynamically generated lipid domains, as well as by cytoskeletal mesh structures bound to the plasma membrane underside. The nanoscale confinement affects the diffusion and aggregation of proteins, which are related to cell membrane function. However, the confinement effects on protein-protein interactions and the diffusivity of protein remain unclear. In this study, we elucidate the effects of nanoscale confinement on protein-protein interactions and membrane phase separation by using a mesoscale simulation combined phase-field model and Brownian dynamics simulation.

2Pos195* 抗菌ペプチドによる膜細孔形成の分子シミュレーション研究
Molecular dynamics simulation study of membrane pore formation by antimicrobial peptides

Issei Kawabata[1], Yusuke Miyazaki[2], Wataru Shinoda[2] ([1]*Grad. Sch. Eng., Univ. Nagoya*, [2]*RIIS., Univ. Okayama*)

Magainin-2 (Mag2) is a pore-forming antimicrobial peptide, though the action mechanism is unclear at the molecular level. We tried to investigate the selectivity of Mag2 action on model bilayers, which mimic bacterial and mammalian cell membranes, by using molecular dynamics simulations. In bacterial membrane, we observed toroidal pores, which remained open for 4 μs. In mammalian cell membranes, however, a disordered pore was detected, but it closed within 1 μs. Moreover, in bacterial membranes, Mag2 formed a pore together with anionic PG lipids, whereas in mammalian cell membranes, Mag2 penetrated into the membrane alone and assembled later to form a distorted pore. The results suggest that PG lipids affect the Mag2 action mode, leading to a stable pore.

2Pos196 光重合性脂質を用いた単分子/二分子のハイブリッド膜
Patterned monolayer/bilayer hybrid membrane composed of polymerized and natural lipids

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Supported lipid bilayers are used for studying the interactions of membrane proteins. We fabricated a hybrid membrane of lipid monolayer and bilayer. A polymerized lipid monolayer was integrated with a natural lipid monolayer and bilayer, acting as an obstacle for the lateral diffusion of membrane proteins. We reconstituted photo-receptor rhodopsin (Rh) and G-protein transducin (Gt) as model transmembrane and peripheral proteins. Rh diffused only in the bilayer region and Gt diffused in both regions. Interestingly, diffusion of Gt and lipids in the hybrid monolayer region was slower than the bilayer region indicating the friction of the polymerized monolayer leaflet. The hybrid membrane provides a unique platform for studying the interactions of membrane proteins.

2Pos197* 分子動力学シミュレーションによるエンドソーム脱出分子機構の解明
Exploring Molecular Mechanism of Endosomal Escape: A Molecular Dynamics Study

Kana Shibata[1], Akhil Pratap Singh[1], Wataru Shinoda[2] ([1]*Grad. Sch. Eng., Univ. Nagoya*, [2]*RIIS., Univ. Okayama*)

Lipid nanoparticles (LNPs) are one of the most promising non-viral gene delivery carriers. The success of transcription is limited by the endosomal escape of LNPs after the cell entry. The nucleic acids must be released into the cytoplasm before being degraded by the drop in pH within the endosome, but often only a few percent of them are released. This molecular mechanism has not been revealed experimentally since it occurs at the nanoscale. Thus, clarification of this event by a molecular dynamics (MD) simulation will lead to higher release efficiency LNP design. This study performed large-scale MD simulations of LNPs fusing to endosomal membranes using the SPICA force field. Mainly, the behavior of LNPs after being connected to endosomal membranes has been examined.

2Pos198* (1SFP-3) Mechanism study of antimicrobial peptide synergistic effects at the molecular level by combining spectroscopy and electrochemical methods

Yuge Hou, Kaori Sugihara (*Institute of Industrial Science, The University of Tokyo,*)

In 2020, Sugihara Group has reported that antimicrobial peptides LL37 and HNP1 cooperatively protects mammalian cell membranes from lysis for minimizing the cytotoxicity in contrast to known synergistic effect against bacteria. Previous study also showed that the synergy among LL37 and HNP1 would greatly increase the killing ability to E. coli. In this project, we study why the LL-37/HNP1 cooperativity enhances the cytotoxicity of E. coli? How the changes in the electric property and composition of membrane will affect the interaction with peptides. Black lipid membrane, circular dichroism, dynamic light scattering and isothermal titration calorimetry measurements will be employed to further understand the interaction mechanism.

2Pos199 電位依存性プロトンチャネルは細胞内 ATP による活性制御を受ける
Intracellular ATP controls the voltage-gated proton channel

Akira Kawanabe, Maki Takata, Yuichiro Fujiwara (*Fac. Med., Kagawa Univ.*)

The voltage-gated proton channel (Hv1) transports protons across the cell membrane in response to the membrane potential [Sasaki et al. 2006]. We reported that intracellular ATP had an effect on the activity of the Hv1 proton channel (58th Annual Meeting of Biophysical Society of Japan). In this study, we tested the dose-response relationship and the effects of ATP analogs on Hv1 using the inside-out patch-clamp technique. The dose-response relationship showed ATP could affect Hv1 within the range of physiological concentrations. ATP analogs (ADP, AMP-PCP) induced a significant increase in the proton current, suggesting that ATP directly controls the Hv1 activity. We are going to discuss the molecular mechanisms and physiological importance of these regulations. COI:No

2Pos200 Smooth 型 LPS を用いたグラム陰性細菌外膜模倣膜への抗菌ペプチドの作用評価
Reconstitution of smooth-type LPS as an outer membrane of Gram-negative bacteria

Wakana Hashimoto, Mitsuki Miyagi, Ryuji Kawano (*Dep. of Biotech. and Life Sci., Tokyo Univ. of Agri. and Tech.*)

Antimicrobial peptides (AMPs) are promising alternatives to traditional antibiotics. To reveal the mode of action of the antimicrobial activities on membrane dysfunction, artificial lipid bilayers have been used as the reconstituted assay. However, the activities of AMPs on the outer membrane consisting of smooth-type LPS (S-OM) of Gram-negative bacteria have not been investigated because of the difficult reconstitution. Here, we attempted to reconstitute the S-OM by the droplet contact method on the microdevice and evaluated the activities of magainin 2, one of the AMPs. As a result, we could reconstitute the S-OM and the magainin 2 mainly showed the penetration in the S-OM. We are attempting to evaluate the effect of the secondary structure of AMPs on the S-OM.

2Pos201* 脂質膜水透過現象の解析: アクアポリン水透過モデルとの比較
Water Permeation through the Lipid Membrane: from the Comparison with Aquaporin Study

Natsuki Fukuda[1], Nozomi Watanabe[1], Mizuki Teraoka[2], Yukihiro Okamoto[1], Hiroshi Umakoshi[1] ([1]*Graduate School of Engineering Science, Osaka University.*, [2]*Doshisha Girl's Senior High School.*)

Aquaporins are transmembrane proteins that can permeate water molecules. The major evaluation method of water permeation through aquaporins is the stopped-flow method, which analyzes permeation phenomena on the millisecond scale. However, considering cellular activities it is necessary to focus on a longer period of time. Although it has been reported that the permeability of aquaporins depends on the membrane, the details of water permeation in lipid membranes remain unclear. In this study, the water permeability on a long-time scale was attempted with proteoliposomes containing E. coli derived aquaporins and various liposomes by fluorescence analysis. Furthermore, the properties of different types of lipid membranes were considered in our evaluation method.

2Pos202 リポソーム型分子ロボットへの標的分子取込み
Transport of the target molecules into liposome-type molecular robots

Harune Suzuki, Kohei Hayashi, Ryuji Kawano (*Grad. Sch. Biotech & Life Sci., TUAT*)

A molecular robot should have three elements to work as a robot: sensor, intelligence, and actuator. Liposome-type molecular robots can encapsulate intelligence and actuators inside of them and sensors in their membranes. We have developed a DNA computing system for autonomous diagnoses and therapy of cancers. The system detected miR-20a (a microRNA from small cell lung cancer) as an input molecule and outputted oblimersen (the tumor antisense that enhances the apoptosis). To adopt this system into the liposome-type robot, the target molecules need to be transported from the outer environment to the inside of the liposomes. We have examined transporting miR-20a into liposomes using nanopores or endocytosis-like mechanisms.

2Pos203 レセプター機能を有する膜中 DNA システムの開発
Construction of a membrane-spanning receptor-like DNA system

Sotaro Takiguchi, Ryuji Kawano (*Dept. Biotech. Life Sci., Grad. Sch. Eng., Tokyo Univ. Agri. Tech.*)

Transmembrane molecular transportation/signal transduction is one of the significant processes in functionalizing molecular robots. Although pore-forming membrane proteins allow the transportation of small molecules, transporting nucleic acids is challenging due to the molecular size. Here, utilizing a 6-helix bundle DNA nanopore structure, we propose a receptor-like DNA system as a transducer for nucleic acid information. To achieve the receptor-like function, we incorporate an across-membrane strand displacement into the DNA sequence design. The structural assembly and strand displacement were confirmed by gel electrophoresis. We are attempting single-molecule observation of the strand displacement-induced structural change using an electrophysiological approach.

2Pos204 細胞性粘菌の cAMP シグナルにおけるレチナールの効果
Effect of retinal on cAMP signaling in *Dictyostelium discoideum*

Kazuki Akiyama, Yusuke Morimoto (*Kyusyu Institute of Technology (Grad. Sch. Comp. Sci. and Sys. Eng., Kyushu Inst. Tech.)*)

Dictyostelium discoideum is a microorganism of interest in drug discovery and developmental biology because of its unique life cycle. *D. discoideum* cells utilize cAMP for cell-to-cell communication. As the cell development progresses, cAMP signals are emitted. We observed the effect of retinal on cAMP signal relay using cAMP fluorescent probe under fluorescence microscope. Addition of retinal induced cAMP signal in *D. discoideum* cells. This result suggests that retinal may accelerate the development of *D. dicoideum* cells or be involved in the cAMP release pathway. This study is an important finding for the utilization of retinal in *D. discoideum* cells.

2Pos205* ヒトアセチルコリン受容体のアロステリック機構の振動分光研究
Vibrational spectroscopic study of Allosteric Mechanism on human muscarinic acetylcholine receptor

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Allosteric ligands have attractive approach to achieve receptor subtype-selective targeting of GPCRs. However, the understanding of mechanisms underlying GPCR allostery from structural basis has still challenged due to low binding affinity between receptor and allosteric ligands. Here, we attempted to obtain structural basis for understanding of allosteric mechanism in human muscarinic acetylcholine receptor (M2R) by using Attenuated Total Reflectance (ATR)-FTIR spectroscopy, which has been utilized to investigate the protein-ligand interaction on M2R in our previous studies. The results showed that binding of alcuronium, one of allosteric ligand, induced the negative allosteric effect for agonist binding and positive allosteric effect for antagonist binding.

2Pos206 センサーキナーゼ BaeS のインドール感知部位の同定
Identification of the indole-sensing region of the sensor kinase BaeS

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The two-component regulatory system BaeS-BaeR of *Escherichia coli* sense indole to induce the expression of various genes, such as *acrD* and *mdtABC* that encode components of RND-type xenobiotic efflux systems. We found that deletion of *tolC*, which encodes the common outer membrane channel of the efflux systems, results in the constitutive expression of *acrD* and *mdtABC*. Such induction was cancelled by the deletion of the tryptophanase gene *tnaA*. A mutant BaeS protein lacking its periplasmic domain and a chimeric BaeS protein with its periplasmic and transmembrane domains replaced by those of another sensor kinase retained the indole-sensing ability. These results indicate that BaeS senses indole by its cytoplasmic domain.

2Pos207 サルモネラクエン酸走性受容体 Tcp のリガンド認識における二価金属イオンの役割
Role of divalent metal cations in ligand recognition by the *Salmonella* citrate chemoreceptor Tcp

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The chemoreceptor Tcp of *Salmonella enterica* has been thought to sense citrate and metal-citrate complexes as distinct attractants. However, crystallography revealed a metal ion accommodated with a citrate molecule in the ligand-binding pocket. The Tcp-mediated citrate responses was inhibited by EDTA, a chelating agent. This inhibition was reversed by the addition of Mg^{2+}. Some mutant Tcp showed a behavioral phenotype that can be accounted for by a decrease in the affinity of Mg^{2+}. Isothermal titration calorimetry revealed that the periplasmic fragment of Tcp does not bind citrate alone but binds it in the presence of Mg^{2+}. These results suggest that Tcp requires a divalent metal cation for citrate recognition.

2Pos208* シナプス後肥厚におけるグルタミン酸受容体と PSD-95 のメソスコピックシミュレーション
Mesoscopic simulation of glutamate receptor and PSD-95 in postsynaptic density

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PSD-95, a major scaffolding protein of postsynaptic density(PSD), is considered an important factor in synaptic plasticity because it interacts with various proteins in PSD, causing liquid-liquid phase separation. However, how the protein network formed by PSD-95 influences receptor behavior on the postsynaptic membrane and subsequent signal transduction remains to be elucidated. This study constructed a mesoscopic model for the interaction between glutamate receptors and PSD-95 and performed reactive molecular dynamics simulations using the software ReaDDy based on the reaction-diffusion system. This model allowed us to analyze the behavior of glutamate receptors on the postsynaptic membrane under various conditions based on the stoichiometry in postsynapse.

2Pos209 海馬興奮性ニューロンにおける NMDA 型イオンチャネル受容体に依存した双方向シナプス可塑性の大規模数理モデルによる研究
Mechanism underlying hippocampal long-term potentiation and depression based on competition between endocytosis and exocytosis of AMPAR

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NMDA receptor-dependent long-term potentiation (LTP) and depression (LTD) are mediated by AMPA receptor (AMPAR) trafficking in postsynaptic neurons. However, the regulatory mechanism of bidirectional plasticity remains unclear. We present a mathematical model of AMPAR trafficking for hippocampal neurons, which reproduces both LTP and LTD. We show that the induction of both LTP and LTD is regulated by the competition between exocytosis and endocytosis of AMPARs, which are mediated by the Ca^{2+}-sensors synaptotagmin 1 and protein interacting with C-kinase 1, respectively. Our result indicates that recycling endosomes containing AMPAR are always ready for Syt1-dependent exocytosis at peri-synaptic/synaptic membranes because of Ca^{2+}-independent myosin V_b transport of AMPAR.

2Pos210 高頻度で持続的なシナプス伝達をささえるシナプス小胞ナノスケール動態
Actin filaments restrict synaptic vesicle movement for high-frequency neurotransmission

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A high rate of synaptic vesicle (SV) reloading to release sites during neuronal activity is required at cerebellar mossy fiber terminals for rapid information processing. However, the mechanism of the rapid reloading remains unknown. By direct observation of SV dynamics with high spatio-temporal resolution, we found that actin disruption abolished the rapid reloading, and decreased the sustained release. Further analysis revealed that SVs under normal conditions had two diffusion states: free-diffusing and trapped, whereas after actin disruption SVs tended to have only the free-diffusion state. Based on these results, we suggest that actin filaments limit SV movement to achieve the rapid tethering which is essential for the sustained activity at the terminals.

2Pos211* 細胞内輸送関連分子の新規解析手法の開発と病態モデルへの応用
A new approach to analysis of intracellular trafficking-related molecules using Cellprofiler and ImageJ in combination

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In the present study, to examine whether intracellular proteins can be discriminated using a combination of CellProfiler and ImageJ, we analyzed neuroblastoma and disease-specific iPS cells (iPSC)-derived neurons. In neuroblastoma lines, we confirmed that our pipelines were applicable both quantitatively and objectively to analysis of membrane trafficking of proteins such as Rab proteins and transferrin. Next, we developed new pipelines for analysis of disease phenotype using familial Parkinson's disease (PD) patient iPSC, harboring the I2020T LRRK2 mutation. Interestingly, Rab4 puncta of PD-iPSC-derived neurons exhibited distinct localization pattern relative to isogenic iPSC-derived neurons.

2Pos212 ダブルＹ字型アガロース微細構造における神経突起同士の相互作用
Interactions of two elongating neurites in double Y-shaped agarose microstructure

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Understanding the interactions of elongating neurites is important for the comprehension of neural network pattern formation in the brain and the arrangement of artificial neurite network patterns. We investigated the interactions of two neurites elongated from isolated hippocampal cells during cultivation exploiting double Y-shaped agarose microstructure, in which the first invert Y-shape for gathering and the second Y-shape for separation, fabricated photothermally on a substrate with a 1480nm infrared laser. The result showed the two gathered elongating neurites at the first invert Y-shaped structure were separated repulsively at the branching point of the second Y-shaped structure, indicating the leading edges of two neurites might have a repulsive tendency.

2Pos213 カルシウムイメージングによるアガロースマクロチャンバー内の神経回路活動の可視化
Visualization of neural circuit activity in agarose micro chamber by calcium imaging

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To understand the brain function, it is necessary to observe how the cells in neural circuits communicate with each other. In this study, we created the neural network in increment of single cell using agarose microfabrication technology and evaluated it by calcium imaging. For construction of the neural network, we seeded neural cells in the cell adhesion area of Agarose Micro Chambers (AMCs) created by this technique. We succeeded in observing neural activity of the cell network on AMCs by calcium imaging. However, synchronous firing could not be confirmed yet. We will try to observe synchronous firing of neural network and to make more complex neural circuits.

2Pos214 海馬が合成する男性・女性ホルモンやストレスホルモンは記憶シナプスを蛋白キナーゼ信号系で制御する
Kinase-dependent modulation of neuronal synapses by hippocampus-synthesized androgen, estrogen and stress hormone

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Neurosteroids (sex steroids and stress steroids) are synthesized in the hippocampus, center for learning and memory. Rapid non-genomic action of neurosteroids has been extensively studied over more than decades, and a significant progress was achieved. Estradiol (E2), testosterone (T), dihydrotestosterone (DHT), and corticosterone (stress hormone) trigger synaptic (membrane) steroid receptors, then inducing kinase signaling (non-genomic), leading to rapid modulation of dendritic spines in the hippocampus. E2 potentiates cognition (LTP), androgen (T, DHT) potentiate spatial memory and stress hormone is responsible for fight-or-flight response. Importantly, both male and female brains synthesize E2, T, DHT, however, several differences are observed in synaptic signaling.

2Pos215 ミトコンドリアβ酸化に関与するHADHが線虫の介在ニューロンにおいて低温馴化を制御する
HADH involved in mitochondrial β-oxidation regulates temperature acclimation in interneurons of *C.elegans*

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We are studying temperature acclimation of *C. elegans* to elucidate mechanism of temperature responses. We isolated the *hadh* gene involved in mitochondrial β-oxidation by RNA sequencing analysis, whose expression level was changed when animals were exposed to higher temperature. HADH encoding an enzyme involved in mitochondrial β-oxidation, was mainly expressed in neurons and located in mitochondria in neurons. *hadh* mutant showed abnormal temperature acclimation, whose abnormality was rescued by expressing *hadh cDNA* in almost all neurons. The candidate functional neural cells were narrowed down to three interneurons by using various neuron-specific promoters for rescue experiment. We are trying to identify functional neuron which HADH regulate temperature acclimation.

2Pos216 全身を周回する神経回路が腸の脂質含量を調節する
Whole-body neural circuit regulates intestinal fat storage

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We are studying neural mechanism underlying temperature acclimation of nematode *C. elegans*. *C. elegans* can be adapted to new temperature condition (Okahata et al., Science Advances, 2019). We show here that whole-body neural circuit, containing ASJ head sensory neuron, PVQ tail interneuron and RMG head interneurons, regulates intestinal gut fat storage and controls temperature acclimation. We examined which neurotransmitter functions between PVQ and RMG, RMG specific knocked down of glutamate receptor caused abnormal temperature acclimation and neural activity of RMG for temperature stimuli.This neural circuit ultimately regulates activity of triglyceride lipase ATGL-1 in intestine via promoting secretion of neuropeptide FLP-7.

2Pos217 環境の酸素情報が温度応答性に影響を与えることで低温馴化多様性が決定される
Cold acclimation diversity is determined by oxygen information, which affect neural activity of thermo sensory neuron in *C. elegans*

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We are studying cold acclimation of natural variants in *C. elegans* to reveal neural circuit regulating temperature signaling. We found that the diversity of cold acclimation between AB1 from Australia and CB4856 from Hawaii were caused by *VH15N14R.1* gene expressing in BAG oxygen sensory neuron. Although AB1 increased cold acclimation compared to CB4856 in 20% oxygen condition, the difference was not exhibited in 5% oxygen condition. Besides, Ca^{2+}imaging analysis suggested that ADL thermo responsivity of CB4856 was affected by oxygen concentration, but AB1 was not affected by oxygen concentration. These results suggested that the cold acclimation diversity is determined by oxygen information from BAG which affects ADL thermo responsivity.

2Pos218 ミミズ非連合学習におけるセロトニンシグナル
Serotonin signaling in non-associative learning in earthworm

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Molecular mechanism of serotonin signaling in non-associative learning of habituation by repeated tactile stimulus in the earthworm was investigated. From previous study shows that this neural activity change is induced due to via serotonin (5-HT) and nitric oxide (NO) signaling, because relatively high concentration of 5-HT or NO accelerated habituation. From our results, several 5-HT receptor antagonists inhibit delay establishment of habituation. Interestingly, non-selective agonist of 5-HT receptor 5-carboxamidotryptamine also showed the same result. In conclusion, non-associative learning such as habituation in the earthworm Eisenia fetida by repeated tactile stimulus to the body wall is due to via 5-HT-NO signaling.

2Pos219 異種混合培養神経回路網における神経情報伝達
Functional connections in a heterologous cultured chimera neuronal network

Ayumi Nishikawa, **Suguru N. Kudoh** (*Dep. of Engineering, Kwansei Gakuin University*)

In xenotransplantation, it is important to confirm functional connectivity of the synaptic transmission between neurons of different species. In this study, we collated the time series of Ca^{2+} peaks in the imaging data and spike events in multisites-extracellular- potentials recorded from a chimera cultured neuronal network, and found that the synaptic transmission between chick and rat neurons. In addition, we provided four types of cultured neuronal networks that combine glial cells and neurons derived from chicken and rat. The results showed that rat glial cells increased spontaneous activity and elongated the lifespan with electrical activity in chicken neurons.

2Pos220 網羅的定量的光計測によるマウス前頭葉前帯状皮質の興奮伝播の解析:膜電位感受性色素 VSD による
Analysis of neural activity propagation in the mouse prefrontal cortex using comprehensive quantitative optical recording: VSD study

Takashi Tominaga[1,2], Pooja Gusain[3], Makiko Taketoshi[1], Yoko Tominaga[1] ([1]*Inst. Neurosci., Tokushima Bunri Univ.*, [2]*Kagawa Sch Pharm., Tokushima Bunri Univ.*, [3]*Dept. Ophth, Sch Med, Keio Univ*)

The prefrontal cortex (PFC) is essential in brain function, and disruption can cause schizophrenic and other neuropsychiatric phenotypes. Here we report the functional dissection of mouse PFC with the quantitative voltage-sensitive dye (VSD) imaging method with high speed-high resolution, with a large field of view. We made serial slices of 350 μm thick from the bregma covering the mouse PFC. We averaged the neural activities of slices to nine stimulation sites and made a functional map of the propagation patterns. The results indicate that the intracortical propagation and directional spread in ACC. The functional anatomy of PFC help evaluates modulations of PFC by neuromodulators related to neuropsychiatric diseases.

2Pos221 咽頭筋のアミノ酸トランスポーター SLC46 は *C. elegans* の低温耐性を制御する
Amino acid transporter SLC46 in pharyngeal muscle regulates cold tolerance of *C. elegans*

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We are using cold tolerance of *C. elegans,* as a model for studying temperature adaptation of animal. We isolated a novel cold tolerance mutant by mutagenesis with EMS. Deep sequencing analyses revealed that the gene responsible for its abnormal cold tolerance is *slcr-46.1*, which encodes a homolog of the human amino acid transporter SLC46A3. SLCR-46.1 was expressed and localized at lysosome in pharyngeal muscle, ASG and BAG sensoryneurons involved in cold tolerance. Tissue specific rescue experiment determined that mutant cold tolerance was caused by at least pharyngeal muscle, and its muscular activity was decreased in the mutant. We are attempting to quantify lysosomal activity in the muscle using optogenetics, to analyze relation to individual cold tolerance.

2Pos222 蟻の探索行動における 3 次元的空間知覚
Three dimensional perception on ant foraging

Tomoko Sakiyama (*Faculty of Science and Engineering, Soka University*)

In this paper, I introduce a visual landmark for Japanese wood ants. The feature of the landmark is that it has different patterns when viewed from an observing angle. Individual foragers were allowed to explore the experimental field and learnt a food position related to a pattern of the landmark. During the learning walk in training phase, they also perceived another pattern of the landmark. During the test phase, another pattern was presented so as ants could see that pattern from the direction of the start position. I found that the ants persisted in approaching the landmark often. Surprisingly, this tendency was disappeared in the control experiment test, where a landmark having a single pattern was introduced on the field during the training phase.

2Pos223 タイリクバラタナゴの赤色に対する特異な行動
Unusual behavior of rosy bitterlings in response to red coloration

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We found out when rosy bitterlings placed in a beaker with a red background were behaved by lying down. We hypothesized that this behavior is a self-protection struggle of behaviors and a meaningful strategy. The results showed that females in a state of readiness to spawn exhibited this behavior the most, and males also exhibited this behavior. The female's rosy bitterlings must lie down to lay their eggs in the shell. These led us to wonder if this collapsing behavior was possibly related to the spawning behavior of the female. We also considered the possibility that the male collapsed sneaking to increase his reproductive success and mimicked the female's behavior to protect himself.

2Pos224 ミクロ社会とマクロ社会におけるカラス属の社会行動が示すカラスの社会性
Crows (*corvus*) society based on crows' behaivor in micro-society and macro-society

Haruki Kon, Kosei Ando, Aoba Sasaki, Hina Nakamura (*Sapporo Kaisei secondary school*)

In this writing, crow collectively means a carrion crow (*Corvus corone*) and a jungle crow (*Corvus macrorhynchos*) that basically lives in Sapporo. Since sociality in general is broadly defined, we will analyze crows' society from two perspectives: micro- and macro-social.
Firstly, we categorized crow's groups into definite groups and indefinite groups, then we observed natural and experimental populations.
We found out that crows could act differently in band and solitary. This fact suggests that local population in fission-fusion society is an emergent property that can only be established through individual negotiations.

2Pos225 シアノバクテリオクロム RcaE におけるユニークな C15 - *E,syn* 型ビリン発色団のラマン分光法による研究
Raman Spectroscopy of an Atypical C15-*E,syn* Bilin Chromophore in Cyanobacteriochrome RcaE

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Cyanobacteriochromes (CBCR) belong to the phytochrome superfamily of photoreceptors, the members of which utilize a linear tetrapyrrole (bilin) as a chromophore. RcaE is a representative member of a green/red-type CBCR subfamily that photoconverts between a green-absorbing Pg and red absorbing Pr states. Our recent crystallographic study showed that the bilin chromophore of RcaE adopts a unique C15-*E,syn* configuration in Pr. In this study, Raman spectra of the Pr state of RcaE were measured and analyzed by quantum chemical calculations and molecular dynamics simulations to explore the structure of the bilin chromophore and their interacting residues under aqueous solution conditions .

2Pos226* 青色光センサータンパク質 SyPixD の C 末端領域による 10 量体構造の安定化
Stabilization of decamer structure by the C-terminal region of the blue light sensor protein SyPixD

Shunrou Tokonami, Yusuke Nakasone, Masahide Terazima (*Grad. Sch. Sci., Univ. Kyoto*)

The oligomeric state of protein is important for regulating biological functions. A blue light sensor protein PixD from *Synechocystis* (SyPixD) acts as a regulator of phototaxis. SyPixD forms a ring-like decameric structure in the dark and dissociates into dimers under blue light exposure, which is considered to be related to its function. We found that few residues at the C-terminal end of SyPixD are indispensable for retaining the decameric form in the dark. It is interesting to note that structural analysis shows the C-terminal end is not located at the interface between each monomeric unit in the decamer. We discuss the stabilization mechanism of the oligomeric state based on experimental results of various mutants of SyPixD.

2Pos227* 新奇塩化物イオンポンプロドプシンの輸送メカニズム研究
Study on the transport mechanism of the novel chloride-ion pump rhodopsin

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Light-driven ion-pumping rhodopsins actively transport ions across the plasma membranes using light energy. This function is induced by conformational changes of the protein accompanying photoisomerization of the retinal chromophore from the all-*trans* to the 13-*cis* form. Previously, several ion pumps have been reported which differ in transporting ion species and the directions of the transport. Here, we conducted transient absorption spectroscopy and site-directed mutagenesis to elucidate the chloride-ion transport mechanism of the novel chloride-ion pump from bacteria. These results were compared with those of known chloride-ion pumps to clarify their similarities and differences, and the molecular mechanism of light-driven chloride-ion pumps will be discussed.

2Pos228* クリプトクロムが触媒する DNA 光修復反応の時間分解分光解析
Time-resolved spectroscopic analysis of DNA photorepair reaction catalyzed by cryptochrome

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CraCRY is animal-like cryptochrome from *Chlamydomonas reinhardtii*. CraCRY is drawing attention due to its bi-functionality *i.e.*, it works not only as photosensor, but also as DNA photolyase to photorepair UV-damaged DNA. This bi-functionality of CraCRY is unique, but its molecular mechanism remains elusive. Here, we focused on the DNA photolyase activity of CraCRY and investigated the photorepair dynamics using a time-resolved UV spectrometer. As results, we succeeded in tracking the photorepair processes from initial electron transfer. Notably, an intermediate of DNA repair, characterized by ~250 nm UV absorption, was detected at 1 ms. In the presentation, we will discuss the photorepair mechanism of CraCRY in comparison to well-studied *Xenopus laevis* (6-4) photolyase.

2Pos229 光と苦味のセンサーとしてはたらくキイロショウジョウバエ Rh7 の赤外分光研究
FTIR study of Drosophila Rh7, a light and bitter taste sensor

Kouhei Watanabe, Kota Katayama, Hideki Kandori (*Grad. Sch. Eng., Nagoya Inst.Tech.*)

The fruit fly, Drosophila melanogaster, senses light and bitter taste using, Rh1, Rh4, and Rh7 opsins. It is intriguing how these Drosophila opsins distinguish and recognize light and bitter compound, and function through signaling cascade. To study this fundamental problem, we attempted to express Drosophila Rh7 in insect cells for structural analysis using FTIR spectroscopy. Purified sample was applied for the measurement of light-induced difference FTIR spectroscopy to elucidate structural changes of the protein upon illumination. In this presentation, we will discuss the Rh7 specific structural changes in comparison to visual rhodopsin. In addition, perfusion-induced difference ATR-FTIR spectroscopy will be further applied to analyze bitter compound-Rh7 interaction.

2Pos230* 霊長類青感受性視物質の 200 K 以上での赤外分光解析
FTIR study of primate blue-sensitive cone pigment at >200 K

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Cone pigments are photoreceptors responsible for color vision, whose structural information is little known compared to rhodopsin for twilight vision. We reported the first structural data of three primate cone pigments, red (MR), green (MG), and blue (MB), where photochromic properties were utilized to accumulate difference FTIR spectra with Batho-state at 77 K. As visual pigments exhibit bleach reaction, structural study for late intermediates is challenging. Here, we report the photochromic property of MB at > 200 K, where the Lumi and Meta-I states are in photoequilibrium with the original state. A comparison of the difference FTIR spectra at 77, 163, 223, and 253 K provided structural information on what happens in the process of transition from originate state.

2Pos231 全トランス型から 11 シス型の光反応を示す新規微生物ロドプシンの分光解析
Spectroscopic analysis of novel microbial rhodopsin showing photoreaction from all-*trans*- to 11-*cis*-retinal

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Bestrhodopsin is a novel microbial rhodopsin subfamily discovered from marine unicellular algae. To date, it was showed that *Tara*-RRB, one of bestrhodopsins, is a pentamer containing two different rhodopsins and bestrophin channel per one protomer. In addition, *Tara*-RRB exhibited photoisomerization from all-*trans* to 11-*cis* retinal like retinal isomerase, one of animal rhodopsins. However, its photoreaction and isomerization mechanisms are unknown. In this study, we measured low-temperature UV-visible and FTIR spectroscopies. From the results, we found that *Tara*-RRB showed photoreaction at >150 K, but not the case at 77-150 K. Based on the spectroscopy combined with protein engineering, unusual photoreaction and isomerization mechanisms on *Tara*-RRB will be discussed.

2Pos232 異なる位置にカウンターイオンを持つクラゲオプシンの光異性化機構解析
Spectroscopic study of photoisomerization mechanism of Jellyfish Opsin having counterion at different position

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All opsins have a negatively charged residue, termed the counterion, to maintain visible light sensitivity and facilitate photoisomerization of their retinal chromophore. The position of the counterion differs between invertebrate and vertebrate opsins, and this counterion displacement is thought to be closely related to the evolution of opsins. Jellyfish Opsin that we focus on in this study acquired the counterion residue in TM2 independently. Here, we measured low-temperature UV-vis and FTIR spectroscopies of Jellyfish Opsin. Based on the obtained spectra, we will discuss the relevance of counterion displacement to similar and/or different manners of retinal photo-isomerization and structural changes with other opsins.

2Pos233* 固体 NMR を用いた Zn^{2+}結合型 TaHeR の脂質二重膜中の構造解析
Solid-state NMR study of membrane embedded TaHeR in the presence of Zn^{2+}

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Heliorhodopsin is a retinal-binding membrane protein with inverted membrane topology that constitutes a new rhodopsin family [1]. *Thermoplasmatales* archaeon HeR (TaHeR) forms a dimer in membranes and binds with Zn^{2+} with only helical structural perturbations [2, 3]. Here, using solid-state NMR spectroscopy, we investigated whether the structure of membrane embedded TaHeR in POPE/POPG is affected by Zn^{2+}-binding. We exhibited changes in ^{15}N chemical shifts of His imidazole rings at 0.15 mM $ZnCl_2$, while that of the protonated Schiff base did not shift. We assume that the binding site of Zn^{2+} is located at the cytoplasmic region.

[1] A. Pushkarev et al. (2018) *Nature*, 558, 595.
[2] W. Shihoya et al. (2019) *Nature,* 574, 132.
[3] M. Hashimoto et al. (2020) *JPC Lett.* 11, 8604.

2Pos234 霊長類の緑色感受性タンパク質の原子構造決定に向けて
Toward determining the atomic structure of primate green cone pigment

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Three cone pigments; red, green, and blue consist of a different protein bound to a common chromophore, 11-*cis*-retinal. Structure determination of cone pigments is needed for a precise understanding of spectral tuning. The principle obstacle to solving the structures is their innate instability in detergent micelles, crystal packing and photo-bleach reaction. To overcome these multiple bottlenecks, we have carried out to engineer primate green cone pigment (MG) such as BRIL-fusion and thermostabilizing mutations to facilitate crystallization. Besides the engineering MG, we used SONICC microscope using second harmonic generation, which allows crystal detection under dim-red light. We would like to discuss further improvements for the goal to determine the structure.

2Pos235 RcPYP と PBP 相互作用における表面電荷の効果
Effects of surface charge on RcPYP and PBP interactions

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Photoactive Yellow Protein from *Rhodobacter capsulatus* (RcPYP) forms a complex with PYP Binding Protein (PBP) in a light-dependent manner. The complex formation ability is reduced under conditions of high ionic strength, suggesting that a cluster of basic residues centered on the K72 surface charge of RcPYP is responsible for the complex formation. In this study, we examined the effect of substituting residues constituting positively charged clusters such as K72 in RcPYP on the interaction. The results showed that the K72Q exhibited a more pronounced ionic strength dependence on the complex formation than that of WT, suggesting that K72 is central to the complex formation and that other surface charges contribute to the complex formation.

2Pos236 固体 NMR による膜中 TAT ロドプシンの構造解析
Solid-state NMR study of membrane-embedded TAT rhodopsin

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The marine bacteria SAR11 contains TAT rhodopsin with specific motif (T82-A86-T93) [1]. The p*K*a (8.4) of the protonated Schiff base (PSB) in TAT rhodopsin is largely lower than the p*K*a (13.2) of bacteriorhodopsin [2]. Here, we observed ^{13}C and ^{15}N solid-state NMR of TAT rhodopsin in POPE/POPG to investigate structure of the retinal chromophore. The ^{15}N signal of PSB at pH 7.0 appeared at 160 ppm, which is the highest magnetic field resonance among other microbial rhodopsins (e.g. BR: 168.8 ppm). It suggested that the PSB forms a weak interaction with surrounding specific motif. We will discuss about unique retinal structure of the membrane-embedded TAT.

[1] A. Philosof & O. Béjà, *Environ. Microbiol. Rep.,* 5, 475 (2013).
[2] C. Kataoka et al, *JPC Lett.*10, 5117 (2019).

2Pos237 低温ラマン分光法による photoactive yellow protein の L 中間体の構造解析
Structural analysis of the L intermediate in the photoactive yellow protein by low-temperature Raman spectroscopy

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Photoactive yellow protein (PYP) is a photosensory protein found in phototrophic bacterium. PYP has a blue light-absorbing *p*-coumaric acid chromophore, which undergoes *trans-cis* isomerization upon photoabsorption. Two isomerization mechanisms, "bi-pedal" and "hula-twist," have been suggested for this photoisomerization, but they are not clearly identified. We study the photoisomerization mechanism of PYP based on the structural anaylysis of the photointermeidate using low-temperature Raman spectroscopy and the isotope-labeled samples.

2Pos238 PELDOR 法により決定した光化学系 II の 2 つの Mn^{2+}親和サイト
Location of the two high-affinity Mn^{2+} site in photosystem II detected by PELDOR

Hiroyuki Mino[1], Mizue Asada[1,2] ([1]*Grad. Sch. Sci., Nagoya Univ.*, [2]*Inst. Molecular Sci.*)

The Mn_4CaO_5 cluster, located in the photosystem II (PS II) protein complex, is the core machinery for photosynthetic oxygen evolution. The location of the high-affinity Mn^{2+}site in apo-Photosystem (PS) II was investigated by pulsed EPR. The electron-electron magnetic dipole interaction of 1.7 MHz between the $Y_D^{\bullet}$ radical and Mn^{2+} ion was observed using the pulsed electron-electron double resonance (PELDOR) technique and the Mn^{2+} ion was bound to one apo-PS II in the absence and presence of Ca^{2+}. The other high-affinity Mn^{2+}site is located at the position denoted by Mn4(A) in the native crystal structure, where the Mn^{2+} is coordinated with axial ligands Asp170 and Glu333 in the D1 polypeptide.

2Pos239 光化学系 II におけるストロマおよびルーメン側における摂動が第一キノン電子受容体 Q_A の酸化還元電位に及ぼす影響
Effects of stromal and lumenal side perturbations on the redox potential of the primary quinone Q_A in photosystem II

Yuki Kato, Takumi Noguchi (*Grad. Sch. Sci, Nagoya Univ.*)

The primary quinone electron acceptor Q_A is a key cofactor in the electron transfer regulation in PSII, and hence accurate estimation of its redox potential (E_m) change upon perturbation is crucial in understanding the regulatory mechanism. We here examined the effects of stromal and lumenal side perturbations on $E_m(Q_A)$ using FTIR spectroelectrochemistry. On the stromal side, replacement of bicarbonate bound to the non-heme iron with formate was found to upshift $E_m(Q_A)$ by ~55 mV, while an E_m gap between binding of different herbicides, DCMU and bromoxynil, at the Q_B site was ~30 mV. As for the lumenal side, removal of the extrinsic proteins downshifted $E_m(Q_A)$ by ~20 mV. We thus suggest that electron flow via Q_A is regulated by the perturbations on both sides of PSII.

Poster

2Pos240* 一分子過度吸収測定による光合成光捕集アンテナ複合体のダイナミクスとエネルギー移動の相関解析
Single-molecule transient absorption spectroscopy of energy transfer in photosynthetic antenna complex

Shun Arai[1], Tomomi Inagaki[2], Chihiro Azai[2], Toru Kondo[1] ([1]*Dept. of Life Sci. and Tech., Tokyo Tech.*, [2]*Grad. Sch. Life Sci., Ritsumeikan Univ.*)

Photosynthetic antenna complexes mediate the excited energy transfer (EET) to reaction centers. Their structures, optimized at the atomic level to carry out the efficient EET, are known to fluctuate under physiological conditions. However, it is still unclear how the conformational dynamics affect the ETT. Single-molecule spectroscopy (SMS) based on fluorescence detection is often utilized to analyze dynamic behaviors because of the high signal-to-noise ratio, but it is not available to observe non- or less-fluorescent processes. In this study, we develop an absorption microscope and perform single-molecule transient absorption spectroscopy of a photosynthetic antenna complex, chlorosome, to reveal relationships between dynamics and ETT rate.

2Pos241 光合成カロテノイドシフォナキサンチンにおける非共役官能基の共役系への影響
Effect of the non-conjugated functional group on the optical properties of a photosynthetic carotenoid, siphonaxanthin

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Siphonaxanthin (Sx) has a conjugated carbonyl group attached to the conjugated chain, which induces the intramolecular charge transfer characters, resulting in efficient energy transfer in photosynthetic systems. Sx has a hydroxy group at the C19 position of the carbonyl side, but its effect has not been considered. Recently, we discovered that a biosynthetic precursor of Sx, 19-deoxy Sx (dS) is accumulated in a marine alga only when irradiated with intense blue-green light. Despite the conjugated structures of dS and Sx being identical, the optical properties are different. In this study, we compared the spectroscopic properties of the Sx-derivatives and discussed the effect of non-conjugated groups on the excited-state characters and the physiological function of dS.

2Pos242 光化学系Ⅱにおける水分解マンガンクラスターの光構築機構の時間分解赤外分光解析
Time-resolved infrared study on the mechanism of photoassembly of the water-oxidizing Mn_4CaO_5 cluster in photosystem II

Shunya Watanabe, Yuichiro Shimada, Takumi Noguchi (*Grad. Sch. Sci., Nagoya Univ.*)

Photosynthetic water oxidation is performed at the Mn_4CaO_5 cluster in photosystem II. The molecular mechanism of the photoassembly of the Mn_4CaO_5 cluster however remains unresolved. Here, we investigated the assembly process of the Mn_4CaO_5 cluster using time-resolved infrared spectroscopy. Photooxidation of the first Mn^{2+} was monitored by detecting the vibrations of carboxylate ligands, showing two phases with ~0.1 ms and ~1 ms, which were attributed to the open and closed conformation of the CP43 lumenal domain interacting with the Mn site. Oxidation was slower at higher pH, likely due to deprotonation of a nearby His. It was thus concluded that the structural fluctuation of CP43 and the His protonation structure are important for the initial oxidation of Mn^{2+}.

2Pos243 光化学系 II の酸素発生中心における S_2 状態の中間体構造の DFT と CC 法による解析
DFT and DLPNO-CC calculation of relative stability and electronic states in the S_2 state of the $CaMn_4O_5$ cluster of the OEC of the PSII

Koichi Miyagawa[1], Takashi Kawakami[2,3], Mitsuo Shoji[1], Hiroshi Isobe[4], Kizashi Yamaguchi[3,5], Yasuteru Shigeta[1] ([1]*Center for Computational Sciences, University of Tsukuba*, [2]*Graduate School of Science, Osaka University*, [3]*RIKEN Center for Computational Science*, [4]*Research Institute for Interdisciplinary Science, Okayama University*, [5]*Center for Quantum Information and Quantum Biology, Osaka University*)

Relative stability and spin structure were investigated by DFT, Domain-based Local Pair Natural Orbital (DLPNO)-CCSD(T), and the exact diagonalization of spin Hamiltonian matrix for the right (R)-opened structures with the low spin (S = 1/2, g = 2) and intermediate spin (S = 5/2, g > 4) state and three left (L)-opened structures with the intermediate spin (S = 5/2, g = 4; S = 7/2, g > 4) and high spin (S = 13/2) state in the S_2 state of the Kok cycle for the oxygen evolving complex(OEC) of photosystem II (PSII). Multiple intermediates in the S_2 state revealed by DLPNO-CCSD(T) are compatible with the experimental results for the S_2 state, indicating proton transfer coupled spin transitions of the $CaMn_4O_5$ cluster in OEC of PSII.

2Pos244 分子動力学シミュレーションによる紅色細菌の光捕集アンテナ LH2 の吸収スペクトルの解析
The analysis of absorption spectra of light-harvesting antenna LH2 in purple bacteria by molecular dynamics simulation

Shunsuke Yabu[1], Hirofumi Sato[1,2], Masahiro Higashi[1] ([1]*Graduate School of Engineering, Kyoto Univ.*, [2]*FIFC, Kyoto Univ.*)

The light harvesting complex 2 in photosynthetic system of purple bacteria, LH2, has two bacteriochlorophyll (BChl) *a* rings; one is B800 composed of separated 8 BChls whereas the other is B850 composed of overlapped 16 BChls. Because of these different spatial configurations, B800 and B850 show different absorption peaks, enabling LH2 to absorb sunlight at a wide range of wavelengths. However, its molecular mechanism is still unknown. To elucidate its mechanism, as a first step, we investigate absorption spectra of LH2 by using molecular dynamics simulation with MMSIC method, an efficient method for calculating QM/MM potential energy function. We found that the charge transfer effect between BChls of B850 is responsible for the wide absorption spectra of LH2.

2Pos245 X 線自由電子レーザーを用いた解析による光化学系 II の基質水分子の取り込みと水分子の酸化に関する構造的知見
Structural insights into the substrate water delivery and water oxidation in photosystem II by analysis with an X-ray free-electron laser

Michi Suga, Yoshiki Nakajima, Hongjie Li, Jian-Ren Shen (*Okayama Univ*)

Photosynthetic water oxidation is catalyzed by the Mn4CaO5-cluster of Photosystem II (PSII) through a linear four oxidation intermediates of the S*i*-state cycle (S*i*, *i* = 0-4). The catalyst becomes a Mn4CaO6-cluster in the S3-state by incorporating additional oxygen O6 nearby a unique central oxo-bridge O5, supporting a dioxygen formation mechanism between O5 and O6. While the insertion of the O6 has been accepted, a pathway to deliver it and the O=O bond formation mechanism remain elusive.
To reveal the molecular details in the water oxidation reaction, we analyzed the X-ray-free laser (XFEL) structures of PSII during the progression of S1-to-S2 and S2-to-S3 states with an XFEL provided by the SACLA. We will present the observed structural changes in the Si-state cycle.

2Pos246* 内向きおよび外向きプロトンポンプロドプシンの駆動力の解明
Driving force of inward and outward proton pump rhodopsins

Akari Okuyama, Shoko Hososhima, Satoshi Tsunoda, Hideki Kandori (*Grad. Sch. Eng., Nagoya Inst. Tech.*)

Proton pump rhodopsins transport protons unidirectionally even against the electrochemical potential gradient upon light absorption. In addition to outward proton pumps, inward proton pumps have been discovered in nature. Which is the superior molecule? It is interesting to compare the performance of various proton pump rhodopsins, which will also help in the development of efficient optogenetics tools. We here determined driving forces of various inward and outward proton pump rhodopsins. They were revealed from the current-voltage relationship (I-V plots) obtained by patch clamp measurements. The effect of pH gradient was also studied. We will discuss the molecular origin of driving forces based on the results of systematic electrophysiological measurements.

2Pos247* Ca^{2+}結合型 TAT ロドプシンの分光研究
Spectroscopic study of TAT rhodopsin bound with Calcium ion

Teppei Sugimoto, Kota Katayama, Hideki Kandori (*Graduate school of Engineering, Nagoya institute of technology*)

TAT rhodopsin contains protonated and deprotonated retinal Schiff bases at physiological pH (pH ~ 8), which absorb visible and UV light, respectively. Visible form has no photoreaction after microseconds, but UV form has long term photocycle, so TAT rhodopsin is UV-dependent pH sensor .Recently, we reported Ca^{2+} binding to TAT rhodopsin, which was achieved for the neutral retinal chromophore with a deprotonated Schiff base. We observed that the equilibrium shifted toward the deprotonated state upon increasing Ca^{2+} concentration. In this study, we examine the photoreaction dynamics of the TAT rhodopsin bound with Ca^{2+} by using various spectroscopic methods. Based on the spectroscopy data, we will discuss the role of Ca^{2+}.

2Pos248* LED 光源を用いた微生物型ロドプシン AR3 による膜電位の長時間イメージング
Long-term membrane voltage imaging by microbial rhodopsin AR3 with LED light source

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Microbial rhodopsin is a photoreceptive membrane protein having a chromophore retinal. It has been reported that a rhodopsin, Archaerhodopsin-3 (AR3) shows voltage-sensitive fluorescence change, leading to voltage imaging in cells with high spatiotemporal resolution although intense laser excitation (~100 W/cm^2) is required [Kralj et al., (2011) Nat. Methods 9, 90.]. Here, using the relatively low intensity LED excitation (0.15 W/cm^2), we successfully detected voltage-sensitive fluorescence of AR3 and its high fluorescence mutant Archon1 in mammalian cells. Of note, the detection system allowed to monitor membrane potential for over 20 minutes with less fluorescence bleaching and less toxicity, implying the high potential of our system for the long-term voltage imaging.

2Pos249* ポンプ型チャネルロドプシン ChRmine のクライオ電子顕微鏡構造解析と次世代光遺伝学ツール開発
Cryo-EM structural analysis of pump-like channelrhodopsin ChRmine and structure guided engineering

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ChRmine, a new type of channelrhodopsin recently discovered, has broadened the application of optogenetics with its large channel conductance, red-shifted action spectrum, and high light sensitivity. Here I present the cryo-electron microscopy structure of ChRmine at 2.0 Å resolution. The structure reveals unusual architectural features never seen before in channelrhodopsins.
Next, by leveraging the structural information, I have engineered two new variants of ChRmine with 1) further red-shifted action spectrum (named rsChRmine) and 2) accelerated on/off channel kinetics (named hsChRmine). Furthermore, I combined rsChRmine with two different Ca2+ indicators and successfully performed a 3-color all-optical interrogation for intact-brain neural circuitry.

2Pos250 光活性化アデニル酸シクラーゼの活性化に伴う構造変化の解明
Structural changes of adenylate cyclase from Oscillatoria acuminata in response to blue light stimulation

Yuki Kitamura, Toru Ide, Minako Hirano (*Grad. Sch. Health Sys,. Okayama Univ.*)

Photoactivated adenylyl cyclase from Oscillatoria acuminata (OaPAC) is an enzyme that creates cAMP from ATP when exposed to blue light. In this study, we examined structural changes of OaPAC depending on light stimulation. We labeled a specific single amino in the adenylate cyclase domain (AC domain) with tetramethylrhodamine which is an environment-dependent fluorescent dye, and measured the fluorescence intensity immediately after blue light stimulation. Changes in fluorescence intensity were detected, which indicated that the environment around the labeled site in the AC domain changed during changes from a light-adapted state to a dark-adapted state. Based on the results, we propose a model for the conformational changes of OaPAC.

2Pos251 藻類シオミドロが持つ 4 種の Aureochrome の類似性と多様性
Similarity and Diversity of aureochromes, *Es*Au1-*Es*Au4, in a brown alga, *E. siliculosus*.

Yuta Nagano, Yumiko Adachi, Osamu Hisatomi (*Grad. Sch. Sci., Univ. Osaka*)

Aureochromes are blue light receptor proteins in yellow plants, and can be classified into four subgroups (Au1~Au4). We have reported that AUREO1 of *V. frigida* (*Vf*AUREO1) belonging to Au1 subgroup is monomeric in the dark state. *Vf*AUREO1 undergoes dimerization upon blue light illumination and increases its affinity for the target DNA. However, aureochromes in Au2~Au4 subgroups have rarely been investigated at the molecule level. In this study, we expressed core regions of *E. siliculosus* Au1~Au4 (*Es*Au1~4) in *E. coli* cells. We found quantitative differences in the photoreactions and in the monomer-dimer equilibria between *Es*Au3 and *Es*Au4. Our results may indicate characteristics of aureochromes among these subgroups.

2Pos252 近赤外光で駆動可能なバイオアクチュエータの創製
Creation of Bioactuators Drivable by Near-Infrared Light

Daisuke Maemura, Son Le The, Mari Takahashi, Kazuaki Matsumura, Shinya Maenosono (*Sch. Mater. Sci., JAIST*)

It has been reported that thin muscle films expressing photoreceptors on their cell surface can contract by irradiating blue light. Therefore a light-drivable bioactuator would be achieved with a combination of optogenetics and tissue engineering. However, since blue light has low biopermeability, it is impossible to stimulate the entire thick skeletal muscle, which is an obstacle to developing high-power light-drivable bioactuators. In this study, we utilized up-conversion nanoparticles (UCNPs) for creating high-power light-drivable bioactuators. Because NIR light has high biopermeability, one can stimulate the entire thick skeletal muscle by binding UCNPs to individual photoreceptors and converting NIR light to blue light in the vicinity of the photoreceptor.

2Pos253 *In vivo* optogenetic system to control deep tissue insulin signaling

Qi Dong, Mizuki Endo, Takeaki Ozawa (*Grad. Sch. Sci., Univ. Tokyo*)

Insulin is a hormone that plays a crucial role in glucose homeostasis To date, the physiological functions of the insulin secretion patterns are not fully understood due to the difficulties in analyzing the signaling in living animals. Aiming to investigate the specific physiological roles of the different temporal patterns of insulin secretion, we have developed an opto-insulin receptor (optoINSR) that enables the optical activation of insulin signaling with blue light illumination in living samples. optoINSR was genetically introduced to mice using AdV vectors. The photoactivation of optoINSR in BALB/c mice liver was confirmed under the illumination of blue LED light ((~440 nm, 10 s min^{-1}) therefore confirming the control of insulin-mediated signaling.

2Pos254 プロトセルの適応度地形
Fitness Landscape of Protocell

Akiko Baba[1], Keidai Sato[1], Kazuki Yokoyama[1], Ulf Olsson[2], Masayuki Imai[1] ([1]*Grad. Sch. Sci., Univ. Tohoku*, [2]*Grad. Sch. Sci., Univ. Lund*)

Evolution, a change shifted toward greater fitness over time, is an essential characteristics for bridging from molecular assemblies to living systems. The evolution began in prebiotic era, when the relationship between genotype and phenotype was primitive. In this study, we have investigated evolution of protocells. In primordial soup, fatty acid vesicles coexisted with numerous primitive molecules such as nucleotides, amino acids, and peptides. We measured growth rate of fatty acid vesicles coupled with peptide as fitness. The obtained fitness landscape show that the growth rate (phenotype) strongly depends on the amino acid sequence of peptide (genotype). Interestingly, the genotype-phenotype relationship is governed by the thermodynamical driving force.

2Pos255* Host-Parasite 分子複製体が織りなす複製反応ネットワークの複雑化過程とその性質
Complexification Process and Property of Replication Network by Host-Parasite Molucular Replicator

Rikuto Kamiura[1], Ryo Mizuuchi[2,3], Norikazu Ichihashi[1,2] ([1]*Grad. Sch. Arts and Sci., Univ. Tokyo*, [2]*Komaba inst., Univ. Tokyo*, [3]*JST, PRESTO*)

How the complexity of primitive self-replication molecules develops through Darwinian evolution remains a mystery with regards to the origin of life. Theoretical studies have proposed that coevolution with parasitic replicators increases network complexity by inducing inter-dependent replication. However, the feasibility of such complexification with biologically relevant molecules is still unknown owing to the lack of an experimental model. Here, we investigated the plausible complexification pathway of host–parasite replicators using both an experimental host–parasite RNA replication system and a theoretical model based on the experimental system.

2Pos256 無細胞翻訳系を用いた DNA 自己複製により成長する相分離液滴の開発
Phase-separated Dex droplets grow coupled with internal DNA self-replication

Moe Yabuta, Yoshihiro Minagawa, Hiroyuki Noji (*Dept. App. Chem., Grad. Sch. Eng., Univ. Tokyo*)

The bottom-up construction of artificial cells will lead us to understand the minimum elements and functions necessary for life. Self-growth is a common phenomenon in living systems and one of the essential properties of autonomous artificial cells. Here we show our new artificial cell system in which compartment growth is coupled with internal DNA self-replication. We focused on the phase-separated droplets of Dextran (Dex) and Polyethylene glycol (PEG) for the compartment, which is stabilized by enriched DNA. We employed a cell-free protein synthesis system and plasmid encoding DNA polymerase inside Dex droplets. The expressed DNA polymerase amplifies the template DNA, and Dex droplets grow as DNA amplification by taking Dex molecules from the surrounding PEG phase.

2Pos257 試験管内の DNA 複製、転写、翻訳反応は最適条件が異なる
Different conditions are optimal for in vitro DNA replication, transcription, and translation

Kaito Seo[1], Norikazu Ichihashi[1,2,3] ([1]*Grad. Sch. Arts. Sci., Univ. Tokyo*, [2]*Komaba Inst. Sci., Univ. Tokyo*, [3]*Res. Cen. Complex Syst. Bio., Univ. Bio. Inst., Univ. Tokyo*)

Construction of artificial cell is a useful strategy to understand life as complex system. In a living cell, DNA replication, transcription, and translation, play crucial roles. To reconstitute these reactions in vitro, isothermal replication by phi29 DNA polymerase and cell free transcription and translation system were combined in previous studies. In this study, we investigated optimal mixture compositions for DNA replication, transcription, and translation, independently. We found that the optimal compositions were significantly different. We will discuss possible methods to overcome the difference of optimal conditions to achieve an efficient transcription and translation-coupled DNA replication system, a required step toward the construction of artificial cells.

2Pos258* RNA 自己複製系を用いた RNA ゲノム再編成を伴う RNA 集団の進化の観察
Observation of RNA population evolution with RNA genome reorganization using RNA self-replication system

Kensuke Ueda[1], Ryo Mizuuchi[2], Norikazu Ichihashi[1,2,3] ([1]*Graduate School of Arts and Science, The University of Tokyo*, [2]*Komaba Institute for Science, The University of Tokyo*, [3]*Universal Biology Institute, The University of Tokyo*)

On a single nucleic acid in organisms, multiple genes are encoded. How did such a structure come into being in the prebiotic world? Several simulation studies have been conducted to answer this question, and it is thought that genetic information on a nucleic acid was expanded by linking nucleic acids with a single gene, resulting in the birth of a longer one. On the other hand, experimental approaches to this question are scarce.

We are addressing this question using an evolvable RNA self-replication system. This system contains two types of RNAs with one gene, and we searched for conditions under which a longer RNA with two genes emerge and is maintained by conducting the long-term self-replication reaction in this system.

2Pos259 Trp を含まない酵素群によって構成される解糖系に依存して生育する大腸菌の作成に向けた活性測定
Activity measurement for the creation of Escherichia coli dependent on glycolysis composed of a group of Trp-free enzymes

Naosato Takagi[1], Mana Hashimoto[1], Akifumi Nishida[1], Kenji Tsuge[2], Daisuke Kiga[1] ([1]*Faculty of Science and Engineering, Waseda University*, [2]*Graduate School of Science, Technology and Innovation, Kobe University*)

Present life synthesizes proteins composed of 20 types of amino acids to maintain living systems. However, it is considered that the primitive earth environment provided not all of the 20 standard amino acids. After emergence of life, the number of available amino acid types increased as life evolved. In this scenario, the last amino acid acquired by life is estimated to be Trp.
In this study, glycolysis, a primitive energy acquisition and storage system, is reconstructed using Trp-free enzymes. For evaluation of growth complementation of E. coli, each glycolytic enzyme with no or a few Trp residues were selected from database. For some of the enzymes with marginal activities, artificial evolution is required to obtained, active variants even without Trp.

2Pos260* (2SHP-4) 新規遺伝子の誕生と機能獲得の進化メカニズムに迫るゲノム計算科学：バイオインフォマティクスのその先に遺伝子の本質を探求する
(2SHP-4) How do *de novo* genes evolve and acquire function?: Computational genomics to revisit the nature of genes beyond bioinformatics

Shun Yamanouchi[1], Wataru Iwasaki[1,2] ([1]*Grad. Sch. Sci., Univ. Tokyo*, [2]*Grad. Sch. Front. Sci., Univ. Tokyo*)

It has recently been shown that novel genes arise from scratch (*de novo* gene birth). Previous studies have focused on identifying and describing *de novo* genes, but their molecular functions and underlying evolutionary mechanisms remain poorly understood. Thus, we systematically evaluated the functional potential of non-coding regions of the yeast and fly genomes. We found that functional motif-like peptides were enriched in some "alternative reading frames" of coding sequences, while they were rarely conserved even at genus level. We then hypothesized that genomes can potentially pool the source of genes, which may contribute to short-term adaptation in microevolution. Here, we aim to obtain new insights that go beyond bioinformatics.

2Pos261 PLA2 産生に関与する遺伝子と経路の同定
Identification of the genes and pathways responsible for PLA2 production

Hiroki Oura[1], Eri Hayashi[1], Yuto Kimura[1], Yusuke Nomura[1], Satoko Nakamura[3], Norimasa Kashiwagi[3], Chiaki Ogino[3], Shuichi Hirose[2], Wataru Nemoto[1] ([1]*Dept. Sch. & Tech., Tokyo Denki Univ*, [2]*NAGASE R & D Center NAGASE & CO*, [3]*Org. of Adv Sci & Tec., Kobe Univ*)

We identified a total of 374 non-synonymous mutations by comparing the genomes of the ten S.lividans mutated strains for the efficient PLA2 production with that of the wild strain. Proteins corresponding to the mutated genes tend to interact with each other on a protein-protein interaction network, and formed three clusters in the early, middle, and late mutation stages where similar GO terms are assigned. This implies the importance of considering mutations to neighboring proteins on the network and their functions to understand the mutation effect. Hence, we have investigated the mechanism of the effective production by using STRING and KEGG pathways, and have investigated the relationship between sequence signature and the impact of the mutations on each protein.

2Pos262* Sequel II を用いた単一インフルエンザウイルス集団中のゲノム配列分布測定
Heterogeneity of Genetic Sequence within Population in Single Plaque of Influenza Virus Revealed by Sequel II analysis

Kenji Tamao[1], Masayuki Suetsugu[2], Hiroyuki Noji[1], Kazuhito Tabata[1] ([1]*Appl. Chem., Grad. Sch. Eng., Univ. Tokyo*, [2]*Dept. Life. Sci., Col. Sci., Univ. Rikkyo*)

Though recent studies have shown phenotypic variety among particles of influenza virus, genomic variety in population remains elusive since a tool for sequencing genome of a single virus particle has not been established. Here, we adopted PacBio single-molecule DNA sequencing system Sequel II to investigate heterogeneity of influenza virus genome. As a result of single-molecule sequencing of influenza A/PR/8/34 virus genome, various mutations were found in population in single plaque. It should include mutations due to viral replication and errors due to sequencing reactions. Thus, this study showed that population in single plaque has significant heterogeneity of genetic sequence, and for more quantitative analysis, the effect of sequence error needs to be studied.

2Pos263* マウス胚性幹細胞の初期分化過程における X 染色体のエピゲノム構造変化は Xic 対合を促進する
Epigenetic-structural changes in X chromosomes promote Xic pairing during early differentiation process from embryonic stem cell of mouse

Tetsushi Komoto, Masashi Fujii, Akinori Awazu (*Grad. Sch. Integrated Sciences for Life, Univ. Hiroshima*)

X chromosome inactivation center (Xic) pairing occurs during the differentiation of embryonic stem (ES) cells from female mouse embryos, and is related to X chromosome inactivation, the circadian clock, intra-nucleus architecture, and metabolism. However, the mechanisms underlying the identification and approach of X chromosome (X chr.) pairs in the crowded nucleus are unclear. To elucidate the driving force of Xic pairing, we developed a coarse-grained molecular dynamics model of intranuclear chromosomes in ES cells and in cells 2 days after the onset of differentiation (2-day cells) by considering intrachromosomal epigenetic-structural feature-dependent mechanics.

2Pos264 Bayesian inference of chromatin folding from Hi-C data and application to enhancer-promoter communication in the Nanog locus

Giovanni Bruno Brandani, Chenyang Gu, Soundhara Rajan Gopi, Shoji Takada (*Grad. Sch. Sci., Univ. Kyoto*)

Recent experimental studies established how chromatin architecture influences key biological processes such as gene regulation, and molecular modeling has the potential to aid our understanding of such interplay. Here, we show how to integrate molecular simulation models of chromatin together with experimental Hi-C data within a Bayesian framework using the metainference approach. Such approach can successfully recover complex synthetic conformational ensembles and the experimental physical distances within the Sox2 and Pou5f1 genomic loci of mouse embryonic stem cells (mESCs) from contact information alone. Finally, we apply our method to the Nanog locus of mESCs to explore the dynamics of enhancer-promoter interactions and the implications for gene regulation.

2Pos265* Polymer physics model of chromatin dynamics during early embryogenesis in *Caenorhabditis elegans*

Yesbolatova Aiya[1], Akatsuki Kimura[1], Takahiro Sakaue[2] ([1]*Grad. Univ. for Adv. Stud., SOKENDAI, National Institute of Genetics*, [2]*Aoyama Gakuin University, Department of Physics and Mathematics*)

During *Caenorhabditis elegans* nematode embryogenesis chromatin mobility significantly decreases, which correlates with nuclear reorganization, such as heterochromatin formation. Nuclear size reduction is another characteristic of nuclear architecture change during nematode embryogenesis. However, the role of nuclear size change in chromatin mobility regulation and its mechanism is unknown. Combining experimental approach and polymer physics theory we propose a new model to explain the reduction of chromatin movement as a function of nuclear size and timescale by the transition from unentangled to entangled state. The results of this study offer new explanations on nuclear size contribution, the spatial-temporal scaling and diffusion effect on chromatin mobility.

2Pos266 Building a Coarse-grained Model of Chromatin

Justin Chan, Hidetoshi Kono (*Molecular Modelling and Simulation (MMS) Team, National Institutes for Quantum Science and Technology (QST)*)

Epigenetics play an important role in regulating gene expression in cells. Nucleosomes which are a complex of histone proteins-DNA, which are involved in DNA packing, are the most common protein-DNA complexes in the eukaryotic genome. Post-translational modifications (PTMs) of nucleosome's histones can affect the interactions between nucleosomes thus affecting the underlying expression of genes that are wrapped within the nucleosomes. However, we lack a method to disentangle the effects of PTMs on chromatin structure. We propose to build a coarse-grained model that can capture the effects of PTMs on the packing of nucleosomes or chromatin structure. Here we will share the latest progress and insights while building the model.

2Pos267 PDB における ATP アーゼ複合体の構造変化
Structural changes of ATPase complexes in the PDB

Ryotaro Koike (*Grad. Sch. Info., Nagoya Univ.*)

ATPases are a group of enzymes that hydrolyze ATP and perform various functions utilizing energy from the hydrolysis. Many ATPases interact with other polypeptide chains, form protein complexes and perform their functions. I focus on the ATPases that form protein complexes, termed ATPase complexes in this study, and survey their structural changes. The two original computational methods, SCPC and Motion Tree, were applied to all available structures of ATPase complexes in the Protein Data Bank (PDB). This extensive analysis revealed that the two complex-specific motions, interface motion and subunit-spanning motion, are more common in ATPase complexes than in homo- or hetero-dimers. I also examine the relationship between these motions and locations of bound ATP.

2Pos268 Accurate modeling and mechanistic investigation of the complexes of the SRK/SP11 proteins of *Brassicaceae*

Hanting Jiang[1], Kentaro Shimizu[1], Tohru Terada[1], Yoshitaka Moriwaki[1], Kohji Murase[2], Seiji Takayama[2] ([1]*Dept. of Biotechnol., Grad. Sch. of Agri. and Life Sci., Univ. of Tokyo*, [2]*Dept. of Appl. Biol. Chem., Grad. Sch. of Agri. and Life Sci., Univ. of Tokyo*)

Self-incompatibility in Brassicaceae is regulated by specific linkage of S-locus protein 11 (SP11) in pollen and S-locus receptor kinase (SRK) in pistil. If the two proteins are derived from the same S-locus, they from a tight complex, which hinders the pollination process to prevent selfpollination. Although the complex structures have been determined experimentally for two haplotypes, the structures of about 30 haplotypes remain unknown. In this study, we predicted the SRK and the SP11 structures with AlphaFold2 for most of the haplotypes and refined them with MD simulations. Our models revealed that several SP11 structures were different from the known structures. We investigated the effect of the difference on the complex formation with SRK.

2Pos269 AlphaFoldDB の予測立体構造と既知の実験立体構造との構造比較
Structure comparison of predicted 3D models in AlphaFoldDB with known experimentally determined 3D structures

Takeshi Kawabata, Kengo Kinoshita (*Grad.Sch.Info.Sci.,Tohoku Univ.*)

The monomeric 3D structural models of model organisms predicted by AlphaFold2 are now available in the database AlphaFoldDB. It stores not only predictions for “easy” target proteins with sequence-homologues of PDB structures, but also those for domains without any sequence-homologues in PDB. It is not clear that these new predictions are based on remote structural homologues of known structures, or structures of new folds. If they have remote homology with known structures, we may deduce their binding molecules from the remote 3D homologues. We compare all the 3D prediction models of human proteome in AlphaFoldDB with known 3D structures of PDB, using the program MATRAS, and discuss the possibility for predicting binding 3D structures for these predicted 3D models.

2Pos270 大和川水系石川におけるオオシマドジョウの生活史
Life History of *Cobitis* sp. BIWAE Type A in the Ishi River in the Yamato River System

Teppei Sakurai[1], Rikiya Ogawa[2] ([1]*Osaka Prefecture Tondabayashi High School*, [2]*Rikijuku Science School*)

Cobitis sp. BIWAE type A is distributed mainly around the Seto Inland Sea inflow rivers. The life history of this species is unknown. Periodic surveys it was conducted in the middle of the Ishikawa watershed (Osaka Prefecture) from February 2020-January 2022. Juveniles with also a larva fish were observed in every early of the month such as June and mid-July 2020, in year 2021 June and August. The gonadal weight index (GSI) of females decreased from May to August. However, it increased from November to April of the following years and remained high results until early summer. From these results, the breeding season is considered from May to July. Moreover, they have reproductive biology in which gonads develop approximately six months before the breeding season.

2Pos271 石川の魚類相の変遷とその要因についての一考察
Transition of fish fauna in Ishi River and a consideration about that factors

Shohei Umegawa[1], Kyoka Matsuo[1], Rikiya Ogawa[2] ([1]*Osaka Prefecture Tondabayashi High School*, [2]*Rikijuku Science School*)

We were interested in how the river environment and fish fauna of the familiars, Ishi River had changed over the years. Through detailed analysis, we attempted to clarify the impact of human activities on the river environment and fish diversity from 1960 to 2021. Lower reaches, there was a decrease in the number of fields and linearization of the river in the first 30 years. The number of fish species continues to decrease for 60 years, despite no notable changes in the river environment in the second half of the 30 years. Therefore, we hypothesized that the number of species is higher in rapids and pools. Conducted a survey we found out the number of species was higher at the sites with riparian vegetation even in the rapids and pools.

2Pos272 自然浄化に必要なものは
What is needed for natural purification?

Kyoka Matsuo[1], Cocona Okada[1], Rikiya Ogawa[2] ([1]*Osaka Prefecture Tondabayashi High School*, [2]*Rikijuku Science School*)

Last year, there was a massive alga in the lower reaches of the Ishi River in the Osaka Pref. These led us to believe that the water quality was deteriorating and to expect that the cause of it would be runoff from the drainage ditches. We conducted a field survey using bioindicators and algae. As a result, water quality deteriorated then the algae increased due to wastewater inflow. They recovered as they moved away from the wastewater inflow. Suggests that rivers have a natural purification effect and that a certain distance and velocity are necessary for this effect to occur. We thought that other conditions of natural purification needed organisms in flow. We are about to conduct a laboratory experiment to prove this.

2Pos273* 皮膚疾患の環状紅斑を対象とした数理解析による炎症調節機構の解明
Mathematical analysis of erythema annulare to elucidate the pattern formation mechanism of skin inflammation

Maki Sudo, Koichi Fujimoto (*Grad. Sch. Sci., Osaka University*)

Inflammation must be regulated to maintain tissue homeostasis. Annular erythema, a disease group of skin inflammation, expands and finally forms six patterns: circle, ring, broken circle, arc, polycycle, and grain. Many mediators spatiotemporally regulate skin inflammation; however, it remains unknown how these mediators develop these patterns. Here, to clarify the development mechanism, we constructed a reaction-diffusion model based on the interaction between pro- and anti-inflammatory mediators. The model succeeds in reproducing six patterns and their expansion. This result suggests that a specific interaction between pro- and anti-inflammatory mediators can develop the pattern of annular erythema in synergy with their diffusion.

2Pos274 嗅覚系における匂い物質・受容体の多対多の相互作用による類似匂い混合物の識別に関する理論的解析
Mathematical analysis of the discrimination of odorant mixtures via collective interactions of multiple odorants and olfactory receptors

Karin Suwazono[1], Tetsuya J. Kobayashi[2] ([1]*Dept. Biophys. and Biochem., Fuc. Sci., Univ. Tokyo*, [2]*Inst. Ind. Sci., Univ. Tokyo*)

The olfactory system recognizes mixtures of odorants from the collective responses of hundreds of olfactory receptors and subsequent neural activities. However, the mechanism of how mixtures are discriminated is rarely investigated compared with the discrimination of individual odorants. In this work, we mathematically model the receptor-odorant interactions and stochastic neural activity of olfactory sensory neurons (OSN) to investigate the conditions under which mixtures of odorants can be discriminable from the OSN activities. We found that OSNs that do not respond to the target mixture become more important when the discrimination task becomes more difficult by an increase in noise intensity or by the increase in the number of shared odorants in mixtures.

2Pos275* 免疫系における予測符号化に基づく適応的な抗原の有害/無害識別
Adaptive discrimination between harmful and harmless antigens based on predictive coding in immune system

Kana Yoshido[1], Naoki Honda[1,2,3] ([1]*Grad. Sch. of Biostudies, Kyoto Univ.*, [2]*Grad. Sch. of Integrated Sciences for Life, Hiroshima Univ.*, [3]*ExCELLS, NINS*)

Immune system discriminates between harmful and harmless antigens based on past experiences; however, the underlying mechanism is largely unknown. Here, we modeled T cell population dynamics by adopting the concept of predictive coding, where prediction is updated based on prediction error. We also hypothesized that prediction error signals induce T cell differentiation to memory T cells. By simulations, we found that the immune system identifies antigen risks depending on the concentration and input rapidness of antigen. Further, our model reproduced history-dependent discrimination, as in allergy onset and therapy. Together, this study provided a novel framework to improve our understanding of how the immune system adaptively learns the risks of diverse antigens.

2Pos276* 化学反応ネットワークの改変がダイナミクスに与える影響の解析
Analyzing the effect of modifications to the chemical reaction network on dynamics

Atsuki Hishida[1], Atsushi Mochizuki[2] ([1]*Grad. Sch. Sci., Univ. Kyoto*, [2]*Inst. Life Med. Sci, Kyoto Univ.*)

In living cells, thousands of chemical reactions are going on simultaneously, and they constitute a large metabolic network. Due to its hugeness, to analyze metabolism mathematically, it is necessary to focus on subsystems such as the glycolytic system. However, no general rule has been obtained for how to decide which reactions or metabolites should be included in the target system to reflect the actual cell properties. In this study, using structural sensitivity analysis, which analyzes the time variation of a chemical reaction system based on the network structure, we examined how modification of the network affects the system dynamics. We found that the system changes in only five ways when a degradation reaction is added to one of the molecules in the system.

2Pos277 新しいパターン伝播機構: 曲率により駆動されるパターン伝播
New mechanism of pattern propagation: Pattern propagation driven by surface curvature

Ryosuke Nishide, Shuji Ishihara (*Grad. Sch. Arts and Sci., Univ. Tokyo*)

Pattern dynamics on curved surfaces are abundant in biological systems. The geometry of surfaces has been shown to influence dynamics and plays a functional role, yet a comprehensive understanding is still elusive. We report for the first time that a static Turing pattern on a flat surface can propagate on a curved surface. To understand the pattern propagation, we investigate reaction-diffusion systems on axisymmetric curved surfaces and reveal that both the symmetries of the surface and pattern participate in the initiation of pattern propagation. This study provides a novel and generic mechanism of pattern propagation that is caused by surface curvature.

2Pos278* ゲノム縮小は内部共生の進化を加速するのだろうか？
Does Genome Reduction Accelerate Evolution of Endosymbiosis?

Yuki Kanai[1], Chikara Furusawa[1,2] ([1]*Grad. Sch. Sci., Univ. Tokyo*, [2]*BDR, Riken*)

Many endosymbionts have extremely small genome sizes. The evolution toward smaller genomes is driven by transposons called insertion sequences, which can also facilitate operon formation (Kanai, Tsuru & Furusawa, NAR, 2022). This implies that genome reduction reduces both the metabolic and the regulatory capacities. How do these two factors influence the evolution of endosymbiosis?
We used a computational toy model of symbionts to tackle this issue. When we reduced the metabolic and regulatory components, some symbionts started to leak nutrients valuable to the host, possibly because the symbionts became susceptible to changes in the host's metabolism. We believe that the statistical property of random matrices could explain this phenomenon.

2Pos279 A mathematical model for emergence of polar order induced by contact following locomotion in a multicellular system

Biplab Bhattacherjee, Masayuki Hayakawa, Tatsuo Shibata (*Laboratory for Physical Biology, BDR, RIKEN*)

Collective behaviour often observed in diverse systems, are important to understand developmental process of living beings. Our group observed Mutant *Dictyostelium discoideum* cells lacking chemotactic activity, exhibiting collective migration and formation of interesting structures like chains and bands.
We present a model of a multicellular system and show that selective adhesion induced contact following locomotion and alignment are the major forces in depicting structures and dynamics, as observed. The asymmetric structures like chains and bands mediate the phenomena of symmetry breaking during the disorder-order transition. A broken action-reaction law provides physical basis of the symmetry breaking for formations of structures like chain and bands in such a system.

2Pos280 ミクロ経済学としての代謝制御の理解：ワールブルク効果とギッフェン財を例として
Microeconomics of Metabolism: The Warburg effect as Giffen behavior

Jumpei Yamagishi, Tetsuhiro Hatakeyama (*Grad. Sch. of Arts and Sci., Univ. Tokyo*)

We developed an exact mapping between metabolic regulation of proliferating cells and the theory of consumer choice in microeconomics, based on the analogy as optimization problems. We thereby revealed that a trade-off and “complementarity” are the minimal requirements for the Warburg effect, a seemingly wasteful but ubiquitous metabolic phenomenon, and its correspondence to a long-lasting mystery in economics, Giffen behavior. Besides, the correspondence implies that respiration is counterintuitively stimulated when its efficiency is decreased by drug administration, mitochondrial dysfunction, etc. We will also show that such results can be extended to arbitrary metabolic systems, leading to a general quantitative law on intracellular metabolic responses.

2Pos281 Growing and competing cell colonies in a hybrid mechanochemical model

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Cells exist together in colonies or as tissues. Their behavior is controlled by an interplay of intercellular forces and biochemical regulation. We develop a model of the cell cycle, the regulatory network controlling growth and division, and couple it to the physical forces arising within the cell collective. We study the model using particle-based simulations and a continuum theory. 2D colonies confined in a channel develop moving growth fronts of dividing cells with quiescent cells in the interior. We then study the competition of two colonies with different rates of programmed cell death (apoptosis) and characteristic cell-cycle control pressures. Synchronisation of cell division/apoptosis events can emerge, causing oscillations in pressure and cell-cycle activity.

2Pos282 人工細胞内で再構成された細胞分裂面を決定する反応拡散波の動態と周期の制御
Tuning dynamics and period of a reaction-diffusion wave for cell division in artificial cells

Sakura Takada[1], Natsuhiko Yoshinaga[2,3], Nobuhide Doi[1], Kei Fujiwara[1] ([1]*Dept. Biosci. Info., Keio Univ.*, [2]*AIMR, Tohoku Univ.*, [3]*MathAM-OIL, AIST*)

Reaction-diffusion coupling (RDc) organizes the location of biomolecules in cells under nonlinear and far-from-equilibrium conditions. However, it is difficult to control the dynamics emerged by RDc such as wave modes and periods due to their unpredictable behaviors derived from the nonlinearity. Here, using the artificial cell system of Min waves generated by the RDc of MinD and MinE, we successfully controlled the two movement modes and periods of Min waves. For the mode control, we found MinD-MinE balance determines the mode and showed varying the balance can regulate the mode. Similarly, we showed mixing rate of two types of energy systems can tune the period of the wave. These results contribute to understanding the mechanism of spatiotemporal patterning in cells.

2Pos283 無細胞発現系における液滴形成のダイナミクス
Dynamics of droplet formation in cell-free expression systems

Shuzo Kato[1], David Garenne[2], Vincent Noireaux[2], Yusuke Maeda[1] ([1]*Dept. Phys., Kyushu Univ.*, [2]*Sch. Phys. Astro., Univ. of Minnesota*)

Liquid-liquid phase separation (LLPS) is an emerging paradigm for subcellular organization. However, intracellular LLPS is often entangled with nonequilibrium, confinement, and crowding effects, which are not fully understood. We study cytoplasmic LLPS using the cell-free expression systems (TXTL), and have shown in previous studies that TXTL exhibits LLPS and synthesized proteins are sequestered in one phase. In this study, we further analyzed the process of droplet formation. We enclosed the solution in cell-sized wells and induced phase separation by evaporation. We revealed that droplet formation depends on the concentration of the crowding agent PEG, changing droplet size and surface tension. We will discuss the experimental results with a theoretical model.

2Pos284 接着力を取り入れたアクティブブラウン粒子モデルによる細胞集団運動のモデル化
Adhesive Active Brownian Particle Model for Collective Cell Motion

Sota Shimamura[1], Nen Saito[2], Shuji Ishihara[1] ([1]*Grad. Sch. Arts and Sci., U. Tokyo.*, [2]*Grad. Sch. of Integrated Sci. for Life, Hiroshima Univ.*)

Cell motility and cell-cell adhesion both play important roles in collective dynamics of cells. We introduced interparticle adhesion into the active Brownian particle model and numerically investigated the macroscopic behaviors by changing the two parameters, motility and adhesion strengths. We found that, when these two parameters are balanced, the particles are divided into clusters, which repeatedly break up and fuse together (semi-aggregation phase). Cluster size distribution shows power law and particles exhibit cooperative motion when escaping from a large cluster, both of which has also observed in cultured cells in vitro. In this presentation, we will discuss the similarities between this semi-aggregation phase and actual cells.

2Pos285* ダイヤモンド量子センサによる単一細胞測定へ向けたピコリットル溶液 NMR 装置の開発
Development of pico-litter liquid NMR for single cell measurement by using diamond quantum sensor

Kohki Morita[1], Izuru Ohki[1,2], Masanori Fujiwara[1], Yuta Nakano[3], Norio Tokuda[3], Norikazu Mizuochi[1,4] ([1]*ICR, Kyoto Univ.*, [2]*QST*, [3]*NanoMaRi, Kanazawa Univ.*, [4]*CSRN, Kyoto Univ.*)

One of the major challenges of life science is to investigate and understand the molecular structure, interaction, and dynamics of living molecules in living cells as they are. NMR is one of the few techniques that makes it possible, but it requires a huge number of molecules and cells to observe, making it difficult to examine individual cells. However, with the progress of diamond nitrogen-vacancy (NV) center as a quantum sensor in recent years, the limitation is being removed. Using this technique, we even succeeded in measuring proton NMR of 1000 or fewer molecules in vitro. In this poster session, I would like to introduce a newly developed NV NMR measuring system that is highly suitable for living molecules and cells and achieved a spectral resolution of 0.9 ppm.

2Pos286* In vitro およびヒト生細胞中における超硫黄分子と S_8 のラマン解析
Raman analyses of supersulfides and S_8 in vitro and in human living cells

Lisa Kageyama[1], Shinji Kajimoto[1,2], Shinya Tahara[1], Takakazu Nakabayashi[1] ([1]*Graduate School of Pharmaceutical Sciences, University of Tohoku.*, [2]*JST PRESTO*)

Catenated sulfur compounds, such as supersulfide and S_8, have been attracting attention in biology. Recently, the possibility that S_8 exists in human cells has been revealed, suggesting that S_8 have a role as the energy source in human. In this study, we present the results of detecting catenated sulfur structure in vitro and in vivo using Raman microscopy. For intracellular detection, we established a label free method for detecting S_8 in cells using Raman microscopy. We showed that S_8 could be introduced into cells using fatty acids, and the Raman signal due to S_8 observed only in lipid droplets. Humans utilize lipids in fat droplets to obtain energy during starvation. The present results may indicate that humans use S_8 as an energy source.

2Pos287* Single Exosome 内包 miRNA 検出に向けた半導体ナノポアを用いた 1 粒子内包物検出法の開発
Development of a single-particle inclusions detection method by solid-state nanopore for miRNA in single exosome detection

Takumi Uchida, Hirohito Yamazaki, Ryo Iizuka, Sotaro Uemura (*Grad. Sch. Sci., The Univ. of Tokyo*)

Exosomes have become attractive candidates for monitoring cellular activities. In particular, inclusions of exosomes such as miRNAs play an important role in cell-to-cell communication. However, the heterogeneity of miRNAs in exosomes has not been investigated in detail. To address this issue, we develop a method for the detection of molecules within single vesicles using a nanopore. In this method, single particles are captured near the nanopore by thermophoresis, ruptured, and then the released inclusions are detected. Using this method, we have confirmed that about 15% of single strand DNA encapsulated in a single liposome can be detected. By applying this method, we are investigating how miRNA are distributed in exosomes.

2Pos288* Nanopore sensing of femtomolar DNAs using the excess complementary probes

Nanami Takeuchi, Ryuji Kawano (*Department of Biotechnology and Life Science, Tokyo University of Agriculture and Technology*)

Nanopore sensing is emerging as a powerful approach for single-molecule detection. Nucleic acid probes are often combined with the nanopores to detect target nucleic acids more efficiently. Here, we report a molecular basis of nucleic acid detection at femtomolar levels using nanopores and DNA probes. First, we detected the target molecules at femtomolar levels when using the excess amount of DNA probes relative to the targets. According to the analysis of the frequency with which nucleic acid molecules are captured in the pore, we found that the part of complementary strands for the target in the nucleic acid probes affects the targets. This phenomenon might point toward new avenues for low-concentration detection of biomarkers using nanopore technology.

2Pos289* ガラスピペットナノポアによるエクソソームの電気的検出
Electrical detection of exosomes by a glass capillary nanopore

Kohei Hayashi, Ryuji Kawano (*Department of Biotechnology and Life Science, Tokyo University of Agriculture and Technology*)

An exosome is a vesicle less than 200 nm in diameter released from a cell and works as a medium for cell-to-cell communication. It is suggested that compositions of encapsulated molecules in exosomes differ despite derived from a same cell population. Single-particle analysis is needed to clarify this difference, but it is still challenging. Nanopore technology will have a potential to detect and to capture the single exosomes. Here, we proposed to use a glass capillary nanopore (~200 nm) prepared by a commercially available material and attempt to capture milk exosomes. As the results, current blockages were observed only in the presence of exosomes, indicating the exosomes translocation through the nanopore. In the future, we will attempt to capture human exosomes.

2Pos290* (2SDA-4) Nanopore direct determination of DNA methylation and demethylation intermediates

Ping Liu[1], Masayuki Honda[1], Ryuji Kawano[2] ([1]*Department of Food and Energy Systems Science, Tokyo University of Agriculture and Technology*, [2]*Institute of Engineering, Tokyo University of Agriculture and Technology*)

This paper describes a nanopore sensing approach method for 5-methylcytosine (5mC) positions with numbers and demethylation intermediates directly. Methylation-demethylation processes are crucial for mammalian development and aberrant methylation patterns could lead to human diseases. However, the general modification methods need chemical conversion or enzymatic reaction and the incomplete reaction may reduce the reliability of the epigenetic analysis. In this work, we utilized the epigenetic modulation of cytosine dynamics in dsDNA which destabilizes the Watson-Crick base pair to allow modified cytosine to interact with the acidic anion acids in nanopore for determining the position with the number of 5mC and three other modifications at the single-nucleotide level.

2Pos291* 原子間力顕微鏡による神経管閉鎖中のホヤ胚の 1 細胞力学特性の測定
Mechanical properties of single cells in ascidian embryo during neural tube closure measured by atomic force microscopy

Yosuke Tsuboyama, Yuki Miyata, Takaharu Okajima (*Graduate School / Faculty of Information Science and Technology, Hokkaido University*)

Zippering is a dynamic embryonic process exhibiting a unidirectional closure of neural tube during neural tube closure. The understanding of mechanical properties of embryonic cells during neurulation is crucial to elucidate the mechanism of the zippering process. In this study, we investigated single cell stiffness in the vegetal pole region of ascidian embryo during the neurulation by atomic force microscopy (AFM), allowing to conduct a less invasiveness measurement of developing embryo at the single cell level. We observed a characteristic spatiotemporal pattern of cell stiffness around the zippering site in the vegetal pole, suggesting that the vegetal cells except zippered cells also mechanically contribute to the zippering process.

2Pos292 Optimization of protocols for metabolomics studies of human breast milk samples using benchtop NMR

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The recent emergence of low-field benchtop NMR using permanent magnets promises a new platform for metabolomics research. It has lower maintenance costs and occupies less space than high-field NMR. But on the other hand, the low resolution and low signal-to-noise ratio of benchtop NMR poses difficulties in quantifying metabolites.
Here, an optimized protocol for metabolomic analysis of human breast milk by benchtop NMR spectroscopy is presented, including the settings of the pre-saturation pulse parameters and the repetition time of the measurements. We also present a reliable automated spectra processing approach for quantification. Our study shows that despite some limitations, low-field benchtop NMR can serve as an excellent platform for metabolomics research.

2Pos293 α-グルコシダーゼ阻害物質を含むクワ葉の投与によるマウス腸内環境への影響の NMR メタボロミクス解析
NMR metabolomics of administration of mulberry leaves containing α-glucosidase inhibitors on the intestinal environment of mice

Li Gan, Yuga Inamura, Zihao Song, Yuki Ohnishi, Yasuhiro Kumaki, Tomoyasu Aizawa (*Grad. Sch. Life Sci., Univ. Hokkaido*)

Mulberry leaf is considered a functional food in many Asian countries. In this study, a nuclear magnetic resonance (NMR)-based metabolomics study was performed on the feces of control and mulberry leaf powder (MLP)-treated mice to reveal the therapeutic effect of long-term MLP intake over 9 weeks. Carbohydrates, amino acids, and propionate were found to be significantly altered after MLP treatment. In the MLP-treated group, glucose and all amino acid levels were lower after week 5, while maltose was significantly increased after week 5. Propionate levels were higher in the treatment group than in the control group from week 1 to week 4. These results suggest that the gut microbiota of mice may be regulated gradually through continued MLP treatment.

2Pos294* Spatiotemporal Dynamics of Small Extracellular Vesicle Nanotopology in Response to Physicochemical Stresses Revealed by HS-AFM

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Small extracellular vesicles (sEVs) native properties is suitable for nanocarriers, vaccines, and theranostic materials. Even though sEVs have been widely studied, an instantaneous assessment on sEVs structure dynamics remains difficult. Here, we use HS-AFM as a nanoscopic assessment to examine sEVs nanotopological changes by manipulating several physicochemical parameters including thermal, pH, and osmotic stresses. At high-temperature, high-pH, and hypertonic conditions the sEVs structure were severely disrupted. In conclusion, our study demonstrated the practicability of HS-AFM for structural characterization and nanoparticle assessment.

2Pos295* 高周波集束超音波スペクトロスコピーによる培養単一細胞への非侵襲局所力学刺激付与システムの開発とヒト iPS 細胞の核の共振による超音波吸収帯
Development of ultrasound spectroscopic imaging system for applying highly controlled local mechanical stimulation on cells

Natsumi Fujiwara, Takaki Matsumotio, Akira Nagakubo, Masahiro Kino-oka, Hirotsugu Ogi (*Graduate School of Engineering, University of Osaka*)

Living cells sense various mechanical stimuli and respond to them by adjusting their tissue morphogenesis, self-renewal, and differentiation. Because stem cells are more sensitive, many studies have been conducted to control their behavior. However, many of these mechanisms remain unexplored, because stimulus extends throughout the cells or causes cell-damaging. In this study, we develop thefocused ultrasound spectroscopic technique for applying a non-invasive localized mechanical stimulation in a single cell to systematically investigate its effects on the function of the cell. For human iPS cells, we found an ultrasound absorption band at ~160 MHz due to resonance of nucleus. This suggests that the technique we developed can stimulate cell nucleus effectively.

2Pos296 神経分化における細胞内温度の貢献
Contribution of Intracellular Thermogenesis to Neural Differentiation

Shunsuke Chuma[1,2], Hirotaka Okita[2], Shingo Sotoma[2], Kohki Okabe[3,4], Yoshie Harada[2,5] ([1]*Dept. Biol. Sci., Grad. Sch. Sci., Osaka Univ.*, [2]*IPR, Osaka Univ.*, [3]*Grad. Sch. Pharm. Sci., The Univ. Tokyo*, [4]*JST PRESTO*, [5]*QIQB Osaka Univ.*)

Neural stem cells differentiate into neurons with neurite outgrowth, regulated by differentiation factors. Although recent studies have shown that temperature influences neural differentiation, the involvement of intracellular temperature remains elusive. Here, we investigated the contribution of intracellular temperature change to neural differentiation. Using a fluorescent polymeric thermometer and nano-diamond, we found that the intracellular temperature increased during differentiation depending on transcription and translation. Additionally, heating the nucleus by laser promoted neurite outgrowth while heating the cytoplasm was less effective. Therefore, we propose that thermogenesis of the nucleus during differentiation contributes to neurite outgrowth.

2Pos297* 高速 AFM の更なる高速化に向けた Z-スキャナの共振制御装置
Resonance-controller of the Z-scanner for faster high-speed AFM

Kazuma Tatsumi[1], Kenichi Umeda[2], Toshio Ando[2], Noriyuki Kodera[2] ([1]*Grad. Sch. Math. & Phys., Kanazawa Univ.*, [2]*WPI-NanoLSI, Kanazawa Univ.*)

In order to study a wider range of biological phenomena with high-speed AFM (HS-AFM), the temporal resolution of HS-AFM should be improved by making a faster Z-scanner. For this, the resonance frequency f_Z must be increased while reducing the mechanical quality factor Q_Z because the response time of Z-scanner τ_Z is defined as $Q_Z/\pi f_Z$. However, no method can simultaneously control both f_Z and Q_Z. Here, we developed a new controller called “resonance-controller” that combines the inverse transfer function and the active damping techniques. As a result, f_Z and Q_S were simultaneously controlled, and τ_Z was improved more than 50 times without changing mechanical parts. The improved performance will be evaluated by HS-AFM imaging of biological samples.

2Pos298 細胞内高速マッピングが細胞内の非伝導性の熱散逸の存在を明らかにする
High-speed Intracellular Temperature Mapping Reveals the Existence of Non-Conductive Heat Dissipation within Cells

Masaharu Takarada[1], Kohki Okabe[1,2], Takashi Funatsu[1] ([1]*Grad. Sch. of Pharm. Sci., The Univ of Tokyo*, [2]*JST, PRESTO*)

Thermometry at single cell level has revealed intracellular temperature variates in both time and space, which has attracted attention in biology. However, real-time temperature mapping has been challenging due to its low spatiotemporal resolution. We developed a method to track intracellular temperature mapping using fluorescent polymeric thermometer and state-of-the-art fluorescence lifetime imaging microscopy, achieving a temporal resolution of 100 ms at a high spatial resolution that reveals the organelle-specific temperature distribution. Furthermore, we found that intracellular heat dissipation is significantly more restricted than in water and demonstrated that this phenomenon cannot be explained by heat conduction.

2Pos299* がん免疫において細胞傷害性指標となる液性因子分泌のライブセルイメージング
Live Cell Imaging of Liquid Factor Secretion as an Indicator of Cytotoxicity in Cancer Immunity

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Cytotoxic T lymphocytes (CTLs) play an important role in cancer immunity by releasing cytotoxic enzymes such as GranzymeB (GrB). However, CTLs are functionally heterogeneous and the genetic background for their efficient cytotoxicity remains unclear. Therefore, we aimed to identify CTLs that can efficiently eliminate cancer cells by observing their cytotoxic and GrB secretion activities at single cell resolution.
In this study, we developed a collagen/anti-GrB antibody bilayer-coated dish suitable for adherent cancer cells. Using this dish, we performed live-cell imaging of GrB secretion of CTLs by real-time fluorescent immunoassay on a TIRF microscope. We found that some, but not all, CTLs showed cytotoxic activity against cancer cells by secreting GrB.

2Pos300* 高速原子間力顕微鏡のさらなる高速化を目指した超微小カンチレバーの開発
Development of ultra-small cantilever for faster high-speed atomic force microscopy

Noriki Katayama[1], Kenichi Umeda[2], Toshio Ando[2], Noriyuki Kodera[2] ([1]*Grad. Sch. Math. & Phys., Kanazawa Univ.*, [2]*WPI-NanoLSI, Kanazawa Univ.*)

High-speed atomic force microscopy (HS-AFM) is a powerful tool for imaging biomolecules in action. To further improve the temporal resolution of HS-AFM, we must increase the resonance frequency of cantilever, the rate-limiting factor in imaging. In this study, we developed an “ultra-small cantilever” via processing a conventional cantilever using focused ion beam. The resonance frequency of the ultra-small cantilever– developed here was about 10 MHz, 20 times higher than that of the unprocessed cantilever. We further developed a stable excitation system with a sufficient excitation efficiency specialized for ultra-small cantilevers. We finally performed HS-AFM observation at higher frame rate than conventional observation to confirm the superiority of the system.

2Pos301 ゴルジ体と小胞体の超解像顕微鏡による可視化解析
Observation and analysis of Golgi body and ER with super resolution microscopy

Kaoru Katoh[1,2], Totai Mitsuyama[2] ([1]*Biomed Res Inst, AIST*, [2]*AIRC, AIST*)

Golgi body is an organelle observed in cytoplasm of eukaryotic cells. Golgi body attaches various sugar monomers to proteins as the proteins move between cis-face and trans-face in the Golgi body. This processing is very important for protein secretion. Here we observed Golgi body of cultured cells with super resolution microscopy (STED and spinning disk (SoRa)). We will show a method to visualize cis and trans side of the Golge body as completely separated two area and to examine distribution of several kinds of proteins in the body. We will also discuss the relationship between Golgi and ER in the 3D images recorded with super resolution microscopy.

2Pos302* 高分解能ライトフィールド顕微鏡の開発によるシングルショット 3D イメージング
Development of high-resolution light-field microscopy for single-shot 3D volumetric imaging

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Light-field microscopy (LFM) enables 'scan-less' acquisition of a 3D volumetric image by postprocessing single 2D camera snapshots recorded. Temporal resolution is 1,000-fold faster than that of confocal microscopy (CM) because LFM can capture 3D in a single camera shot. Yet, its spatial resolution is 10-fold lower because LFM requires recording all XYZ '3D' information with a limited number of pixels by the '2D' sensor. Here we overcame this problem and developed high-resolution LFM with submicron XY and 2um Z resolutions. In this LFM, a novel optical system and 3D postprocessing algorithm were built for sampling 20-fold more pixels than conventional LFM. This LFM enables high-resolution 3D volumetric imaging at 1,000-fold faster than CM in freely behaving *C. elegans*.

2Pos303* (2SBA-2) ヒト生細胞の局所クロマチン動態は細胞周期を通して一定である
(2SBA-2) Single-nucleosome imaging reveals steady-state motion of interphase chromatin in living human cells

Shiori Iida[1,2], Soya Shinkai[3], Yuji Itoh[1], Sachiko Tamura[1], Masato Kanemaki[2,4], Shuichi Onami[3], Kazuhiro Maeshima[1,2] ([1]*Genome Dynamics Lab., Natl. Inst. of Genet.*, [2]*Dept. of Genet., Sch. of Life Sci., SOKENDAI*, [3]*RIKEN BDR*, [4]*Mol. Cell Eng. Lab., Natl. Inst. of Genet.*)

Dynamic chromatin behavior plays a critical role in various genome functions. However, it remains unclear how chromatin behavior changes during interphase, where the nucleus enlarges and genomic DNA doubles. We unveil that local chromatin motion captured by single-nucleosome imaging remained steady throughout interphase in live human cells. A defined genomic region also behaved similarly. Our results of Brownian dynamics modeling suggest that this steady-state chromatin motion was mainly driven by thermal fluctuations. Steady-state motion temporarily increased following a DNA damage response. The observed steady-state chromatin motion allows cells to conduct housekeeping functions, such as transcription and DNA replication, under similar environments during interphase.

2Pos304 High-speed atomic force microscopy mapping of *Bacillus subtilis'* mechanical properties

Christian Ganser[1], Shigetaka Nishiguchi[1], Takayuki Uchihashi[1,2] ([1]*ExCELLS, NINS*, [2]*Grad. Sch. Sci., Nagoya Univ.*)

Atomic force microscopy (AFM) is a unique imaging technique as it probes surface topography by physically contacting a sample with a sharp tip. One of the advantages of AFM is the availability of a multityde of imaging modes such as mapping mechanical properties on the nanometer scale. However, long imaging times obscure dynamic effects.
High-speed AFM (HS-AFM), on the other hand. is typically focussing on fast topography imaging. By utilizing the high imaging speed of HS-AFM with the flexibility of force mapping, a multitude of information can be obtained and used to study also dynamic effects. In this study, I will present the application of HS-AFM force mapping to *Bacillus subtilis* to visualize dynamic effects such as softening upon lysozyme addition.

2Pos305* 高速 AFM 観察を用いた E6AP/E6/p53 複合体の構造ダイナミクスの解明
Structural dynamics of E6AP/E6/p53 complex revealed by high-speed AFM (HS-AFM)

Kazusa Takeda[1], Ikumi Muro[1], Hiroki Konno[2] ([1]*Grad. Sch. of Nat. Sci. & Technol., Kanazawa University*, [2]*WPI Nano Life Sci. Inst. (WPI-NanoLSI), Kanazawa Univ*)

Ubiquitin conjugation to target proteins (ubiquitination) is a post-translational modification that regulates numerous cellular processes. It is known that E6AP (E6-associated protein), a kind of ubiquitin ligase, interacts with E6 protein derived from oncogenic human papilloma virus (HPV 16/18) and the enzyme complex induces ubiquitination of p53 resulting p53 degradation by ubiquitin-proteasome system. To reveal that how the E6AP/E6/p53 complex is constructed and how E6 promotes the ubiquitination activity of E6AP, we investigated the structural dynamics of E6AP/E6 and E6AP/E6/p53 complex using HS-AFM. We also investigated the importance of E6AP N-terminal region for the E6AP/E6/p53 complex formation by using of N-terminal truncated E6AP mutant ($E6AP_{\Delta 1\text{-}225}$).

2Pos306 透過型電子顕微鏡の最大感度をもたらす新規ヒルベルト位相板
Novel Hilbert Phase Plates for Maximum Sensitivity in Transmision Electron Microscopy

Kuniaki Nagayama (*N-EM Laboratories Inc.*)

The phase plate (PP) method in TEM began to be replaced by the conventional Scherzer defocus method due to the severe electron loss via PP, recently recognized as a DQE. We have found a novel class of PP that can yield a sensitivity higher than that of the Scherzer defocus method, namely twin φ-Hilbert PPs (HPPs) method, where twin means the use of symmetric (left and right) two φ-HPPs and φ means the HPP phase smaller than π. A theoretical analysis based on the CTF theory clarified the sensitivity maximized around φ= π/2. It was computationally confirmed using a commertial TEM simulator (Elbis™). The agreement between the theory and the simulation was particularly good in the high-resolution condition, demonstrating the effectiveness of the novel HPP method.

2Pos307* Dynamic unfolding of the laminin coiled-coil domain revealed by high-speed AFM

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Laminins are trimeric glycoproteins with important roles in cell-matrix adhesion and tissue organization. However, dynamic conformational changes of laminin have so far not been studied at the single-molecule level. Using high-speed atomic force microscopy (HS-AFM) imaging we observe dynamic unfolding of a ~35 amino acid stretch of the laminin α-chain, leading to temporary unraveling of the C-terminus of the laminin triple coiled-coil domain. We further identified laminin isoform-specific amino acid sequences required for α-chain unfolding. Interestingly, the C-terminus of the laminin coiled-coil domain also contains binding sites for integrin receptors, suggesting that reversible α-chain unfolding may regulate the cell adhesion properties of some laminin isoforms.

2Pos308 脂肪細胞内脂質分布の TOF-SIMS 解析
Subcellular lipid analysis in a 3T3-L1 adipocyte by TOF-SIMS

Noritaka Masaki (*National Institute of Genetics*)

Time-of-Flight Secondary-Ion Mass Spectrometry (TOF-SIMS), which uses focused primary ion beam for ionization, has an advantage in the spatial resolution with tens of nanometers. By combining Gas Cluster Ion Beam for sputtering, TOF-SIMS can reveal 3D chemical map even in intra-nuclear structures [1]. However, it also clarifies a problem that fresh frozen samples popularly used in mass spectrometry imaging cannot maintain subcellular chemical distributions, especially about lipids. To overcome this, fixation to maintain lipid signals in TOF-SIMS spectrum [2] is modified. Adipocytes prepared with this method successfully shows lipid distributions consistent with electron microscopy observations.
[1] Masaki *et al*. *Sci. Rep.* 2015
[2] Nagata *et al. Surf. Interface Anal.* 2014

2Pos309 Development of genetically encodable tool for live-imaging and manipulation of endogenous RNAs in living cells

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In this study, we report the development and application of designer RNA-binding protein (dRBP), which is designable to bind to the RNA of interest. By using an ELISA-like assay combined with our bright bioluminescent protein Nano-lantern (Takai et al., PNAS 2015), we showed our dRBPs specifically bind to target RNAs with high affinity. We also showed our dRBPs can be used for the visualization of the endogenous RNAs such as Actb mRNA and lncRNA Neat1_2 in living cells. Furthermore, by using the dRBP fused to constitutively active kinesin, we succeeded in the manipulation of the localization of endogenous Actb mRNA. These data suggest that our dRBP would serve as a powerful tool for visualization and manipulation of endogenous RNAs in living cells.

2Pos310* 表面形状計測システムに向けた生体ナノポアプローブの特性
Characteristics of Biological Nanopore Probes as a Topological Imaging System

Shuta Nomi, Kan Shoji (*Nagaoka University of Technology*)

Scanning ion conductance microscopy (SICM) using biological nanopore probes (BNP), that a biological-nanopore-reconstituted lipid bilayer is prepared at the tip of glass pipettes, has been proposed as a simultaneous imaging system of chemicals and topography. In addition, because BNs have smaller pore diameters and lengths than glass pipettes, SICM using BNPs potentially provides higher spatial-resolved topographic images. However, the spatial resolution of topographic images was limited by the micrometer-scale tip of the pipette. In this study, we developed BNPs using a hydrogel-filled nanopipette. Then, we evaluated the topographic imaging ability of the BNP incorporated SCIM by conducting approach curve experiments.

2Pos311 Raman spectral analysis of induced pluripotent stem cell during spontaneous differentiation

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To observe a cell state transition in non-labeling and non-destructive manner, we have developed a technique to collect Raman scattering spectra with high reproducibility, independent of experimental date, analyst, and optical aberrations. Using this method, we observed the cooperative differentiation of human iPS cells. A predominant change was observed in the Raman scattering spectrum of the cells from the fourth day after differentiation induction. We succeeded in identifying a group of peaks that fluctuated significantly from the first to the second day of differentiation induction and then quenched, even though the spectral intensity remained unchanged. This result indicates that fluctuation analysis can detect the onset of singularity phenomena at an early stage.

2Pos312* 真核細胞における翻訳活性変化の温度シグナリング機構の解明
Thermal Signaling Mechanisms of Translational Control in Eukaryotic Cells

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The translation rate of ribosomes is known to be non-constant. Because the physicochemical mechanism of the rate switching is not known, this study aimed to reveal the thermal signaling mechanism of the steady-state translation in eukaryotic cells. The temperature-sensitive fluorescence imaging of cells with different translation activity suggested that translation is an exothermic reaction. In addition, the fluorescence imaging to measure translation activity in cells whose temperature gradient was inhibited suggested that localized heat in the cytoplasm should promote the activity of translation. These results will provide a parametric mechanism that regulate the rate of translation.

2Pos313 Structure mechanism for color tuning of red-colored chromoprotein, R-Velour

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GFP-like chromoproteins with non-fluorescence have been used for bioimaging indicators. At the last meeting, we reported a novel chromoprotein, R-Velour, and its color variants. Through the survey for residues surrounding the chromophore by mutagenesis, we found a key residue, S155, for color change. Based on the recently proposed spectrum shift theory, we explained the spectrum shift with the difference in the state of the hydrogen bonds from the chromophore phenolate oxygen. That was further supported by disruption of the hydrogen bond in the crystal structure of the variants M-Velour-537 and M-Velour-554 with the bathochromic shift. These findings may support further development of R-Velour variants with useful absorption characteristics for bioimaging.

2Pos314 統合情報理論に基づいたスイッチング DNA 論理回路の構築
Construction of Switching DNA Logic Circuit based on Integrated Information Theory

Fumika Kambara[1], Sotaro Takiguchi[1], Hiroki Watanabe[2], Masahiro Takinoue[2], Ryuji Kawano[1] ([1]*Department of Biotechnology and Life Science, Tokyo University of Agriculture and Technology / Japanese*, [2]*Department of Life Science and Technology, Tokyo Institute of Technology / Japanese*)

DNA computing has attracted attention as a tool for implementing a wide range of information processing. The next step in advanced computation is constructing and theoretically systemizing an automatically controllable molecular system, which requires information feedback. Benefitting from Integrated Information Theory (IIT), we here propose a switching DNA logic circuit with a feedback function. Our designed circuit switches from AND to OR circuit depending on an output strand and its feedback. The feedback function was theoretically confirmed by IIT-based quantitative analysis. After the theoretical examination, we experimentally confirmed the respective behaviors of the AND and OR circuits by gel electrophoresis, producing the output strand following the truth table.

2Pos315 (2SDA-5) ATP を検出可能な DNA ナノポアセンサの開発
(2SDA-5) ATP-detectable DNA nanopore sensor

Hiromu Akai, Kan Shoji (*Nagaoka University of Technology*)

Nanopore sensors, that can electrically detect target molecules, are a powerful tool for single molecular analysis. However, the molecular selectivity and usable conditions of biological nanopores were limited. Thus, DNA-based nanopores are expected as alternative nanopores because of their high designability and robustness. Here, we proposed DNA nanopores, that can repeatedly open and close in response to ATP, as a model for molecular-selective DNA nanopores. DNA aptamers, which specifically bind to a molecule, were applied as a molecular-recognition domain of the molecular-responsive DNA nanopore. In this study, we investigated the molecular response-ability of the DNA nanopore by measuring the channel currents through the nanopore with multiple ATP concentrations.

2Pos316* カスケード反応における酵素複合体形成の寄与
Contribution of three-enzyme complex via 3-way junction DNA to activity of the cascade reaction

Aoi Mameuda, Koki Kamiya (*Grad. Sch. Sci. Tech. , Gunma Univ.*)

A proximity of enzymes into a cytoplasm causes efficient cascade reactions of enzymes. Hence, enzyme efficiencies *in vitro* will be improved by a local increase in concentration of enzyme. In this study, we attempt to closely assemble three enzymes using 3-way junction DNA. We prepared single stranded DNAs (ssDNAs) which can form the triply-branched structure by a hybridization reaction. The ssDNA with terminal amino group was conjugated to NHS ester-PEG_4-maleimide. To obtain ssDNA-PEG_4-Protein, three types of thiolated enzymes (horseradish peroxidase, glucose oxidase and β-galactosidase) were conjugated with three different ssDNA-PEG_4-maleimide, correspondingly. Activity of the three-enzyme complex in the cascade reaction was higher than that of free enzymes.

2Pos317 様々な形状の DNA 検出のための β ストランド数変化した改変型 β バレルナノポアタンパク質の構築
Modified β-barrel nanopore-forming protein with changed the number of β-strands for detection of various-shaped of DNA

Toshiyuki Tosaka, Koki Kamiya (*Grad. Sch. Sci. Tech. Gunma Univ.*)

Recently, nanopore-forming protein has attracted attention as biological sensors for single-molecule detection and sequencing of single-stranded DNA or polypeptide chain. OmpG in outer membrane of the gram negative bacteria forms a stable β-barrel nanopore composed of 14 β-strands. In this study, to create mutant OmpGs with various size of nanopores for detection of various-shaped DNA, we prepare mutant OmpGs from different number of β-strands. The ion permeability and the pore size of mutant OmpGs were measured using a patch clamp method of the artificial lipid bilayer. A change of ion permeability and pore size depends on the number of β-strands. In addition, we tried to the detection of various-shaped DNA using a mutant OmpGs.

2Pos318 塩基配列の設計による DNA 液滴の安定化
Stabilization of DNA droplets by designing base sequences

Kazuki Kobayashi[1], Satoshi Takahashi[2], Masahiro Takinoue[1,2] ([1]*Dept. Life Sci. Tech., Tokyo Tech*, [2]*Dept. Computer Sci., Tokyo Tech*)

The DNA droplet is a fluid state of the DNA self-assembly system consisting of branched nanostructures such as X-shaped DNA motifs. The programmability of DNA sequences and controllability of molecular interactions allow DNA droplets various applications such as miRNA biosensing and artificial cell construction. However, DNA droplets cannot exist stably except under certain conditions, making it difficult to apply the DNA droplets in vivo. Therefore, we have been attempting to stabilize DNA droplets by strengthening the interaction between DNA molecules using long single-stranded DNA (ssDNA). We believe that our study will contribute to the development of molecular devices for biomedical applications.

2Pos319* 液-液相分離に基づく分子検出ための DNA 液滴コンピュータ
Computational DNA droplets based on liquid-liquid phase separation for molecular detection

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Phase-separated biomolecular droplets are formed in cells to regulate various biological processes. Programmable phase-separated droplets, called DNA droplets, have recently been reported as artificial intracellular compartments. We constructed a computational DNA droplet that can recognize specific combinations of tumor marker microRNAs (miRNAs) as molecular inputs and output the results of DNA logic operations through physical DNA droplet phase separation. We demonstrated that the computational DNA droplet could perform miRNA pattern recognition represented by the logical formula ((miRNA-1 ∧ miRNA-2) ∧ (miRNA-3 ∧ ¬miRNA-4)). Research is underway to enable observation using microwells to observe multiple samples simultaneously and promote the development of chips.

2Pos320* 油中水滴を活用した新規蛍光 RNA アプタマー創出法の開発
Feasibility study of the method for obtaining fluorogenic RNA aptamers using water-in-oil microdroplets

Keisuke Ito, Ryo Iizuka, Sotaro Uemura (*Dept. Biol. Sci., Grad. Sch. Sci., The Univ. Tokyo*)

Fluorogenic RNA aptamers (FRs), which specifically bind to nonfluorescent dyes and drastically enhance fluorescence, are useful for live cell RNA imaging. Most FRs were engineered through repeated rounds of *in vitro* selection based on the binding to the target dyes; the selected RNAs do not always enhance fluorescence upon the binding to the dyes. We then developed a method to obtain FRs using fluorescence-based *in vitro* selection with water-in-oil microdroplets. To confirm the feasibility of the method, a pilot experiment was performed using Spinach2 and DHFBI-1T. DNA constructs encoding Spinach2 and noncognate RNA were mixed at a ratio of 1:100 to prepare a model library. We successfully recovered the sequence encoding Spinach2 from the library.

2Pos321 有殻アメーバの頑健な卵型被殻構築過程の 4D イメージングおよび模型作成
4D Imaging and 3D modeling of the robust egg-shaped shell construction process of testate amoeba

Mami Nomura[1], Yukinori Nishigami[2], Josephine Galipon[3], Masatoshi Ichikawa[4], Takuro Nakayama[5], Keisuke Ohta[6], Kei-ichiro Nakamura[6] ([1]*Fac. Sci., Yamagata Univ.*, [2]*RIES, Hokkaido Univ.*, [3]*IAB, Keio Univ.*, [4]*Dept. Phys., Kyoto Univ.*, [5]*CCS, Univ. Tsukuba*, [6]*Sch. of Med., Kurume Univ.*)

The testate amoeba *Paulinella micropora* has a robust egg-shaped shell composed of about 50 scales. The extracellular scales are manipulated by thick pseudopodium to construct a shell for the daughter cell, which is the same shape as the shell of the maternal cell. Our purpose is to reveal how a single-celled testate amoeba manipulates and arranges extracellular scales to construct a robust shell. Using confocal laser microscopy, we observed the movement of scales during shell construction and found that the scales changed direction and position quite dynamically before they were placed in the correct position. A model of the shell was then printed using a 3D printer, and a model of the capsule was built from the 52 printed scales.

2Pos322* ナノダイヤモンドを用いたアミロイド β 蛋白への新規標的治療法の検証
Verification of a new targeted therapy against amyloid-β using nanodiamonds

Miwa Shintani[1,2], Shin-ichiro Yanagiya[2], Hiroki Takanari[2] ([1]*Grad. Sch. opt., Uni. Tokushima / Japanese*, [2]*Post-LED Photonics Inst., Uni Tokushima / Japanese*)

New treatments for Alzheimer's disease targeting Amyloid β (Aβ), such as photothermal therapy (PTT) using metal nanoparticles, have been actively investigated. We examined the potential of PTT against Aβ using nanodiamond (ND) and ND with nitrogen-vacancy center (NVND). Aβ (190 μg/mL) dissolved in Tris-HCl (pH 8.0) and dimethyl sulfoxide was mixed with colloidal solutions of ND or NVND and irradiated with an 800-nm femtosecond pulsed laser (600 mW). Western blot experiments showed that NVND significantly reduced Aβ in the solution, and ND also transiently reduced Aβ immediately after laser irradiation. Although the mechanism is still unclear, the results indicate the potential of nanodiamond as a biocompatible carbon-based material for targeted therapy of Aβ.

2Pos323 関西におけるアカハライモリの警戒色の斑紋パターンの多様性
Diversity of warning coloration pattern in Kansai red-bellied newts

Sora Kazumi[1], Rikiya Ogawa[2] ([1]*Osaka Prefecture Tondabayashi High School*, [2]*Rikijuku Science School*)

Cynops pyrrhogaster in Japan is known to have some different populations based on morphological studies. The boundary of populations is ambiguous. I'm interested in difference of pattern of warning coloration. I compare complexly of it and compare red area of abdomen to study about factor varies the patterns in Kansai area. I measured length of speckles, head and body length, and the red area of abdomen each newts. Then, I made boxplots to compare each sampling points. Comparation of the red area of abdomen between populations with genetically different populations. Showed differences in the scatter of numerical values, different populations are thought to have different coloration. Two populations distance between the two sampling points didn't differ the complexly.

2Pos324 クサカゲロウの翅の反射防止性能
Anti-reflectivity in green lacewing wings

Yuro Katsurashima[1], Leona Takahashi[2], Kazunari Yoshida[1] ([1]*Grad. Sch. Sci. Eng., Univ. Yamagata*, [2]*Grad. Sch. Sci. Eng., Univ. Aoyama Gakuin*)

The structures and the functionality of various insect wings have been studied. For instance, an anti-reflective moth-eye structure has been attracting attention and is quite famous. As a part of such research themes, we focused on the green lacewing wings. The green lacewing wings are transparent and have fine structures consisting mainly of oil and fat. The transparent wings of insects tend to have anti-reflective functions. However, the optical properties of the green lacewing wings are still unclear. In this study, we used the finite-difference time-domain (FDTD) method to calculate the behavior of light penetration through the wings. It was found that the concentration of light on the surface protrusions of the wings suppressed reflections.

2Pos325 Enzymatically controlled micro-patterning of self-assembled nanoparticles by surface-bound ATP

Ekta Shandilya, Subhabrata Maiti (*Indian Institute of Science Education and Research (IISER) Mohali, Punjab, India - 140306*)

Non-equilibrium surface patterning of catalytically active soft matter or nano/microparticles is vital in diverse areas. Here, we used affinity between specific enzyme (alkaline phosphatase, ALP) and its substrate (mostly ATP), which is non-covalently bound to a nanoparticle surface, **to prompt assembly of overall ensemble in a spatiotemporally controllable way under flow or no flow conditions.** for this, we used a cationic nanoparticle aggregation phenomenon taking place in presence of multivalent anionic nanoparticle binding ATP and ALP. Overall, this work merges patterning of nanoparticles and enzyme in one platform **(theoretically and experimentally),** just by self-assembled nanoparticles, demonstrating a unique method for macrobiopatterning with potential applications.

3Pos001 全原子シミュレーションを用いた βαβ モチーフのレジスタシフトルールの解明
Explaining empirical rules of register shift of βαβ-motif by physical interactions

Senji Mishima, Hiroto Murata, George Chikenji (*Dept. of App. Phys., Grad. Sch of Eng., Nagoya Univ.*)

A register shift in a β-sheet is defined as a residue offset between terminal residues of adjacent β-strands. Previously, we reported that register shift rules are important for *de novo* design of β-sheet proteins; according to the PDB analysis, preferred register shifts in a βαβ-motif strongly depend on the loop torsion types; and the empirical rule of the register shifts of the most frequently observed loop-type (GB-loop) was explained by physical interactions. To deepen our understanding of the relationship between loop-types and register shifts from a physical viewpoint, we performed all-atom calculations for βαβ-motifs with another popular loop-type (GBA-loop). Detailed results will be reported in the presentation.

3Pos002 Structural Validation Properly Regulates Boost Potentials in the Biased Sampling of Proteins

Takunori Yasuda[1], Rikuri Morita[2], Yasuteru Shigeta[2], Ryuhei Harada[2] ([1]*University of Tsukuba, Doctral Program in Biology*, [2]*University of Tsukuba, Center for Computational Sciences*)

Free energy landscapes (FELs) of proteins are indispensable for evaluating their thermodynamic properties. Molecular dynamics (MD) simulation is a computational method to calculate the FELs. However, conventional MD simulations often fail to search broad conformational subspaces. While well-designed external biases allow for the broad conformational sampling of proteins, improper ones tend to collapse their structures due to unreasonably strong perturbations. To prevent the collapse, we focused on a structural validator called G-factor, and it was used to properly regulate the external biases. Based on the G-factor, we proposed a scheme for regulating biased sampling, which is referred to as a G-factor-based external bias limiter (GERBIL).

3Pos003 補酵素結合と二量体化による細菌の 3α - ヒドロキシステロイド脱水素酵素（3αHSDs）の構造揺らぎ変化に対する MD シミュレーション
MD simulation study of fluctuation changes of bacterial 3a-Hydroxysteroid Dehydrogenases (3aHSDs) by coenzyme binding and dimerization

Kahoru Amakawa[1], Hiroki Suzuki[2], Ayako Shiota[2], Masayuki Oda[2], Juha Lintuluoto[3], Masami Lintuluoto[2] ([1]*Fac. Life and Env., Univ. Kyoto Prefectural*, [2]*Grad. Sch. Life and Env. Sci., Univ. Kyoto Prefectural*, [3]*Grad. Sch. Eng., Univ. Kyoto*)

Bacterial 3aHSD catalyzes the conversion of hydroxysteroid with coenzymes NADH and/or NADPH. The 3aHSDs from Pseudomonas sp. B-0831 (Ps3aHSD) and from Comamonas testosteroni (Ct3aHSD) with high sequence homology showed high structural similarities, while their coenzyme specificities and their binary complex manners with coenzymes have been reported to be different from the experimental studies. In this work, we examined the dimer interactions and coenzyme specificities of Ps3aHSD and Ct3aHSD by using MD simulations. The dimerization of apo-monomer subunits reduced the fluctuation around the binding site in Ps3aHSD, while the fluctuation in apo-dimer of Ct3aHSD increased. The NADH binding also affected the structural stability and the fluctuation around the binding site.

3Pos004 Structural determinants for distinguishing frequently and rarely occurring psi-loop motifs

Tomoki C. Terada, Takumi Nishina, George Chikenji (*Dept of Appl. Phy., Grad. Sch. of Eng., Nagoya Univ.*)

The psi-loop motifs are defined by consecutive three beta strands on the amino acid sequence that include hairpin connection with one intervening strand, and they have four possible distinct connecting topologies. Although these four psi-loop topologies are structurally very similar to each other, the frequencies of these topologies in PDB are largely different: only the two of them are observed frequently and the others are rare. Addressing a question why their observed frequencies are so different is important for understanding structure-sequence relationship of proteins, but a consensus has not been reached. Here we study the origin of the difference by the database analysis and physics based simulations.

3Pos005 蛋白質の荷電性残基が液-液相分離に及ぼす影響に関する粗視化分子動力学法による検討
A Coarse-Grained Molecular Dynamics Study to elucidate the effect of charged residues of proteins on liquid-liquid phase separation

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Certain intrinsically disordered proteins are known to form droplets by liquid-liquid phase separation (LLPS) and have important biological functions. To solve the formation mechanism, we have applied coarse-grained molecular dynamics (CG-MD) simulations to a part of the low-complexity domain of protein FUS (57 resides peptide, positions 39 to 95). In this study, three residues in various positions were mutated to three negatively charged Glu residues to verify the effect of the electrostatic interaction. As the model of LLPS, the formation of the aggregates was investigated in a system consisting of the 100 peptide molecules by using CG-MD. From these results, we examined the effect of the distribution of charged residues on the LLPS.

3Pos006 3D Convolutional Neural Network を用いたタンパク質-ペプチドドッキングモデルの評価
Structure evaluation for protein-peptide docking models using 3D convolutional neural networks

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Protein-peptide interactions play critical roles in a wide variety of biological processes, such as cell signaling and immune response. The tertiary structures of their complexes can provide valuable clues to elucidate the molecular mechanisms. The structural determination of the protein-peptide complex through experimental procedures is often challenging because of its flexibility. The computational docking method could be one of the promising approaches to tackle the hurdle. However, the practical use has been hampered by the poor accuracy in the scoring function. Here, we address to develop a 3D convolutional neural network model to evaluate the probability of protein-peptide complex models with high accuracy and low computational costs.

3Pos007 深層学習を用いたタンパク質ドメインの予測研究
A deep-learning model for the prediction of protein domains

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Predicting the conformational changes of proteins from their structures and amino-acid sequences would be useful for drug design. As a first step, we developed a deep-learning model for predicting protein domains from their amino acid sequences. The Transformer, which is a method in the field of natural language processing, was employed for the deep-learning model. As the training and testing of the deep-learning model, proteins before and after the conformational change upon ligand binding were taken from Protein Structural Change Database. The domain of each protein was defined using the Motion Tree, and each residue of proteins labeled with domain A or B. In our presentation, details of our deep-learning model and results of the test will be discussed.

3Pos008 Structure of the IscB–ωRNA ribonucleoprotein complex, the likely ancestor of CRISPR-Cas9

Kazuki Kato[1], **Sae Okazaki**[1], Soumya Kannan[2], Han Altae-Tran[2], Yukari Isayama[1], Junichiro Ishikawa[1], Rhiannon K Macrae[2], Tomohiro Nishizawa[3], Kira S Makarova[4], Eugene V Koonin[4], Feng Zhang[2], Hiroshi Nishimasu[1] ([1]*RCAST.,Univ.Tokyo*, [2]*MIT*, [3]*Grad.Sch.Medical Life Science.,Univ.Yokohama City*, [4]*NCBI*)

IscB is an RNA-guided nucleases, and likely ancestors of Cas9 in the type II CRISPR-Cas adaptive immune system. IscB associates with ωRNA to form a ribonucleoprotein complex that cleaves DNA targets complementary to an ωRNA guide segment. Here, we report the cryo-EM structure of an IscB–ωRNA–target DNA complex. The structure shows how the IscB protein assembles with the ωRNA and mediates RNA-guided DNA cleavage. The ωRNA structurally and functionally compensates for the nucleic-acid recognition lobe of Cas9, and participates in the recognition of the guide RNA–target DNA heteroduplex. These findings provide insights into the mechanism of the programmable DNA cleavage by the IscB–ωRNA complex and the evolution of the type II CRISPR-Cas9 effector complexes.

3Pos009 Benchmark of force fields to characterize the short intrinsically disordered region of FUS-LC domain

Maud Chan-Yao-Chong, Justin Chan, Hidetoshi Kono (*Molecular Modelling and Simulation (MMS) Team, National Institutes for Quantum Science and Technology (QST)*)

Amyloid fibrils formations are involved in neurodegenerative diseases such as Alzheimer's disease, Amyotrophic Lateral Sclerosis (ALS). The proteins associated with the formation of amyloid fibrils are Intrinsically Disordered Proteins (IDP) in the native state.
The FUS Low-complexity (LC) domain is such an IDP. This domain is of interest because in ALS patients, mutants in this domain enhance amyloid fibrils and increase stability. Unfortunately, not all the force fields (FF) used in molecular dynamics simulation well describe the behavior of IDPs. To study the mechanism of FUC-LC fibril, we benchmarked 12 all-atom FFs to evaluate if they can sample both IDP and amyloid fibrils structures. We report how well the FFs reproduce the structures of the FUS-LC domain.

3Pos010 Photon Factory における BioSAXS 測定システムの高度化
Upgrade of BioSAXS measurement system at the Photon Factory

Nobutaka Shimizu, Hideaki Takagi, Yasuko Nagatani, Takeharu Mori, Keiko Yatabe, Masatsuyo Takahashi, Noriyuki Igarashi (*PF, IMSS, KEK*)

Three beamlines, BL-6A, BL-10C, and BL-15A2, are dedicated to small-angle X-ray scattering (SAXS) experiments at the Photon Factory (PF). SAXS for biological macromolecules (BioSAXS) is utilized to understand the properties and structural states of molecules in solution. Recently, advanced measurement systems such as the SAXS systems combined with gel filtration (SEC-SAXS) have also made possible polydisperse complex analysis. We, PF support BioSAXS measurement and analysis for BioSAXS unfamiliar users under the new AMED's platform project, BINDS (Phase II, 2022~), at BL-10C and BL-15A2. This presentation will introduce not only the upgrades of our BioSAXS measurement systems but also the latest collaborative works as model studies.

3Pos011 Structure determination of Ferritin at room temperature in microfluidic chips

Yusuke Kono, Leonard Chavas (*Dept of Appl. Phys., Grod. Sch. of Eng., Nagoya Univ.*)

he structure of a protein provides an understanding of how the protein works.
At low temperature the high quality structural data of Ferritin is available. However, Structure determination of Ferritin at room temperature is not finished. Here, we use microfluidic chips to observe Ferritin at room temperature.

3Pos012 分子動力学計算による FtsZ の構造変化機構の解析
Molecular dynamics simulations on the conformational stability of FtsZ with the different bound nucleotides

Taichi Takasawa[1], Go Watanabe[2,3], Yoshio Kodera[2,4], Takashi Matsui[2,4] ([1]*Grad. Sch. Sci., Kitasato Univ.*, [2]*Sch. Sci., Kitasato Univ.*, [3]*KISTEC*, [4]*Cent. Disease Proteomics*)

FtsZ is a prokaryotic tubulin homolog and is an essential role in bacterial cell division. FtsZ bound with GTP polymerizes into tubulin-like protofilaments accompanied by the conformational change of the subunit from Relaxed to Tensed states. While the head-to-tail polymerization, the upper subunit hydrolyzes GTP accommodated in the next one to GDP may also cause the conformational change of the subunit subsequently FtsZ with bound GDP depolymerizes. However, the molecular cycle of this conformational change has been unveiled. In this study, molecular dynamics simulations of monomeric FtsZ derived from *Staphylococcus aureus* in the Relaxed and Tensed states bound with GTP or GDP were performed. Here we discuss the conformational stability difference among them.

3Pos013 (2SEA-7) Optineurin の E50K 緑内障変異はオリゴマー粒径を増大させる
(2SEA-7) The E50K mutation of optineurin increases the oligomer size

Rintaro Kawamura[1], Soya Uetsuki[1], Takehito Tanzawa[2], Takayuki Kato[2], Masataka Kinjo[3], Akira Kitamura[3] ([1]*Grad. Sci. Life Sci., Hokkaido Univ.*, [2]*Inst., for Proteins Res., Osaka Univ.*, [3]*Fac. Adv. Life sci., Hokkaido Univ.*)

Optineurin (OPTN) is a coiled-coil-rich oligomerization protein. E50K mutant of OPTN (EK), associated with glaucoma, forms larger foci in the cytoplasm than its wild type (WT). However, little is known about their oligomerizing mechanism. The oligomeric states of purified recombinant WT and EK were analyzed using Native-PAGE, Dynamic light scattering (DLS), and negative stain transmission electron microscopy (TEM). Native-PAGE showed that WT mainly formed pentamers, whereas EK was heptamers. DLS showed that EK formed oligomers of larger and diverse particle size than WT. Furthermore, ring-like structures of OPTN were observed using TEM. Consequently, the higher order of EK oligomers may be because the assemble angle between intermolecular coiled-coils would be shifted.

3Pos014 鶏卵白リゾチームの D/H コントラスト法を利用した中性子結晶解析
Neutron crystallography of hen-egg white lysozyme using D/H contrast technique

Toshiyuki Chatake[1], Ichiro Tanaka[2], Katsuhiro Kusaka[3], Satoru Fujiwara[4] ([1]*Inst. Integ. Rad. Nucl. Sci., Kyoto Univ.*, [2]*Grad. Sci. Eng., Ibaraki Univ.*, [3]*Front. Res. Cent. App. Atom. Sci., Ibaraki Univ.*, [4]*Inst. Quantum Life Science, QST*)

Neutron scattering lengths of hydrogen and its isotopes are comparable to non-hydrogen atoms. Hence, neutron crystallography has an advantage on observing hydrogen atoms in proteins. In addition, a large difference of scattering lengths between hydrogen (H) and deuterium (D) provides high detectability of hydrogen atoms, in the contrast map between D_2O- and H_2O- solvent crystals. The technique of calculating the contrast map, in which the subtraction of D and H was carried out in real space, was developed previously. In the present study, a neutron D/H contrast crystallographic analysis of hen-egg white lysozyme was performed, to reveal the details of protonation states and hydration of this protein.

3Pos015 多分散溶液中の生体高分子の構造解析のための超遠心分析と小角散乱による統合アプローチ
Integrated approach to biomacromolecular structure in polydisperse solution with analytical ultracentrifugation and small-angle scattering

Ken Morishima, Rintaro Inoue, Aya Okuda, Nobuhiro Sato, Masahiro Shimizu, Yasuhiro Yunoki, Reiko Urade, Masaaki Sugiyama (*Institute for Integrated Radiation and Nuclear Science, Kyoto University*)

To build a reliable structural model of a biomacromolecule in a solution with small-angle X-ray and neutron scatterings (SAS), it is indispensable to obtain a SAS profile purely from a target molecule. However, in spite of a purification, non-specific aggregates often remain in the solution. Even if the weight fraction of the aggregates is a few percent, the experimental SAS profile is deteriorated by the aggregates, and it leads to an incorrect structural model as the target molecule. To overcome this problem, an integrated approach, “AUC-SAS”, was developed with analytical ultracentrifugation (AUC) and SAS. AUC-SAS derives the SAS profile of a target molecule from the deteriorated experimental profile using the information provided by AUC.

3Pos016 クライオ電子顕微鏡による高精度構造解析
High-precision structural analysis by cryo-electron microscopy

Tasuku Hamaguchi[1], Keisuke Kawakami[2], Saori Maki-Yonekura[2], Koji Yonekura[1,2] ([1]*IMRAM, Tohoku Univ.*, [2]*RIKEN SPring-8 Center*)

Single-particle cryo-EM collects movies of protein particles embedded in thin vitreous ice. Dose-dependent weighting for movie frames can give high-resolution reconstructions, but the scheme is not ideal for proteins containing cofactors with metallic ions, which are extremely susceptible to electron radiation. We investigated conditions to minimize radiation damage for a membrane protein complex photosystem I, which contains many chlorophylls and other cofactors. We found that an electron dose of 1.3 $e^-/Å^2$ (equivalent to ~ 4.8 MGy) kept most of the cofactors in intact conformations. We will also introduce high-resolution 3D maps of other examples, whose images were acquired from gold-sputtered grids and by an AI-assisted system, and discuss the merits of our approach.

3Pos017 Preparation of phosphorylated FROUNT protein, a regulator of chemokine receptors, for structural and functional analyses

Keisuke Uchida[1], Sosuke Yoshinaga[1], Takafumi Sato[1], Mitsuhiro Takeda[1], Yuya Terashima[2,3], Etsuko Toda[2,3,4], Kouji Matsushima[2,3], Hiroaki Terasawa[1] ([1]*Fac. Life Sci., Kumamoto Univ.*, [2]*Grad. Sch. Med., Univ. Tokyo*, [3]*RIBS, Tokyo Univ. Sci.*, [4]*Nippon Med. Sch.*)

Chemokines released from inflamed sites, are recognized by chemokine receptors on leukocytes, thus triggering leukocyte cell migration. It has been found that cancer diseases occur when these chemokine signals are disturbed. Therefore, anticancer agents can be developed by controlling the chemokine signals. We found a cytoplasmic signaling protein, FROUNT, which binds to a chemokine receptor CCR2 (*Nature Immunol.*, 2005). Recently, FROUNT was found to be phosphorylated in the cell migration tips. The aim of this study is to prepare the phosphorylated proteins and analyze the effects of the phosphorylation on the structure and the chemokine-binding capacity. Based on the structural information, we will develop compounds that regulate FROUNT for cancer therapeutics.

3Pos018 Computational analysis on the effects of active-site reduction on structures and dynamics of plant-type ferredoxin

Tomoki Nakayoshi[1], Yusuke Ohnishi[2], Hideaki Tanaka[2], Genji Kurisu[2], Yu Takano[1] ([1]*Grad. Sch. Inf. Sci., Hiroshima City Univ.*, [2]*Inst. Protein Res., Osaka Univ.*)

Plant-type ferredoxin (Fd) contains [2Fe–2S] clusters in the active center, which is ligated with four cysteine (Cys) residues. In physiological conditions, [2Fe–2S] cluster mainly takes two electronic states, and plays a role as a single-electron carrier. Conformational changes in Fds associated with electron transfer change the interaction between electron donor and acceptor, and accelerate the formation and dissociation of electron donor-acceptor complexes. Analysis of the structures and behaviors of Fds contributes to the elucidation of the electron-transfer mechanisms. In this study, we computationally analyzed the detailed effects of active-site reduction in Fds on the structures and dynamics using the recently determined high-resolution X-ray crystal structures.

3Pos019 Efficient Conformational Sampling with an Adaptive Coarse-Grained Elastic Network Model using Dynamic Cross-Correlation Coefficient

Ryo Kanada[1], Kei Terayama[2], Atsushi Tokuhisa[1], Shigeyuki Matsumoto[3], Yasushi Okuno[1,3] ([1]*RCCS, RIKEN*, [2]*Grad. Sch. Medical Life Sci., Yokohama City Univ.*, [3]*Grad. Sch. Medicine, Kyoto Univ.*)

Coarse-Grained simulation based on structure based model are unsuitable for sampling structures that depart significantly from the initial structure without any biased force. We developed a new adaptive CG elastic network model (ENM), in which the dynamic cross-correlation coefficient based on short-time AA-MD of at most ns order is considered. To evaluate the performance of adaptive CG-ENM, we applied the new methodology to several proteins such as glutamine binding protein (GBP) in the apo state. The results showed that the structural ensembles explored by adaptive CG-ENM could be considerably more diverse than those by conventional ENMs with enhanced sampling such as temperature replica exchange MD and long-time AA-MD.

3Pos020 Structural basis of actin-microtubule crosstalk mediated by GAS2

Jiancheng An, Tsukasa Makino, Masahide Kikkawa (*The University of Tokyo*)

Crosstalk between actin filament (F-actin) and microtubule mediated by crosslinking proteins is crucial for cell shape and polarity. Members of the growth arrest-specific 2 (GAS2) protein family mediate crosstalk between F-actin with microtubules and consist of a putative actin-binding (CH) domain and microtubule-binding domain (GAR) and play crucial roles in various cellular processes.
To understand the structural basis of the GAS2, here, we solved the structures of the GAR-domain-MT complex and CH-domain-F-actin complex using cryo-electron microscopy and single-particle analysis. Based on these results, I will discuss a simple interaction model for actin-microtubule cross-talk mediated by GAS2.

3Pos021 Cryo-EM structure of an osmotically sensitive Ca^{2+} ion channel

Honoka Hosoki, Tatsuya Hagino, Kanae Demura, Wataru Shihoya, Tsukasa Kusakizako, Osamu Nureki (*Grad.Sch.Sci.,Univ.Tokyo*)

Organisms sense and respond to various physical stimuli from the outside world, such as thermal, mechanical, and chemical stimuli via plasma membrane. In particular, mechanical stimuli, including osmotic pressure and stretch stimuli, are sensed by mechanosensitive channels. Some of the mechanosensitive channels are Ca^{2+}-permeable and function as sensor molecules. Here, we determine the cryo-EM structure of an osmotically sensitive Ca^{2+} channel at 2.7 Å resolution. Compared with homologues of known structure, our structure contains distinctive features, which might explain the difference in sensitivity to osmotic pressure between the homologs of this channel. In this conference, I discuss the structural features of this channel and comparisons with homologues.

3Pos022 結晶構造から明らかになったシゾロドプシンの内向きプロトン輸送機構
Crystal structure of schizorhodopsin reveals mechanism of inward proton pumping

Wataru Shihoya[1], Akimitsu Higuchi[1], Masae Konno[2], Tatsuya Ikuta[1], Hideki Kandori[3], Keiichi Inoue[2], Osamu Nureki[1] ([1]*Grad. Sch. Sci., The Univ of TOkyo*, [2]*ISSP, The Univ of TOkyo*, [3]*Life Sci. Appl. Chem., Nagoya Inst. Tech.*)

We present a high-resolution structure of schizorhodopsin (SzR), a new rhodopsin family identified in Asgard archaea. SzRs work as light-driven inward H^+ pumps as bacterial xenorhodopsins. Although SzRs are phylogenetically located at an intermediate position between type-1 microbial rhodopsins and heliorhodopsins, the structure of SzR resembles that of bacteriorhodopsin. Notably, the cytoplasmic parts of the transmembrane helices in SzR are shorter than those in other microbial rhodopsin, and thus the putative H^+ acceptor E81 is located near the cytosol. Thus, we propose a model of untrapped inward H^+ release through a water-mediated transport network.

3Pos023 タンパク質中性子回折実験における水素高感度検出のための技術開発
Technological development for high-sensitivity detection of hydrogen in protein neutron diffraction experiments

Ichiro Tanaka[1,2], Hideki Yamauchi[1], Yohei Noda[1,2], Tomoki Maeda[2], Satoshi Koizumi[1,2] ([1]*Grad. Sch. Sci. Eng., Ibaraki Univ.*, [2]*Frontier Res. Center Appl. Atomic Sci., Ibaraki Univ.*)

The dynamic nuclear polarization(DNP) technique in neutron diffraction can increase the hydrogen detection sensitivity. This is because the relative scattering length of hydrogen becomes about 8 times larger at maximum can be obtained. This technique will be useful for obtaining the positional information of active hydrogen atoms in the molecules. By using a super-conducting 7 T magnet installed at BL20 in MLF in J-PARC, nuclear polarization experiments of protein polycrystal were conducted. Using samples in H_2O and D_2O buffers, different diffraction patterns between both buffers were observed, this suggests neutron scattering length of hydrogen could be changed successfully. And the maximum polarization rate was achieved at 68%.

3Pos024 FAP47, HYDIN, and CPC1 in the central pair apparatus of *Chlamydomonas*

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Motile cilia have nine doublet microtubules and central pair apparatus (CP). CP is thought to control the flagellar beating. Recently the components of CP are identified, but the mechanism how it contributes to the ciliary motility has much to be revealed. We focused on high molecular weight components of the central pair apparatus of *Chlamydomonas* flagella and studied the localization and the function of these components. FAP47-deficient cells have phototaxis defect. FAP47-deficiency makes the speed of the cells with CPC1 or HYDIN deficiency slower. In indirect immunofluorescence microscopy we observed FAP47 in the entire length of *Chlamydomonas* axonemes. Cryo-electron tomography revealed partial lack of C1-C2 bridge structure in FAP47-deficient strain.

3Pos025 昆虫由来不凍タンパク質は哺乳動物細胞を−5℃でも生存可能にする
Insect-derived antifreeze protein allows mammalian cells to survive at −5°C

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Mammalian cells for therapeutic use are often preserved at +4°C and the storage period is limited to a few days. Here, we examined the survival rate (%) of adherent rat insulinoma cells after 1, 3, 5, 10 and 20 days of “nonfreezing” preservation at −5°C, −2°C, or +4°C by employing commercial cell storage solutions, in which we dissolved fish- or insect-derived antifreeze protein (AFP). Our results show that the survival rate of the cells preserved with Euro-Collins solution containing insect AFP was always higher than that of the fish AFP solution after any preservation period at −5°C, −2°C, or +4°C. Significantly, insect AFP dissolved in University of Wisconsin solution kept 53% of the cells alive, even after 20 days of preservation at −5°C.

3Pos026 Integration of *In Silico* Strategies for Drug Repositioning towards P38α Mitogen-Activated Protein Kinase (MAPK) at the Allosteric Site

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P38α MAPK has been identified its pivotal role regulating physiological processes and inhibition of this target could provide therapeutic outcomes for various diseases. Herein, by using docking- and dynamic-based screening from 3,210 FDA-approved drugs, we found that lomitapide (a lipid-lowering agent) and nilotinib (a Bcr-Abl fusion protein inhibitor) could alternatively inhibit phosphorylation of p38α MAPK. The predicted binding affinity of two screened drugs suggested a high potential of being a successful inhibitor. Moreover, key influential amino acids and binding patterns were also elucidated in comparision to BIRB796. Altogether, our contributions might be exploited as attractive starting points for future drug development disrupting MAPK signaling pathway.

3Pos027 Designed darunavir derivatives against HIV-1 protease: A computational study

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Darunavir (DRV) is one of the potent human immunodeficiency virus type-1 (HIV-1) protease inhibitors (PIs). However, the protease mutations decrease DRV susceptibility. Hence, we designed and screened 232 DRV analogs *in silico*. The docking results showed the top 10 analogs interacting with the protease at the active site better than the DRV. Then these analogs were investigated by 500-ns molecular dynamics (MD) simulations. The root-mean-square deviation (RMSD) values and the number of H-bonds of DRV and their analogs were stable throughout the MD simulations. The lowest binding affinity of darunavir 1-3-2-1 was -26.29 kcal/mol compared to DRV. The analogs with strong interaction with the HIV-1 protease could serve as potential candidates for developing effective PIs.

3Pos028 Structural effects of spike variants that reshaped the pandemic

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Mutations in Spike (S) protein alter SARS-CoV-2 virus transmissibility, infectivity, and immune evasion. One single mutation, emerged in 2020, has dominated all circulating variants to date. Similarly, the recent antigenic drift in Omicron variants has taken over within a month. Both D614G and Omicron show higher infectivity rate. Here, we employed classical and enhanced sampling molecular dynamics simulations to dissect the underlaying mechanisms in both variants. Starting from wild-type, we induce structural changes in S-protein upon D614G mutation and 630 loop rigidification. The loss of anionic charge has local and global effects on S-protein stability and ACE2 accessibility. Similarly, the introduction of several mutations in Omicron alters Spike conformations.

3Pos029 コレラ菌走化性受容体 Mlp3 のリガンド認識機構
Ligand recognition mechanism of Mlp3, a chemoreceptor of *Vibrio cholerae*

Yuka Ueda[1], Yuzuki Yabunaka[1], Norihiro Takekawa[1], So-ichiro Nishiyama[2], Hirotaka Tajima[3], Ikuro Kawagishi[3], Katsumi Imada[1] ([1]*Dept. Macromol. Sci., Grad. Sch. Sci., Osaka Univ.*, [2]*Dept. Appl Life Sci, Niigata Univ of Pharm and Appl Life Sci.*, [3]*Dept. Front Biosci., Hosei Univ.*)

Toxigenic *Vibrio cholerae* has at least 45 genes for methyl-accepting chemotaxis protein-like proteins (MLPs). Among them, Mlp3 is involved in chemotactic response to amino acids, especially to serine, but does not bind serine. However, co-expression of Mlp3 with a putative periplasmic amino acid binding protein, in vmlp201 cells, a mutant strain of *V. cholerae*, showed an enhanced chemotactic response to serine. These results suggest that Mlp3 recognizes serine with the periplasmic protein. In this study, to reveal the ligand recognition mechanism of Mlp3, we determined the crystal structure of the periplasmic region of Mlp3 (Mlp3p). Surprisingly, Mlp3 bound a putative propionic acid. We will discuss the ligand recognition mechanism of Mlp3 based on the structure.

3Pos030 HIV 逆転写酵素の薬剤耐性変異に対する動的残基間相互作用ネットワーク解析
Dynamic Residue Interaction Network Analysis of HIV-1 Reverse Transcriptase for Drug Resistance Mutations

Ryuki Hashimoto, Norihumi Yamamoto (*Chiba Tech*)

Human immunodeficiency virus type 1 (HIV-1) is the pathogen of acquired immunodeficiency syndrome (AIDS), a disease that can be controlled in the long term by anti-HIV drugs. However, there are serious concerns about the emergence of viral mutants that are resistant to anti-HIV drugs. Some amino acid mutations in the HIV-1 reverse transcriptase are known to directly and substantially reduce drug efficacy against anti-HIV drugs. These mutations are referred to as drug resistance mutations. In this study, we used dynamic residue interaction network (dRIN) analysis based on molecular dynamics simulations to clarify dynamic correlations in the intermolecular interactions between drug-resistant mutants of HIV-1 reverse transcriptase and anti-HIV drugs.

3Pos031 HIV-1 の Nelfinavir 耐性プロテアーゼ D30N/L90M 変異体に対する動的残基間相互作用ネットワーク解析
Dynamic Residue Interaction Network Analysis of the Protease D30N/L90M Mutant Conferring Nelfinavir Resistance in HIV-1

Ryoga Miyawaki, Norihumi Yamamoto (*Chiba Tech*)

Human immunodeficiency virus type 1 (HIV-1) is the pathogen of acquired immunodeficiency syndrome (AIDS), a disease that can be controlled in the long term by anti-HIV drugs. However, there are serious concerns about the emergence of viral mutants that are resistant to anti-HIV drugs. The D30N mutant of the HIV-1 protease is known to be resistant to Nelfinavir. In adittion, the D30N/L90M dual mutation is known to significantly reduce the viral replicative capacity. In this study, we investigated the dynamic correlation between the binding of D30N/L90M mutant HIV-1 protease to Nelfinavir using dynamic residue interaction network (dRIN) analysis based on molecular dynamics simulation.

3Pos032 イオタ毒素 Ia-GFP キメラのタンパク質膜透過の確認と構造解析
Confirmation of protein membrane translocation and structural analysis of Iota toxin Ia-GFP chimera

Shun Tomoda, Tomohito Yamada, Hideaki Tsuge (*Graduate School of Life Science, Kyoto Sangyo University*)

Iota toxin from Clostridium perfringens is a binary toxin consisting of two components: Ia, which is an enzymatic component, and Ib, which is a membrane-transport component. In an acidified endosome, Ia translocates into cells via Ib-pore using the pH gradient, thereby causing cell toxicity. However, the detailed conditions for protein membrane-translocation are not known yet. In this study, Ia-GFP chimeras were prepared and studied the conditions under which Ia translocates. The structure of the chimera with and without translocation conditions were analyzed using cryo-EM. In addition, cell experiments would be conducted to determine whether the chimeras translocate the membrane or not.

3Pos033 酸化還元感受性の鉄硫黄クラスターを利用する tRNA 硫黄修飾酵素の反応機構
The reaction mechanism of tRNA sulfur modification enzymes using redox-sensitive iron-sulfur clusters

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tRNA requires sulfur modification and its disruption is linked to diseases. We previously reported the complex structure of the tRNA sulfur modification enzyme TtuA with sulfur donor protein TtuB, showing that TtuA has a redox-responsive co-factor [4Fe-4S]. However, it was unknown whether [3Fe-4S]-TtuA is an active form because [4Fe-4S] seems to be easily changed to [3Fe-4S]. Also, two different groups reported that TtuA homolog enzyme Ncs6 has [4Fe-4S] and [3Fe-4S], respectively.
Here, we controlled the redox conditions and analyzed the structure of iron-sulfur clusters and the enzymatic activity of TtuA in time-course. Our results proposed that the cross-validation of [4Fe-4S] and [3Fe-4S] is important to reveal the exact catalytic mechanism with iron-sulfur clusters.

3Pos034 A new enzyme from tardigrades which consists of ferritin-like and IgG-like domains

Subaru Kato, Yota Fukuda, Tsuyoshi Inoue (*Graduate School of Pharmaceutical Sciences, Osaka University*)

Some tardigrades can tolerate various extreme environments in the state called anhydrobiosis. They have proteins regarding these tolerances. Some of them are also found among a wide variety of organisms showing stress tolerances, implying the presence of an unknown ubiquitous mechanism to survive environmental stresses. We determined a crystal structure of one of such tardigrade proteins. It consists of ferritin- and IgG-like domains. The ferritin-like domain preferentially interacts with Zn ions, although ferritin-like domains normally accommodate Fe ions. We also found that it has a phosphatase activity albeit low. It has a hydrophobic and negatively charged path toward the metal binding site, suggesting its substrate has high hydrophobicity and positive charges.

3Pos035 生物発光タンパク質イクオリンのアロステリックな発光反応制御機構についての理論的研究
Theoretical study on allosteric control mechanism of a luminescent reaction of bioluminescent protein aequorin

Tomohiro Ando, Shigehiko Hayashi (*Grad. Sch. Sci., Kyoto Univ.*)

Aequorin is a blue light emitting protein of which a luminescent reaction is triggered by binding of calcium ions. In this study, we analyzed the allosteric correlation between the luminescent reaction of the luminescent substrate, coelenterazine, and structural changes of the protein through QM/MM free energy calculations. The calculations accurately determined molecular interaction between the substrate and the surrounding amino acid side chains that are important for the reaction, and also revealed dynamics of protein structural changes upon the binding of calcium ions which is expected to affect a proton transfer reaction that controls formation of the luminescent state. We will discuss energetics of the allosteric control mechanism of luminescent reaction.

3Pos036 Structural dynamics and kinase inhibitory activity of tyrosine kinase inhibitors against wild-type and mutant forms of EGFR

Rungrotmongkol Thanyada[1,5], Todsaporn Duangjai[1], Mahalapbutr Panupong[2], P. Poo-arporn Rungtiva[3], Choowongkomon Kiattawee[4] ([1]*Center of Excellence in Biocatalyst and Sustainable Biotechnology, Department of Biochemistry, Faculty of Science, Chulalongkorn University, Bangkok 10330, Thailand*, [2]*Department of Biochemistry, and Center for Translational Medicine, Faculty of Medicine, Khon Kaen University, Khon Kaen 40002, Thailand*, [3]*Biological Engineering Program, Faculty of Engineering, King Mongkut's University of Technology Thonburi, Bangkok, Thailand*, [4]*Department of Biochemistry, Faculty of Science, Kasetsart University, Bangkok 10900, Thailand*, [5]*Program in Bioinformatics and Computational Biology, Graduate School, Chulalongkorn University, Bangkok 10330, Thailand*)

Mutations in the tyrosine kinase domain of epidermal growth factor receptor (EGFR) are major causes of acquired resistance towards EGFR targeted drugs. In this work, a combination of molecular modeling and in vitro kinase inhibition assay was used to unravel the mutational effects of EGFR. The binding affinity of all studied inhibitors towards EGFR mutations was in good agreement with the experimental data, ranked in the order of osimertinib > afatinib > dacomitinib > erlotinib > gefitinib. Hot-spot residues at the hinge region (M790, M793, and C797) were involved in binding osimertinib and afatinib, enhancing their inhibitory activity towards mutated EGFRs. This work paves the way for further design of the novel EGFR inhibitors to overcome drug resistance.

3Pos037 RNA-seq 解析によるセイヨウイトスギの新規アレルゲン候補の探索
Searching for new allergen candidates in European cypress by RNA-seq analysis

Tomona Iizuka[1], Hélène Sénéchal[2], Pascal Poncet[3], Tomoyasu Aizawa[1] ([1]*Grad. Sch. Life Sci., Hokkaido Univ.*, [2]*Allergy & Environment, Armand Trousseau Children Hospital, Paris, France*, [3]*Immunology Department, Institute Pasteur, Paris, France*)

Identification of causative allergen components is important for accurate diagnosis and treatment of pollinosis. In this study, we sought to identify the amino acid sequence of a novel allergen candidate protein from European cypress (*Cupressus sempervirens*), one of the major pollinosis-causing trees in Europe. RNA-seq data from pollen and male flowers were analyzed to search for homologous proteins of allergens identified in other trees. By targeting transcripts, comprehensive analysis can be performed for proteins that are difficult to extract directly or only contain small amounts. The expression levels and tissue distribution were also examined, and data were obtained that will lead to future analysis at the protein level.

3Pos038 分子動力学法による自己集合性ペプチドの配列最適化
Sequence optimization of self-assembly peptides by using MD simulations

Koya Sato[1], Kota Kasahara[2], Hiroshi Imamura[2], Takuya Takahashi[2] ([1]*Grad. Sch. Life Sci., Univ. Ritsumeikan*, [2]*Coll. Life. Sci., Univ. Ritsumeikan*)

We discovered a 12-residue peptide (peptide A) with a β-sheet-like self-assembling structure from PDB. To obtain a guideline for designing a stable multimer structure (i.e., dimer, trimer and so on.), we performed MD simulations of the 12 different peptides, which were created by alanine scanning on the peptide A. Then, from the secondary structure propensity and the frequency of contact between atoms, the important sites for the stable dimer structure were obtained. The K12A, in which the 12th Lys is replaced by an Ala residue, showed an increase in the β-sheet structure and contact frequency. That is, the Lys12 residue seems to suppress self-assembly. We will further investigate mutations to various residues and optimize the sequence to enhance self-assembly.

3Pos039 緑色蛍光タンパク質のループ領域の静電ポテンシャルに影響を及ぼす部位特異的アミノ酸置換と分子構造および発光特性の相関
Correlation of amino acid substitutions affecting the electrostatic potential of loop region with structure and luminescence properties

Kaori Chiba, Kokomi Takanashi (*Indust. Eng. Natl. Inst. Tech, Ibaraki Coll. Japan*)

Peptide bind planarity is one of the most fundamental restrains for structure analysis of proteins. We have studied the correlation between the effect of the proton/deuteron near the main-chain carbonyl oxygen, localized by intramolecular electrostatic potentials and observed in neutron crystallography, on site-specific relaxation of the planarity of the peptide bond, and the ^{15}N chemical shift of the main-chain amide by NMR. In this presentation, we report on the effects of amino acid substitutions designed to alter the electrostatic potential near the main chain of the loop region of the β-barrel protein Green Fluorescent Protein, resulting in local changes in the physical properties of the peptide bond and its effects on molecular structure and optical properties.

3Pos040 分子動力学計算によるダイナミンの誘電アロステリー解析
Dielectric allostery of dynamin studied by molecular dynamics simulation

Masataka Yaguchi[1], Jun Ohnuki[2], Mitsunori Takano[1] ([1]*Dept. of Pure & Appl. Phys., Grad. Scl. Adv. Sci. & Eng., Waseda Univ.*, [2]*Inst. for Mol. Sci.*)

Dynamin, which plays a critical role in membrane fission in endocytosis, assembles into a large helical structure that constricts the membrane using the GTP hydrolysis energy. However, the force-generating mechanism for the constriction remains unclear. Interestingly, dynamin has a GTPase domain (G-domain) and such a lever-arm-like domain as in myosin, which is supposed to exhibit a power-stroke in the course of GTP hydrolysis. In the case of dynamin, nucleotide-dependent G-domain dimerization is also important. To shed light on the force-generating mechanism of dynamin in light of our previous study of myosin, we here investigate the dielectric response (i.e., dielectric allostery) of dynamin induced by the GTP binding and subsequent hydrolysis.

3Pos041 HIV-1 Vif タンパク質によるヒト抗ウイルス因子 APOBEC3 タンパク質のマルチファセットな無力化: ユビキチン化と脱アミノ化阻害
HIV-1 Vif drived multifaceted neutralization against human APOBEC family proteins: ubiquitination/degradation and deamination inhibition

Keisuke Kamba[1], Li Wan[1,2], Kentaro Tozawa[1,2], Ryo Iwaoka[1,2], Satoru Unzai[3], Ryo Morishita[4], Akifumi Takaori-Kondo[5], Takashi Nagata[1,2], Masato Katahira[1,2] ([1]*Inst. of Adv. Energy, Kyoto Univ.*, [2]*Grad. Sch. Energy Sci., Kyoto Univ.*, [3]*Frontier Bioscience, Hosei Univ.*, [4]*CellFree Sciences Co.,Ltd.*, [5]*Grad. Sch. Med., Kyoto Univ.*)

HIV-1 Vif protein neutralizes the antiviral activities of human APOBEC proteins (A3s). Vif hijacks four host proteins, a transcription factor CBFβ (β) and E3 ubiquitin ligase components, elongine B (B), elongine C (C), and culin5 (c), to form a five-membered complex, VβBCc. VβBCc had been known to degrade A3s via ubiquitin-proteasome proteolysis. We combined biophysical and NMR techniques and newly found that VβBCc directly inhibits the deaminase activities of various A3s, which is independent of above-mentioned proteolysis. Additionally, VβBCc were found to use all the components to bind A3s for deamination inhibition. Our study revealed that VβBCc uses different binding modes against A3s for its neutralization through proteolysis and deamination inhibition.

3Pos042 タンパク質構造の熱揺らぎと進化しやすさは相関している
Dynamics-Evolution Correspondence in Protein Structures

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The genotype-phenotype mapping of proteins is a fundamental question in structural biology. With a large dataset of proteins from hundreds of protein families, we quantitatively demonstrate the correlations between the noise-induced protein dynamics and mutation-induced variations of native structures, indicating the dynamics-evolution correspondence. Based on the investigations of the linear responses of proteins, the origin of such a correspondence is elucidated. As confirmed from the data, the noise- and mutation-induced deformations of the proteins are restricted on a common low-dimensional subspace. These results suggest an evolutionary mechanism of the proteins gaining both dynamical flexibility and evolutionary structural variability. [PRL, 127, 098103 (2021).]

3Pos043 シアン化物結合シトクロム酸化酵素の結晶構造から示唆される、金属中心の酸化状態変化による活性制御機構
Crystallographic cyanide-probing of cytochrome oxidase provides insights into its activity regulation by the redox change of metal sites

Atsuhiro Shimada[1], Kazumasa Muramoto[2], Kyoko Shinzawa-Itoh[2], Tomitake Tsukihara[3], Shinya Yoshikawa[2] ([1]*Dept. Appl. Life Sci., Fac. Appl. Biol. Sci., Gifu Univ.*, [2]*Grad. Sch. Sci., Univ. Hyogo*, [3]*Inst. Protein Res., Osaka Univ.*)

Cytochrome *c* oxidase (CcO) pumps protons via the proton conducting pathway, H-pathway, coupled with O_2 reduction reaction. It has been reported that each proton is transferred by sequential electron transfer from low potential metal sites to O_2 reduction site comprised of Fe_{a3} and Cu_B. Crystal structures determined at fully oxidized and reduced state suggest that, for unidirectional proton transfer, the structures of amino acids near the metal sites or H-pathway are changed upon the oxidation states of metal sites. In this study, effect of cyanide, which stabilizes specifically the ferric Fe_{a3}, on the crystal structures of CcO at various oxidation states were explored for identifying the metal sites triggering structural changes involved in its activity regulation.

3Pos044 アクチンフィラメントの張力依存的な構造変化の解析
Analysis of the tension dependent structural changes of actin filament

Fumito Matsuzaki, Tao Q.P. Noguchi (*National Institute of Technology, Miyakonojo College*)

Actin takes multiple molecular structures, which are thought to be deeply involved in the functions of actin-binding proteins (ABPs). Some ABPs showed tension to F-actin-dependent binding, suggesting that tension-depending structural changes of actin subunits affect the affinity of ABPs. In this study, we aim to clarify the relationship between force-stimulated conformational changes and changes in binding protein affinity. F-actin containing FRET actin, in which donor and acceptor dyes were attached, was pulled by micro-needles, resulting in altered FRET efficiency. This means the tension induces a structural change of actin. Similar experiments will be performed in the presence of fluorescently labeled ABPs to investigate changes in affinity for ABPs.

3Pos045 Kai 時計システムにおける分子の統合運動
Orchestration of proteins in a Kai clock system

Masaaki Sugiyama[1], Ken Morishima[1], Yasuhiro Yunoki[1], Rinatro Inoue[1], Nobuhiro Sato[1], Hirokazu Yagi[2], Koichi Kato[3] ([1]*KURNS*, [2]*Grad. Sch. Phar., Nagoya City Univ.*, [3]*ExCELLS*)

The circadian clocks in Cyanobacteria consists of KaiA, KaiB and KaiC. Kai clock has two rhymes, phosphorylation-oscillation of a KaiC molecule and association-dissociation kinetics between three proteins. In the clock, base units are KaiA dimer (A_2), KaiB tetramer (B_4) and KaiC hexamer (C_6). The standard picture describes the association-dissociation kinetics as follows: $A_2+B_4+C_6$(fully dissociation phase)$\rightarrow A_2C_6\rightarrow B_6C_6\rightarrow A_xB_6C_6$ (x will reaches 12: fully association phase)$\rightarrow A_2+B_4+C_6$. We examined this process and found that there should be unknown complexes even in the fully dissociation phase. The standard picture described only a part of clock oscillation of a Kai clock system. In this presentation, we will report what all proteins are doing in the clock oscillation.

3Pos046 高分子クラウディング環境下での蛋白質溶解度の進化
Evolution of protein solubility in macromolecular crowding

Yasuhiro Isogai[1], Hiroshi Imamura[2], Tomonari Sumi[3], Tsuyoshi Shirai[4] ([1]*Dept. Pharmaceutical Engineering, Toyama Prefectural Univ.*, [2]*Dept. Bio-Science, Nagahama Inst. Bio-Science and Technology*, [3]*Research Inst. Interdisciplinary Science, Okayama University*, [4]*Dept. Computer Bioscience, Nagahama Inst. Bio-Science and Technology*)

The inside of living cells is crowded by extremely high concentrations of biomolecules, and thus globular proteins should have been developed to increase their solubility under such crowding conditions during organic evolution. Myoglobin (Mb) is known to be expressed in myocytes of diving mammals in much larger quantities than those of land mammals. We have resurrected ancient whale and pinniped Mbs, and demonstrated that the diving animal Mbs have evolved to maintain high solubility under the crowding conditions. Here, we investigated pH dependence of the precipitant tolerance (β) of extant and ancestral Mbs, and demonstrated that β was approximated by the square of Z_{Mb}. This effect of Z_{Mb} can be explained by electrostatic repulsion between Mb molecules.

3Pos047 Dispersion Effect of Molecular Crowding on Ligand-Protein Surface Binding Sites of *Escherichia coli* RNase HI

Chikashi Ota[2], Hikari Suzuki[1], Shun-ichi Tanaka[1], **Kazufumi Takano[1]** ([1]*Kyoto Prefectural University*, [2]*Ritsumeikan University*)

To elucidate the detailed molecular mechanism underlying the ligand-protein interactions with flexible binding sites on a protein surface in crowded environments, we studied the interaction between the basic protrusion of *E. coli* RNase HI and ANS. RNase HI concentration-dependent ANS fluorescence was measured to characterize a typical self-crowding environment. The results show that ANS molecules bind to the additional binding sites because of the destabilization of the main sites by the excluded volume effect in a crowding environment. This suggests that the decrease in the ΔG difference between the main and minor sites due to destabilization of the main site could lower the potential barrier between them, inducing the dispersion of binding pathways.

3Pos048 線維形成前駆状態 β2 ミクログロブリンの残余構造がアミロイド線維のモルフォロジーに与える影響
The residual structure of acid-denatured β_2-microglobulin is relevant to an ordered fibril morphology

Ryosuke Tomiyama[1], Masatomo So[2], Yohei Miyanoiri[3], **Kazumasa Sakurai[1,4]** ([1]*Graduate School of Biology-Oriented Science and Technology, Kindai University*, [2]*Astbury Centre for Structural Molecular Biology, University of Leeds*, [3]*Institute for Protein Research, Osaka Univeristy*, [4]*Institute of Advanced Technology, Kindai University*)

SS bond-oxidized β_2-microglobulin (β2m) forms rigid fibrils, whereas reduced β2m forms amorphous fibrils, suggesting that the SS bond alters the residual structure of the monomer and the morphology of resultant fibril. Our NMR experiments revealed that oxidized β2m contained a residual structure throughout the molecule, though its range did not coincide with that of the fibril core. These results indicate that acid-denatured β2m has variable conformations. Most of them cannot participate in fibril formation because their core residues are hidden by residual structures. However, when hydrophobic residues are exposed, polypeptides competently form an ordered fibril. This conformational selection phase may be needed for the ordered assembly of amyloid fibrils.

3Pos049 透析アミロイドーシスの発症機構における分子夾雑環境の役割
Role of macromolecular crowding in the onset mechanism of dialysis-related amyloidosis

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Dialysis-related amyloidosis (DRA) is the specific amyloidosis for dialysis patients caused by amyloid fibrils of β_2-microglobulin (β2m). Although the onset mechanism of DRA has been investigated for several decades, it remains unclarified due to the complexity of amyloid fibril formation in a crowded milieu. In this study, we investigated β2m amyloid fibril formation in a crowded milieu using sera collected from dialysis patients. The result showed that macromolecular crowding in serum inhibited amyloid formation, indicating that reduced serum components by long-term dialysis treatment are one of the risk factors for the onset of DRA. Moreover, we comprehensively discussed the onset mechanism of amyloidoses based on the unified theoretical model.

3Pos050 異種フィブロイン混合系におけるナノファイバー/前駆体形成評価
Evaluation of nanofiber/precursor formation in heterogeneous fibroin mixtures

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Fibroin is a structural protein that forms spider silk. The protein consists of a repetitive region and two terminal regions. In the repetitive region, the Poly-Ala alternates with other amino acid residues. We have revealed the existence of a precursor composed of three fibroins and nanofibers (NFs) composed of the precursor. Poly-Ala stacking is involved in their formation. However, it is unclear how Poly-Ala intervals contribute to NF/precursor formation. To elucidate the structure of NFs and Precursors, we evaluated their formation in mixed solutions of fibroin with different Poly-Ala intervals. The results showed that NF/precursor formation is likely between homologous fibroins. Based on this fact, a new structural model of NFs and precursors will be discussed.

3Pos051 アラニンスキャン変異解析による c-Myb–KIX 間相互作用に重要なアミノ酸残基の同定
Identifying key residues of c-Myb–KIX interaction by alanine scanning mutagenesis

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Many human diseases are attributed to undesired protein-protein interactions (PPIs). The transcriptional activator c-Myb interacts with the KIX domain of the transcriptional coactivator CBP, and its aberrant expression causes leukemia. To develop PPI inhibitors, identifying key residues known as “hot spots” is an important issue. Here, we performed computational and experimental alanine scanning mutagenesis of the KIX binding with c-Myb. We found that three residues of KIX are essential for its interaction with c-Myb. In particular, the Y658A mutant significantly reduced the binding affinity with c-Myb, indicating that Y658 is a key residue for the interaction. These results will provide important insights into drug discovery targeting the c-Myb–KIX interaction.

3Pos052 高温条件下における耐熱化デンプンブランチングエンザイムの MD シミュレーションによる構造解析
Molecular Dynamics Simulation of Heat-Resistant Starch Branching Enzyme under High Temperature Conditions

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Starch Branching Enzyme (SBE) is an enzyme used industrially to improve the water solubility of starch and the stability of its aqueous solution. The optimum temperature of SBE is lower than the temperature at which starch is highly reactive, and improvements in the heat resistance of SBE are being investigated. Based on the report that the heat resistance of SBE derived from *Cyanidioschyzon merolae* (CmeBE) was improved by introducing an ancestral sequence, we analyzed the structure of wild-type (WT) and ancestral sequence-introduced mutant-type (MT) of CmeBE under high temperature conditions using MD simulations. Analysis of the residues that form hydrogen bonds with the introduced ancestral sequence showed differences between WT and MT.

3Pos053 分子シミュレーションにおける高次項を用いた補間による自由エネルギー地形の推定
Estimation of Free-Energy Landscape for Molecular Simulations by Interpolation with Higher-Order Terms

Shohei Toyama[1,2], Yuji Higuchi[3], Hiroshi Noguchi[1] ([1]*ISSP., Univ. Tokyo*, [2]*Dept. Phys., Univ. Tokyo*, [3]*RIIT., Univ. Kyushu*)

We propose a method for estimating the approximate shape of free energy landscapes from molecular simulations such as protein folding with small cost. In this study, we improved the reweighting process of umbrella sampling. The local landscapes calculated in each window is fitted to a polynomial equation to obtain the differential coefficients of free energy. By interpolating and integrating these coefficients, we were able to estimate landscapes at a significantly smaller cost than the previous methods.

3Pos054 アミロイド β タンパク質の分子構造動態に D-アスパラギン酸が与える影響
Effect of D-Aspartic Acid on the Conformational Dynamics of Amyloid-$\beta_{1\text{-}42}$ Protein

Yu Fukuda[1], Takeru Kameda[1], Shin-ichi Tate[3], Yuichi Togashi[1,2] ([1]*Coll. Life Sci., Ritsumeikan Univ.*, [2]*Riken BDR*, [3]*Grad. Sch. Integ. Sci. Life, Hiroshima Univ.*)

The pathogenic mechanism of Alzheimer's disease is thought to be related to the aggregation of amyloid-β protein (Aβ) in the brain; some studies have reported that aspartic acid at position 23 is isomerized to the D-form (D-Asp23), forming a β-sheet at the C-terminus and initiating Aβ aggregation. It has also been reported that D-Asp1 and D-Asp7 promote or inhibit β-sheet formation by D-Asp23. Therefore, in this study, we investigated whether isomerization of these residues is involved in β-sheet formation. Replica-exchange molecular dynamics simulation was used for efficient structural sampling. The results suggest that D-Asp1 and D-Asp23 are involved in the formation of α-helix. Stable β-sheet formation was not observed in the mutants used in this study.

3Pos055 タンパク質複合体における複数残基間相互作用の解析
Analysis of multiple residue interactions in protein complexes

Masaki Koyama, George Chikenji (*Dept. of Appl. Phys., Grad. Sch. of Eng., Nagoya Univ.*)

In recent years, many successful examples of de novo protein design have been reported, but the success of the de novo design of protein binders that can function as therapeutics is limited. This limitation may be due to the insufficient understanding of the physical principle of protein-protein interfaces, which is largely different from the principle of protein core. To accelerate de novo design researches of protein binders and deepen our understanding the physical principle of interfaeces, we performed a protein structure database analysis, examining not only interface interactions, but also geometric features. We will talk about the details on the day.

3Pos056 蛍光タンパク質イクオリンとカルシウムの結合に関する熱力学的解析
Thermodynamic analysis of the calcium binding with photoluminescence protein; aequorin

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The photoluminescence protein; aequorin (AQ) has three Ca^{2+} binding sites with loop structure and the binding induces the transient emission of blue light. Stepwise Ca^{2+} binding has been proposed, but the affinity of each site has not been evaluated. In this study, thermodynamic analyses of the AQ-Ca^{2+} binding were performed based on the heat changes along the Ca^{2+} titration in real-time manner by using isothermal titration calorimetry. First binding site showed that it binds with one Ca^{2+} with the dissociation constant of 2 mM, and negative enthalpy/entropy changes. These results suggests that the electrostatic interactions between the loop and Ca^{2+}, which fixes the loop structure. Additional Ca^{2+} titration would enable us to monitor the affinity of other two loops.

3Pos057 CHARMM C36m 力場のタンパク質-水相互作用の強化によるタンパク質の水溶液環境及び混雑環境における拡散性及び熱力学的特性の改善
Improved diffusive and thermodynamic properties of proteins with modified interactions between water and protein in CHARMM c36m

Daiki Matsubara[1], Kento Kasahara[2], Hisham Dokainish[3], Hiraku Oshima[1], Yuji Sugita[1,3,4] ([1]*Kobe Inst., RIKEN*, [2]*Grad. Sch. Eng., Univ. Osaka*, [3]*Wako Inst., RIKEN*, [4]*Kobe Inst., RIKEN*)

Atomistic structures and molecular interactions between biomolecules are important for understanding their molecular functions. Using the conventional force fields, intrinsically disordered proteins tend to be more compact and proteins in crowded solutions can be aggregated too strongly, mainly due to the imbalance of interactions between protein and water. To overcome these problems, Lennard-Jones potential between protein and water is modified by introducing the NBFIX scaling parameter for CHARMM c36m. In this poster, we propose the optimized NBFIX parameter, which can keep protein stability in solution as the original c36m, while avoiding too strong aggregations between proteins in crowded solution.

3Pos058 Structural Characteristics Investigation of Hero Peptides Using All-atom Molecular Dynamics Simulations

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Molecular chaperones regulate protein folding and prevent aggregation or misfolding of client proteins, protecting proteins after stress shocks. Recently, among the intrinsically disordered proteins (IDPs), heat-resistant obscure (Hero) proteins are found to function as “molecular shields”. However, the molecular mechanism of their function is unknown. In this study, we perform all-atom molecular dynamics (MD) simulations and protein biophysical experiments to investigate the structural properties of the Hero proteins. Through their structural characterization, we intend to demonstrate how the features of the amino acid sequence are related to the properties of the disordered structure, and their heat resistance and anti-aggregation activity for client proteins.

3Pos059 乾燥耐性生物クマムシのミトコンドリア局在性熱可溶性タンパク質 MAHS ・LEAM における乾燥誘導性 LLPS
Dehydration inducible LLPS of the mitochondria localized heat-soluble protein MAHS & LEAM of an anhydrobiotic tardigrade

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Water is essential for life; however, some tardigrades can enter anhydrobiosis, an ametabolic dehydrated state. Intrinsically disordered proteins (IDP) are considered to be related to anhydrobiotic ability and are assumed to protect other proteins and membrane structures from denaturation upon desiccation. Here, we focused on tardigrade mitochondrial IDPs, LEAM and MAHS, which confer osmotic stress tolerance to human cultured cells. We first confirmed these GFP-fused proteins formed LLPS with desiccation, and the addition of PEG promoted the LLPS formation, especially on LEAM. Moreover, we observed GFP-fused MAHS proteins formed a giant aggregate after long-term incubation. Besides LLPS formation, tardigrade-unique proteins probably have high self-association ability.

3Pos060 ベイズ学習による格子タンパク質模型のデザイン
Lattice protein design using Bayesian learning

Tomoei Takahashi[1], George Chikenji[2], Kei Tokita[1] ([1]*Grad. Sch. Inf. Nagoya Univ.*, [2]*Grad. Sch. Eng. Nagoya Univ.*)

Protein design is the inverse approach of the three-dimensional (3D) structure prediction for elucidating the relationship between the 3D structures and amino acid sequences. In general, the computation of the protein design involves a double loop: A loop for amino acid sequence changes and a loop for an exhaustive conformational search for each amino acid sequence. Herein, we propose a novel statistical mechanical design method using Bayesian learning, which can design lattice proteins without the exhaustive conformational search. As a result, on applying the 2D lattice hydrophobic-polar (HP) model, our design method successfully finds an amino acid sequence for which the target conformation has a unique ground state.

3Pos061 がん抑制タンパク質 p53 のアモルファス凝集体・アミロイド凝集体への新たなる知見
New insights into morphous & amyloid aggregates of the tumor suppressor p53

Emi Hibino[1], Reiji Hijikata[2], Takeshi Tenno[1,3], Hidekazu Hiroaki[1,3] ([1]*Grad. Sch. Pharm. Sci., Nagoya Univ.*, [2]*Sch. Sci., Nagoya Univ.*, [3]*BeCellBar*)

Retention of function of the tumor suppressor protein p53 is important in inhibiting tumorigenesis. The DNA-binding domain of p53 (p53-DBD) is reported to be aggregation-prone. However, since p53 functions intracellularly, we hypothesized that there are factors affecting the p53 aggregation in the cell. In this study, we investigated the effects of intracellular osmolytes on p53-DBD aggregation and function. p53-DBD aggregation was detected by thioflavin T and 8,1-ANS fluorescence, DNA binding by gel shift assay, and structural transition by tryptophan fluorescence. This study revealed that intracellular osmolytes inhibit amorphous aggregation of p53-DBD, inhibit p53 denaturation and loss of DNA binding ability, and promote amyloid aggregation in some cases.

3Pos062 細胞質中のヌクレオチド三リン酸によって改変される生体高分子の相互作用と安定性
Stability and interaction of macromolecules altered by nucleoside triphosphates in cytoplasm

Isseki Yu[1], Ryuto Yamazaki[1], Michael Feig[2], Yuji Sugita[3] ([1]*Maebashi Institute of Technology Information Systems Program*, [2]*Michigan State University Department of Biochemistry and Molecular Biology*, [3]*Riken Theoretical Molecular Science Laboratory*)

Recently, ATP, one of the most abundant metabolites in cell, was found to inhibit the aggregation of intrinsic disordered proteins. On the other hand, how ATP and other nucleoside triphosphates (NTs) change the stability and interaction of macromolecules in the cytoplasm is not fully understood yet. To understand the physicochemical role of NTs in cell, we performed all-atom molecular dynamics (MD) simulations of cytoplasms. The simulations indicated that the presence of NTs reduces the interaction of macromolecules. The mechanism was analyzed by calculating the non-bond interaction energies between macromolecules under the presence of NTs. In addition, the effect of NTs on the structural stability of proteins was also investigated.

3Pos063 自由エネルギー解析によるトリプトファン合成酵素におけるアロステリックなトリプトファン合成機構の解明
Allosteric regulation mechanism of tryptophan synthesis in tryptophan synthase by free energy analysis

Shingo Ito, Kiyoshi Yagi, Yuji Sugita (*Theor. Mol. Sci. Lab., CPR, RIKEN*)

Tryptophan synthase (TRPS), which consists of an αββα heterodimer, synthesizes L-tryptophan (L-Trp). The ligand binding at the α subunit affects conformation and ligand-binding affinity at the β-subunit to regulate the enzymatic reaction at the α-active site. The allosteric communication in TRPS have been investigated for a long time but the mechanism is not clear at the atomistic level. We perform molecular dynamics (MD) simulations with umbrella sampling of TRPS in the apo, α ligand bound, and α & β ligand bound states. The free energy and hydrogen bond analysis revealed that gradual switches of hydrogen bond interactions at the interface between the α and β-subunits regulate conformational change of domain structures and ligand-binding affinities.

3Pos064 Cryptdin-4, a mouse α-defensin, with multiple antibacterial mechanisms regulated by its redox structure and environmental conditions

Yi Wang, Yuchi Song, Rina Hiramine, Tomoyasu Aizawa (*Grad. Sch. Life Sci., Hokkaido Univ.*)

Cryptdin-4 (crp4), an enteric mouse α-defensin, is one main effector to confer immunity to oral infections and define the composition of the ileal microbiota. Structurally, crp4 performs two states—oxidized form (crp4oxi) constrained by disulfide bonds and reduced form (crp4red) with six thiol groups. Crp4red would induce rapid membrane depolarization, in which the loss of intracellular components led to irreversible bacteria death. *E. coli* treated by crp4oxi exhibited more complicated changes in membrane permeabilization, the release of membrane vesicles, and the induction of oxidative stress. Our data proposed different antimicrobial activities and mechanisms by one peptide, which was dependent on their redox structure and environmental situations.

3Pos065 Insights into the allosteric modulation of catalysis via a single surface mutation on a flexible loop in dihydrofolate reductase

Sandhya Premnath Tiwari, Shinichi Tate (*Grad. Sch. of Integrated Sciences for Life, Hiroshima University*)

Dihydrofolate reductase has served as a well-studied example for exploring the role of conformational fluctuations and allostery in function. We investigate the poorly characterized surface amino acid mutation at Gly67 which altered the catalytic rate when substituted to Trp and Ala. NMR experiments showed a significant reduction in the hydride transfer rate for the mutants despite limited chemical shift changes, and a shift in closed to occluded states. Through MD simulations, we found increased rigidity in the active site region for the mutants with a loss of collective motions. We also investigate if the mutants expose hidden allostery not easily identified by current prediction methods.

3Pos066 大腸菌フェリチンの鉄酸化とミネラル化に与えるリン酸の効果
Effect of phosphate on the iron oxidation and mineralization in *Escherichia coli* ferritin

Takumi Kuwata, Kazuo Fujiwara, Masamichi Ikeguchi (*Dept. of Biosci., Grad. Sch. of Sci and Eng., Soka Univ*)

Ferritin is a protein cage capable of storing up to 5000 iron atoms as a mineral core. It has been known that the iron cores of ferritins from archaea, bacteria, and plants contain the comparable amount of phosphate. However, the role of phosphate in the oxidation and mineralization is not fully understood. In this study, we investigated the effect of phosphate on the ferroxidase activity and mineralization in non-heme ferritin A from *Escherichia coli* (EcFtnA). Rapid kinetic experiments showed two oxidation phases when 96Fe/shell or more were added. Phosphate accelerated the slow phase but did not affect the fast phase. Sequential mixing experiments showed that phosphate promoted the regeneration of the ferroxidase center in EcFtnA.

3Pos067 テロメアブーケ形成における Mps3、Rpf2-Rrs1、Ebp2-Brx1 間の結合関係
Binding relationships among Mps3, Rpf2-Rrs1 and Ebp2-Brx1 in telomere bouquet formation

Hao Li[1], Takuma Eguchi[1], Isao Tanaka[1,2], Toyoyuki Ose[1,2], Min Yao[1,2] ([1]*Graduate School of Life Science, Hokkaido University*, [2]*Faculty of Advanced Life Science, Hokkaido University*)

Meiosis is an important process that chromosomes are replicated, recombined and distributed into daughter cells. Meiotic cell pairs its chromosomes by formation of telomere cluster at the nuclear membrane called “telomere bouquet” during meiosis.
In Saccharomyces cerevisiae, telomeres are anchored to nuclear envelope by interaction with Mps3 which is located on the nuclear envelope. Also, protein Ebp2 and Rrs1 was found to work as initiation factors of telomere bouquet formation through binding to N-terminal of Mps3(Mps3NTD).
For the moment, how Ebp2, Rrs1 and Mps3NTD work together is unclear. In this research, we aim to understand the role of each protein by their interaction assay and structure analysis of protein complex around Ebp2, Rpf2-Rrs1 and Mps3NTD.

3Pos068 IL-6 刺激下における非リン酸化型 STAT3 動態の解析
Analyses of the unphosphorylated STAT3 dynamics in the IL-6 activated pathway

Rin Tanaka[1,2], Michio Hiroshima[2], Masahiro Ueda[1,2] ([1]*Grad. Sch. Sci., Univ. Osaka*, [2]*Osaka Inst., Riken*)

STAT3 is phosphorylated on tyrosine residue (Y705) to form dimer, followed by nuclear translocation in activated signaling pathway. Recently, the unphosphorylated STAT3 (uSTAT3) has been reported to translocate into the nucleus in the basal state, which regulates the specific gene expression and heterochromatin formation. However, the dynamics and significance of uSTAT3 in the activated signaling pathway remains unknown. Here, we analyzed the undetectable uSTAT3 dynamics by quantitative measurements of the STAT3 localization and phosphorylation with biochemical and imaging methods. Our results showed the active uSTAT3 nuclear translocation after IL-6 stimulation, suggesting that there are novel mechanisms to regulate STAT3 dynamics in the activated signaling pathway.

3Pos069 A simple coarse-grained model for ADP binding to HSP90

Kazutomo Kawaguchi, Hidemi Nagao (*Inst. Sci. Eng., Kanazawa University*)

Functional cycle of HSP90 assisting protein folding is driven by association/dissociation of ADP and ATP. All-atom molecular dynamics (MD) studies have investigated the free energy profile for association/dissociation of ADP. It is difficult to proceed association/dissociation process for protein molecules in all-atom MD simulations, due to high computational cost of all-atom MD. In this work, we develop our coarse-grained model for ADP binding and apply it to the Langevin dynamics simulations for HSP90-ADP binding. We show that binding conformation of HSP90 and ADP obtained from our simulations is consistent with the X-ray structure. It is suggested that ADP is trapped at the entrance of the binding pocket of HSP90 and cannot enter the binding pocket without Mg^{2+}.

3Pos070 分子動力学に基づく混雑環境がタンパク質-リガンド結合に与える影響の速度論的解析
Kinetic analysis of the crowder effects on protein-ligand processes based on the molecular dynamics

Kento Kasahara (*Grad. Sch. Engr. Sci., Osaka Univ.*)

Many proteins function upon substrate (ligand) binding. In a cell, both protein and ligand molecules are surrounded by a number of macromolecules. Such crowded environments strongly affect the protein-ligand binding kinetics. In the present study, we quantify the rate constants for a protein-ligand binding in the dilute and polymer crowded solutions using molecular dynamics (MD) simulation and returning probability (RP) theory, a rigorous diffusion-influenced reaction theory. The binding rate constant in the crowded solution is found to be ~10 times slower than that in the dilute solution. The systematic analysis based on the RP theory reveals that the slow-down of the state transitions around the intermediate state contributes to decreasing the rate constant.

3Pos071 ジアゾ化酵素 Fur5 のジアゾ化反応機構の計算化学的解析
Computational analysis of the diazotization reaction mechanism of diazo-forming enzyme Fur5

Shota Kaneko, Yoshitaka Moriwaki, Tomohiro Noguchi, Tomohisa Kuzuyama, Tohru Terada, Kentaro Shimizu (*Grad. Sch. of Agri. and Life Sci., Univ. of Tokyo*)

Recently, enzymes that catalyze nitrogen–nitrogen bond formation have been discovered and their reaction cascades have been proposed. Fur5 is one of these enzymes identified in the furaquinocin-producing *Streptomyces* sp. strain KO-3988. It catalyzes the diazotization of 8-amino-flaviolin (8-AF) in the presence of $NaNO_2$ and ATP. Since the tertiary structure of neither Fur5 nor the other diazo-forming enzymes has been reported, the reaction mechanism remains elusive. In this study, the tertiary structure of Fur5 was predicted by AlphaFold, and a structural model of the complex with 8-AF was constructed by molecular docking and MD simulation. Based on the results of QM/MM calculations, the reaction mechanism of Fur5 will be proposed.

3Pos072 二重スピンラベル-ESR 分光法による ABC トランスポーターの膜貫通ドメインのコンフォメーション変化
Conformational changes in transmembrane domain of ABC transporter revealed by double spin label-ESR spectroscopy

Ayaka Naka[1], Yasuhiro Kobori[1,2], Motonari Tsubaki[1], Yoshitsugu Shiro[3], Hiroshi Sugimoto[3,4], Tetsunari Kimura[1] ([1]*Grad. Sch. Sci., Kobe Univ.*, [2]*Mol. Photo. Res. Cent., Kobe Univ.*, [3]*Grad. Sch. Sci., Univ. Hyogo*, [4]*SPring-8, RIKEN*)

The allocrite transport through transmembrane domain (TMD) of ABC transporters should be realized by the binding and hydrolysis of ATP in the nucleotide binding domain (NBD). In an importer, an additional periplasmic binding protein (PBP) delivers allocrite to the TMD. Such allocrite transport should be regulated by the conformational changes in TMD, but the chemical events causing the structural changes are still unclear. We introduced the spin-labels into the TMD of the heme importer; BhuUV-T, and analyzed their mobility along the binding with PBP or nucleotide by ESR spectroscopy. Binding of PBP increased motility of the periplasmic side of the TMD but decreased that of the cytoplasmic side, indicating that the TMD opens against the PBP to catch the allocrite.

3Pos073 時間分解分光測定を用いた ABC トランスポーター BhuUV-T におけるヘム輸送機構の解析
Tire-resolved spectroscopic analysis of allocrite transport mechanism in heme ABC transporter; BhuUV-T

Akiho Hara[1], Yoshitsugu Shiro[2], Hiroshi Sugimoto[2,3], Tetsunari Kimura[1] ([1]*Grad. Sch. of Sci., Kobe Univ.*, [2]*Grad. Sch. Sci., Univ. of Hyogo*, [3]*SPring-8, RIKEN*)

ABC transporters are proteins involved in membrane transport of allocrite upon ATP binding and hydrolysis. Their molecular mechanisms are poorly understood because of the difficulty in the observation of allocrite transport. A heme transporter, BhuUV-T, enabled us to follow the transport by the time-resolved UV/vis absorption spectroscopy with stopped-flow method based on spectral changes upon binding states of heme. The transport was initiated by the mixing of BhuUV-T/heme complex with ATP, and the spectrum at 2 s showed the interaction between heme and the detergent micelles in solution, suggesting that heme was released from BhuUV-T complex into solution within 2 s after ATP mixing. The detailed mechanism will be discussed based on the millisecond time-scale data.

3Pos074 Refinement of MD-derived conformational ensemble by referring to experimental SANXS data in framework of Bayesian statistics

Tomotaka Oroguchi[1,2] ([1]*Faclt. Sci. Tech., Keio Univ.*, [2]*RIKEN SPring-8 Center*)

The information on protein conformational ensemble is important to understand mechanism of protein function. MD simulation is useful to obtain such information at an atomic level. However, it is often difficult to obtain the MD ensemble that can account experimental data because of problems in validity of force fields and sampling efficiency of simulations. In this study, we have developed the method to refine MD-derived ensemble by referring to experimental SANXS data in framework of Bayesian statistics. By employing relative entropy of model ensemble against the MD-derived ensemble as a prior function, the self-consistent equation for optimization of the model is constructed. The validity of the method is examined using the simulated and experimental SANXS data.

3Pos075 蛍光相関分光法を用いたリボソーム-新生鎖複合体と相互作用する大腸菌 **Trigger Factor** シャペロンの動態観察
Application of fluorescence correlation spectroscopy to investigate dynamics of a ribosome-associated trigger factor chaperone in *E. coli*.

Tatsuya Niwa[1,2], Koki Nakazawa[1], Kensuke Hoshi[1], Hisashi Tadakuma[3], Koichi Ito[4], Hideki Taguchi[1,2] ([1]*Dept.of Life Science and Technology, Tokyo Tech.*, [2]*Cell Biology Center, IIR, Tokyo Tech.*, [3]*Sch. of Life Science and Technology & Gene Editing Center, ShanghaiTech University*, [4]*Dept. of Computational Biology & Medical Sciences, Grad. Sch. of Frontier Sciences, Tokyo University*)

Co-translational protein folding is one of the central topics in molecular biology. In *Escherichia coli*, trigger factor (TF) is a primary chaperone that facilitates co-translational folding by directly interacting with nascent polypeptide chains on translating ribosomes. We applied fluorescence correlation spectroscopy (FCS), which can analyze the diffusion properties of fluorescent molecules, to investigate the interaction between TF and a ribosome-nascent-chain complex. The FCS analysis with a reconstituted cell-free translation system confirmed that the interaction of TF with a nascent chain depended on the emergence of the nascent chain from ribosomes. Furthermore, the translation-dependent behavior of GFP-fused TFs was also observed in living *E. coli* cells.

3Pos076 BLI 法を用いた変性 LDL と LDL 関連受容体との結合特性
Binding properties of LDL to recombinant receptors were investigated by biolayer interfere layer method

Seiji Takeda[1], Nozomu Sato[1], Ao Hamamuki[1], Kanako Usirogata[2], Taichi Takasuka[2] ([1]*Dept. Pharm., Hokkaido Univ. of Sci.*, [2]*Grad. Sch. GFR., Hokkaido University*)

Modification changes low-density lipoprotein (LDL) properties and it alters affinity to the modified LDL receptors that are related to the development of various diseases. So that the evaluation of the ratio or amount of modified LDL recognized by these receptors are of great interested. Although some recombinant LDL related receptors such like LOX-1, CD36 are commercially available, the properties of these recombinant were not investigated in-depth. In this study, we investigated the binding properties of the recombinant LOX-1 and CD36 against oxidized LDL using a biolayer interfere layer method. We would like to show some results showing the binding selectivity of the recombinants against various LDL and temperature dependency of their binding.

3Pos077 一定力下での非平衡分子動力学シミュレーションの再検討
Non-equilibrium molecular dynamics simulation under constant force revisited

Shinji Iida, Tomoshi Kameda (*National Institute of Advanced Industrial Science and Technology*)

We discuss constant-Force steered MD (CF-SMD) simulation where constant external forces are applied to a system to enhance the dissociation events of molecules from a protein. Unlike velocity-dependent SMD, CF-SMD has the potential to give dissociation rate directly. However, the ability of CF-SMD to estimate kinetics has not been well investigated for biomolecules. Here, we demonstrate that (i) dissociation rates under various constant forces are correlated with experimental binding free energy, (ii) absolute dissociation rates under zero force (i.e., in equilibrium) can be estimated by CF-SMD simulation combined with a kinetic model, and (iii) there exists the limitation that dissociation rates in equilibrium for strong binders are significantly overestimated.

3Pos078 量子ビームを利用した膜タンパク質分子内ダイナミクスの直接検出
Direct detection of intramolecular dynamics of membrane proteins using X-ray based analysis techniques

Kazuhiro Mio[1,2], Tatsunari Ohkubo[1,2], Shoko Fujimura[1,3], Tatsuya Arai[3], Hiroshi Sekiguchi[4], Yuji C. Sasaki[1,3,4] ([1]*Operand OIL, AIST*, [2]*Grad. Sch. Med. Sci., Yokohama CU*, [3]*Grad. Sch. of Front. Sci., The Univ of Tokyo*, [4]*JASRI*)

We adopted diffracted X-ray tracking (DXT) to analyze internal motion of membrane proteins. DXT analyzes trajectories of Laue spots generated from the attached gold nanocrystals, which provides microsecond-time scale and picometre-spatial information. Although twisting motion of transmembrane helices was enhanced in TRPV1 both by capsaicin and antagonist, a life-time filtering method clearly distinguished them. A diffracted X-ray blinking (DXB) uses monochromatic X-ray source. DXB analyses the continuation of signals by calculating the auto-correlation function of intensity of each pixel. Due to the reduced flux dose, DXB minimizes damage to the samples. By combination of DXT and DXB, we succeeded in extracting two different modes of 5-HT2A motion on live cells.

3Pos079 ノイズのある原子間力顕微鏡像からの探針形状推定法の開発
Development of blind tip reconstruction method for noisy atomic force microscopy images

Ryuhei Oshima (*Grad. Sch. Sci. Eng., Saitama Univ.*)

Atomic force microscopy (AFM) uses a tip to scan the surface of a sample molecule. Since the measured heights depend not only on the sample molecular surface but also on the tip shape, it is necessary to know the tip shape for more detailed information on the molecular surface. The blind tip reconstruction (Villarrubia 1997) is an algorithm to estimate the tip shape by analyzing AFM images. However, this method is susceptible to noise. To overcome this problem, we are developing a novel reconstruction method. A current drawback of our method is that it is computationally time-consuming. Here, to accelerate the computation, we introduce a more efficient optimization technique and GPGPU in the method. In the poster, we report detailed benchmarks of computational speed.

3Pos080 木探索分子動力学法による Interleukin-2-inducible T-cell kinase 活性化経路の探索
Activation Pathway of Interleukin-2-inducible T-cell kinase Explored by Tree-Search Molecular Dynamics

Yukina Nakai[1], Toru Ekimoto[1], Tsutomu Yamane[2], Naoki Ogawa[1], Masao Inoue[1], Kei Terayama[1], Mitsunori Ikeguchi[1,2] ([1]*Dept. of Med. Life Sci., Yokohama City Univ.*, [2]*R-CCS, Riken*)

Interleukin-2-inducible T cell kinase (ITK) is a non-receptor tyrosine kinase that mediates T cell receptor signaling. In this study, we applied a new enhanced pathway-search method, termed tree-search molecular dynamics (TS-MD), to explore conformational changes during the activation event of ITK. TS-MD successfully sampled a conformational pathway from active to inactive states. In addition, multiple short MD simulations (~100 μs in total) from the structures sampled by TS-MD were performed, and those trajectories were integrated using a Markov state model for free-energy analysis. From the free-energy landscape, stable inactive and intermediate states and an energy barrier between them were observed.

3Pos081 微分可能な多状態ベネット受容比法を用いたシミュレーションモデルパラメータの効率的なチューニング
Efficient parameter tuning of simulation models by differentiable multistate Bennett's acceptance ratio method

Haruto Uchino, Yasuhiro Matsunaga (*Grad. Sch. Sci. Eng., Saitama Univ.*)

The MBAR method is widely used for estimating not only free energy differences but also ensemble averages of physical quantities from molecular dynamics simulation data. Since the method can interpolate/extrapolate ensemble averages of unsampled states, it is often used for parameter tuning of simulation models or conditions (such as the parameters of a Go-model, folding temperature. Shinobu et al. BPPB 2019). In order to achieve further efficient parameter tuning, we here implemented the differentiable version of the MBAR. Our implementation allows us to easily compute the gradient of ensemble averages over parameters. Using several toy models as test cases, we will demonstrate the efficiency of parameter tuning based on the gradient information.

3Pos082 深層学習によるグリッドベースの水和自由エネルギー計算
A deep-learning model for Grid-based Solvation Free Energy

Yusaku Fukushima, Takashi Yoshidome (*Dep. of Appl. Phys., Tohoku Univ.*)

In computational drug discovery, the affinity between a ligand and a protein is estimated using the free energy change upon ligand binding. However, in the estimation, water is often treated implicitly because computation of the solvation free energy requires a long computational time of a few days. To improve the performance of docking programs by explicitly treating water, we develop a deep-learning model that can calculate the solvation free energy within a minute. As the training and testing of the deep-learning model, solvation free energy of 90 proteins was computed using the Grid Inhomogeneous Solvation Theory (GIST). In this presentation, we discuss the prediction performance of our deep-learning model.

3Pos083 生体分子による液-液相分離とその環境要因を予測する機械学習モデルの開発
Development of machine learning models to predict liquid-liquid phase separation of biomolecules and its environmental factors

Kayin Chin, Shoichi Ishida, Kei Terayama (*Grad. Sch. Med. Life Sci., Yokohama City Univ.*)

Liquid-liquid phase separation (LLPS) of biomolecules is regulated by environmental factors, such as pH, temperature, and concentrations, and much effort has been devoted to understanding LLPS behavior. Recently, machine learning (ML) models have been developed to predict LLPS behavior and to discover novel LLPS biomolecules. However, the environmental factors have not been sufficiently predicted and analyzed by the ML models because the required data for such prediction was limited. Here, we constructed a detailed database of the biomolecules and environmental factors curated from published literature. We also developed a model using the collected data and analyzed the factors which could regulate LLPS behavior.

3Pos084 自由エネルギー摂動法を用いた VHH 抗体の等電点の制御
In silico control of isoelectric point of VHH using free energy perturbation method

Soichiro Oda, Yasuhiro Matsunaga (*Grad. Sch. Sci. Eng., Saitama Univ.*)

VHHs or nanobodies are single domain antibodies, recently attracting attention as an alternative to conventional antibodies in therapeutic applications. An important issue for developing VHH-based drugs is the control of isoelectric points to avoid aggregations of VHHs in specific conditions. To control isoelectric point, we need to optimize the sequence of titratable residues in VHH. Here, to search possible mutation sites by titratable residues in silico, we applied the free energy perturbation method to VHH. By calculating the free energy difference upon mutation with titratable residues, we found several candidates for mutation sites. These candidates are further verified with long-time molecular dynamics simulations.

3Pos085 X 線構造解析とラマン分光によるテトラペプチド結晶中の水素結合ネットワークの解析
Hydrogen network in a tetrapeptide crystal characterized by X-ray diffraction and Raman spectroscopy

Kazunori Motai[1], Masaki Kawano[2], Yuji Mochizuki[3,4], Takehiko Mori[1], Yuhei Hayamizu[1] ([1]*Department of Materials Science and Engineering, Tokyo Tech*, [2]*Department of Chemistry, School of Science, Tokyo Tech*, [3]*Department of Chemistry and Research Center for Smart Molecules, Faculty of Science, Rikkyo University*, [4]*Institute of Industrial Science,The University of Tokyo*)

Hydrogen bonds play an essential role in stabilizing protein conformation leading to their functional properties. The strength of hydrogen bonds has been investigated through structural analysis and spectroscopy. A previous work found a linear relationship between the interatomic distances and the vibrational frequency involving hydrogen bonds. However, these studies have been limited to small molecules, such as amino acids. In this study, we employed tetrapeptide as a model system to investigate peptide crystals. Single crystal X-ray structure analysis and Raman spectroscopy exhibited that the formation of hydrogen networks and the correlation of vibrational frequency of amide bonds with their interatomic distance.

3Pos086 気軽に試せる計算機タンパク質デザインに向けて
Towards easy-to-try computational protein design

Naoya Kobayashi, Shun Hirota (*NAIST, Mat. Sci.*)

This study provides a freely accessible and customizable web user interface to allow many people to computationally design a protein easily. The web user interface of protein design is available on Google Colaboratory. It allows users to get a sequence profile predicted by a deep neural network based on a backbone structure of an input protein and to design amino acid sequences using PyRosetta based on the predicted sequence profile. In this presentation, examples of this web user interface application will demonstrate sequence redesigns of proteins with/without a cofactor, a design of an interface of a symmetric oligomer, a design of a hetero protein complex, and *de novo* designs of monomeric proteins.

3Pos087 phi29 ファージ DNA 複製を用いた人工 DNA ゲノム進化系の構築
Development of an artificial DNA genome evolution platform using the phi29 DNA replication

Taro Furubayashi[1,2], Yoshihiro Minagawa[1], Hiroyuki Noji[1] ([1]*Grad. Sch. Eng., Univ. Tokyo*, [2]*JSPS*)

Design and evolution of gene-encoding DNA (= genome) is crucial to understand molecular evolution and engineer biomolecules. However, there is still no established platform for running efficient design-build-test-learn cycles of artificial evolution. Here we report our progress for constructing such an in vitro evolution platform consisting of the linear DNA replication scheme of phi-29 phage (genome), reconstituted cell-free translation (cytosol), and water-in-oil emulsion (compartment). We discuss applications of the proposed system for evolutionary genome optimization and RNA/protein engineering.

3Pos088 RNA メチル基転移酵素の配列特異性および補酵素選択性を改変する進化分子工学的手法の開発
Development of a directed evolution method for changing sequence specificity and cofactor selectivity of RNA methyltransferases

Yoshiki Ochiai, Paola Laurino (*Protein Engineering and Evolution Unit, OIST*)

RNA methyltransferases (RNMTs) play essential roles in RNA stability, processing, and translation. RNMT-based tools will be powerful in investigating the RNA methylation status and manipulating the regulation of RNA in a live cell. However, natural RNMTs were limited to use for tools due to their narrow sequence specificity and cofactor selectivity. Also, there is no engineering method for RNMTs to change their sequence specificity and selectivity of a synthetic cofactor. Here, we propose a novel directed evolution method for engineered RNMTs of specific RNA substrate using a synthetic cofactor. These engineered enzymes will ultimately be used as tools for changing RNA methylation states and epigenetic regulations in cells and *in vivo*.

3Pos089 ヘリックス-ループ-ヘリックスペプチドを分子基盤とする細胞内タンパク質間相互作用阻害剤の分子設計
A Cyclized Helix-Loop-Helix Peptide as a Molecular Scaffold to Design Inhibitors against Iintracellular Protein-Protein Interactions

Daisuke Fujiwara, Masataka Michigami, Ikuhiko Nakase, Ikuo Fujii (*Grad. Sch. Sci., Osaka Metropolitan Univ.*)

The design of inhibitors of intracellular protein–protein interactions (PPIs) remains a challenge in chemical biology and drug discovery. We propose a cyclized helix-loop-helix (cHLH) peptide as a scaffold for generating cell-permeable PPI inhibitors through bifunctional grafting: epitope grafting to provide binding activity, and arginine grafting to endow cell-permeability. To inhibit p53–HDM2 interactions, the p53 epitope was grafted onto the C-terminal helix and six Arg residues were grafted onto another helix. The designed peptide cHLHp53-R showed high inhibitory activity for this interaction and cell-membrane permeability. This strategy of bifunctional grafting could facilitate the generation of inhibitors for intracellular PPIs.

3Pos090 cDNA display 法により取得されたペプチドアプタマーの迅速かつ最適なダイマー化への新しいコンビナトリアル手法の開発
High-throughput identification of bivalent peptide aptamers selected by cDNA display with a newly combinatorial approach

Taro Noguchi[1], Kanako Nakao[1], Shigefumi Kumachi[1], Masayuki Tsuchiya[1], **Naoto Nemoto**[1,2] ([1]*Epsilon Molecular Engineering, Inc.*, [2]*Grad. Sch. Sci. & Eng., Saitama Univ.*)

Bivalent peptides, which consists of two peptide aptamers connected with flexible linker, possess potent binding activities and unique biological activities. However, it is very difficult to identify the appropriate length of aptamers between the different binding sites of a target antigen. In our study, we performed the combination with *in vitro* selection named cDNA display and subsequent a new combinatorial reaction method to identify the bivalent peptides which consist of two peptides binding to the same antigen all at once. The novel method based on the combinatorial-based dimerizing reaction of the monomeric peptides showed that the specific peptide pairs and linker length increased the binding response of bivalent peptides.

3Pos091 Model screening of a peptide by individual evaluation and separation using a combination of FACS and peptide ligase display (PL display)

Shingo Ueno, Fumi Toshioka, Takanori Ichiki (*iCONM, Kawasaki Inst. Industry. Promo.*)

Peptide ligase display (PL display) is a recently developed bead surface protein display method that uses peptide ligase for the linking of proteins and their DNA immobilized on beads. The unique feature of this method is that the proteins and DNA are covalently linked via short peptide only, without the use of large protein tags that causes steric hindrance. The proof of principle of this method using a single gene was reported in the previous meeting. In this meeting, we report on a model screening of peptides using a combination of PL display and FACS. The method enables quantitative and clear separation of affinity peptides by evaluating and manipulating each peptide in a library separately.

3Pos092 CRISPR-Cas ファミリータンパク質のデザインと標的探索の解明
Engineering and elucidation of target search by CRISPR-Cas family proteins

Trishit Banerjee[1,2], Hiroto Takahashi[2], Kiyoto Kamagata[1,2] ([1]*Grad.Sch.Sci., Tohoku Uni.*, [2]*IMRAM, Tohoku Uni.*)

The genome editing protein Cas9 faces engineering challenges in improving off-target DNA cleavage and low editing efficiency. Thus, we aimed to engineer Cas9 to be able to slide along DNA, which might facilitate genome editing and reduce off-target cleavage. Two approaches were used to achieve this: reducing the sliding friction along DNA by removing Cas9-DNA interactions and facilitating sliding by introducing the sliding-promoting tail of Nhp6A. The attachment of the tail to Cas9 mutants enhanced sliding along DNA by 8-fold in the presence of sgRNA. Further, we would elucidate the target search mechanism of other Cas family proteins such as Cas1-Cas2 which play a crucial role in the acquisition of viral DNA in bacteria and storing it as a memory of past infection.

3Pos093 (1SEP-5) Control of small G-protein Ras using calmodulin-based ionochromic molecular device

Yassine Sabek, Nobuyuki Nishibe, Kazunori Kondo, Shinsaku Maruta (*Graduate school of science and engineering , department of biosciences , soka university, Hachioji TOKYO*)

A small G-protein (RAS) which leads to the stimulation of downstream pathways, playing an important role in cell proliferation, and differentiation among others may also promote tumorigenesis. We have been studying to control Ras function using photochromic molecular devices. In this study, we used Calmodulin as an ionochromic molecular device to control Ras with Ca^{2+} ions. Calmodulin fusion protein with inhibitory peptide for Ras and M13 calmodulin target peptide (CAM-I-M13) was designed and prepared by the E.coli expression system. CAM-I-M13 exhibited different inhibitory activities for Ras GTPase between the conditions in the presence and absence of Ca^{2+}. Ca^{2+}-dependent reversible binding of CAM-I-M13 was also examined by size-exclusion-HPLC

3Pos094 ヒト・ノイラミニダーゼの構造解析に向けたハイブリッドモデル作成
The investigation of hybrid models for the structure determination of human Neuraminidases

Takeru Nakajima (*Dept. Appl. Phys., Nagoya Univ. / Japanese*)

Neuraminidases are widespread enzymes found in a range of organisms. Four human neuraminidases (HNEU1, HNEU2, HNEU3, and HNEU4, respectively) have been identified with distinct functions. Particularly, HNEU1 is involved in multiple pathogenecities including human disorders, tumor progression, and metastasis repression. Understanding the exact structure of the enzyme would help clarify its specificities toward substrate selectivity, eventually clarifying its implications for the diseases.
In our research, we attempt to design and express structurally stable hybrid forms of HNEU1 based on amino acid similarities with the cytosolic HNEU2, the only human and mammalian neuraminidase for which the structure is known.

3Pos095 Deciphering the signal transmission of activation mechanism for chemokine CXCL12-bound receptor CXCR4 in complex with G_i-protein

Ting-Yu Hu[1], Hao-Jen Hsu[1,2], Chun-Chun Chang[3,4] ([1]*Department of Life Sciences, College of Medicine, Tzu chi University*, [2]*Department of Biochemistry, School of Medicine, Tzu Chi University*, [3]*Department of Laboratory Medicine, Hualien Tzu Chi Hospital, Buddhist Tzu Chi Medical Foundation*, [4]*Department of Laboratory Medicine and Biotechnology, College of Medicine, Tzu Chi University*)

In this study, various ligands were respectively docked to CXCR4 and Gi-protein to study the molecular switches and internal downstream signals. MD simulation results showed that the tyrosine toggle distance of CXCR4 in the agonist-bound system was much lower than in the antagonist-bound system, which caused TM7 inward tilt. We also found TM6 outward tilt only in the agonist-bound active system. The residues $Y256^{6.52}$ and $W252^{6.48}$ were observed to play a crucial role in regulating the water molecule flowing. The internal water molecules were found to form a continuous water channel only in the active CXCR4 system. This study provides atomic-level insights into the structural and functional importance of CXCR4 and can be applied in the design of the anti-cancer drugs.

3Pos096 GPCR の相互作用ネットワーク解析
Interaction Network Analysis of GPCRs

Yusuke Higaki[1], Wataru Nemoto[2], Yoshihiro Yamanishi[3], Hiroyuki Toh[1] ([1]*Dept. of Bio. Med. Sci., Grad. Sch. of Sci., Univ. of Kangaku*, [2]*Dept. of Life. Sci. Eng., Grad. Sch. of Sci., Univ. of Touden*, [3]*Dept. of Biosci. Bioinfo., Grad. Sch. of Com. Sci., Univ. of Kyukou*)

G-protein-coupled receptors (GPCRs) constitute a very large family of proteins, of which there are more than 800 genes in the human genome. GPCRs have been found not only as monomers, but also in complexes, where they change their functions. However, the overall picture of GPCR interactions has not yet been clarified. In this study, we will examine the interactions of GPCRs by network analysis to identify hub GPCRs that play a central role in the interaction network and to elucidate their functions and characteristics. The results showed that many GPCRs interacted with each other. Among them, a large number of interacting GPCRs were found. The GPCR network was divided into 10 communities, with multiple hubs per community.

3Pos097 全反射赤外分光法による GPCR のリガンド認識機構研究
ATR-FTIR study of ligand recognition on GPCRs

Seiya Iwata[1], Kota Katayama[1], Kohei Suzuki[1], Ryoji Suno[2], Chiyo Suno[2], Takuya Kobayashi[2], Hirokazu Tsujimoto[3], So Iwata[3], Hideki Kandori[1] ([1]*Grad. Sch. Eng., Nagoya Inst. Tech.*, [2]*Grad. Sch. Med., Kansai Med. Univ.*, [3]*Grad. Sch. Med., Kyoto Univ.*)

Stimulus-induced difference FTIR spectroscopy is a powerful method to investigate local protein structure related to its molecular function. We recently applied this method to muscarinic receptor (M2R), and clarified its ligand binding mechanism. Although we succeeded in distinguishing different type of ligands such as agonist and antagonist in M2R, all of them that we used are water-soluble ligands. Here, to demonstrate the general applicability of our method to a wide range of other GPCRs, we measured ligand binding-induced difference FTIR spectroscopy on Kappa opioid receptor (KOR) and Orexin receptor 2 (OX2R) of which they recognize mainly water-insoluble ligands. Based on the results obtained, future problems and improvements in this method will be discussed.

3Pos098 ソラベグロンおよびイソプレテレノールに結合した β3 アドレナリン受容体のクライオ電顕構造
Cryo-EM structures of the β3 adrenergic receptor bound to solabegron and isoproterenol

Ikko Nureki[1], Tatsuki Tanaka[1], Kazuhiro Kobayashi[1], Asuka Inoue[2], Wataru Shihoya[1], Osamu Nureki[1] ([1]*Grad. Sch. Sci., Univ. Tokyo*, [2]*Grad. Sch. Pharm. Sci. Univ. Tohoku*)

We report the cryo-electron microscopy structures of the β_3AR-G_s signaling complexes with the selective agonist, solabegron and the nonselective agonist, isoproterenol. Comparison of the isoproterenol-, mirabegron-, and solabegron-bound β_3AR structures revealed that the extracellular loop 2 changes its conformation depending on the bound agonist and plays an essential role in solabegron binding. Moreover, β_3AR has an intrinsically narrow exosite, regardless of the agonist type. This structural feature clearly explains why β_3AR prefers mirabegron and solabegron, as the narrow exosite is suitable for binding with agonists with elongated shapes.

Poster

3Pos099 The Off-Axis Rotor of *Enterococcus hirae* V-type ATPase by Volta Phase Contrast and Conventional Phase Cryo-EM

Raymond N. Burton-Smith[1], Jun Tsunoda[1,2], Chihong Song[1,2], Hiroshi Ueno[3], Takeshi Murata[4], Ryota Iino[5], Kazuyoshi Murata[1,2] ([1]*ExCELLS, Okazaki, Japan*, [2]*SOKENDAI, Okazaki, Japan*, [3]*Univ. Tokyo, Tokyo, Japan*, [4]*Chiba Univ. Chiba, Japan*, [5]*IMS, Okazaki, Japan*)

The V-type ATPases are large membrane complexes which utilise ATP hydrolysis to power ion transport across cell membranes, in this case the alkali metal ion Na^+ is transported. *E. hirae* is a Gram-positive zoonotic bacterium, with implications for both human health and the farming industry.
Here we report our extension of earlier Zernike-type phase contrast cryo-EM analysis with Volta-type phase contrast, and further extended this using a JEOL CRYOARM 300 and a Gatan K3 detector. Upon addition of ATP to the purified V-ATPase, we are able to isolate several states of the *E. hirae* V-ATPase, with three states corresponding to the widely reported rotor orientations from other ATPases, and some intermediate states corresponding to the "sub-pauses" exhibited by this V-ATPase.

3Pos100 PANX1 の K346E 変異型の発現系の確立と構造的基盤の検討
Establishment of the expression system and structural basis of the K346E mutation of PANX1

Kana Taniguchi, Taiichi Tsuyama, Ken Yokoyama (*Department of Molecular Biosciences, Kyoto Sangyo*)

PANX1 is a large pore channel responsible for the permeation of small molecules, including ATP. Its gating is tightly regulated to prevent the permeation of metabolites across the cell membrane. For instance, the cytoplasmic inhibitory C-terminal region maintains the closed state, and its cleavage results in opening the channel; however, the structural basis of the gating remains unclear.
Here, we focus on the K346E mutation in *PANX1*, one of the causative mutations of infertility, which is reported to activate the channel. We are attempting to purify the mutant channel and determine its structure. The structure of mutant PANX1 may provide a structural basis for the mechanism of pore opening by the K346E mutation.

3Pos101 Structural insights into the HBV receptor and bile acid transporter NTCP

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Roughly 250 million people are infected with hepatitis B virus (HBV) worldwide. Ten years ago the HBV receptor was identified as NTCP, which interacts with the N-myristoylated preS1 domain of the viral large protein. Despite the pressing need for therapeutic agents to counter HBV, the structure of NTCP remains unsolved. Here we present the structure of NTCP clearly showing the transporter has no equivalent to the first transmembrane helix of other SLC10 models, leaving the N-terminus exposed on the extracellular face. Comparison of the different structures indicates a common mechanism of bile acid transport, but the NTCP structure also displays a pocket formed by residues known to interact with preS1, presenting enticing opportunities for structure-based drug design.

3Pos102 インフルエンザ菌アドヘシンの膜貫通ドメインのナノディスクへの挿入における BamA の役割
Role of BamA on the insertion of the transmembrane domain of *Haemophilus Influenzae* adhesin into nanodiscs

Eriko Aoki[1], Kazuo Fujiwara[2], Masamichi Ikeguchi[2] ([1]*GaLSIC, Soka Univ.*, [2]*Dept. Biosci., Soka Univ.*)

Bacterial outer membrane proteins (OMPs) are thought to be inserted into the outer membrane by a β-barrel assembly machinery (BAM) complex. BamA is essential for function of BAM complex and thought to assist OMPs membrane insertion. In this study, we investigated the membrane-insertion mechanism of *Haemophilus Influenzae* adhesin transmembrane domain (HiaTD), using BamA-embedded nanodiscs. The insertion of HiaTD into nanodiscs was enhanced by embedding BamA into nanodiscs. BamA consists of a 16-strand transmembrane β-barrel and five periplasmic POTRA domains. The truncation of POTRA domains from BamA showed that POTRA domains contribute to the BamA function. The role of POTRA domains in the BamA-assisted HiaTD assembly will be discussed.

3Pos103 大腸菌 UvrD C 末端アミノ酸欠損変異体の DNA 結合・巻き戻しダイナミクス
Dynamics of DNA binding and unwinding by *Escherichia coli* UvrD lacking C-terminal amino acids

Hiroaki Yokota (*Grad. Sch. Creation New Photon. Indust.*)

Escherichia coli UvrD protein is a non-hexameric superfamily I DNA helicase required for DNA-repair mechanisms. To understand the role of the C-terminus amino acids of UvrD that are crucial to dimerization and unwinding activity, single-molecule direct visualization has been performed for UvrD mutants lacking the C-terminal amino acids. I have reported that a UvrD mutant lacking the C-terminal 40 amino acids (UvrDΔ40C) unwound DNA in the form of an oligomer (dimer or trimer) (*Biophys. J.* 2020) as wildtype UvrD (*Biophys. J.* 2013). I will show experimental results that indicate that a UvrD mutant lacking longer C-terminal amino acids can still oligomerize and unwind DNA. I also will discuss the results by referring to past relevant studies (*Biophys. Physicobiol.* 2022).

3Pos104 転写因子 Nanog についての粗視化および全原子分子動力学シミュレーション
Coarse-grained and all-atom molecular simulations for transcription factor Nanog

Azuki Mizutani[1], Cheng Tan[2], Yuji Sugita[2], Shoji Takada[1] ([1]*Grad. Sch. Sci., Univ. Kyoto*, [2]*RIKEN, Comput. Sci.*)

Nanog is a master transcriptional factor for the maintenance of pluripotency in mammalians. Biochemically, Nanog forms a condensate via liquid-liquid phase-separation (LLPS) *in vitro*, and to form oligomers via its tryptophan repeat (WR) region in the C-terminal tails. We performed coarse-grained molecular simulations of mouse Nanog mixture. In the simulation, we found that Nanog forms a micelle-like oligomer via its WR region. We further investigate the system that contains oligomer and DNA. Moreover, motivated by recent CD spectra data that showed β-sheet formation in Nanog oligomer, we performed all-atom MD of the WR monomer to see β sheet. We also investigate oligomer structure of WR region.

3Pos105 スピンラベル ESR による HP1 天然変性ヒンジ領域と DNA 相互作用の動的構造解析
Dynamics of HP1 intrinsic disorderd hinge region with DNA measured by site-directed spin labeling-ESR spectroscopy

Isao Suetake[2,4], Kazunobu Sato[3], Tohru Kawakami[4], Tomoaki Sugishita[4], Risa Mutoh[5], Yuichi Mishima[4], Takeji Takui[3], Toshimichi Fujiwara[4], Hironobu Hojo[4], Makoto Miyata[1], **Toshiaki Arata**[1,4] ([1]*Dept.Biol. Grad. Sch. Sci. Osaka Met.Univ.*, [2]*Nakamura Gakuen Univ.*, [3]*Dept.Chem. Grad. Sch. Sci. Osaka Met.Univ.*, [4]*IPR. Osaka Univ.*, [5]*Fac. Sci. Toho Univ.*)

We examined the residual dynamics of IDRs (HR, N/C-tails) of HP1 with DNA by spin-labeling ESR [Suetake et al 2021] using domain truncation. It was suggested that all the residues of HR and tails were loosely arranged by the weak interaction of HR with two tails between monomers in auto-inhibited state, as previously assumed. Multi-interspin distances from pulse ESR also showed that HR was loosely but regularly arranged. Spin label at HR remained the same very high rotational mobility at subnsec upon DNA addition. In contrast the dynamics of both CD/CSD of HP1 was clearly restricted at the same nsec correlation time with DNA, suggesting that HP1 diffuses very rapidly along DNA as a fuzzy complex, and that CD/CSD are tethered with similar dynamics on DNA[Watanabe, 2018].

3Pos106 Through the Looking-Glass: Functional ‘Ambidexterity’ in an Ancient Nucleic Acid Binding Protein

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For nearly 4 billion years, evolution has operated exclusively on just one of the two possible mirror images of proteins and nucleic acids. As a result, any biopolymer that manages to jump ‘through the looking glass’ becomes out of step with Earth biology and suffers a complete distortion of its functional profile. We present an intriguing counterexample to this dogma of biological homochirality: An ancient nucleic-acid binding domain that retains its function upon chiral inversion. If the evolutionary constraints of early biology are indeed written into the most ancient protein domains, we must now grapple with the question: Could the divide between mirror worlds be narrower than is usually assumed – either today or in the past?

3Pos107 分子動力学法を用いたシニョリン及び変異体周囲の水和ダイナミクスの解明
Elucidation of hydration dynamics around chignolin and mutants using molecular dynamics

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In this study, we clarified the effect of structural differences in the peptides on the surrounding hydration dynamics of chignolin (1UAO) and four mutants of the same sequence length (2E4E, 2RT4, 2RVD, 5AWL). For the structural comparison, we used the original stable β-sheet structure obtained from the Protein Data Bank and the heat-denatured disordered structure. As a result, hydration water showed high motility on the surface of the disordered peptides. That is, the structural disorder and exposure to solvent strongly correlated with the high motility of the solute, and this high motility correlated with the high motility of the hydration water. We also analyzed other physical properties of the peptide-solvent systems and found some correlations.

3Pos108 溶質周囲の水分子の配置・立体構造の歪みを解析するツール開発
Development of a program to analyze water's structure around solutes and the applications

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The water's structures around solutes have been studied by various methods, and molecular dynamics (MD) simulation is one of them. In this study, we have developed a program that can analyze the water's structures in the respective layers (i.e., hydration layer, layer I, and layer II) around the solute surface by calculating the q-value, which is an index of the tetrahedral water's structure, . To verify the validity of this program, MD simulations were done using five water models (SPC/E, TIP3P, TIP4P, TIP4P2005, TIP5P) and using urea as a solute. Then, the water's structures were analyzed and compared with the previous studies (e. g., Bandyopadhy et al., 2013). Furthermore, we also apply this program to larger solutes such as antifreeze proteins.

3Pos109 データ駆動的に構築した記述子を用いた液相水分子の静的・動的構造の研究
Static and dynamic structure of liquid water investigated by means of data-driven atomic descriptor

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Water is a ubiquitous liquid, and shows a variety of anomalies, as 1) molecular low diffusivity near the protein surface 2) spatially heterogeneous dynamics of water near the glass transition temperature. Under the motivation to biomolecular researches, we investigate the behavior of water molecule by means of MD simulation and machine-learning method. The data-driven atomic environmental descriptors were built from water-water coordination geometry and that of water transfer. The descriptors of every atom in all frameshots were calculated from the trajectories of MD simulations of supercooled water. The clusterization and dimensionality reduction technique were applied on the descriptor space, and the static and dynamic structure of liquid water were discussed.

3Pos110 サブテラヘルツ波照射によるタンパク質水和の非熱的促進：誘電緩和測定による解析
Nonthermal acceleration of protein hydration by sub-terahertz irradiation: Analysis of dielectric relaxation measurements

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At physiological temperatures, collective dynamics of biomolecules and the coupled water molecules have been observed in the sub-terahertz (THz) frequency range. We demonstrate that the applied sub-THz radiation energy leads to a decrease in the dielectric permittivity of an aqueous protein solution by developing novel experimental system combining 0.1-THz excitation and the reflection method of dielectric relaxation measurements. This finding is associated with an enhancement of protein hydration in terms of the lower orientation polarization of water dipoles. We also observed a decrease in the permittivity specifically for high frequencies during the 0.1-THz irradiation, which did not occur by isotropic heating, and thus can be explained to be nonthermal.

3Pos111 濃厚な糖溶液の構造：単糖類と二糖類の特性の比較とトレハロースの特異性
Structures of concentrated sugar solutions: Comparison of characteristics of mono- and disaccharides and specificity of trehalose

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Trehalose has received considerable attention in the context of cryptobiosis. In spite of the importance of understanding cryptobiosis, even basic knowledge of structures of sugar solutions such as intermolecular interactions and/or correlation is still ambiguous. Using a wide-angle X-ray scattering method, we clarified the characteristics of the structures of sugar solutions (glucose, fructose, mannose, sucrose, and trehalose), over a wide concentration range of 0.05–0.65 g/mL. Trehalose prefers a more disordered arrangement in solution compared to other sugars, i.e., bulky arrangement. The present findings will afford new insight into the molecular mechanism of the protective functions of the sugars relevant to cryptobiosis, particularly that of trehalose.

3Pos112 MD と 3D-RISM 理論による SARS-CoV-2 スパイクタンパク質と ACE2 タンパク質間相互作用の研究
MD and 3D-RISM study of the interaction between SARS-CoV-2 spike and ACE2 proteins

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We investigated the binding process of angiotensin converting enzyme 2 (ACE2) to the SARS-CoV-2 spike protein receptor binding domain (RBD) using MD simulation and 3D-RISM methods. As a structural feature, it was shown that the sugar chain of ACE2 first forms a hydrogen bond with the RBD when the proteins approach. Then, the number of hydrogen bonds between proteins increased due to conformational changes in the amino acid side chains of the binding site. The spatial distribution function of the solvent revealed the presence of hydrogen bonds bridged by water molecules at the RBD-ACE2 interface. Principal component analysis revealed that ACE2 exhibits significant structural changes during the bonding process, while RBD shows no such changes.

3Pos113 ガン関連タンパク質 MDM2 のリガンド結合能に対する共溶媒効果の定量的評価
Quantitative evaluation of cosolvent effects on ligand binding abilities of cancer-associated protein MDM2

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MDM2 is a protein reducing the activity of the tumor suppressor p53. Anticancer drugs are often targeted to inhibit the MDM2 activity by occupying its binding pocket. For drug design, it is important to understand the effects of cellular environments which contain various molecules (cosolvents) such as other proteins, nucleic acids, and metabolites on the binding affinity. Here, we investigate the cosolvent effects on the binding affinities of MDM2 with p53 and a well-known inhibitor nutlin-3a, using molecular dynamics simulation and energy representation theory. It is found that the same trend was observed for both MDM2-p53 and MDM2-nutlin-3a as follows; while urea, DMSO, and 1,6-hexanediol promote dissociation, ethanol and PEG increase the binding affinity.

3Pos114 タンパク質およびその多量体の共溶媒添加に伴う安定性変化のエネルギー解析
Free-energy Analysis of Stability Change of Proteins and Their Oligomers upon Addition of Cosolvent

Yuka Hamada, Kento Kasahara, Nobuyuki Matubayasi (*Division of Chemical Engineering, Graduate School of Engineering Science, Osaka University*)

Although the aggregation equilibrium of proteins is altered by the addition of cosolvents, the detailed mechanism is still largely unknown. In this study, we focused on the aggregation equilibrium between monomeric and dimeric forms of lysozyme. Using molecular dynamics (MD) simulations and energy representation (ER) methods, we analyzed the effect of cosolvent addition on the aggregation equilibrium in terms of intermolecular interactions. The clarification of the effect of co-solvent addition on the aggregation equilibrium at the molecular level is expected to lead to systematic knowledge on protein crystallization.

3Pos115 統計熱力学に基づくペプチド薬デザイン法の開発
Computational study for designing peptide drugs based on statistical thermodynamics

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Computational strategies are widely used to design the peptide drugs with high affinity to the target proteins. The rapid modeling of the native-like poses of a protein-peptide complex is difficult but crucial. Our strategy is as follows: (1) the complex structures with a wide variety of binding poses of a peptide are generated using the molecular dynamics simulation or the sampling algorithms employed in the protein-peptide docking programs, (2) our physics-based free-energy function (FEF) is applied to the structures and the protein-peptide complex giving the lowest value to FEF is identified. By using our FEF, the microscopic structural information of a complex is rapidly correlated with thermodynamic properties through statistical mechanics.

3Pos116 *C. elegans* のスプライシング因子 AQR の温度耐性への関与
A homolog of splicing factor AQR, *emb-4*, is involved in high and low temperature tolerance in *C. elegans*

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Analysis of plant polymorphic strain showed polymorphisms in the splicing factor AQR are involved in heat tolerance (Isono *et al.* unpublished). *emb-4* is a C. elegans homolog of AQR and *emb-4* mutant showed a weaker heat tolerance abnormality than wild-type, whereas they showed a stronger cold tolerance. Phenotypes of another allele and RNAi knocked-down animals also suggested that EMB-4 positively regulates heat tolerance and negatively regulates cold tolerance. We found 55 genes significantly differentiated expression levels in *emb-4* by RNA-seq. Among of these genes, *asm-3* and *scrm-4* mutants showed abnormalities in both heat and cold tolerance. We expect to elucidate the temperature adaptation mechanism related to EMB-4.

3Pos117 Photocontrol of small GTPase Ras using its regulatory factor GEF modified with photochromic azobenzene derivative

Yuichi Imamura, Nobuyuki Nishibe, Kazunori Kondo, Shinsaku Maruta (*Grad.Sch.Sci.,Univ.Soka/Japanese*)

Ras is a central regulator of cellular signal transduction processes. GEF exchange GDP in Ras to GTP and Ras transmit signal to downstream effectors. In this study, azobenzene derivatives was incorporated into the functional region of GEF in order to control GDP-GTP exchange of Ras photo-reversibly. We have designed the Ras mutants which have a single cysteine at the functional region and prepared by E. coli expression system. 5 kinds of mutants were prepared. Azobenzene derivative (PAM) was incorporated into the cysteine of each mutant. Photocontrol of Ras GTPase activity with the PAM modified GEF mutants was examined under UV and visible light irradiations.

3Pos118 (2SAP-4) グラフニューラルネットワークによる細胞間の時空間相互作用の推定
(2SAP-4) Graph-based machine learning reveals rules of spatiotemporal cell interactions in tissues

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Robustness in developing and homeostatic tissues is supported by various types of spatiotemporal cell-to-cell interactions. Although live imaging and cell tracking are powerful in providing direct evidence of cell coordination rules, extracting and comparing these rules across many tissues requires a versatile framework of analysis. We demonstrate that graph neural network (GNN) models are suited for this purpose, by showing how they can be applied to predict cell fate in tissues and utilized to infer the cell interactions. Analyzing the live mammalian epidermis data, where spatiotemporal graphs constructed from cell tracks and cell contacts are given as inputs, GNN discoveres distinct neighbor cell fate coordination rules that depend on the region of the body.

3Pos119 ニワトリ胚心臓の発生にエタノールが与える影響の SS-OCT 観測
Heart development of chick embryo under ethanol exposure imaged by Swept Source OCT

Taichi Furuta, Takashi Yamaoka, Keisuke Matsubara, Yuuta Moriyama, Toshiyuki Mitsui (*Dept. Phys. Sch. Sci. Aogaku Univ.*)

Recently, it has been statistically demonstrated that alcohol is a factor in congenital heart disease (CHD). However, the development of the heart under alcohol exposure that triggers CHD cannot be visualized. We developed a system to observe the heart development of chicken embryos using swept source optical coherence tomography (SS-OCT). To culture chick embryos without a shell, we used a state-of-the-art shell-less culture method. The heart development of the chick resembles that of humans. Moreover, it is completed after about four days, and the heart is small enough to be examined by SS-OCT. In this study, we present the abnormalities in heart development caused by ethanol exposure of embryos and discuss the functioning of the heart in the context of CHD.

3Pos120 Observation of calcium and mitochondrial activity in mouse sperm state changes

Yuichi Hiramatsu, **Takashi Ijiri** (*Dept. of Lif. Sci., Fac. of Sci. and Eng., Setsunan Univ.*)

AMP-activated protein kinase (AMPK) is a sensor of cellular energy. Therefore, we have investigated the effects of two AMPK activators, metformin and AICAR, on mouse sperm, to understand the mechanisms of energy metabolism in sperm. Our previous results suggest the treatment of mouse sperm with these activators promoted an increase in acrosome reaction and the ATP amount. To investigate the reason why the addition of AMPK activator increased the acrosome reaction induction rate, imaging of sperm with AMPK activator and inhibitor for calcium was performed using the calcium indicator Fluo8-AM. Also, the role of mitochondria in sperm function remains largely unknown. The mitochondrial membrane potential in sperm is also being analyzed by imaging using JC-1.

3Pos121 Analysis of the gene expression fluctuation and post-differentiation state in the differentiating human pluripotent stem cells

Kensuke Sasaki, Sayaka Yamamoto, Yasuhiro Maeda, Tomonobu Watanabe (*RIKEN Center for Biosystems Dynamics Research*)

Intrinsic state of the pluripotent stem cells spontaneously fluctuates. During differentiation, the fluctuation is suppressed by or spread to surrounding cells via cell-cell interaction, leading the collective state transition of the cell population. To observe the gene expression fluctuation in relation to post-transition state, we cultured human induced pluripotent stem cells (hiPSCs) on a circular micropattern substrate, where the differentiated cells are aligned to a concentric circle. Immunohistochemical staining of Oct4, Nanog, Sox2 and Brachyury (BRA), showed the spatial fluctuation in Sox2 expression resembles the pattern of BRA distribution. our results suggest the gene expression fluctuation can predetermine the cell state transition of hiPSCs.

3Pos122 深層学習を利用した電子線トモグラフィー法による心筋サルコメア構造のタンパク質分類の検討
Classification of muscle tissue components elucidated by electron tomography and deep learning

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The smallest and essential repeating structure in the muscle hierarchy is the sarcomere. In sarcomere, actin filaments and myosin filaments are arranged in a regular pattern and slide with each other in active contraction. Previous studies suggested that the interaction between the proteins cMyBP-C and Fhod3 in cardiac sarcomere is involved in structural maintenance. To visualize these structures in 3D architecture of cardiac muscle, we performed automatic segmentation of actin filaments and myosin filaments in the 3D maps of cardiac muscle acquired by electron tomography using 3D U-Net, one of the deep learning models. As a result, we found the 3D U-net should be valuable to improve the efficiency of manual segmentation.

3Pos123 滑り運動中のアクチン繊維内に沿って生じる局所的な内部コンフォメーション変化とその伝播
Local conformational changes and the propagation along an actin filament during in vitro motility assay

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Actin and myosin molecules are essential for various force generation events in living cells. An approach to imitate the actomyosin interaction is called an *in vitro* motility assay (IVMA). It allows us to observe the sliding movement of fluorescently labeled actin filaments (F-actin) on the glass surface that bound Heavy Mero Myosin in the presence of ATP by using the light microscope.
A previous study of IVMA (Hatori et al., 2004, PMID:15110932) showed that lateral fluctuation of F-actin unidirectionally propagates along its filament, suggesting that the internal load of F-actin regulates the surrounding myosin heads.
Here, we observed the structural changes of FRET-F-actin associated with actomyosin motility by using F-actin labeled with 2 different fluorescent dyes.

3Pos124 温められた心筋は安定性と不安定性を併せ持った収縮リズムを刻む
The warmed myocardium creates a contractile rhythm that combines stability and instability

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As a result of efficient search by deep learning type symbolic regression using experimental data as input, we were able to discover interesting properties of the myocardium. We found that warmed myocardial sarcomere carves a contractile rhythm that combines stability and instability. When the sarcomere in the cardiomyocytes is warmed, the sarcomere becomes an oscillation state in which it repeatedly contracts and relaxes (HSOs). This study revealed that HSOs chaotically change the phase state and oscillation amplitude between adjacent sarcomere. However, the oscillation period of HSOs remains constant. From the discussion by mathematical models, we have predicted that this chaotic instability produces periodicity and responsiveness to changes in calcium concentration.

3Pos125 コフィリン結合によるアクチン繊維のアロステリック応答解明に向けた分子動力学計算
Molecular dynamics simulation to study the long-range allostery of an actin filament due to cofilin binding

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Cofilin binds cooperatively to an actin filament and forms a cluster on the filament, which promotes severing the filament. The AFM observation demonstrated that cooperative and asymmetric binding of cofilin to an actin filament is realized by a long-range allostery. However, the long-range allostery of the actin filament remains controversial, and if it does exist, its physical mechanism remains elusive. In this study, to see how the cofilin binding affects the physical state of the actin filament, we conducted molecular dynamics simulation of a cofilin-bound actin filament. We focused on not only the structural responses but the dielectric response (i.e., dielectric allostery), which might underlie the long-range allostery of actin filaments.

3Pos126 マウス心筋細胞で認める高静水圧誘発性緩徐収縮
High hydrostatic pressure induces slow contraction in mouse cardiomyocytes

Yohei Yamaguchi[1], Masayoshi Nishiyama[2], Hiroaki Kai[3], Toshiyuki Kaneko[1], Keiko Kaihara[3], Gentaro Iribe[1], Akira Takai[1], Keiji Naruse[3], Masatoshi Morimatsu[3] ([1]*Dept. Physio., Asahikawa Med. Univ.*, [2]*Dept. Physics, Kindai Univ.*, [3]*Dept. Cardio. Physio., Grad. Sch. Med. Dent. Pharm., Okayama Univ.*)

Cardiomyocytes are contractile cells. Ca^{2+} flux activates actomyosin interactions, leading to the contraction, which is modulated by hydrostatic pressure. We evaluated the mechanism triggering slow contractions using a high-pressure microscope to characterize changes in cell morphology and $[Ca^{2+}]_i$ in mouse cardiomyocytes under high hydrostatic pressures. We found that cardiomyocytes contracted slowly, while a myosin ATPase inhibitor interrupted its slow contractions. Transmission electron microscopy also showed that the pressure of 20 MPa did not collapse cellular structures. Our results suggest that pressure-induced slow contractions in cardiomyocytes are driven by the activation of actomyosin interactions without an acute transient increase in $[Ca^{2+}]_i$.

3Pos127 クライオ電子顕微鏡による ATP 合成酵素 FoF1 の化学力学共役機構の解明
Molecular Basis of the Chemo-Mechanical Coupling Mechanism in the ATP-Driven Rotation of ATP Synthase FoF1

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The ATP synthase FoF1 can rotate using the hydrolysis energy of ATP. ATP hydrolysis by FoF1 consists of four processes: ATP binding, ATP hydrolysis, phosphate release, and ADP release, and in each process the catalytic subunit is conformationally changed to rotate the axis of rotation. In this study, we attempted to determine the structures corresponding to all reaction processes using single-particle analysis by cryo-EM, and to reveal the structural changes corresponding to the hydrolysis reaction cycle. Structural analysis under two substrate conditions yielded multiple structures with different rotation angles. From the obtained structures, the chemo-mechanical coupling mechanism in the F1 part will be discussed.

3Pos128 (2SCA-4) 1 分子回転操作実験によって解明されたミトコンドリア由来 ATP 合成酵素における阻害因子 IF_1 の一方向制御機構
(2SCA-4) Unidirectional regulation of ATPase factor 1 in mitochondrial ATP synthase studied by single-molecule manipulation experiments

Ryohei Kobayashi[1,2], Hiroshi Ueno[1], Kei-ichi Okazaki[2], Hiroyuki Noji[1] ([1]*Appl. Chem., Grad. Sch. Eng., Univ. Tokyo*, [2]*Inst. for Mol. Sci.*)

IF_1 is a regulatory protein for mitochondrial ATP synthase (F_oF_1), which inserts its N-terminus into the $\alpha_3\beta_3$ interface of F_1. One of the unique features of IF_1 is the unidirectional regulation: it inhibits ATP hydrolysis but does not inhibit ATP synthesis. To elucidate how IF_1 is released from F_1, we have performed single-molecule manipulation experiments of IF_1-inhibited F_1. The "stall-and-release" experiment showed the strong angle dependence of IF_1 release in the clockwise direction, but no activation in the counter-clockwise direction. Further, to explore the origins of the unidirectionality, we have conducted experiments with the N-terminal truncated IF_1, suggesting that the entrance part of the long helix of IF_1 contributes most to the unidirectionality.

3Pos129 Drug binding to the mycobacterial ATP synthase – mechanistic implications

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Mycobacteria are to able cause diseases, such as tuberculosis or skin infections, which can be treated by antibiotics. However, multidrug resistance is a current problem, rendering many first line antibiotics ineffective. Here, we study binding of recently developed therapeutic compounds to the F_o domain of the mycobacterial ATP synthase. Using molecular dynamics simulations, we clarify the binding modes of these drugs and characterize the associated energetics. Based on the obtained results, we provide additional insights into the mechanistic action of these drugs.

3Pos130 Single-molecule analysis and engineering of rotary V-ATPase

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V-ATPases (V_oV_1) actively transport H^+ or Na^+ in V_o motor by using torque generated by ATP hydrolysis in V_1 motor. To understand the energy transduction and ion transporting mechanism of V_oV_1, we performed single-molecule analysis and engineering of *Enterococcus hirae* V-ATPase (EhV_oV_1) which pumps Na^+. Our high-speed/high-precision single-molecule imaging simultaneously visualized rotational pauses and steps of EhV_o and EhV_1 and revealed rigid coupling between two motors for the first time. Furthermore, we are engineering the ion-binding rotor c-ring of EhV_o to change the ion selectivity from Na^+ to H^+, and to double the number of transported ions per turn. Based on these results, we will discuss the mechanism of EhV_oV_1.

3Pos131 Acrive structures of V/A-type rotary ATPase reveal the rotary catalytic mechanism

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V/A-ATPase is a motor protein that function with a rotary catalytic mechanism. When powered by ATP hydrolysis, the V_1 moiety rotates the central rotor against the A_3B_3 hexamer, composed of three catalytic AB dimers adopting different conformations. The catalytic intermediates of the V_1 moiety of V/A-ATPase under different reaction conditions reveal that the rotor does not rotate immediately after binding of ATP to the V_1. Instead, three events proceed simultaneously with the 120˚ rotation of the shaft: hydrolysis of ATP, zipper movement along with the binding ATP, and unzipper movement in along with release of both ADP and P*i*. This indicates the unidirectional rotation of V/A-ATPase by a ratchet-like mechanism owing to ATP hydrolysis.

3Pos132 全原子分子動力学計算による KIF1A の微小管への結合過程の解析
All-atom molecular dynamics simulation analysis of KIF1A binding to microtubule

Koki Adachi, Mitsunori Takano (*Dept. of Pure & Appl. Phys., Grad. Scl. Adv. Sci. & Eng., Waseda Univ.*)

KIF1A moves on the microtubule (MT) toward the plus end. Our previous coarse-grained (CG) molecular dynamics (MD) simulation showed a plus-end-directed biased binding of a KIF1A monomer on a single MT protofilament, which was realized by the Coulomb interaction between K-loop of KIF1A and the C-terminal tail (CTT) of tubulin. In this study, we conducted the all-atom MD simulation of KIF1A binding to MT that consists of multiple protofilaments in order to see whether the plus-end-directed biased binding can be observed in more accurate model. We also pay attention to the lateral movement of KIF1A to the adjacent protofilaments and the role of CTT in the biased binding and the lateral movement.

3Pos133 微小管とキネシンによる三次元のモティリティアッセイの実現
Realization of three-dimensional motility assay with microtubules and kinesin

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Biomolecular motors, which are used for material transport and structural deformation in cells, have attracted much attention for their use as actuators for molecular robots. One such example is the two-dimensional movement of microtubules on a glass slide on which kinesin is immobilized (motility assay). Using this method, observation of intelligent movement, such as large-scale herd movement, has been reported. However, existing methods place kinesins only in a two-dimensional plane, limiting the spatiotemporal information that can be obtained. In this study, we aim to realize three-dimensional motion of microtubules by spatially arranging kinesins. This research will lead to the observation of more advanced movements, such as flocking of birds.

3Pos134 KIF5A の ALS 関連遺伝子変異は KIF5A のオリゴマー化と凝集を促進し神経毒性を引き起こす
An ALS-associated KIF5A mutant forms oligomers and aggregates and induces neuronal toxicity

Kyoko Chiba[1], Juri Nakano[2], Shinsuke Niwa[1] ([1]*FRIS, Tohoku Univ.*, [2]*Grad. Sch. of Life Sci., Tohoku Univ.*)

KIF5A is a kinesin superfamily motor protein that transports various cargos in neurons. Mutations in Kif5a cause familial amyotrophic lateral sclerosis (ALS). It has been suggested that ALS is caused by loss of function of KIF5A. However, the precise mechanisms regarding how mutations in KIF5A cause ALS remain unclear. Here, we show that an ALS-associated mutant of KIF5A, KIF5A(Δexon27), is predisposed to form oligomers and aggregates in vivo and in vitro. Moreover, KIF5A(Δexon27)-expressing Caenorhabditis elegans neurons showed morphological defects. These data collectively suggest that ALS-associated mutations of KIF5A are toxic gain-offunction mutations rather than simple loss-of-function mutations.

3Pos135 ADP 解離の遅い変異体を用いたキネシン 1 の連続的歩行能を決める要因の研究
High-speed single molecule study of the determinant of kinesin-1's processivity using mutants with slow ADP-release

Yuta Miyazono, Hiroki Hayano, Tukasa Enomoto, Michio Tomishige (*Grad. Sch. Sci. Eng., Aoyama Gakuin Univ.*)

Kinesin-1 is a motor protein that moves along microtubules to transport intracellular cargoes. Kinesins has been shown to take ~100 steps before dissociating from microtubule, which is important for long-range transport, however the underlying mechanism is still unknown. Here, we investigated the effect of ADP release on kinesin-1's processivity using heterodimers consisting of wild-type and mutant heads that have defects in ADP release. Using high-speed single molecule microscopy, we found that the mutant leading head often prematurely dissociated from microtubule, especially prior to the dissociation of both heads from microtubule. These results suggest that prompt release of ADP from the leading head is important for kinesin-1 to maintain the stepping motion.

3Pos136 KIF1A/ダイニンが制御する軸索内小胞プールサイズ
Vesicle pool sizes controlled by axonal transport of KIF1A/dynein

Yuki Kagawa[1], Ryo Sasaki[1], Yuzu Anazawa[2], Shinsuke Niwa[3], Kumiko Hayashi[1] ([1]*Grad. Sch. Eng., Tohoku Univ.*, [2]*Grad. Sch. Life Sci., Tohoku Univ.*, [3]*FRIS., Tohoku Univ.*)

KIF1A/dynein transports synapse vesicle precursors (SVPs) in neuron axons; additionally, its genetic mutation causes hereditary spastic paralysis (HSP). In this study, we used HSP models of *C. elegans*. Fluorescence microscopy revealed en passant synapse distribution in the DA9 motor neurons of the HSP worms, indicating abnormal synapse distributions in HSP. Then, we investigated the difference of dynamics between the WT and mutants. Specifically, we investigated the capture and dissociation events of SVPs at the vesicle pools, considered immature synapses. We found the vesicle pool sizes largely depended on the KIF1A/dynein dynamics. We aim to reproduce the dependence by using the mathematical model of axonal transport and understand the abnormal synapse distributions.

3Pos137 Dpcd ノックアウトマウスの側脳室における内腕ダイニンの遺伝子発現と脳室内の流れの解析
Analysis of inner arm dynein gene expression and intraventricular flow in the lateral ventricle of Dpcd knockout mice

Hironori Ueno[1], Daiki Yamamoto[2], Kazuhito Takeuchi[2], Yuichi Nagata[2], Fumiharu Ohka[2], Atsushi Natsume[2], Ryuta Saitou[2] ([1]*Aichi Univ. of Edu.*, [2]*Grad. Sch. of Med., Nagoya Univ.*)

The purpose of this study is to elucidate a part of the cause of hydrocephalus. We added tracer particles to the surface of the ventricles and analyzed their behavior. As a result, it was found that the velocity of particles was reduced in the lateral ventricle. It's revealed that the electron density of inner arm dynein in axoneme decreased by the electron microscopy. The expression level of some inner arm dynein gene also decreased by qPCR analysis, which was in agreement with the result of electron microscopic observation. In addition, we found changes in the ciliary waveform. These results suggested that such abnormalities in inner arm dynein might be the cause of hydrocephalus.

3Pos138 ミュータントの S1 による F アクチンの協同的構造変化の伝播距離の推定
Estimation of propagation distance of cooperative conformational changes in F-actin induced by a mutant S1

Masahiro Miura, Taro QP Uyeda (*Department of Pure and Applied Physics, Graduate School of Advanced Science and Engineering, Waseda University*)

Sparse binding of G680V-mutant S1 to F-actin accelerates the actin movement on muscle HMM ~2-fold in vitro (Iwase et al. 2017). Acceleration occurred even when the binding ratio of G680VS1 to actin was a few tenths, suggesting that this acceleration is due to a cooperative conformational change of actin. To estimate the propagation distance of the conformational change, we created a fusion protein of actin nanobody (AN) and G680V S1, because, unlike G680V S1, AN-G680V S1 is expected to bind to F-actin randomly and uniformly. The maximum velocity was observed when the molar ratio of AN-G680VS1 to actin was in the range of 1:100~1:1000. We thus speculate that the conformational change of actin by G680V S1 propagates several hundred actin protomers.

3Pos139 ダイニンによる細胞内輸送が細胞質動態から受ける影響について
Effect of cytoplasmic dynamics on dynein-dependent transports

Takayuki Torisawa[1,2], Akatsuki Kimura[1,2] ([1]*Cell Arch. Lab., Natl. Inst. Genet.*, [2]*Dept. Genet., SOKENDAI*)

Intracellular transport driven by molecular motors is essential for various cellular functions. Although many *in vitro* studies have revealed several aspects of transporting activities, there remain discrepancies between *in vivo* and *in vitro* transports, evoking the importance of considering the cytoplasm-specific factors. In this study, we focused on the transport of early endosomes in *C. elegans* early embryos, which is mainly driven by cytoplasmic dynein, and examined how the cytoplasmic dynamics affect the transport properties. We found that the transport speed depended on the cell size and the activity of the actomyosin network. These results suggest that the active dynamics in the cytoplasm are a crucial factor in explaining *in vivo* transports.

3Pos140 減圧顕微鏡法によって測定されたバクテリア運動能
Bacterial motility measured by depressurization microscopy

Masayoshi Nishiyama (*Kindai Univ.*)

I have developed a depressurization chamber for optical microscopy. The chamber could be combined with an inverted microscope. The biological sample was prepared in a glass-bottomed dish or glass coverslips, and then enclosed in the chamber. The air pressure in the chamber could be decreased to ~0.015 MPa (0.15 bar) by a vacuum pump. Even at reduced pressure conditions, microscopic observation could be done while changing the focus position and observation area. At the poster presentation, I will share with experimental results about bacterial motility at reduced pressure conditions.

3Pos141 The relative motion of MotA around MotB in bacterial flagellar stator

Phuoc Duy Tran, Akio Kitao (*Sch. Life Sci. Tech., TokyoTech*)

Although the recent structures of flagellar stator complex MotA/B have been published, their motion to trigger the rotation of the baterial flagellar motor has not been thoroughly understood. Here, we applied the metadynamics to sample the structure of MotA rotating around MotB. The results exhibit the complicated relative motion between MotA and MotB is not likely to be the rotation of a ring around an well defined axis.

3Pos142 Single particle cryo-EM of *Paenibacillus* stator complex reveals the flexibility of the pentameric MotA1 ring

Sakura Onoe[1], Tatsuro Nishikino[2], Nobuhiro Takekawa[3], Jun-ichi Kishikawa[2], Takayuki Kato[2] ([1]*FBS, Osaka Univ.*, [2]*IPR, Osaka Univ.*, [3]*Dep. Macromol. Sci., Osaka Univ.*)

Bacterial flagellar has multiple stator complexes that act as ion channels to rotate a rotor. The type of ions utilized are monovalent cations, but the MotA1B1 stator complex of *Paenibacillus sp*. TCA20 was suggested to use divalent cations. However, the functional analysis using the chimeric complex suggested that the MotA1B1 is an H^+-driven stator. The structure of chimeric MotA1B1 was solved at 3.4 Å resolution by single-particle Cryo-EM and the MotA1 formed a pentameric ring, as the other stator complexes. The dimeric MotB1 penetrated the ring, and the plug helices of MotB1 were observed at the periplasmic tip of the MotA1 ring. In addition, several different conformational structures were obtained. The results strongly suggest the flexibility of the MotA1 ring.

3Pos143 (2SFA-6) SLC26 陰イオントランスポーターによる電気→運動エネルギー変換
(2SFA-6) SLC26 ion transporters act as electricity-driven motor proteins

Tomohiro Shima (*Grad. Sch. Sci., Univ. Tokyo*)

Outer hair cells in the inner ear of vertebrates greatly change their cell length in response to membrane potentials and amplify sound signal. The energy conversion efficiency from electricity to physical motion by the outer hair cells is approximately 10,000 times higher than that of man-made piezoelectric devices. Prestin, a unique member of SLC26 anion transporter family, is the motor protein responsible for this highly efficient energy conversion. By combining sensitive electrophysiological assays with light microscopy techniques, we found that prestin and other SLC26 proteins share voltage-sensing and motile abilities. Based on our results, we would like to discuss the currently conceivable mechanism that drives the large movement of outer hair cells.

3Pos144 速く動く DNA ナノ粒子モーターはつくれるか？シミュレーションによる検討
How to engineer fast-moving DNA-nanoparticle motor? A simulation study

Takanori Harashima, Akihiro Otomo, Ryota Iino (*Institute for Molecular Science*)

DNA-modified nanoparticle (DNA-NP) shows super-diffusion on RNA-modified surface as a burnt-bridge Brownian motor driven by enzymatic RNA hydrolysis. However, velocity of the DNA-NP motor is only a few nanometers/s and much lower than that of the biological counterpart such as processive chitinase. Here, to improve the velocity of DNA-NP motor, we perform a simulation considering the binding, hydrolysis, and dissociation rates of DNA/RNA duplex, enzyme concentration, and particle size. Interestingly, our preliminary results suggest that both the velocity and linearity of motion increase with the increase of the particle size. We will perform more detailed analyses and verify simulation results experimentally by using high-speed/high-precision single-particle tracking.

3Pos145 Fimbrin の協同的相互作用による F-actin の長さの変化
Changes in actin filament length induced by the cooperative interaction of fimbrin

Ryosuke Tsunabuchi[1], Naoki Hosokawa[1], Rika Hirakawa[1], Masahiro Kuragano[1], Taro Q.P Uyeda[2], Kiyotaka Tokuraku[1] ([1]*Graduate School of Engineering, Muroran Institute of Technology*, [2]*Department of Physics, Faculty of Science and Engineering, Waseda University*)

Cooperative interaction between actin-binding proteins (ABPs) and F-actin (FA) leads to functional differentiation of FAs but remains unknown. We have successfully observed cooperative interactions of myosin and fimbrin to FAs loosely immobilized on a positively charged lipid membrane. These ABP-FA interactions accompanied by long-range allostery on FA. We also found that the interaction of fimbrin induced the shortening of FAs. In this study, we observed whether the length of FA shortened by fimbrin binding was recovered by fimbrin dissociation by washing with buffer. The results showed that the length of FA after fimbrin dissociation returned to the length before fimbrin binding. We are currently analyzing the time it takes for this FA length to recover.

3Pos146 魚類ケラトサイトのストレスファイバ直動回転変換メカニズム
Linear contraction of stress fibers kicks the substratum for their rotation

Chika Okimura[1], Shu Akiyama[1], Tatsunari Sakurai[2], Yoshiaki Iwadate[1] ([1]*Dept.Biol., Yamaguchi Univ.*, [2]*Dept.Math.Eng., Musashino Univ.*)

Crawling migration plays an essential role in a variety of biological phenomena, including development, wound healing, and immune system function. Keratocytes are wound healing motile cells in fish skin. Recently, we showed that multiple contractile stress fibers are arranged around the nucleus, and are rotating. It is reminiscent of a novel mechanism that converts linear contraction into rotation. To see the mechanism is feasible, we made a “soft” mechanical model that mimics the cell body of keratocyte from silicone gel and contractile coils. The motion analysis of the model predicted that the stress fibers in keratocyte cell body would rotate by kicking the substrate. As predicted, we detected keratocytes kicking the substrate.

3Pos147 G146V とそのサプレッサー変異は酵母のアクチンダイナミクスに影響する
G146V and its suppressor mutations in yeast actin suggested to affect actin dynamics in vivo

Tenji Yumoto[1], Taro QP Uyeda[1], Takehiko Yoko-o[2] ([1]*Department of Pure and Applied Physics, Graduate School of Advanced Science and Engineering, Waseda University*, [2]*Cellular and Molecular Biotechnology Research Institute, AIST*)

G146V mutant actin dominantly inhibits cofilin binding to copolymer with WT actin and slows actin movement on myosin II in vitro. In vivo, the G146V mutant actin is dominantly lethal to yeast. To investigate how G146V affects yeast viability and actin functions, we previously conducted intragenic suppressor screening against G146V actin and identified seven suppressor mutations. Here, we analyzed effects of these novel actin mutations to yeast cells. Cells expressing these suppressor mutant actins showed abnormal actin cytoskeleton, multinucleation, and mitochondrial misorganization. These phenotypes and the locations of the suppressor mutations in the actin molecule suggested that the lethality of cells expressing G146V actin is mainly due to defective actin dynamics.

3Pos148 気管形成におけるアクチン骨格のミクロ相分離と自己組織化構造の転移ダイナミクス
Microphase separation and transition dynamics of self-organized structures of actin cytoskeleton during tubulogenesis

Mitsusuke Tarama[1], Sayaka Sekine[2], Tatsuo Shibata[1], Shigeo Hayashi[1] ([1]*RIKEN BDR*, [2]*Grad. Sch. Life Sci., Tohoku Univ.*)

Cytoskeleton molecules organise into various mesoscale structures that are responsible for force generation of macroscopic cells. During the development of the tracheal tube in Drosophila embryo, actin cytoskeleton cables appear at half-micrometer intervals to control the tubular size. In our experiment using high resolution imaging at an earlier stage of development, we found sporadic actin signals of 200-300 nanometers. To understand the emergence of these actin structures, we developed a theoretical study based on a coarse-grained molecular dynamics model. We found the clusters and stripes are reproduced through microphase separation. The transition dynamics of the self-organised structures predicted theoretically is also confirmed experimentally.

3Pos149 アクトミオシンの収縮による膜変形の再構成
Morphological transitions of lipid vesicles driven by the contraction of actomyosin networks

Makito Miyazaki[1,2,3,4], Fahmida Sultana Laboni[5], Masatoshi Ichikawa[2], Taeyoon Kim[5] ([1]*Hakubi, Kyoto Univ.*, [2]*Dept. Phys., Kyoto Univ.*, [3]*Inst. Curie*, [4]*PRESTO, JST*, [5]*Biomed. Eng., Purdue Univ.*)

The actomyosin network beneath the cell membrane, generally called the actin cortex, regulates various cellular functions through inducing morphological transitions. To elucidate the mechanism, we encapsulated purified proteins in lipid vesicles and sought conditions in which actomyosin networks induce the vesicle deformation. This bottom-up approach identified the key parameters regulating the probability and magnitude of the membrane blebbing. Time-lapse observation clarified that the bleb was induced by either membrane detachment from the actin cortex, or rupture of the actin cortex, and the actin-membrane interaction determined which case was dominant. These findings will bring us general insights into the physical mechanism of morphological transitions of the cell.

3Pos150 人工細胞内アクチン光操作が可能にする細胞運動の再構成
Synthesizing motility in artificial cells by asymmetrically reconstituted actin polymerization

Hideaki Matsubayashi[1,2], Shiva Razavi[2,3], Hideki Nakamura[2,4,5], Daniel A. Kramer[6], Tomoaki Matsuura[7], Baoyu Chen[6], Takanari Inoue[2] ([1]*Frontier Research Institute for Interdisciplinary Sciences, Tohoku University*, [2]*Department of Cell Biology, School of Medicine, Johns Hopkins University*, [3]*Department of Biological Engineering, School of Engineering, Massachusetts Institute of Technology*, [4]*Hakubi Center for Advanced Research, Kyoto University*, [5]*Department of Synthetic Chemistry and Biological Chemistry, School of Engineering, Kyoto University*, [6]*Roy J. Carver Department of Biochemistry, Biophysics and Molecular Biology, Iowa State University*, [7]*Earth-Life Science Institute, Tokyo Institute of Technology*)

Cell migration is a dynamic process represented by neutrophils chasing pathogens. Although molecules involved in the reorganization of the actin cytoskeleton at the leading edge of migrating cells have been identified, it remained elusive what the minimal factors are to support the unidirectional motion of lipid vesicles. Aiming to reconstitute cell motility, we developed a novel light-inducible system inside giant vesicles where reversible and asymmetric actin polymerization/depolymerization can be achieved. We further identified a biochemical condition to guide lipid vesicles with light. Our functionally reconstituted biomechanical system embodies the longstanding model of cell migration and offers new avenues to both basic and applied sciences of cell motility.

3Pos151 Probing the influence of geometrical constraints on collective cell dynamics in diameter-varying 3D gelatin tube structures

Mitsuru Sentoku, Kenji Yasuda (*Dept. Pure & Appl. Phys., Grad. Sch. Adv. Sci. & Eng., Waseda Univ.*)

While the collective cell migration of a two-dimensional epithelial sheet has been studied extensively, the guidance mechanism of cellular rearrangement remains elusive for three-dimensional platforms. Here, the behavior of endothelial cells is examined inside successive transitions across diameter-varying tube structures (30-150 μm) in gelatin substrate. The transition from a narrow to the wider region caused a decrease in migration velocity following in direct proportion to the ratio of the diameter increase, whereas narrowing the diameter of the microtube increased the speed with no apparent correlation. Our findings provide insights into the dominant geometric factor in migratory modes corresponding to fluid-like profiles in the borderless cylindrical cell sheets.

3Pos152 プリント化したフィブロネクチン勾配に対する好中球の走触性の解析
Analysis of neutrophil haptotaxis on printed fibronectin gradients

Yoshino Tanaka[1], Gen Honda[2], Masahito Uwamichi[3], Satoshi Sawai[3] ([1]*Grad. Sch. Sci., Univ. Tokyo*, [2]*Komaba institute for science, Grad. Sch. Arts & Sci., Univ. Tokyo*, [3]*Grad. Sch. Arts & Sci., Univ. Tokyo*)

Haptotaxis is a form of directed cell migration based on surface-bound chemical cues. Despite its assumed importance for cell guidance in vivo, its exact nature in immune cell is unclear and largely remains untested even in vitro. Here we show, by using photo-printed gradient of fibronectin density on a glass substrate, neutrophil-like HL60 cells exhibit positive haptotaxis. Quantitative analysis of the centroid trajectories indicates large orientational bias towards higher density of fibronectin ranging from 1.7 to 6.6 μg/ml mean density. The velocity on the other hand tapered off at an intermediate density thus giving rise to a swarming-like effect. We will discuss details of the analysis as well as localization of some of the key intracellular moleculars.

3Pos153 細胞性粘菌の運動において bleb モードへの転換は Ca^{2+}流入に依存しない
The transition to bleb mode is independent on extracellular Ca^{2+} influx in *Dictyostelium discoideum* motility

Hitomi Takeuchi, Taro QP Uyeda (*Department of Pure and Applied Physics, Graduate School of Advanced Science and Engineering, Waseda University*)

Motility of amoeboid cells often switch between the pseudopod mode and bleb mode depending on their environment. In *Dictyostelium discoideum,* bleb mode is induced experimentally by pressure. Srivastava et al. (2019) concluded that extracellular Ca^{2+} influx through Piezo stretched-activated Ca^{2+} channel induces the bleb mode, whereas we previously showed that extracellular Ca^{2+} is dispensable for the pressure-induced conversion to the bleb mode motility. Here, we observed conversion to the bleb mode in both Piezo channel-knock out cells and wild type cells even when extracellular Ca^{2+} was chelated, suggesting that extracellular Ca^{2+} influx is unnecessary for the conversion. We are currently examining the source of discrepancy between Srivastava et al. and us.

3Pos154 Velocity field dynamics under blurring in fluorescent images of dictyostelium discoideum colonies

Md Mohiuddin[7,8], Md Motaleb Hossain[1,2], Sulimon Sattari[1], Udoy S. Basak[1,3], Mikito Toda[4], Kazuki Horikawa[5], Tamiki Komatsuzaki[1,6,7] ([1]*Research Institute for Electronic Science, Hokkaido University, Japan*, [2]*University of Dhaka, Bangladesh*, [3]*Pabna University of Science and Technology, Bangladesh*, [4]*Nara Women's University, Japan*, [5]*Tokushima University Graduate School, Japan*, [6]*Institute for Chemical Reaction Design and Discovery (ICReDD), Hokkaido University, Japan*, [7]*Graduate School of Chemical Sciences and Engineering, Hokkaido University, Japan*, [8]*Mathematics Discipline, Comilla University, Bangladesh*)

cAMP (chemoattractant) drives collective motion.On starvation, cells signal by emitting cAMP and nearby cells move towards the cAMP gradient and release cAMP.New imaging tool is developed to monitor cell & cAMP together.Velocity flow field(VFF) of image sequences can be generated by PIV.The VFF of original images follows the underlying cell motion, when blurred images provide cAMP motion.The angle of cell velocities & cAMP waves is nearly 180^0.cosq among PIV of original and blurred images and cAMP motion are computed to infer the direction of cAMP motion. On wave peaks cosq between cell motion and cAMP motion ($\sigma=50$) is lowest.This reverses upon increase in the blurred parameters σ.cosq is flipped when $\sigma=50$,it indicates $\sigma=50$ blurred image represents cAMP motion.

Poster

3Pos155 The dominant factor of shapeshifts of collective cell migration between sheet form and clusters in flexible 3D tunnel structures

Wataru Hanamoto[1], Miki Takei[1], Masaharu Endo[2], Kaito Asahi[2], Mitsuru Sentoku[2], Kenji Yasuda[1,2] ([1]*Dept. Pure & Appl. Phys., Sch. Adv. Sci. & Eng., Waseda Univ*, [2]*Dept. Pure & Appl. Phys., Grad. Sch. Adv. Sci. & Eng., Waseda Univ.*)

Collective cell migration is a factor of lumen formation in organs, but it has been difficult to create three-dimensional lumen structures with a wider interior using conventional methods. We have developed an infrared laser processing of gelatin to fabricate flexible lumenal structures. We formed a cone-shaped narrowing tunnel connected to the inverse cone-shaped widening tunnel through their cone points. The migrating cell sheet in the narrowing cone region was shifted to the densely packed form at 25 μm in diameter and was recovered to the cell sheet form again at 25 μm in diameter in the widening reverse cone region. The results suggest the conversion of shapes between cell sheets and clusters is a simple reversible tunnel-diameter-dependent phase shift.

3Pos156 二次元制限空間内を進行する細胞集団の流体的振る舞いの計測
Measuring the fluid-like behavior of collective cell migration in two-dimensional restricted structures

Miki Takei[1], Masaharu Endo[2], Mitsuru Sentoku[2], Kaito Asahi[2], Wataru Hanamoto[1], Kenji Yasuda[1,2] ([1]*Dept. Phys., Sch. Adv. Sci. & Eng., Waseda Univ.*, [2]*Dept. Pure & Appl. Phys., Grad. Sch. Adv. Sci. & Eng., Waseda Univ.*)

To understand the fluid-like behavior of collective cell migration, we analyzed the change of cell migration during pathway width changes (e.g., wide-narrow-wide) in agarose microstructures. Cell velocity increased as cells moved from wider to narrower pathway regions, satisfying the mass conservation law. However, the degree of change in path width did not correlate with the rate of increase in cell velocity caused by the change in cell shapes—Higher-ratio of the wide-narrow-wide structure generated isolated single cells at the widening point of the narrow-wide part. The results suggest the shape of the confinement structure can control not only the fluid-like manner of the cell sheet but also the cell-to-cell connections for cell shape change and isolation.

3Pos157 CheZ 局在の大腸菌走化性に及ぼす影響のキャピラリーアッセイによる解析
Analysis for the effect of CheZ localization on chemotaxis of *Escherichia coli* by capillary assay

Sawako Matsuda[1], Yong-Suk Che[1], Akihiko Ishijima[1], Masaru Kojima[2], Hajime Fukuoka[1] ([1]*Grad. Sch. Frontier Biosci. Osaka Univ*, [2]*Grad. Sch. Engineering Sci. Osaka Univ*)

Previously, we evaluated the chemotactic response by the rotational direction of flagellar motor of *E. coli*. But this method is insufficient to quantitatively evaluate chemotaxis by cellular swimming. Therefore, we made an experimental system using micropipette and compared the temporal changes in chemotactic responses of wild-type and CheAshort-deficient mutant cells by swimming. Wild-type cells assembled (time constant, ~30s) and dispersed (time constant, ~20s) around pipette depending on the serine-release and stop of it. The assembly and disperse of mutant cells were slower than those of wild-type cells. CheAshort is the binding target for CheZ to receptor array, therefore this binding is important for cells to reach their target environment quickly in chemotaxis.

3Pos158 CheB の極性局在を利用した異種走化性受容体の忌避刺激に対する応答性の比較
Comparison of responses to repellent stimulus at heterogeneous MCPs through polar localization of CheB

Shinnosuke Kawahara, Yumiko Uchida, Yong-Suk Che, Akihiko Ishijima, **Hajime Fukuoka** (*Grad. Sch. Frontier Biosci. Osaka Univ.*)

E. coli adapt to external stimuli by sensory adaptation system. In previous meeting, we reported that, in a cell expressing Tsr as a sole receptor, CheB assembled to cell pole by repellent (isoleucine) and dispersed by adaptation. In this study, we investigated whether other types of chemoreceptors recognize isoleucine. In Tar-expressing cell, CheB-localization was increased in response to isoleucine, but the amount and duration of localization were less and shorter than in Tsr-expressing cells. In Trg-expressing cell, no change in CheB-localization was observed. The cellular responses monitored by bead assay are consistent with CheB-localization in all cell lines. These results suggest Tsr may have a mechanism that strongly recognizes isoleucine as a repellent.

3Pos159 バクテリアの群れ運動における局所的な細胞間相互作用と運動制御
Local cell interaction and motility regulation for swarm motility of bacteria

Kodai Suzuki, Ikuro Kawagishi, Masatoshi Nishikawa (*Grad. Sch. Fun., Univ. Hosei*)

Vibrio alginolyticus undergoes morphological changes, namely cell elongation and synthesis of lateral flagella, Laf, and exhibits collective motion to spread rapidly, on the surface of solid. The surface swarming is emergent from complex interplay between local cell interaction mediated by Laf and chemotaxis signaling pathway, but its underlying mechanisms remain to be largely unexplored. In this poster, we studied the swarming motility of the heterogeneous populations that consist of wild-type and swarm mutants. We found that the small fraction of chemotaxis mutant induce severe defect of swarm motility, while laf mutant does not interfere. This suggests the importance of local interaction between cells in which the motility is under regulation by chemotaxis pathway.

3Pos160 クラミドモナス繊毛交互打ち変異株の解析
Analysis of a *Chlamydomonas* mutant showing alternate ciliary beatings

Kazuma Sakamoto[1,2], Atsuko Isu[1], Toru Hisabori[1,2], **Ken-ichi Wakabayashi[1,2]** ([1]*Lab. Chem. Life Sci., Tokyo Tech.*, [2]*Sch. Life Sci. Tech., Tokyo Tech*)

Chlamydomonas reinhardtii is a unicellular green alga that swims by beating two cilia simultaneously like human's breaststroke. The simultaneous beatings of two cilia are essential for *C. reinhardtii* cells to show phototaxis because they change their swimming direction by beating one of the two cilia stronger than the other. However, the mechanism of how the two cilia beat simultaneously is a long-standing question. By screening for phototaxis mutants, we accidentally isolated mutants that beat cilia alternately (termed *alt* mutants). We identified a causative gene for a mutant tentatively named *alt6*. Localization of Alt6p will be discussed.

3Pos161 海洋性ビブリオ菌におけるべん毛本数制御因子 FlhF と MS リング構成因子 FliF の相互作用解析
Interactions between the flagellar number regulator FlhF and the MS ring protein FliF in *Vibrio alginolyticus*

Yuria Fukushima, Seiji Kojima, Michio Homma (*Div. Biol. Sci., Grad. Sch. Sci., Nagoya Univ.*)

Vibrio alginolyticus forms only a single flagellum at the cell pole by regulators FlhF and FlhG. FlhF belongs to the signal recognition particle type GTPase family, regulates positively the formation of flagella and is required for polar positioning of the flagellum. FliF, the two transmembrane (TM) segments and a large periplasmic region, forms the MS ring of flagellar basal body in the membrane. Previous studies suggest that FlhF interacts with FliF to facilitate MS ring formation at the cell pole, but the interaction has not been detected. Here, we show the possibility that FlhF interacts with FliF at residues 55 to 108, including the first TM segment and following periplasmic region. The hydrophobic residues of this region may be important for the interaction.

3Pos162 Functional and structural analyses of FlaK, a master regulator of the genes involved in polar flagellar formation in marine *Vibrio*

Seiji Kojima[1], Tomoya Kobayakawa[1], Yuxi Hao[1], Tatsuro Nishikino[2], Michio Homma[1] ([1]*Div. of Biol. Sci., Grad. Sch. Sci., Nagoya Univ.*, [2]*Inst. for Prot. Res., Osaka Univ.*)

Marine *Vibrio* has a polar flagellum at cell pole and genes involved in its formation are regulated hierarchically with several classes. FlaK is an ortholog of *Pseudomonas* FleQ, the AAA+ ATPase that functions as a master regulator. We conducted mutational analysis of FlaK to examine its function in flagellation, ATPase activity, and the ability to form multimeric structure. Mutations at the ATP binding/hydrolysis sites abolished not only FlaK function to express downstream flagellar genes but also their ATPase activity. Chemical crosslinking and size exclusion chromatography showed that FlaK alone forms mainly dimer in solution independent of ATP. The negative regulator FlhG reduced FlaK ATPase activity, whose detailed mechanism will be discussed in the meeting.

3Pos163 カルシウム感受性があるクラミドモナス鞭毛内部構造のラセン配置
The Calcium Sensitive Helical Arrangement of Axonemal Structures in Chlamydomonas Flagella

Hitoshi Sakakibara[1], Kenta Ishibashi[1], Hiroyuki Iwamoto[2], Hiroaki Kojima[1], Kazuhiro Oiwa[1,3] ([1]*Bio-ICT, Nat. Inst. Inf. Com. Tech.*, [2]*SPring-8, JASRI*, [3]*Life Sci. Univ. Hyogo*)

Chlamydomonas incleases intracellular Ca^{2+} by intense light stimulation and changes its flagellar waveform. In its axoneme, the 9 peripheral microtubules (PMTs) are arranged so that their associated structures are arranged helically. From X-ray fiber-diffraction studies, we recently revealed that this helical arrangement is disturved by the addition of Ca^{2+} (BPJ2019). Here, we analyzed this arrangement in detail in the conditions of +/- Ca^{2+} by negative-staining electron tomography. Images of PMTs were extracted from tomograms and arrangements of those structures were compared. In the absence of Ca^{2+}, PMTs were arranged so as to be offset by about 32 nm in one direction to the next PMT. On the other hand, the arrangement was disturbed in the presence of Ca^{2+}.

3Pos164 大腸菌べん毛モーター間の回転方向転換同調を阻害する走化性受容体クラスター内における野生型/変異体比率の見積もり
Estimation of mutant/WT receptors ratios in receptor array that disrupts the switching coordination between flagellar motors of *E. coli*

Yumiko Uchida, Hajime Fukuoka, Akihiko Ishijima, Yong-Suk Che (*Grad. Sch. Frontier Biosci. Osaka Univ.*)

E. coli cells exhibit coordinated switching of flagellar motors by fluctuating CheYp concentrations. We speculate this coordination involves spontaneous activation/inactivation of receptor array (array blinking). This study tested whether array blinking occurs by changing the expression ratio of mutant receptors that lack cooperativity in the receptor array. The switching coordination was disrupted when the mutants' ratio exceeded only about 10%. These results suggest the insertion of a small number of receptor mutants disrupts the cooperative manner in the receptor array, so that array could not blink to produce significant fluctuation of CheYp concentration.

3Pos165 回転する大腸菌べん毛モーター中の GFP-FliL 局在の定量解析
Quatitative analysis of GFP-FliL localization at rotating flagellar motor of *E. coli.*

Miyuto Miyazaki, Yumiko Uchida, Hajime Fukuoka, Akihiko Ishijima, Yong-Suk Che (*Grad. Sch. Frontier Biosci. Osaka Univ.*)

E. coli swim in liquid environment by rotating flagellar motor. FliL is thought to localize at flagellar motor with stator and to assist the rotation. In this study, we investigated the intracellular dynamics of GFP-FliL under TIRF microscopy. GFP-FliL localized at the rotational center of tethered cell, indicating FliL acts directly on the motor. Based on comparison with the fluorescence intensity of FliM-GFP, tens of FliL molecules were estimated to be bound to the motor. Furthermore, FliL molecules seemed to be replaced on the order of tens of seconds without the change in rotational speed of flagellar motor. These results indicate that the replacement of FliL is independent of that of stator. We want to discuss these quantitative parameters at annual meeting.

3Pos166 キイロショウジョウバエの精子鞭毛の波形と鞭毛打頻度
The waveform and beat frequency of a sperm flagellum of *Drosophila melanogaster*

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A flagellum of *Drosophila melanogaster* spermatozoon is extremely long (ca 2mm) and has a characteristic internal structural feature, i.e., 9 + 9 + 2 architecture instead of conventional 9 + 2. To characterize its waveform, we isolated spermatozoa from the testis and recorded their swimming with a high speed camera. The spermatozoon swims in a spiral pathway, and the beating pattern consists of minor waves superimposed on major waves. Although its physiological significance is unclear, the double-wave nature of the beating pattern could be related to the 9 + 9 + 2 architecture. When combined with the genetic resource of *Drosophila*, the precise observation will provide a powerful clue for studying the structure-function relationship of eukaryotic flagella in general.

3Pos167 ピエゾ駆動対物レンズを用いたホヤ精子遊泳の 3 次元的解析
3D analysis of ascidian sperm swimming using a piezoelectric Z-scanner attached to a microscope objective

Kogiku Shiba, Kazuo Inaba (*Shimoda Marine Research Center, Univ. Tsukuba*)

Most studies on sperm motility have been performed in only two-dimensions due to the difficulty with capturing free-swimming sperm. To understand sperm motility regulation, we analyzed ascidian sperm swimming in three-dimensions using a piezoelectric device. Free-swimming sperm in a glass-bottomed dish were observed under the inverted phase contrast microscope with the objective lens actuated by a high-speed piezo Z-scanner. The images were recorded at 8,000 frames per second by a high-speed camera with an LED strobe light. We obtained the sperm head position in the Z-axis within 150 μm depth and reconstructed the 3D swimming trajectory. This allowed us to analyze the direction of helical swimming and sperm chemotactic behavior in three-dimensions.

3Pos168 蛍光共鳴エネルギー移動(FRET)によるタウ–微小管相互作用の熱力学的解析
Thermodynamic analysis of tau–MT interaction by Forster resonance energy transfer (FRET)

Riku Kiyonaka, Hideyuki Komatsu (*Dept. of Bioscience and Bioinformatics, Kyushu Inst. Tech.*)

A microtubule (MT)-associated protein tau stabilizes microtubules. Our previous study using isothermal titration calorimetry shows that the interaction between MT and tau is endothermic reaction at 35°C. Although the tau-bound MT has a high enthalpy state, the MT is energetically stabilized. Thus the energetic property of tau-induced stabilization of MT and its mechanism are interesting. The endothermic interaction primarily exhibits that the binding affinity of tau to MT increases with increasing temperature. In this report, effect of temperature on the dissociation constant of the tau–MT interaction will be investigated using FRET between Green fluorescent taxol-bound MT and rhodamine-labeled tau.

3Pos169 FRET 計測系を用いた低濃度セリンに対する単一大腸菌受容体の協同作用による 2 種類の適応
Two behaviors of adaptation by cooperative action of a single *E. coli* receptor to low concentrations of serine using FRET measurement

Yuki Takada, Akihiko Ishijima, Hajime Fukuoka, Yong-Suk Che (*Graduate School of Frontier Biosciences Osaka University*)

In chemotaxis system of *E.coli*, CheYp concentration ([CheYp]) and motor-rotation are closely related. In this study, we simultaneously measured the motor-rotation and FRET ratio between CheY and CheZ, which represents [CheYp], in a single cell; FRET ratio rapidly decreased after adding serine and then recovered to original level by adaptation, and the motor-rotation was consistent with the time trace of FRET ratio. We also detected two types of cells that exhibited steep or gradual recovery in FRET ratio only at low serine concentration (< 1 μM). We simulated this phenomenon by MWC model, and the number of cooperativity in the process of adaptation might be able to explain this phenomenon. In annual meeting, we will discuss this mechanism occurred in E. coli cell.

3Pos170 BAR ドメインタンパク質による細胞間接着の維持
Maintenance of cell-cell adhesions by BAR domain proteins

Yosuke Senju (*RIIS, Univ. Okayama*)

The generation of membrane curvature is essential for the formation of membrane protrusions and invaginations during cell migration, morphogenesis, and endocytosis. The BAR (Bin/Amphiphysin/Rvs) domain proteins can sense/generate membrane curvatures, and deform the membranes into protrusions or invaginations through phosphoinositide binding. Here, we revealed that MIM (missing-in-metastasis), one of the BAR domain proteins, localizes at adherens junctions in polarized MDCK cells. To elucidate the molecular mechanism by which MIM is responsible for the maintenance of adherens junctions, we identified several putative interaction partners of MIM. We now verify their physiological relevance for the actin and membrane dynamics at adherens junctions in epithelial cells.

3Pos171 スパイロプラズマの細胞分裂タンパク質の機能解析
Functional analysis of Spiroplasma cell division proteins

Taishi Kasai[1], Yuhei Tahara[2], Makoto Miyata[2], Daisuke Shiomi[1] ([1]*Rikkyo University, College of Science*, [2]*Osaka Metropolitan University, Graduate School of Science*)

The bacterial cell division is regulated by the tubulin homolog protein FtsZ. FrsZ forms the ring like structure (Z-ring) with the other cell division proteins and the Z-ring drives cell wall synthesis. Spiroplasma are cell wall-less bacteria, lacking most genes involved in cell wall synthesis except ftsZ and sepF genes. We analyzed the GTPase activity of FtsZ and the interaction between FtsZ and SepF. The GTPase activity of FtsZ was estimated from released phosphate in sample solution. The rate of GTP hydrolysis was increased in the presence of SepF. The interaction was measured by the bio-layer interferometry. The presence of GTP decreased the affinity of FtsZ for SepF, suggesting that the polymerized FtsZ reduces the interaction to SepF.

3Pos172 細胞外小胞の受容細胞への内在化と膜融合効率の検討
Investigation of the efficiency of internalization of extracellular vesicles and their membrane fusion with recipient cells

Hisaaki Hirose, Yusuke Hirai, Shiroh Futaki (*ICR, Kyoto Univ.*)

Extracellular vesicles (EVs), such as exosomes and microvesicles, contribute to cell-cell communication. EVs physiologically encapsulate various proteins, nucleic acids, and metabolites as cargos. In general, it has been thought that EVs release their cargos into recipient cells by “membrane fusion” with the plasma membrane or the endosomal membrane of the cells. However, the details have remained unknown on how EVs release their cargo. Here, we sought to establish two methods to 1) visualize EVs internalization and membrane fusion by fluorescence live cell imaging and 2) quantitatively analyze the amount of internalized and fused EVs by bioluminescence. We would like to discuss the possibility of membrane fusion between EVs and the recipient cells.

3Pos173 レプトスピラの運動性や物性、病原性に与える外膜分子の影響
Effect of the outer membrane (OM) molecules on the motility, physical property, and pathogenicity of *Leptospira*

Keigo Abe[1], Nobuo Koizumi[2], Shuichi Nakamura[1] ([1]*Grad. Sch. Eng., Univ. Tohoku*, [2]*Dept. of Bacteriology I, National Inst. of Infectious Disease*)

Leptospira is a zoonotic bacterium, infecting various mammalian hosts. It's suggested leptospiral pathogenicity somehow involved motility, but how the pathogen uses the motility within the host is unknown. Here, we investigated the leptospiral motility and physical property by using OM-component-related mutants to understand the role of OM on pathogenicity. First, we will report implementation of the new image processing method using Bayesian estimation to detect *Leptospira* on kidney cells from unclear images. The result of motility assay shows the mutation in OM proteins affects leptospiral crawling on the cultured kidney cells. In addition, we will discuss the OM-molecules dependence of the rigidity and its effect on the motility and pathogenicity.

3Pos174 自律拍動心筋細胞ネットワークにおける強制発火周期の記憶化
Memorization of forced firing intervals in spontaneous beating cardiomyocyte networks

Akira Nishizaki[1], Yoshitsune Hondo[2], Suguru Matsumoto[2], Kazuhumi Sakamoto[2], Kenji Yasuda[1,2] ([1]*Dept. Pure & Appl. Phys., Sch. Adv. Sci. & Eng., Waseda Univ.*, [2]*Dept. Pure & Appl. Phys., Grad. Sch. Adv. Sci. & Eng., Waseda Univ.*)

We examined the cell number dependence on the adaptation process of forced stimulation intervals in spontaneous beating cardiomyocyte networks exploiting our originally designed stimulation device. We used square electric field waveforms to stimulate single isolated cardiomyocytes and their networks and compared them. Both beating intervals of single cells and those of networks increased as the stimulation intervals increased. After forced stimulation stopped, single cells recovered to their original spontaneous beating intervals, whereas the cardiomyocyte networks maintained their faster spontaneous beating intervals. These results suggest that the forced beating intervals are memorized easier in the network form of cardiomyocytes than in single isolated cells.

3Pos175 Plasticity of synchronized beating during connecting and separating of cardiomyocyte networks

Suguru Matsumoto[1], Kazufumi Sakamoto[1], Akira Nishizaki[2], Kenji Yasuda[1,2] ([1]*Dept. Pure & Appl. Phys., Grad. Sch. Adv. Sci. & Eng., Waseda Univ.*, [2]*Dept. Pure & Appl. Phys., Sch. Adv. Sci. & Eng., Waseda Univ.*)

Fast firing regulation is a dominant rule of cardiomyocyte synchronization. However, the slower spontaneous beating clusters were conserved when attached to the faster beating cells. To unveil this phenomenon, we constructed a pair of spontaneously beating 25-cell cardiomyocyte networks and connected them and then separated them to measure their synchronization and adaptation in beating intervals. The beating intervals after their connection were new and original from those of component networks, against the fast firing regulation. Beating intervals of each network after their separation also showed a tendency to maintain beating intervals close to those of the connected, indicating beating intervals can be memorized in the networks regardless consisting cell number.

3Pos176 緩やかな温度上昇による心筋細胞の拍動揺らぎの抑制
Depression of beating fluctuation in cardiomyocytes by gradual temperature rising

Kohei Oyama, Masahito Hayashi, **Tomoyuki Kaneko** (*LaRC., Dept. Frontier Biosci., Hosei Univ.*)

Arrythmia can be caused by cold temperatures from cooling the heart during heart transplantation. To clarify the transition process of the beating pattern in temperature change, we investigated Inter-Spike Interval (ISI) and Short-Term Variability (STV) of ISI in cardiomyocytes from 37 to 5°C and from 5 to 37°C by using Multi-Electrode Array (MEA) system. ISI, stabled at 37°C, increased to at 13°C and disappeared. Stopped beating at lower temperatures resumed at 26°C and ISI decreased to at 37°C. STV decreased with temperature drop too, however, STV increased at around 30°C. More gradual temperature rise to 30°C resulted in decreasing of STV at all temperatures. It is considered that gradual temperature change can inhibit arrythmia caused by temperature change.

3Pos177 哺乳動物細胞におけるコレステロール依存的な熱吸収機構
Cholesterol-dependent mechanism underlying heat absorption in mammalian cells

Akira Murakami[1,2], Tasuku Sato[1], Kohki Okabe[1], Takashi Funatsu[1] ([1]*Grad. Sch. Pharm. Sci., Univ Tokyo*, [2]*Grad. Sch. Pharm. Sci., Univ Shizuoka*)

The body temperature has long been believed to be determined by the balance between heat production and dissipation. While recent intracellular thermometry has revealed the mechanism of heat production at the single cell level, the process by which the produced heat dissipates to the extracellular environments remains unknown. In this study, the heat flow and the intracellular heat transfer of living HeLa cells were analyzed using differential scanning calorimetry (DSC) and fluorescent polymeric thermometer (FPT), respectively. We identified that cholesterol, a membrane lipid, inhibits the heat efflux from inside to outside of cells. Our findings might provide new evident that the intracellular generated heat is absorbed in cells.

3Pos178 自己融解酵素によるグラム陽性細菌の溶菌過程の高速 **AFM** 観察
High-speed AFM observation of the lysis process of Gram-positive bacterial cell by autolysin

Yumu Ota[1], Hayato Yamashita[1], Kotaro Higashi[2], Masaya Yamaguchi[2], Shigetada Kawabata[2], Masayuki Abe[1] ([1]*Grad. Sch. of Eng. Sci., Osaka Univ.*, [2]*Grad. Sch. of Den., Osaka Univ.*)

Gram-positive bacteria *Streptococcus pneumoniae* is the main pathogen causing pneumonia. Autolysin LytA is considered to be a virulence factor that facilitates the spread of toxins by lysing the bacterial cell wall [1]. However, the relationship between the cell wall architecture and the lysis mechanism by LytA remains unclear. In this study, we applied high-speed AFM (HS-AFM) to observe *Streptococcus mitis*, *S. pneumoniae*-close relative. We successfully visualized the band-like structure of cell wall peptidoglycans along the short axis of the cells. Furthermore, HS-AFM movies showed the binding of LytA on the cell wall surface and the lysis of the bacterial cell. We will discuss the lysis process by autolysin LytA.
[1] P. Mellroth et al., *J. Biol. Chem.* (2012)

3Pos179 Application of three-dimensional holotomography in label-free living cells

Seongsoo Lee, **Jae-Hyuk Lee** (*Korea Basic Science Institute Gwangju Center, Gwangju 61751, South Korea*)

Holotomography (HT) is a new promising technique for label-free imaging of living biological samples. Using laser interferometry and holographic method, HT technique can measure three-dimensional (3-D) refractive index (RI) distribution of a living cell and reconstruct a dynamic 3-D image with high contrast spatial resolution (resolved to 110 nm). Here, we will present the recently developed 3-D multimodal imaging system, which simultaneously analyzes the quantitative phase and fluorescence images in a label-free living cell. We will also discuss various biological applications including cell biology, immunology, pathology and infection diseases. HT technique as a new approach in imaging system will enhance our interest in the biophysiology of cells and tissues.

3Pos180 細胞応答評価のためのマルチモーダル刺激可能なマイクロハンドの開発
Development of microhand with multimodal stimulus system for evaluation of cellular response

Masaru Kojima[1], Kazuma Koshide[1], Yasushi Mae[2], Tatsuo Arai[3] ([1]*Grad. Sch. Eng.Sci., Osaka Univ.*, [2]*Fac. of Eng. Sci., Kansai Univ.*, [3]*UEC*)

In recent years, there has been an increasing demand to measure cell and tissue characteristics. In particular, various techniques have been proposed to measure specific cellular responses to various external stimuli and to achieve unprecedented analysis. In our laboratory, we are developing a compact micro-hand system that can approach cells dexterously and rapidly. Furthermore, based on this micro-hand technology, we are developing a new end-effector that can apply not only force stimulation but also various other types of stimulation such as chemical and thermal stimulation. Herer, we report on the development and evaluation of a micro-hand end-effector that can apply multimodal stimuli such as force stimulation as well as local chemical stimulation.

3Pos181 皮膚線維芽細胞の長期培養による粘弾性への影響
Effect of long-term culture of skin fibroblasts on viscoelasticity

Kosuke Matsumura[1], Akira Kabasawa[1], Sayaka Miyoshi[3], Michiya Matsusaki[4], Arif Md. Rashedul Kabir[1,2], Teruki Yanagi[5], Kazuki Sada[1,2], Akira Kakugo[1,2], Kaori Shigetomi (Kuribayashi) [3] ([1]*Grad. Sch. of Chem. Sci. and Eng., Hokkaido Univ.*, [2]*Fac. of Sci., Hokkaido Univ.,*, [3]*Institute for the Advancement of Higher Education, Hokkaido Univ.*, [4]*Grad. Sch. of Eng., Osaka Univ.*, [5]*Department of Dermatology, Faculty of Medicine and Graduate School of Medicine, Hokkaido Univ.*)

Interactions between cells and the extracellular matrix (ECM) contribute significantly to cell functions such as cell division and cell adhesion, as well as wound healing and ECM remodeling. However, it is not well understood how the restructuring of ECM through cell division and metabolism in cell culture affects the viscoelasticity of ECM.
In this study, human skin fibroblasts were cultured in TG gels, in which gelatin is cross-linked with transglutaminase (TGase), and their viscoelasticity was measured. The results showed that the viscoelasticity of the TG gels changed depending on the number of culture days and cell concentration. This may be due to the effect of cell adhesion, metabolism, and degradation of gelatin molecules in the gel.

3Pos182 細胞性粘菌の生細胞での膜タンパク質分子の多状態側方拡散運動の細胞膜フィールドモデルの構築
Field model for lateral diffusion of transmembrane proteins in *Dictyostelium* cells

Kazutoshi Takebayashi[1], Yoichiro Kamimura[2], Masahiro Ueda[1,3] ([1]*BDR., RIKEN*, [2]*Nara Med. Univ.*, [3]*Grad. Sch. Front. Biosci., Osaka Univ.*)

The lateral diffusion of various transmembrane proteins was studied in lower eukaryote *Dictyostelium* cells by a Hidden Markov model for single-molecule trajectories. As common features, all membrane proteins with one to ten transmembrane regions adopted three free diffusion states with similar diffusion coefficients regardless of their structural variability. These species-independent properties of multistate free diffusion were explained quantitatively by a simple free-diffusion model based on three membrane fields. These results indicate a basal structure for heterogeneous mobility commonly observed in all transmembrane proteins and suggest an ancestral form of raft domains, in contrast to the complex diffusion behaviors of transmembrane proteins in higher eukaryotes.

3Pos183 Unraveling the host-selective toxic interaction of cassiicolin with lipid membranes and its cytotoxicity

Kien Xuan Ngo[1], Phuong Doan N. Nguyen[1], Hirotoshi Furusho[1], Makoto Miyata[2], Tomomi Shimonaka[2], Nguyen Ngoc Bao Chau[3], Nguyen Phuong Vinh[4], Nguyen Anh Nghia[4], Tareg Omer Mohammed[1], Takehiko Ichikawa[1], Noriyuki Kodera[1], Hiroki Konno[1], Takeshi Fukuma[1], Nguyen Bao Quoc[5] ([1]*WPI-NanoLSI, Kanazawa University, Kanazawa*, [2]*Grad. Sch. Sci., Osaka City University, Osaka*, [3]*Facult. Biotech., Ho Chi Minh City Open University, Ho Chi Minh City, Vietnam*, [4]*Rubber Res. Inst. Vietnam, Ho Chi Minh City, Vietnam*, [5]*Res. Inst. Biotech. Environ., Nong Lam University, Ho Chi Minh City, Vietnam*)

Cassiicolin (Cas), a toxin produced by *Corynespora cassiicola*, is responsible for corynespora leaf fall disease in susceptible rubber trees. Currently, the molecular mechanisms of the cytotoxicity of Cas and its host selectivity have not been fully elucidated. We analyzed the binding of Cas1 and Cas2 to membranes consisting of different plant lipids and their membrane-disruption activities by high-speed AFM and confocal fluorescence microscopy. Indeed, the negative phospholipids, glycerolipids, and sterols are more sensitive to membrane damage caused by Cas1 and Cas2 than neutral phospholipids and betaine lipids. Cryo-SEM analyses of necrotic leaf tissues treated with Cas1 confirm that cytoplasmic membranes are vulnerable to the toxin (Phytopathology, 2022).

3Pos184 分子動力学シミュレーションを用いた脂質膜におけるメリチンの抗菌作用の研究
Investigation for antimicrobial action of melittin on a lipid membrane using molecular dynamics simulation

Yusuke Miyazaki, Wataru Shinoda (*Research Institute for Interdisciplinary Science, Okayama University*)

We performed a series of coarse-grained molecular dynamics (CG-MD) simulations to investigate actions of melittin, a representative antimicrobial peptide (AMP) derived from honey bee venom, on a lipid membrane. As a result of the simulations, three different modes; toroidal pore formation, lipid extraction/budding, and bursting, were observed depending on a peptide-to-lipid ratio and local arrangement of peptides on the membrane. Our observations are consistent with fragmental pictures extracted from experimental data. Finally, we found that the local arrangement and density of melittin peptides and the area expansion rate due to membrane deformation were crucial for the initiation of and competition among the multiple pore formation mechanisms.

3Pos185 細胞膜糖鎖構造によるウイルス感染のメカニカルな制御
Mechanical modulation of virus infection by cell membrane glycocalyx

Yoshihisa Kaizuka, Rika Machida (*National Institute for Materials Science*)

Cell membrane glycocalyx has been suggested to mechanically inhibit viral infections. To measure such negative roles of glycoproteins in viral infections, we first made a list of highly glycosylated proteins from database. Then, we analyzed mechanical properties of multiple glycoproteins in cells or artificial membranes, and investigate the roles of glycosylation in infections at tissue level by experiment and by reanalyzing single cell transcriptome data of COVID-19 patients. Our analyses suggest that highly glycosylated proteins can mechanically inhibit viral infection at physiologically relevant density and that the density of total glycocalyx on cell membrane surface is a factor that is negatively correlated with the viral infection progressions.

3Pos186 (2SBP-3) エンベロープ型ウイルス粒子の粗視化シミュレーション：B 型肝炎ウイルス
(2SBP-3) Coarse-grained Molecular Dynamics Study of Enveloped Virus Particle: Hepatitis B Virus

Ryo Urano, Wataru Shinoda (*Res. Inst. Interdiscip. Sci., Okayama Univ.*)

Coarse-grained molecular dynamics simulation has been performed for Hepatitis B virus (HBV) particle to investigate the structure and dynamics of the enveloped capsid at molecular level. The envelope is a lipid membrane containing viral membrane proteins, though which structure was not determined at the molecular level. Thus, the structural role of viral membrane protein in the envelope is unclear. By constructing a reasonable HBV envelope model, our simulations clarified the role of envelope protein in the interaction with capsid spike and surrounding lipids. The details will be reported on the day.

3Pos187 曲率誘導タンパク質の膜曲率応答の平均場理論
Mean field theories of curvature sensing and generation of isotropic and anisotropic curvature-inducing proteins

Hiroshi Noguchi (*ISSP, Univ. Tokyo*)

We have studied the binding of curvature-inducing proteins using mean-field theories. Proteins generating spherical buds are modeled as laterally isotropic objects, and those generating membrane tubes are modeled as anisotropic objects of a crescent elliptic shape.
For the binding to cylindrical tubes, the isotropic proteins exhibit symmetric force-dependence to the force point, in which the tube curvature matches the protein (sensing) curvature. In contrast, the anisotropic proteins exhibit asymmetric dependence and the sensing curvature is varied. The former and latter have first-order transitions twice and once, respectively. These theories reproduce the meshless membrane simulation results of homogeneous phases very well.

3Pos188 高分子をグラフトした脂質三成分ベシクルの膜粘度
Viscosity of polymer grafted ternary lipid vesicle

Yuka Sakuma (*Grad. Sch. Sci., Tohoku Univ.*)

In cell membranes, the mobility of the functional constituents such as peptides, proteins, and polysaccharides in a sea of lipids controls the cell functions. Therefore, the membrane viscosity has been investigated with model biomembrane (vesicle). In this study, among the functional constituents, we focus on glycolipids which extend their polysaccharide chains from the phospholipid bilayer to the external solution and play role of cellular recognition. To understand the effect of the polysaccharide chains on the membrane fluidity, we estimated the apparent membrane viscosity of a polymer grafted ternary vesicle. This study will reveal the dynamics of glycolipids in the cell membrane, which might be responsible for their functionality.

3Pos189 脂質三成分ベシクルにおける膜粘度の温度依存性
Viscosity Landscape of Ternary Vesicles in Composition-Temperature Space

Juria Tanaka, Kenya Haga, Masayuki Imai, Yuka Sakuma (*Grad. Sch. Sci., Tohoku Univ.*)

The fluidity of cell membrane controls the diffusion of functional constituents, such as peptides, proteins, and polysaccharides. Therefore, the membrane viscosity has been studied with model biomembrane (vesicle). The domain formed by phase separation of ternary lipid vesicle might be responsible for the lipid raft which is the platform for cellular functions. By decreasing temperature from the miscibility transition temperature, ternary vesicle shows phase separation and forms the domain structure. In this study, we measured the membrane viscosity in the process of decreasing temperature for several compositions of ternary vesicles. The obtained phase diagram in temperature-composition space will reveal the relation between membrane fluidity and domain formation.

3Pos190 細胞内反応拡散波の再構成に向けた膜流動性の制御手法
Improvement of the membrane fluidity to reconstitute the intracellular reaction-diffusion waves

Gen Honda[1], Nao Shimada[2], Satoshi Sawai[2,3], Miho Yanagisawa[1,2,3] ([1]*Komaba Institute for Science, Graduate School of Arts and Sciences, University of Tokyo*, [2]*Department of Basic Science, Graduate School of Arts and Sciences, University of Tokyo*, [3]*Research Center for Complex Systems Biology, Graduate School of Arts and Sciences, University of Tokyo*)

Signaling cascades to regulate F-actin polymerization, involving small GTPases and phosphoinositides, generate spatio-temporal pattern of traveling waves on cell membrane in many organisms. The actin wave induces cell deformation such as migration and phagocytosis but what triggers it and how it depends on the membrane shapes have been unclear. To address these questions, we employed the reconstitution approach using artificial membrane and cell extracts from *Dictyostelium discoideum*. Similarly to the previous studies using Xenopus egg extracts, membrane fluidity was completely lost when exposed to cell extracts in vitro. We established the method to maintain the membrane fluidity and found that it was also critical to diffusion of small GTPase.

3Pos191 抗菌ペプチドの抗菌および殺菌活性の単一細胞解析
Single cell analysis for antimicrobial and bactericidal activities of antimicrobial peptides (AMPs)

Farzana Hossain[1], Masahito Yamazaki[1,2,3] ([1]*Res. Inst. Ele., Shizuoka Univ.*, [2]*Grad. Sch. Sci. Tech., Shizuoka Univ.*, [3]*Grad. Sch. Sci., Shizuoka Univ.*)

We have developed a method to examine the antimicrobial activities of AMPs at single cell level (single cell analysis). In this method, we monitor the proliferation of single cells and measure the distribution of the number of cells in each microcolony. In the method A, we incubate cells in the presence of various concentrations of AMPs. The minimum concentration where the fraction of microcolonies containing only a single cell, P_{single}, becomes 1 corresponds to the MIC. In the method B, after the interaction of a cell suspension with AMPs for a specific time, an aliquot is sufficiently diluted with fresh medium, and then monitor the proliferation of single cells. The time when P_{single} becomes 1 corresponds to the minimum interaction time for bactericidal activity.

3Pos192 浸透圧ストレス下における脂質二重膜の挙動に対し、F-actin が及ぼす影響
Effect of F-actin on the behavior of lipid bilayers under osmotic stress

Ken Bessho, Moka Ito, Kingo Takiguchi (*Dept. Biol. Sci., Grad. Sch. Sci., Nagoya Univ.*)

Cells are constantly exposed to external stimuli, and osmotic pressure is one of the most important environmental factors concerning in membrane homeostasis.
Liposomes stressed by osmotic pressure are known to show various responses depending on the magnitude of the stress, thus using them, we try to construct an observation system suitable for quantitative analysis.
As the first attempt, the effect of the encapsulation of F-actin, as expecting to work as a membrane beneath structure, on the liposomal response was examined.
The F-actin-encapsulation prevented liposomes from breakdown and contraction or prolonged the time required for these responses, suggesting that F-actin reinforced the membrane.

3Pos193 クロモグリク酸ナトリウム液晶封入リポソーム上の 3 本縞様膜相分離
Three-stripe pattern of lipid domains on spindle-shaped liposome containing liquid crystal of disodium cromoglycate

Kaori Udagawa, Masahito Hayashi, Tomoyuki Kaneko (*LaRC., Dept. Frontier Biosci., Hosei Univ.*)

We have found that DSCG encapsulating liposome transforms from spherical to spindle shape due to the phase transition of the DSCG from isotropic to liquid-crystal phase. In order to investigate the relationship between its shape and the localization of lipid domains on its surface, we visualized the phase separation pattern of its membrane induced by addition of water-soluble cholesterol. Spherical liposomes exhibited random dot pattern, whereas spindle-shaped liposomes exhibited three-stripe pattern across its long axis. In order to elucidate the self-organization mechanism of lipid domains corresponding to the shape of liposome, we will try to control the phased separation pattern through the change of temperature and the concentration of cholesterol.

3Pos194 クラミドモナス含有リポソームの鞭毛運動と膜運動の高速イメージング
High-speed imaging of the flagellar beating and membrane motion of *Chlamydomonas* containing liposome

Shunsuke Shiomi, Masahito Hayashi, Tomoyuki Kaneko (*Graduate School of Science and Engineering, Hosei University.*)

We develop moving liposomes using microorganisms as its engine. We have found that *Chlamydomonas* containing liposomes (Chlamylipos) move forward. In order to clarify the moving mechanism, we observed the flagellar beating and membrane motion of a Chlamylipo with a high-speed camera (600 Hz), which is 10 times faster than the flagellar beating (60 Hz). Flagellar beating caused the membrane protrusion in the effective stroke and the membrane repulsion in the recovery stroke. We will visualize the external flow to understand how the moving force is generated.

3Pos195 コリネ型細菌の機械受容チャネル MscCG の人工脂質膜リポソームへの再構成と電気生理学的特性
Liposome reconstitution and electrophysiological characterization of *Corynebacterium glutamicum* mechanosensitive channel MscCG.

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Bacteria release osmolytes, including L-glutamate, when MscS-like mechanosensitive channels are activated by membrane tension resulting from an increase in turgor pressure.Specifically, the MscCG channel, an MscS homolog in *Corynebacterium glutamicum,* plays a role in L-glutamate efflux.To understand the gating mechanism of MscCG, we recorded channel currents from liposomes fused with the native membrane vesicles and reconstituted with the purified channel.The purified MscCG channels reconstituted into 100% azolectin liposomes exhibited a very high threshold of activation.Our data suggest that mechanosensitivity of the MscCG channels is strongly dependent on the lipid content and confirmed that modulation of the channel activity follows the force-from-lipids paradigm.

3Pos196 KcsA カリウムイオンチャネルにおける膜張力感知部位の探索
Exploring the membrane tension sensing sites in the KcsA potassium channel

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The KcsA potassium channel is known as the acidic pH-gated channel, but the activation gate is also modulated by the lipid bilayer tension. In this study, we explored the molecular mechanism of tension sensitivity of the KcsA channel. The KcsA channels reconstituted in the contact bubble bilayer are subjected to membrane tension changes, in which each monolayer tension rather than the bilayer tension was separately controlled. Mutant channels were examined to identify the tension-sensing sites. The single-channel current and the fluorescence measurements revealed the functional and structural effects of tension on the channel. Based on these results, we will discuss the tension-sensing modality of the KcsA channel.

3Pos197 KcsA カリウムチャネルゲーティングに対する膜厚と膜張力の作用
Concurrent effect of the membrane thickness and tension on the gating of the KcsA potassium channel

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At the channel-membrane interface, the hydrophobic surface of a channel often mismatches with the hydrophobic core of the membrane. This leads to local deformation of the surrounding membrane, from which the channel is subjected to stress. Moreover, conformational changes upon channel gating alter the adaptation of the membrane interface. To examine the effect of membrane thickness and tension on the gating, the KcsA channel was embedded in lipid bilayers having variable thickness by using phospholipids of different acyl lengths, and arbitrary bilayer tension was applied using the contact bubble bilayer method. The open probability varied with the membrane thickness and tension changes. The data were analyzed for the concurrent action of thickness and tension.

3Pos198 *C.elegans* の低温耐性を制御する転写伸長因子 TCEB-3 のトランスクリプトーム解析
Transcriptome analysis of a transcription elongation factor TCEB-3 that is positive regulator of cold tolerance in *C.elegans*

Hiroaki Teranishi[1], Toshihiro Iseki[1], Natsune Takagaki[1], Yohei Minakuchi[2], Atsushi Toyoda[2], Akane Ohta[1], Atsushi Kuhara[1,3] ([1]*Grad. school of Nat. Sci., Konan Univ, Japan*, [2]*National Institute of Genetics, Japan*, [3]*PRIME, AMED*)

Temperature is an important factor affecting the biological environment. In this report, we describe the analysis of a transcription elongation factor TCEB-3 that positively regulates cold tolerance in C. elegans found in sequential genetic analysis. TCEB-3 is expressed in many neurons, and the results of a rescue experiment of tceb-3 mutant with abnormal cold tolerance showed that expression of TCEB-3 in 130 neurons in the mutant rescued abnormal cold tolerance. However, narrowing down to a smaller number of functional cells was difficult. Therefore, we report the current status of this study, since we tried to identify functional cells of TCEB-3 by transcriptome analysis of transgenic rescue strains and knockdown strains.

3Pos199 GPCR SRX は線虫の低温耐性に関わる温度受容体候補である
GPCR SRX is a thermoreceptor candidate in cold tolerance of *C. elegans*

Chinatsu Morimoto[1], Chie Miyazaki[1], Kohei Ohnishi[1], Tohru Miura[1], Akane Ohta[1], Atsushi Kuhara[1,2] ([1]*Inst. for Integrative Neurobio., Konan Univ., Japan*, [2]*PRIME, AMED*)

We are using cold tolerance of *C. elegans* to analyze thermosensation. Since G-protein is involved in the thermosensing (Ohta et al., Nat commn, 2014), we performed exhaustive RNAi screening of GPCR, resulting on 86 GPCR were involved in cold tolerance. Among them, *srx* gene was expressed in a pair of olfactory neurons. *srx* mutant showed reduced odortaxis, which was rescued by expressing *srx* cDNA in *srx* mutant. By Ca^{2+} imaging, the olfactory neuron pair was responsive to warming as asymmetric manner, which was diminished in *srx* mutant. Expressing SRX in non-warm sensitive gustatory neuron resulted in acquisition of warm sensitivity, indicating that GPCR SRX maybe sufficient to confer warm sensitivity. We are trying to introduce reconstructive analysis with cultured cell.

3Pos200 脳-腸連関によって制御された脂質代謝が線虫の温度順化を引き起こす
Lipid metabolism regulated by brain-gut interaction causes temperature acclimation in *C. elegans*

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Cold tolerance and temperature acclimation, one of the temperature response mechanisms in *C. elegans*, are regulated by the nervous system. To clarify the temperature acclimation mechanism, we investigated the downstream physiological output of the neural circuit. Neuropeptide FLP-7, which is secreted from the neuron and received in the gut, upregulates the expression of triglyceride lipase ATGL-1 in the gut in a cultivating temperature-dependent, promoting lipolysis. In addition, mutants of a gene that works in the neural circuit controlling temperature acclimation showed abnormalities in lipid metabolism. In other words, neuron-regulated lipid depletion may cause cold death.

3Pos201 拡散追跡による脂質膜上の初期の Aβ 凝集過程に対する開放系の効果
Effect of Open System on Early Aggregation Process of Amyloid β on Lipid Membrane by Diffusion Tracking

Akane Iida[1], Hideki Nabika[2] ([1]*Graduate School of Science and Engineering, Yamagata Univ.*, [2]*Faculty of Science, Yamagata Univ.*)

Alzheimer's disease (AD) has the feature of amyloid β (Aβ) aggregation on the surface of the brain cells. Although Aβ interacts with the cell membrane under interstitial fluid which keeps the brain in an open system, many studies investigated the Aβ aggregation ignored in closed system. Especially, the behavior of most toxic oligomers on the membrane under open system has not been clarified. In this study, we constructed the open system that can track the single Aβ molecule on the membrane to elucidate the initial aggregation behavior of the oligomer. The open system promoted the Aβ aggregation more than closed system as a result of the increased diffusion rate of Aβ on the membrane. Thus, it is necessary to elucidate the mechanism of AD under open system.

3Pos202 インスリン刺激時のモノアラガイ単離脳に対するリン酸化プロテオミクス解析
Phosphoproteomic analysis of the pond snail's CNS stimulated by insulin

Junko Nakai, Etsuro Ito (*Dept. Biol., Waseda Univ.*)

Insulin plays an important role in learning and memory ability in the pond snail. However, the physiological mechanisms of how insulin promotes learning and memory are unknown. To clarify the insulin signalling pathway (IIS) in the central nervous system (CNS) of the pond snail, an LC-MS/MS phosphoproteomic analysis of the CNS stimulated by insulin was performed. Phosphorylation/dephosphorylation occurred in IIS-related proteins (e.g., phosphorylation of Akt) and cytoskeleton-related proteins (e.g., phosphorylation of intermediate diameter filaments). A series of molecular cascades activated by insulin in the CNS will be also discussed.

3Pos203 fMRI データに対する行列分解による脳情報コーディング
Brain information coding in fMRI data via matrix factorization

Yusuke Endo, Koujin Takeda (*Grad. Sch. Eng., Univ. Ibaraki*)

In brain, there is a hypothesis that sparse coding is realized in information representation of external stimulus (Olshausen, Field). In addition, by physiological experiments with two-photon microscope calcium imaging (Ohki, Yoshida), they found that visual stimulus can be reconstructed from activities of a small number of neurons in primary visual cortex. As described, information representation in specific functional region in brain has been investigated, whereas representation in the whole brain has not been clarified in general. In this study, we investigate validity of sparse coding in information processing in the whole human brain by applying sparse matrix factorization to fMRI (functional magnetic resonance imaging) data of neural activities in the whole brain.

3Pos204 機能的神経クラスタ推定のためのベイズ生成モデルの一般化
Generalization of Bayesian generative model for functional neuronal ensembles inference

Shun Kimura, Koujin Takeda (*Grad. Sch. Sci. and Eng., Ibaraki Univ.*)

Brain functions are realized by information transfer through interactions among large number of neurons. Hence, inference of interaction among neurons, i.e., strength of functional connections and neuronal ensemble structure, is significant for revealing the mechanism of brain functions. In fact, a method to infer neuronal ensemble structure from activity data has been proposed using a Bayesian generative model under the assumption that neurons with similar roles exhibit similar neuronal activities. However, this method requires binary input activity data and assumes stationarity of the ensemble structure and activity state. Therefore, we attempt to resolve these problems by enhancing representability of the Bayesian generative model in the prior study.

3Pos205 アガロースマイクロチャネル構造における単一神経突起の分化に必要な定量的条件
Quantitative requirement for single neurite differentiation of neurons in agarose microchannel structures

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Regulation of neurite outgrowth and differentiation control is essential for constructing the minimum unit of artificial neuronal networks.To design the connections of the desired neuronal networks, we need to acquire the required minimum length of axonal differentiation in straight agarose microchannels. We isolated and elongated the first neurites from the second and following neurites from neurons with a 20 μm-diameter cell body holding region and connected five μm-width microchannels. The results showed the first neurites of neurons differentiated into axons after they reached 100 μm in length. From the results, we expect to be able to construct the smallest unit of artificial neuronal circuits having at least 100 μm distances between neighboring neurons.

3Pos206 Evaluation of agarose microfabrication technology using Joule heat of micrometer-sized ionic current for cell network formation

Yuri Kamiya[1], Kenji Shimoda[2], Yoshitune Hondo[2], Haruki Watanabe[2], Nanami Abe[1], Ryohei Yamazaki[2], Kenji Yasuda[1,2] ([1]*Dept. Phys., Sch. Adv. Sci. & Eng., Waseda Univ.*, [2]*Dept. Pure and Appl. Phys., Grad. Sch. Adv. Sci. & Eng., Waseda Univ.*)

For the constructive approach of cell network analysis, we have used a photothermal etching technology for forming desired agarose microstructures during cell cultivation. However, it still has limitations, such as the unexpected structure formation caused by the absorption of permeable ITO wiring patterns on the multielectrode array chip. To overcome these limitations, we developed a new method to form agarose microstructures exploiting a micrometer-sized Joule heat of ion current at the tip of the microcapillary tube. We used cardiomyocytes and neurons to construct their networks in the agarose microstructures and formed additional microstructures. The results showed Joule heat of micro ionic current is enough for agarose microfabrication without any damage to cells.

3Pos207 線虫の神経活動解析における擬似相関の除去
Eliminating spurious correlation in neural activity analysis of *C. elegans*

Harutaka Takeshita, Yuishi Iwasaki (*Grad. Sch. Sci. Eng., Ibaraki Univ*)

In time series analysis such as neural activity analysis, eliminating spurious correlation is important to detect actual relationship between observed data. The partial cross mapping (PCM; Leng *et al*., Nature Comm., 2020) is applied to analyze neural activity data of *C. elegans*. PCM is a model-free method to eliminate indirect causal influences and is applicable to non-linear data. In *C. elegans*, whose synaptic connectivity is completely determined, whole-brain activity is measured by calcium imaging (Toyoshima *et al*., BMC Biol., 2020). In our analysis, many spurious correlation are detected between the neural activities. We compare the estimated causality between the neurons with the synaptic pathway in *C. elegans*.

3Pos208 遺伝子発現に基づく神経回路形成のデータ駆動型解析
Data-driven analysis of the formation of neural circuit based on gene expression

Jigen Koike[1], Kana Yoshido[1], Naoki Honda[1,2,3] ([1]*Graduate School of Biostudies, Kyoto University*, [2]*Graduate School of Integrated Science for Life, Hiroshima University*, [3]*Explatory Research Center on Life and Living Systems, ExCells*)

Neural circuits are formed by the process of axonal projection, where each axon of a neuron extends to the proper location and makes synapses with other neurons. The target location of this axonal projection is known to be determined based on the concentration gradients of the ligands and their receptors responsible for axon guidance. However, it is still unknown how the complex wiring of the entire brain is formed. To solve this problem, we developed a new machine learning method, which can infer the genes contributing to neural circuit formation from datasets of axonal projections and gene expression distribution. We aim to reveal the design principle of brain circuit by applying this method to experimental data in database such as Allen Brain Atlas.

3Pos209 ヨーロッパモノアラガイの摂食中枢ニューロン CGC 近傍における電気生理学的性質に対する緑茶由来カテキンの影響
The effect of green tea-derived catechin on electrophysiological properties around the CGC in the pond snail *Lymnaea stagnails*

Hideki Matsuoka[1], Ayaka Itoh[2], Terumasa Amano[2], Ken Lukowiak[3], Minoru Saito[2], Yoshimasa Komatsuzaki[4] ([1]*Dept. Phys., Grad. Sch. Sci. and Tech., Nihon Univ.*, [2]*Dept. Corr. Study in Phys. and Chem., Grad. Sch. Integ. Basic Sci., Nihon Univ.*, [3]*Hotchkiss Inst., Cumm. Sch. Med., Univ. of Calgary, Canada*, [4]*Dept. Phys., CST, Nihon Univ.*)

Green tea-derived catechin promotes long-term memory formation in the pond snail *Lymnaea stagnalis*. In this study, we examined the effect of relatively low-dose catechin on long-term memory formation in snails. We showed that snails treated with 1.5 mg/L epicatechin exhibited memory retention for 72 hours, but there was no significant difference compared to control snails. Next, we have developed a local field potential (LFP) measurement method to record the activity of the Cerebral Giant Cells (CGCs), which are involved in feeding behavior in snails, and its peripheral neurons. An administration of 1 mM GABA to the preparations from “poor learner” snails increased spike activities of LFP around the CGC. Further evaluation by using another bunch of snails will be discussed.

3Pos210 エピカテキンはナメクジ嗅覚中枢シナプスの長期抑圧現象を惹起する
Effects of epiatechin on synaptic plasticity of the olfactory center in the land slug *Limax valentianus*

Aya Nagata, **Yoshimasa Komatsuzaki** (*Dept. Phys., CST, Nihon Univ.*)

Epicatechin, a flavonoid which is abundantly contained in green tea, improves cognitive functions in various animals including invertebrates. Here, we investigate the effects of epicatechin (EpiC) on the synaptic plasticity in the synaptic pathway between the olfactory nerve and the procerebral cortex (PC) in the land slug *Limax valentianu*. We found that the amplitude of excitatory post-synaptic potentials in the PC increased within ten minutes after administration of EpiC. High frequency stimulation of the olfactory nerve induced long-term depression in the presence of EpiC but did not in the absence of EpiC. These results suggest that EpiC directly affects a synaptic connection between olfactory organ and olfactory central nervous system to cause memory enhancement.

3Pos211 神経細胞内シナプス小胞群の光捕捉下における神経活動測定
Neuronal activity measurement under optical trapping of synaptic vesicles in neurons

Taketo Yasuda, Wataru Minoshima, Kyoko Masui, Chie Hosokawa (*Grad. Sch. Sci., Osaka Metro. Univ. / Osaka City Univ.*)

Neurons in the brain communicate through synapses. Neurotransmitters stored in synaptic vesicles are released from the pre-synapse and received by neurotransmitter receptors at the post-synapses. Synaptic vesicles play an important role for neuronal communication. The assembling of synaptic vesicles by optical trapping has been demonstrated to modulate the synaptic function. In this study, we evaluated neuronal activities of cultured hippocampal neurons during optical trapping of synaptic vesicles by using multi-electrode arrays. The frequency of neuronal activity increased during the optical trapping of synaptic vesicles, implying that optical trapping of synaptic vesicles can modulate the synaptic transmission.

3Pos212 集光フェムト秒レーザーの短時間照射により誘発された神経活動
Neuronal activities induced by short-time irradiation of a focused femtosecond laser

Kan Otani, Yumi Segawa, Wataru Minoshima, Kyoko Masui, Chie Hosokawa (*Grad. Sch. Sci., Osaka Metro. Univ. / Osaka City Univ.*)

In the neuronal network, synaptic connectivity associated to the brain functions is modified by external stimuli. We have demonstrated that the femtosecond laser irradiation for 8 ms induced neural activity in the single neurons. Since laser irradiation time was much longer than the time scale of neuronal activities (~2 ms), short-time laser irradiation seems necessary for stimulation. Here, a femtosecond laser (center wavelength 800 nm, pulse width ~100 fs, repetition rate 82 MHz) was focused to single neurons for less than 3 ms, and Ca^{2+} influx into the neurons was confirmed. The probability of Ca^{2+} elevation was found to depend on the irradiation time. Our results indicate that femtosecond laser irradiation is expected to induce the single neuronal activity.

3Pos213 Dynamical systems model of the development of action differentiation and memory in early infancy

Ryo Fujihira, Gentaro Taga (*Grad. Sch. Edu., Univ. Tokyo*)

What is the origin of goal-directedness in our movement? Infants come to differentiate their actions: increase their limb movements when they cause environmental events and otherwise decrease them between 2 and 3 months of age. This is evidence of the infants' ability to learn circular causality between self-generated movements and environmental changes. Infants also remember the self-generated events. To reveal the underlying mechanisms of such ability, we made a dynamical systems model composed of the brain, the limb oscillator, and a toy in the environment. Simulation showed that the model generated movement differentiation and memory in terms of bifurcation dynamics. We discuss how internal state dynamics create goal-directed actions.

3Pos214 ゾウリムシの走化性はレヴィウォークを通じて現れる
Chemokinetic responses of *Paramecium tetraurelia* through Lévy walks

Azusa Kage[1], Takeru Wakano[1], Masato S. Abe[2], Takayuki Nishizaka[1] ([1]*Dept. Physics, Gakushuin Univ.*, [2]*Facl. Culture and Information Science, Doshisha Univ.*)

Movement is a fundamental characteristic of living organisms. From bacteria to large animals, motile cells and organisms obey a universal law of movement: Lévy walks. Lévy walk is a class of random walks that is characterized by the equation $P(l) \sim l^{-\mu}$ ($1<\mu<3$), where P is the probability and l is the length of a step, which means a trajectory with long straight walks and occasional turns. In this study, we first examined if the ciliate *Paramecium* showed Lévy walks. We analyzed trajectory step sizes of *P. tetraurelia*, and found that about 20-40% of Paramecia showed Lévy walks. Paramecia with food in the environment swam slower and showed a higher proportion of Lévy walks than those without food, suggesting the mechanism of chemokinesis through Lévy walks.

3Pos215 Near wall rheotaxis of ciliates, *Tetrahymena pyriformis*.

Yukinori Nishigami[1], Takuya Ohmura[2], Masatoshi Ichikawa[3] ([1]*RIES, Hokkaido Univ.*, [2]*Biozentrum, Univ. Basel*, [3]*Dept Phys., Kyoto Univ.*)

Freshwater ciliates need to swim against the external flow to stay in suitable environments. Although qualitative descriptions of the ciliate's positive rheotaxis have been described so far, no quantitative studies had been conducted. Therefore, we observed the behavior of the ciliates, *Tetrahymena pyriformis*, in a flow using a microfluidic device. As a result, *T. pyriformis* swam against the flow near the walls. The frequency of dorsal ciliary beating was normal, but the frequency of ventral ciliary beating near the wall was decreased. Based on this observation, a fluid simulation was performed using a squirmer model. As a result, rheotaxis is achieved if the cell shape is a prolate ellipsoid and the ciliary beating stops near the wall.

3Pos216 **Photoactive Yellow Protein** における酸性アミノ酸に置換した **52** 番目の残基のプロトン化状態
Protonation state of 52nd residue replaced by an acidic amino acid in Photoactive Yellow Protein

Kento Yonezawa[1,2], Yoichi Yamazaki[2], Mikio Kataoka[2], Hironari Kamikubo[1,2] ([1]*NAIST, CDG*, [2]*NAIST, MS*)

We previously revealed that the hydrogen bond (HB) between the chromophore (pCA) and E46 in Photoactive Yellow Protein (PYP) is an LBHB and that R52 near the LBHB is electrically neutral. Furthermore, we also found that R52 is protonated by replacing the LBHB with a normal HB. The pK_a of arginine is about 14, and it is usually not electrically neutral in solution. R52 locates at the bottom of the cleft. We assumed that R52 is partially protected from exposure to solvents. To verify the effect of the environment in the cleft on pK_a, we measured the pK_a of D52 by mutating R52 to aspartic acid. The pK_a of D52 is estimated to be 7.5 larger than that in the aqueous solution (3.8). The fact implies that the environment in the cleft is hydrophobic.

3Pos217 RcPYP と PBP の複合体形成に及ぼす PBP C 末端部位の役割
Role of PBP C-terminal region on the complex formation between RcPYP and PBP

Daiki Takenaka[1], Yoichi Yamazaki[1], Kento Yonezawa[1,2], Sachiko Toma-Fukai[1], Hironari Kamikubo[1,2] ([1]*NAIST, MS*, [2]*NAIST, CDG*)

The photoreceptor protein RcPYP (Rhodobacter capsulatus photoactive yellow protein) binds to PBP (PYP binding protein) in a light-dependent manner. It has been suggested that the interaction site involved in this binding is K72 of PYP. However, the site on PBP is still unknown. In this study, we focused on the C-terminal region of PBP to identify the interaction site and prepared a PBP lacking the C-terminal region (PBP ΔC). PBP ΔC showed the same level of interaction ability with RcPYP as PBP WT in 100 mM NaCl, but in high-salt conditions, the binding ability of PBP ΔC was significantly reduced. Based on the fact that the salt concentration-dependent behavior can be seen between RcPYP K72Q and PBP WT, the PBP C-terminal site was implied to be interacted with K72.

3Pos218 青色光センサー TePixD の光可逆的な分子集合反応
Light-dependent reversible molecular assembly of a blue light sensor protein TePixD

Yusuke Nakasone, Yusuke Masuda, Shunrou Tokonami, Masahide Terazima (*Grad. Sch. Sci., Kyoto Univ.*)

TePixD is one of BLUF (blue light sensor using flavin) proteins and exists as a decamer in solution. It dissociates into pentamers upon weak light illumination. In this study, we have newly found that TePixD associates to form a giant cluster under strong light condition and this cluster recovers to the original oligomeric state (decamer) in the dark. To understand the molecular mechanisms of the assembly, we investigated this light dependent association reaction using turbidity measurement, mutational analysis and time-resolved transient grating (TG) method. We found that the cluster is stabilized by electrostatic and cation-p interactions, and light-induced nucleation process is detected by the TG method as a significant decrease of the diffusion coefficient.

3Pos219 深海エビ *Rimicaris hybisae* が持つオプシン類の分子特性
Molecular properties of opsins from the deep-sea hydrothermal vent shrimp *Rimicaris hybisae*

Keiichi Kojima[1], Yuya Nagata[2], Norio Miyamoto[3], Keita Sato[1], Yuji Yamanaka[4], Yosuke Nishimura[5], Susumu Yoshizawa[5], Ken Takai[3], Hideyo Ohuchi[1], Takahiro Yamashita[6], Yuki Sudo[1] ([1]*Med, Dent & Pharm Sci, Inst of Acad. & Res., Okayama Univ.*, [2]*Grad. Sch. of Med. Dent. & Pharm. Sci., Okayama Univ.*, [3]*X-STAR, JAMSTEC*, [4]*Fac. of Pharm. Sci., Okayama Univ.*, [5]*AORI, Univ. Tokyo*, [6]*Grad. Sch. Sci., Kyoto Univ.*)

Opsins are universal photoreceptive membrane proteins which underlie the molecular basis of photoreception in animals. The vent shrimp *Rimicaris hybisae* lives near the hydrothermal vent in the deep-sea where very dim light from the black-body radiation is present. It is suggested that the vent shrimp detect the dim light using its dorsal enlarged eye. In this study, we performed transcriptome analysis and identified six opsin genes from the vent shrimp. We analyzed light-dependent G protein activity and photochemical properties of the six opsins using recombinant proteins expressed in mammalian cultured cells. Based on the results, we will discuss the molecular basis of photoreception of the vent shrimp in the deep-sea.

3Pos220 Investigation of spectral properties and spectral tuning mechanisms of anthozoan-specific opsins from a reef-building coral

Yusuke Sakai, Mitsumasa Koyanagi, Akihisa Terakita (*Department of Biology, Graduate School of Science, Osaka Metropolitan University*)

Opsins serve as light-sensitive G-protein-coupled receptors by binding to chromophore retinals. Anthozoans including corals possess a set of phylogenetically unique opsins, anthozoan-specific opsins (ASOs), of which molecular characteristics such as absorption spectra, yet, have not been uncovered. In this study, we conducted spectroscopic analyses of ASOs of a reef-building coral and found that each ASO had an ability to absorb light in a specific wavelength between UV to visible region. We investigated the amino acid residues that are involved in spectral tuning of visible light-sensitive ASO(s) by analyzing a series of site-directed mutants. On the basis of the obtained results, we discuss a possible spectral tuning mechanism for visible light-sensitive ASOs.

3Pos221 光駆動型 Cl^-ポンプ・ハロロドプシンの細胞質型ハーフチャンネルにおける高速 Cl^-輸送のメカニズム解明
Probing the mechanism of fast Cl^- transport in the cytoplasmic half channel of light-driven Cl^- pump halorhodopsin

Yubo Zhai[1], Anna Shimosaka[1], Takashi Tsukamoto[1,2], Makoto Demura[1,2], Takashi Kikukawa[1,2] ([1]*Grad. Sch. Life Sci., Hokkaido Univ.*, [2]*Fac. Adv. Life Sci., Hokkaido Univ.*)

Halorhodopsin (HR) has a highly hydrophobic half channel on its cytoplasmic (CP) side. Despite this hydrophobicity, HR can quickly transport Cl^- toward the CP medium. Exploring the residues critical for this transportation of *N. pharaonis* HR, we found that the replacements of Phe211 and Leu214 significantly slowed down the latter half of the photocycle, at which Cl^- is released to the CP medium. For L214 mutants, their slow photocycles were significantly accelerated by simultaneous replacements of the adjacent Lys215 with a neutral residue. Thus, the L214 mutations might induce an unfavorable interaction between K215 and Cl^-. We will present the results of simultaneous mutations of F211 and K215 and then discuss the mechanism of Cl^- transport in the CP channel.

3Pos222 光駆動 Cl^-ポンプ halorhodopsin の基質放出・取込み中間体の同定
Identification of substrate release and uptake intermediates of light-driven Cl^- pump halorhodopsin

Chihaya Hamada[1], Keisuke Murabe[1], Takashi Tukamoto[1,2], Makoto Demura[1,2], Takashi Kikukawa[1,2] ([1]*Grad. Sch. Life Sci., Hokkaido Univ.*, [2]*Fac. Adv. Life Sci., Hokkaido Univ.*)

Substrate release and uptake reactions are major events for membrane transport proteins. In this study, the relevant intermediates for these events were examined for the light-driven Cl^- pump halorhodopsin (HR). We herein compared the time courses of two different signals. One was the flash-induced absorption change that reflects the formation and decay of intermediates. The other was the flash-induced potential change of a Cl^- selective membrane, which reflects the Cl^- concentration change due to Cl^- release and uptake reactions of HR. The latter signal became negligible at higher bulk Cl^- concentration. Thus, two signals were compared up to 30 mM Cl^-. The results indicated that Cl^- release and uptake occur during the formation and decay of the HR' intermediate.

3Pos223 光駆動イオントランスポーターハロロドプシンの理論的研究
Theoretical study on molecular mechanism of a light-driven ion transport of Halorhodopsin

Tomo Ejiri, Ryo Oyama, Shigehiko Hayashi (*Grad. Sch. Sci., Univ. Kyoto*)

Halorhodopsin from Natronomas pharaonis functions as an inward light-driven chloride pump and is utilized to silence neurons in optogenetics technique. The chromophore retinal isomerizes from all-trans confomation to 13-cis one upon photoabsorption, and triggers a photocycle during which one chloride ion is transported across the membrane. We have performed QM/MM RWFE-SCF methods to examine the functional coupling of the structual change of the chromophore described at an ab initio quantum chemistry level with the protein large conformational changes described by MD simulations. We explore changes of the protein conformations and titration states in the conduction pore that allow a chloride ion to be taken up into the intracellular region in the photo-activated state.

3Pos224 低温ラマン分光法による光駆動 Cl^-ポンプ NMR3 の発色団構造変化の研究
Low-temperature Raman study of chromophore structural changes in a light-driven Cl^- pump NMR3

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NMR3 is a microbial rhodopsin discovered from a marine bacterium *Nonlabens marinus*. NMR3 functions as a light-driven inward Cl^- pump via a series of chemical steps that start from the photoisomerization of the retinal chromophore. The previous transient absorption study revealed the multiple reaction intermediates to realize the Cl^- pumping. However, the structures of these intermediates are not yet known. In this study, we use low-temperature Raman spectroscopy to clarify the ion pumping mechanism based on the molecular structures of the reaction intermediates.

3Pos225 異なるプロトン化状態のアニオンチャネルロドプシン GtACR1 とその変異体の吸収波長に関する理論的研究
Theoretical study on absorption wavelengths of anion channelrhodopsin GtACR1 in different protonation states and their mutants

Takafumi Shikakura, Cheng Cheng, Shigehiko Hayashi (*Grad. Sch. Sci., Kyoto Univ.*)

Channelrhodopsins are photoreceptor ion channel proteins with a retinal chromophore. Photo-isomerization of retinal leads to ion conduction. Recently an atomic model of the anion-conducting channelrhodopsin, GtACR1, was determined by X-ray crystallography. We created all-atom models with different protonation states and their mutants and performed structural optimizations by the QM/MM RWFE-SCF method. Photo-excitation energies were then calculated with the MC-QDPT methods in the protein electrostatic environment. The results show the position of the chloride anion and titratable acidic residues affect the absorption wavelength. The presence of the chloride anion may explain the property of GtACR1 that the absorption wavelength is kept unchanged over a wide pH range.

3Pos226 新奇酵素ロドプシン(NeoR)の特異な光化学特性
Unique photochemical properties of novel enzyme rhodopsin (NeoR)

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Enzyme-rhodopsins are a photoactivatable membrane protein composed of a rhodopsin domain and enzyme domain at cytoplasmic side. In 2020, novel enzyme rhodopsin, NeoR, was discovered. NeoR absorbs a far-red light and shows guanylyl cyclase activity by forming heterodimer, both of which are unique features in microbial rhodopsins.
Detailed analysis by vibration spectroscopy has not been reported so far. Therefore, we applied FTIR spectroscopy and HPLC analysis to reveal its light-induced structural changes and photochemical properties. We succeeded in capturing unique features including changes in protonation state of amino acids and a characteristic photoisomerization.
In this presentation, we would like to discuss the molecular mechanism of NeoR.

3Pos227 近赤外光吸収型ロドプシンの波長制御機構
Color tuning mechanism of near-infrared light absorbing rhodopsins

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Rhodopsin is a photoreceptor protein with a retinal as a chromophore. Rhodopsins absorb light whose wavelength ranges from 300 to 700 nm. Absorption wavelength is tuned by the amino acids surrounding the chromophore. The critical amino acids for color tuning have been studied in visible light-absorbing rhodopsins. We have recently identified several novel rhodopsins absorbing near-infrared light (NeoRs), two of which absorb 692 nm and 640 nm light. Even though they have a high sequence homology, the difference in absorption maxima is about 50 nm. Here, we perform mutation study to understand color tuning mechanism of the NeoRs. We identified several amino acids which cause absorption shift. We provide novel insights into the color determination mechanism.

3Pos228 表面増強赤外分光法を用いた Heliorhodopsin の O 中間体構造変化解析
Structural change upon O intermediate formation of Heliorhodopsin analyzed by using SEIRA spectroscopy

Soichiro Kato[1], Jingyi Tang[1], Insyeerah Binti Muhammad Jauhari[2], Hideki Kandori[1,3], Yuji Furutani[1,3] ([1]*Graduate School of Engineering, Nagoya Institute of Technology*, [2]*Nagoya Institute of Technology*, [3]*OptoBio, Nagoya Institute of Technology*)

SEIRA is an infrared spectroscopic method that utilizes the phenomenon of increase of the infrared absorption about 100 times by adsorbing molecules on a gold film. The closer the molecule to the gold film, the stronger the enhancement. Another characteristic of SEIRA is that the infrared absorption of molecular vibrations with vibrational dipole moments in the direction perpendicular to the gold film is selectively enhanced. Heliorhodopsin (HeR) is a newly discovered unique microbial rhodopsin. Although most of the physiological functions remain unknown, characteristic amide I change in the long lived O intermediate may relate to its functioning. In this study, we applied SEIRA on a HeR and its mutants and discuss the O intermediate structural changes in detail.

3Pos229 ヘリオバクテリア反応中心における Chl-a_F から BChl-g への励起エネルギー移動速度の理論的解析
Theoretical analysis of rate of excitation energy transfer from Chl-a_F to BChl-g in heliobacterial reaction center

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Excitation Energy Transfer (EET) reaction is essential in the initial process of photosynthesis. Type I reaction center of Heliobacteria (hRC) contains two types pigments, bacteriochlorophyll g (BChl-g) and chlorophyll a_F (Chl-a_F as A_0). The structure of hRC was revealed in 2017 [1]. We studied the EET mechanism on hRC initiated by the selective excitation of Chl-a_F using the theoretical model [2] constructed by using the structural information. We calculated the EET rates using the (generalized) Förster equation considering the $Q_y(0, 1)$ transitions of the pigments. Each model reproduced the experimentally observed reaction time (1.4 ps) [3] well.
[1] C. J. Gisriel et al. *Science* 2017.
[2] A. Kimura et al., *J. Phys. Chem. B* 2021.
[3] S. Neerken et al. *Biochemistry* 2000.

3Pos230 ヘリオバクテリアにおける cyt *bc* 複合体から光合成反応中心への電子伝達反応の分子機構
Molecular mechanism of the electron transfer reaction from cyt *bc* complex to the photosynthetic reaction center in heliobacteria

Hirozo Oh-oka[1,2], Hiraku Kishimoto[2], Yuki Makino[2], Risa Kojim[1], Akihiro Kawamoto[3], Hideaki Tanaka[3], Genji Kurisu[3] ([1]*CELAS, Osaka Univ.*, [2]*Grad. Sch. Sci., Osaka Univ.*, [3]*Inst. Protein Res., Osaka Univ.*)

Heliobacteria are anaerobic and anoxygenic photosynthetic bacteria. The cyt *bc* complex oxidizes menaquinol, with which proton translocation across membranes is coupled to produce proton motive force essential for the ATP synthesis. The membrane-bound cyt *c*-553 serves as an electron donor to the P800 in the type-1 reaction center (RC) by mediating electron transfer from the cyt *bc* complex. This cyt *bc* complex is a unique one consisting of Rieske protein, cyt b_6, subunit IV, and di-heme cyt *cc*. In the present study, the 3D structures of di-heme cyt *cc* and cyt *c*-553 were determined with the X-ray crystallography to investigate the molecular interaction mechanism between them. The complex formation between the RC and cyt *c*-553 was also analyzed with the Cryo-EM.

3Pos231 緑色光合成硫黄細菌における Rieske/cyt*b* 複合体と *c* 型シトクロムとの構造機能相関
Structure-function relationships between the Rieske/cyt*b* complex and *c*-type cytochromes in photosynthetic green sulfur bacteria

Hiraku Kishimoto[1], Ryoga Kawanami[1], Chihiro Azai[2], Risa Mutoh[3], Hideaki Tanaka[4], Yohei Miyanoiri[4], Genji Kurisu[4], Hirozo Oh-oka[1] ([1]*Grad. Sch. Sci., Osaka Univ.*, [2]*Col. Life Sci., Ritsumeikan Univ.*, [3]*Fac. Sci., Toho Univ.*, [4]*Inst. Protein Res., Osaka Univ.*)

Cytochrome (cyt) *bc* complexes functioning in photosynthetic electron transport chain conducts electron transport reactions coupled with proton translocation across membranes, resulting in the production of proton motive force to synthesize ATP. Photosynthetic green sulfur bacteria are supposed to contain the most primitive Rieske/cyt*b* complex.
Flash-induced absorption changes of cytochromes indicated that an efficient coupling reaction between the Rieske/cyt*b* complex and the reaction center complex could be realized through membrane-bound cyt *c*-556. We constructed the electron transfer model of the Rieske/cyt*b* complex interacted with cyt *c*-556 based on NMR measurements, and have also tried to purify the Rieske/cyt*b* complex in order to reveal its molecular structure.

3Pos232 低温顕微鏡による藻類細胞内光捕集調節機構の空間・波長・時間分解解析
Study on light-harvesting regulation mechanism in algal cells by space-wavelength-time-resolved analysis by cryogenic microscope

Yuki Fujita, XianJun Zhang, Shen Ye, **Yutaka Shibata** (*Grad. Sch. Sci., Tohoku Univ.*)

State transitions is a regulation mechanism of oxygenic photosynthetic organisms to maintain the excitation balance between photosystem (PS) I and II. Shuttling of light-harvesting complexes (LHCs) between PSI and PSII underlies the ST mechanism. We have conducted study of ST in algal cells based on the spatial resolution of the intracellular PSI-rich and PSII-rich domains realized by the self-developed cryogenic microscope. We extend our system to measure time-resolved fluorescence spectra of selected regions of a cell by using a streak-camera as an additional detection port. Acquisitions of the fluorescence spectrum and decay enabled to specify highly quenched and red-shifted (to 695 nm) LHCs colocalizing with PSI. The red shift suggested the aggregation of LHCs.

3Pos233 紅色光合成細菌の辺縁アンテナタンパク質の B800 バクテリオクロロフィル *a* の改変：色素酸化と色素置換
Conversion of B800 bacteriochlorophyll *a* in peripheral antenna proteins of purple photosynthetic bacteria by oxidation and reconstitution

Yoshitaka Saga, Kohei Hamanishi, Yuji Otsuka, Madoka Yamashita (*Fac. Sci. Eng., Kindai Univ.*)

Changing the functional relationship between energy donor and accepter in photosynthetic light-harvesting antenna proteins is promising to better understanding of their excitation energy transfer mechanisms. Here we report selective conversion of B800 bacteriochlorophyll (BChl) *a*, which acts as an energy donor in peripheral light-harvesting antenna proteins, LH2 and LH3, of purple photosynthetic bacteria, by oxidation and reconstitution methods. This conversion induced shifts of the lowest excitation energy band (Qy band) of the energy donor in the B800 site of the peripheral light-harvesting proteins without structural change. We discuss the effects of the conversion of B800 BChl *a* on the photofunctions of the peripheral light-harvesting proteins.

3Pos234 タンパク質間相互作用による光合成集光システムの調節
Regulation of light-harvesting systems by protein-protein interactions in plants

Eunchul Kim, Jun Minagawa (*National Institute for Basic Biology*)

Photosynthesis is a fundamental energy conversion process that sustains the Earth's ecosystem. As the environment has changed, photosynthetic systems of photosynthetic organisms have diversified and optimized. Recent research has shown that photosynthesis was developed not only for its "efficiency" in energy conversion, but also for its "flexibility" in sustaining itself in a changing environment. In particular, its light-harvesting system was found to have the greatest diversity and flexibility to cope with the changing light conditions. In this presentation, I would like to introduce my recent studies on the regulation of light-harvesting systems by protein-protein interactions in plants.

3Pos235 紅藻 *Porphyridium purpureum* のフィコビリソームロッドにおける最低第１励起状態をもつ発色団の特定
Identification of chromophores with the lowest first excited state in the phycobilisomal rod of the red alga *Porphyridium purpureum*

Hiroto Kikuchi (*Dept. of Phys. Nippon Med. Sch.*)

The molecular mechanisms of excitation energy transfer within the phycobilisome (PBS), the antenna system of cyanobacteria and red algae, is the superior function of living organisms. The energy state of each chromophore in the PBS, which is determined by electrical influences from the surrounding environment, is an important factor in revealing the excitation energy transfer mechanism. The three-dimensional structure of PBS containing the linker protein of the red alga *Porphyridium purpureum* was determined by cryo-electron microscopy at 2.82 angstrom resolution. On that basis, we report that the chromophore with the lowest first excited state in the rod of Porphyridium purpureum PBS has been identified by quantum chemical calculations.

3Pos236 太古岩石試料中の光合成色素の顕微分光分析
Microspectroscopic analysis of photosynthetic pigments in ancient rock samples

Tomohiro Ishikawa[1], Ryosuke Saito[2], Toru Kondo[1] ([1]*Dept. of Life Sci. and Tech. Tokyo Tech.*, [2]*Dept. of Earth Sci., Yamaguchi Univ.*)

Photosynthetic organisms have been evolved over long years under global environmental changes. Understanding antient photosynthetic systems leads to reveal a coevolutionary process of life and earth, which is an essential interest in both biology and geology. Here, we demonstrate a spectroscopic analysis of photosynthetic pigments left in geological samples in order to directly investigate ancient photosynthetic systems. We develop a confocal microscope with a wavelength-tunable laser source and measure several geological samples obtained from stratums from seven million to two hundred fifty million years old. Based on fluorescence and excitation spectra and fluorescence lifetime, we will discuss photosynthetic materials remaining in rock samples and their functions.

3Pos237 反復回分培養による紅色非硫黄細菌の光合成を利用した水素生成能について
Photosynthetic hydrogen production performance of purple non-sulfur bacteria in repeated batch culture

Masahiro Hibino, Sota Suzuki (*Div. Sust. Enviro. Eng., Muroran Inst. Tech.*)

Hydrogen has gained attention as clean energy due to its clean, recyclable, and more environmentally-friendly nature. Photosynthetic bacteria have ability to produce hydrogen from organic compounds under photosynthetic and anaerobic conditions. In this study, hydrogen production on the carbon source of acetate using repeated batch culture with purple non-sulfur bacteria was investigated. The maximum H_2 conversion efficiency of ~40 % was obtained at the first photo-hydrogen reaction cycle. The efficiencies decreased as the number of the reaction cycles increased. These results indicate that the hydrogen production using repeated batch culture can be continuously obtained at ~80 % of the maximum H_2 conversion efficiency under the optimal conditions.

3Pos238 Photo-control Small GTPase Ras Using Photochromic Peptide inhibitor

Nobuyuki Nishibe, Yuichi Imamura, Kazunori Kondo, Shinsaku Maruta (*Department of Bioinformatics, Soka University Graduate School of Engineering, Hachioji, Japan*)

The function of Small GTPase Ras is regulated by GEFs and GAPs. Previously, we have shown that GDP-GTP exchange of Ras with GEF is photo-regulated by peptide inhibitor crosslinked with azobenzene-di-maleimide. Recently, GEF proteomimetic inhibitor was reported that inhibits Ras-GEF interaction. This inhibitor consists of two peptide,αH and αI mimic which are intermolecularly crosslinked with dibenzylether. In this study, GEF mimic peptides and KRpep-2d modified with azobenzene derivative were prepared in order to photocontrol Ras GTPase. KRpep-2d inhibited the GTPase cycle in a concentration-dependent manner. Intact GEFαH peptide did not show inhibitory activity in GTPase cycle assay. Subsequently photo-reversible control of Ras GTPase was examined.

3Pos239 陸生アクチノバクテリア由来の新規微生物ロドプシン群
A novel clade of microbial rhodopsins in terrestrial *Actinobacteria*

Mako Ueno[1], Fumio Hayashi[2], Takashi Kikukawa[3], Masashi Sonoyama[1,4,5] ([1]*Grad. Sch. Sci. Tech., Gunma Univ.*, [2]*Ctr. Inst. Anal., Gunma Univ.*, [3]*Fac. Adv. Life Sci., Hokkaido Univ.*, [4]*GIAR, Gunma Univ.*, [5]*GUCFW, Gunma Univ.*)

Microbial rhodopsins are 7-transmembrane photoreceptors, and advances in metagenomics have led to their diversity. Currently, most experiments have been done just about sourced aquatic environments. In this study, proteorhodopsin was used as a query sequence in PSI-BLAST to find out rhodopsins encoded in terrestrial bacteria. As a result, we identified 102 sequences, all of which comprised a novel clade absent from known microbial rhodopsins by phylogenetic analyses. The identified sequences are mainly encoded in terrestrial *Actinobacteria* and commonly have longer C-terminus. Some of them achieved expression as colored rhodopsins. Clarified functions and structures of the identified sequences would broaden our knowledge of bacterial habitat and adaptability.

3Pos240 Gs 共役型オプシンを用いた二状態安定型光操作ツールの作製
Development of bistable optical control tools based on a Gs-coupled opsin

Akinari Sakayori[1], Yusuke Sakai[2], Mitsumasa Koyanagi[2], Akihisa Terakita[2], Hisao Tsukamoto[1] ([1]*Department of Biology, Kobe University*, [2]*Department of Biology, Osaka Metropolitan University*)

Animal opsins, light-sensitive G protein-coupled receptors (GPCRs), have been used as optogenetic tools to regulate GPCR-related cellular responses. In particular, many opsins in invertebrates have a property called bistability, which allows them to be activated or inactivated by different color of light. This bistable property of invertebrate opsins would be useful as optical control tools. In this study, we introduced amino acid substitutions on a Gs-coupled opsin from coral in order to change the spectral properties, and obtained opsin mutants that are activated by green light and inactivated by orange light. We propose these functionally modified opsins can function as valuable optical control tools that can regulate Gs-dependent cAMP responses by visible light.

3Pos241 光活性化転写因子「光ジッパー」の分子機構
Molecular mechanism of a light-activatable transcription factor, Photozipper

Osamu Hisatomi, Yuta Nagano, Yumiko Adachi (*Grad. Sch. of Sci., Osaka Univ.*)

Photozipper (PZ) is a light-activatable bZIP transcription factor composed of the C-terminal region of *V. frigida* AUREO1. We have investigated the photoreaction, dimerization and DNA-binding properties of site-directed PZ mutants, and found that blue light induces a conformational change of LOV core through several amino acids close to the chromophore, FMN, and causes deformation of the hydrophobic surface on the β-sheet of LOV core. It further induces the detachment of A'α helix at the N-terminal side of LOV core and the subsequent dimer formation of PZ, which results in the increment of its affinity for the target DNA. Our studies clearly indicated the molecular mechanism essential for aureochromes.

3Pos242 高速原子間力顕微鏡による光制御型転写因子 Photozipper の二量体形成過程の観察
Dimerization processes of a light-regulated transcription factor, Photozipper, observed by high-speed atomic force microscopy

Akihiro Tsuji[1], Hayato Yamashita[1], Osamu Hisatomi[2], Masayuki Abe[1] ([1]*Grad. Sch. Eng. Sci., Osaka Univ.*, [2]*Grad.Sch. Sci., Osaka Univ.*)

Dimerization is crucial for transcription factors (TFs) to bind DNA and control various cellular functions in living organisms. However, its single-molecular mechanism has been poorly clarified. To solve this problem, we observed Photozipper (PZ), a blue light (BL)-regulated TF module, by high-speed AFM (HS-AFM). Light-controlled HS-AFM experiments visualized the reversible dimerization process of PZ. Also, the lifetime of dimers under light were found to be longer than that in the dark. Furthermore, HS-AFM revealed that the DNA-binding bZIP domain in PZ is entangled under dark, but loosens up and increases its fluctuation by BL. Our data unravel the molecular mechanism of BL-induced activation of PZ, and may provide valuable insights to understand the TF activity.

3Pos243 光受容タンパク質を用いた液液相分離の光制御システムの作製
Creation of a light-control system for liquid-liquid phase separation using a photoreceptor protein

Mizuki Takasugi[1], Yoichi Yamazaki[1], Kento Yonezawa[1,2], Sachiko Toma-Fukai[1], Hironari Kamikubo[1,2] ([1]*NAIST, MS*, [2]*NAIST, CDG*)

Liquid-liquid phase separation (LLPS) is formed by multiple interactions. We attempted to create a photo-reversible LLPS system by utilizing the light-dependent association-dissociation reaction between Photoactive Yellow Protein (PYP) and PYP Binding Protein (PBP). PYP associates with PBP upon UV-A light irradiation and dissociates upon blue light irradiation. We produced a PBP and FUS fusion protein (FUS is known as a LLPS protein). While the PYP and PBP-FUS mixture did not show LLPS under dark, UV-A irradiation resulted in increased turbidity and droplet formation. Subsequent blue light irradiation resulted in a decrease in turbidity and disappearance of droplets, indicating photo-reversible LLPS was achieved.

3Pos244 集束超音波による生体分子への影響
Focused ultrasound induced denaturation of biomolecules

Takumi Akiu[1], Kotarou Takeda[2], Wakako Hiraoka[1] ([1]*Grad. Sch. Sci. & Tech., Meiji Univ.*, [2]*Sch. Sci. & Tech., Meiji Univ.*)

Focused ultrasound is a promising noninvasive treatment that complements current standard therapies such as surgery, radiation, gene therapy, immunotherapy, and chemotherapy. The high pressure produced by focused ultrasound generates efficient and powerful cavitation, and its physicochemical effects are expected to have therapeutic efficacy. The purpose of this study is to investigate the effects of focused ultrasound on biological macromolecules, which are considered essential and basic information for therapy. We will report of focused ultrasound-induced denaturation and functional modification of biomolecules, such as amino acids, peptides, proteins, genes and cell membrane.

3Pos245 Elucidation of intracellular temperature changes induced by external stress using fluorescent nano diamonds

Kiichi Kaminaga, Chihiro Suzuki, Yanagi Tamami, Hiroshi Abe, Takeshi Ohshima, Ryuji Igarashi (*Institute for Quantum Life Science, Quantum Life and Medical Science Directorate, QST*)

Temperature is an important physicochemical parameter that changes the rate of chemical and enzyme reaction in cells.This study attempted to elucidate the intracellular temperature change after external stress (X-ray irradiation). As a preliminary study, the intracellular temperatures of human cancer cells (HeLa) and human normal fibroblasts (BJ 5ta) were measured by Fluorescent Nano Diamond at 1-2 hours after X-ray (10 Gy) irradiation. As a result, irradiated cells show higher temperature in both cell lines than the non-irradiated group. In the presentation, I would like to discuss about chronological changes, dose dependency, and the mechanism.

3Pos246 ヒトプリオンタンパク質オクタリピート領域におけるレドックス調節
Redox regulation in octarepeat region of human prion protein

Wakako Hiraoka[1], Osamu Inanami[2], Satoru Tsuri[3] ([1]*Grad. Sch. Sci. & Tech., Meiji Univ.*, [2]*Grad. Sch. Vet. Med., Hokkaido Univ.*, [3]*Sch. Sci. & Tech., Meiji Univ.*)

Neurodegenerative disease-related proteins have been implicated in possible association with oxidative stress. Physiological function of human prion protein (hPrP) is still unknown, however its metal-binding potentials are meaningful and viewed as metal reservoir and redox regulation. We have studied the stability of divalent metals at binding site using a single octarepeat peptide of hPrP. In this report, the reactivity of octarepeat peptide with oxidative metabolite such as reactive oxygen species and organic peroxides was studied using ESR-spin trapping and several biochemical methods. The binding of divalent metal ions to peptides is suggested to have a significant effect on the property of prion protein in vivo.

3Pos247 Coexistence of crystals and membraneless polyester microdroplets in a primitive complex system

Chen Chen[1], Ruiqin Yi[1], Motoko Igisu[2], Afrin Rehana[1], Takazo Shibuya[2], Yuichiro Ueno[2,3], Anna Wang[4], Andre Antunes[5], Kuhan Chandru[6], Tony Z. Jia[1,7] ([1]*Earth-Life Science Institute, Tokyo Institute of Technology, Japan*, [2]*Institute for Extra-cutting-edge Science and Technology Avant-garde Research (X-star), Japan Agency for Marine-Earth Science and Technology (JAMSTEC), Japan*, [3]*Department of Earth Science and Planetary Sciences, Tokyo Institute of Technology, Japan*, [4]*School of Chemistry, UNSW Sydney, Australia*, [5]*State Key Laboratory of Lunar and Planetary Sciences, Macau University of Science and Technology, China*, [6]*Space Science Center (ANGKASA), Institute of Climate Change, Level3, Research Complex, National University of Malaysia (UKM), Malaysia*, [7]*Blue Marble Space Institute of Science, USA*)

α-Hydroxy acids (αHAs) like phenyllactic acid (PA) or leucic acid (MA) are abundant prebiotic monomers and can condense to form gel-like polyesters forming membraneless droplets via LLPS upon aqueous rehydration. These droplets are essential to biochemical reactions and origins of life. However, limited αHAs monomers were used previously. To explore the chemical diversity with various αHAs amongst many other organic compounds, we selected tartaric acid (TA) as a negatively charged αHA to incorporate with PA or MA. Finally, we found minor changes of chemical diversity make a new phase coexisting with droplet compartments, suggesting that the messy prebiotic chemical milieu could have formed an abundance of such co-existing macrostructures on the early Earth.

3Pos248 Exploring ancient origins of the circadian clock system through molecular evolution

Atsushi Mukaiyama[1,2], Yoshihiko Furuike[1,2], Shuji Akiyama[1,2] ([1]*Inst. for Mol. Sci. CIMoS*, [2]*SOKENDAI*)

Circadian clocks are endogenous time-management systems that organisms have acquired during the course of evolution in order to adapt to periodic environmental changes on Earth. We have reported that the rhythmic frequency in the cyanobacterial clock is encoded within the clock protein KaiC (Abe et al. ***Science*** , 2015), but a key question of when KaiC acquired its oscillatory ability remains unanswered. To address this question, we attempted to reconstruct ancient circadian clock systems by restoring ancestral KaiCs using a molecular evolution approach. Our results suggest that the circadian rhythm first appeared in the earliest cyanobacteria together with KaiC. We discuss the emergence of the circadian clock in relation to Earth's history.

3Pos249 Development of a translational field in the artificial cell by the shell of multiphase droplets

Kanji Tomohara, Yoshihiro Minagawa, Hiroyuki Noji (*Dept. Appl. Chem., Grad. Sch. Eng., Univ. Tokyo*)

In the research field of the artificial cell, individual cellular functions have been reconstituted in cell-sized droplets. In integrating such functions in a single droplet as a next step, we can refer to natural cells' strategy of spatially compartmentalizing each reaction. Thus, we focused on creating an artificial organelle that works as a field of enzymatic reactions and enables the rectification of biochemical pathways. Here, we prepared core-shell structured droplets by LLPS of three polymers: PEG, dextran, and IDP. After confirming that the transcription can be carried out in the IDP-phase located at the core, we are now trying to perform the translation in the dextran-phase located at the shell, thereby mimicking the nucleus and the cytosol of eukaryotic cells.

3Pos250 アミノ酸熱重合物を用いた代謝様反応
Metabolism-like reactions using proteinoid

Shunsuke Ito[1], Shigeru Sakurazawa[2] ([1]*Future University Hakodate*, [2]*Department of Complex and Intelligent Systems, Future University Hakodate*)

Metabolism is a reaction cycle that extracts energy from organic matter and is the basis of life phenomena, and chemical oscillatory reaction is reaction system that model the metabolic system of life. Proteinoid is a macromolecule modeled for abiotic primitive proteins, and has functions related to various reactions. However, a reaction cycle using proteinoid has not yet been realized. In this study, we aim to realize a reaction cycle using proteinoid, which is a model of primitive biomolecules. In this study, substrate was replaced by proteinoid for BZ and BR reaction. Oscillating reactions were observed in both reactions with proteinoids of different compositions. These results suggest that proteinoid can have potential for primitive metabolism.

3Pos251 触媒反応ネットワークにおけるコンパートメントの進化的獲得
Catalytic reaction networks evolve compartmentalization and compartment-specific reactions

Shunsuke Ichii[1], Yusuke Himeoka[1], Chikara Furusawa[1,2] ([1]*Grad. Sch. Sci., Univ. of Tokyo*, [2]*BDR, RIKEN*)

From prokaryotes to multicellular organisms, various compartments such as organelles and biomolecular condensates are commonly observed in cells; those compartments regulate specific reactions. Though molecular mechanisms of compartments are well studied, the evolutional benefit remains unclear. In this study, we analyze the evolution of regulations in catalytic reaction networks within compartmentalized spaces by numerical simulation. As a result, we found that compartmentalization can acquire compartment-specific reactions and increase evolutional fitness under certain conditions of the reaction network and chemicals that are exchangeable between compartments. We will discuss the conditions for the evolution of regulations to acquire compartment-specific reactions.

3Pos252 緩慢凍結融解サイクルによるベシクル融合実験：原始細胞生成過程への示唆
Vesicle fusion via slow freeze-thaw cycles and its implications for the emergence of a protocell

Natsumi Noda[1], Tatsuya Shinoda[1], Kazumu Kaneko[1], Yoshikazu Tanaka[2], Yasuhito Sekine[1], Tomoaki Matsuura[1] ([1]*ELSI, Tokyo Tech.*, [2]*Grad. Sch. Life Sci., Tohoku Univ.*)

Condensations of biomolecules must have played an important role on the emergence of the primitive cell system on early Earth. Here, we propose vesicle fusion through freeze-thaw (FT) cycles as a plausible mechanism to assemble and concentrate various biomolecules into a single compartment. While eutectic solution formed at a slow freezing rate (< ~1 K min^{-1}) may affect the dynamics of lipids, its effect on the vesicle concentration or fusion has hardly been studied. We prepared large unilamellar vesicles (LUVs, ~100 nm) with egg phosphatidylcholine (eggPC) and subjected them to slow-FT cycles. We found that LUV has grown to ~1000 nm, suggesting slow-FT can induce vesicle fusion. We also discuss the role of slow-FT on the concentration of extravesicular biomolecules.

3Pos253 核スペックルの構造形成・動態のシミュレーション
Simulations of structural dynamics of nuclear speckle

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Nuclear speckle is the populations of molecular droplets broadly distributed in nucleus, that is one of nuclear bodies playing various roles of intranuclear processes in multi-cellular organisms. Each droplet contains various proteins and noncoding RNAs working as splicing factors to synthesize mRNAs. The droplets of nuclear speckle were known to gather to forms large spherical structures when the transcriptions pause. On the other hand, it was also known these droplets cannot be maintained when the noncoding RNA called MALAT1 is depleted. However, the mechanism of such transcription activity-dependent features has not been clarified.
In this study, we proposed and simulated a coarse-grained model to explain such structural-dynamical properties of nuclear speckles.

3Pos254 Hi-C データからの直感的なヘテロクロマチンとユークロマチンの識別法
An intuitive discrimination method of heterochromatin and euchromatin from Hi-C data

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Hi-C, a technique giving contact frequencies between pairs of loci in chromosomes, has been revealed the structure and dynamics of chromosomes such as topologically associated domains (TADs) and looping. Plaid patterns in TADs are closely related to heterochromatin and euchromatin regions. However, the way to discriminate heterochromatin and euchromatin from Hi-C data is complicated and not intuitive. Recently, Fujishiro and Sasai suggested that they can be discriminated by correlations with neighboring regions in Hi-C data: heterochromatin regions have high correlations with neighbors. Here, we propose another simple and intuitive way. Summation of a column of Hi-C matrices is found to give vectors that highly correlate with the eigenvectors used for discrimination.

3Pos255 Modeling heterogeneous chromatin structure ensembles using metainference from Hi-C data

Chenyang Gu, Giovanni Brandani (*Grad. Sch. Sci., Univ. Kyoto*)

Chromosome conformation capture techniques like Hi-C provides huge amount of information about chromatin conformations. However, the chromatin conformation is usually highly heterogeneous, and contacts from different structures are mixed in Hi-C data. In this study we use metainference, a Bayesian inference framework integrated with molecular dynamics simulation, to infer the heterogeneous chromatin structures from Hi-C data. Applycation of this method on the mESC Nanog locus reconstructs different structure clusters related to enhancer-promoter interaction dynamics.

3Pos256 改良 MSA を用いたアブラナ科植物の SRK/SP11 複合体構造のハプロタイプ網羅的な予測
Haplotype exhaustive prediction of SRK/SP11 complex structure in Brassicaceae using a modified MSA

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S-locus receptor kinase (SRK) in pistil and a small ligand protein, *S*-locus protein 11 (SP11) in pollen are responsible for *Brassicaceae* self-incompatibility. If both proteins are derived from the same S-locus, the pollen will be rejected to prevent self-pollination. Although two haplotypes of their complex crystal structures have been determined, there remain many haplotypes with unknown structure. AlphaFold2, which is highlighted for its high accuracy, is expected to be effective for the problem, but the prediction of SP11 was still difficult due to its shallow MSAs. Here we report a modified MSA considering well-conserved disulfide bond pairs for SP11s could generate more plausible SP11 and SRK-SP11 complex structures using AlphaFold2.

3Pos257 深層学習を用いた、電子顕微鏡画像からの骨格筋小胞形態判別
Skeletal muscle vesicle morphology discrimination from electron microscope images using deep learning method

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The sarcoplasmic reticulum is important device in muscle contraction. Three main morphologies are observed in the electron microscope image (EMI) of the isolated sarcoplasmic reticulum. The relationship between the appearance frequency of these morphologies and the surrounding environment leads to the molecular mechanism of the muscle contraction. However, it is difficult to manually classify the vesicles from a huge number of EMIs. Therefore, we studied a method for automatically detect and classify vesicles using deep learning method(CNN). EMIs of vesicles isolated from scallop skeletal muscle were increased by rotation processing to make 7050 training data. The trained CNN model made it possible to classify three morphologies with high accuracy of mAP = 72.83%.

3Pos258 新しいタンパク質立体構造がミスセンスバリアントの評価に与える影響の評価
Evaluating the impact of new three-dimensional structures for interpretation of missense variants in human genome

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Although new protein structures are solved every week, how they contribute to the interpretation of amino acid changes caused by human genome variations has not been well described. By weekly updating data from PDB, we observed recent rapid increase of the human proteins covered by PDB structures, contributed by cryo-EM methods. About half of the most constrained proteins have at least partial experimental structure in April 2022. Compared to predicted models with AlphaFold, structures in PDB involve a variety of protein-protein interaction interfaces and ligand-binding sites, which are critical for interpretation of variants. These results highlight the importance of new protein structures for bridging the gap between human genotypes and phenotypes.

3Pos259 Structural characteristics of coregulated phosphorylation sites

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Phosphorylation is a fundamental protein modification that modulates protein function in accordance with cellular signaling. Phosphorylation sites are known to be often clustered on protein sequences; however, it is unclear whether there exist spatial clusters of multiple phosphorylation sites regulated together. Here I employed AlphaFoldDB models to investigate the structural features of coregulated phosphorylation sites. With a phosphoproteomics dataset, cophosphorylated site pairs were identified and mapped onto AlphaFold models. Phosphosite pairs with stronger correlation slightly tend to avoid structured regions, namely high pLDDT scores. Based on the PAE values, positively coregulated phosphosite pairs were weakly clustered compared to negatively coregulated ones.

3Pos260 微生物群集は普遍的に極めて安定な形質組成を持つ
Microbial communities are universally characterized by extremely stable trait compositions

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Rules that govern community structures are central issues in community ecology. While adaptation processes of each organism have been studied rigorously, how phenotypic traits of the entire communities adapt to environments has not been investigated systematically. Here, we conducted meta-analysis of 1,525 bacterial communities from three popular environments (soil, marine, and human gut) using our comprehensive trait-based analysis of various microbial traits. Surprisingly, we found that microbial communities universally exhibit very stable trait compositions within each environmental category. At the community level, microbial trait compositions are under strong and universal selection pressures, which affect the flexible dynamics of trait evolution of each species.

3Pos261 乳腺組織のがん化により染色体内相互作用を維持する遺伝子の遺伝子オントロジーの特定
Identification of gene ontologies of genes with intra-chromosomal interactions in the breast cancer tissue

Yuta Shintani (*Fac. Adv. Math. Sci., Meiji Univ*)

It is known that cancerization decreases inter-chromosomal (trans) interactions more dramatically than intra-chromosomal (cis) interactions in the cell. In this study, we aimed to identify gene ontologies (GOs) of genes which maintain cis interaction in the breast cancer tissue. First, 3,918 of Differentially Expressed Genes (DEGs) were extracted by Significance Analysis of Microarrays. Next, the correlation network by DEGs in normal and cancer cells was generated to predict cis/trans interactions. Finally, GOs of genes which form cis/trans interactions were extracted by enrichment analysis. As a result, genes with OGs related to mitotic cell cycle, DNA metabolic process, and regulation of cell cycle process were maintained the cis interaction even after cancerization.

3Pos262 出芽酵母プロテオームからの新規 PLP 結合タンパク質の予測
Prediction of novel PLP-binding proteins from budding yeast proteome

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Although many comprehensive experiments have been conducted, more than 10% of proteins encoded in the *Saccharomyces cerevisiae* genome are annotated as uncharacterized proteins. To characterize their molecular functions, we focused on the binding ability to pyridoxal 5'-phosphate (PLP), a crucial coenzyme in organisms. To predict the PLP-binding ability, we employed ProLMS-GNN. This graph neural network-based method trains the prediction model using simple features of coenzyme-binding residues, such as amino acid types and surface geometry. We chose predicted PLP-binding proteins with high reliability from yeast uncharacterized proteins and verified their PLP-binding ability by a microbiological assay. As a result, at least one of them was confirmed to bind PLP.

3Pos263 膜タンパク質クラスター形成とそのシグナル伝達系における機能的意義に関する数理的研究
A Mathematical study for membrane protein cluster formations and its functional significance in signal transduction systems

Hiroaki Takagi (*Sch. Med., Nara Med. Univ.*)

In cell signaling systems, it has become clear through advanced single-molecule measurements that protein molecules such as receptors on the plasma membrane perform their functions while adopting non-uniform and non-trivial spatial structures on the 100-nm-scale. In order to explore the mechanism of such spatial distribution of membrane molecules and its functional significance, we mathematically studied models of cluster formation and its extension in several spatial point processes. We will discuss the conditions required for various statistical properties of non-Poisson distributions such as power-law, and the relationship between spatial distributions of membrane proteins and their advantages in signal transduction.

3Pos264 主成分分析を用いた希少/遺伝性疾患に対する human phenotype ontology からの特徴抽出
Feature extraction from human phenotype ontology for rare/hereditary disease using principal component analysis

Yoshino Jibiki[1], Toyofumi Fujiwara[2], Takanori Sasaki[1] ([1]*Fac. Adv. Math. Sci., Meiji Univ.*, [2]*DBCLS*)

There are more than 300 million patients worldwide with rare/hereditary diseases, and early and proper diagnosis for these diseases is difficult. In this study, we investigated the relationship between diseases and phenotypes using the Human Phenotype Ontology (HPO), a symptom ontology, to support diagnosis for these diseases. First, disease groups were clustered using the Mondo Disease Ontology. Next, a principal component of the HPOs whose occurrence frequency was counted for each disease group was analyzed. By this feature extraction, clarification of the relationship between disease-causing genes/tissues and specific phenotypes is expected. In this presentation, we will discuss the possibility of predicting disease candidates based on medical record information.

3Pos265 クロマチンポリマーモデルにおける結合分子によるクラスターの寿命
Lifetime of Bridging Induced Cluster in Chromatin Polymer Model

Ryo Nakanishi[1], Koji Hukushima[1,2] ([1]*Graduate School of Arts and Sciences, The University of Tokyo*, [2]*Komaba Institute for Science*)

The SBS (Strings and Binders Switch) model [1] is a polymer model that takes into account the phase separation of chromatin induced by its binding molecules. The binding molecules can bind multivalently to chromatin and switch between two states, one in which it can bind chromatin and one in which it does not, at a constant rate. In this model, chromatin forms clusters due to the effective attraction between chromatin segments via the binding molecules[1,2,3]. We analyzed the processes of cluster formation and measured the lifetime of clusters from the results of molecular dynamics simulations of the SBS model.
[1] Mariano Barbieri et al., PNAS, 2012.
[2] Andrea M. Chiariello et al., Sci. Rep., 2016.
[3] Chris A Brackley et al., Biophys J., 2017.

3Pos266 遺伝子発現制御ネットワークモデルの応答ダイナミクス次元圧縮
Dimensional compression of response dynamics on a gene regulatory network model

Masayo Inoue[1], Kunihiko Kaneko[2] ([1]*Grad. Sch. Eng., Kyushu Inst. Tech.*, [2]*Niels Bohr Inst.*)

Because biological networks are composed of a large number of closely interacting elements, it is difficult to quantitatively analyze their response dynamics (information transmission process). In order to realize quantitative analysis and to understand the flow of information in a large network, we performed two types of dimensional compression methods using a gene regulatory network model as an example; "dynamic mode decomposition" (DMD) which works on state space and “Koopman mode decomposition" (KMD) which takes place in observable space. We will also report how the primary modes (information transfer pathways) are formed as the network evolves.

3Pos267 細胞配置替え過程におけるアクトミオシンケーブルの剥離と接着の数理モデル
Mathematical model for detachment and attachment of cortical actin cable in cell rearrangement

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Cell rearrangement, one of the fundamental processes responsible for tissue deformation, involves the exchange of junctions. The mechanism behind the exchange of junctions remains elusive. We previously identified a cytoskeleton structure that could be critical in the junction exchange: myo-II gap, a small structure of cortical actin cable detached from adherence junction (AJ), transiently appears during the junction exchange. Here, we propose a mathematical model based on wetting theory and determine the mechanical and geometrical conditions for the appearance and disappearance of the myo-II gap. The model reveals the mechanical roles of molecules such as myosin-II, actin-AJ linker Jub, tricellular junction protein M6, and PTEN in the junction exchange.

3Pos268 Which asymmetry leads to genitalia rotation: Direction-dependent interfacial tension vs effective cellular torque

Sonja Tarama[1,2], Sayaka Sekine[3], Erina Kuranaga[3], Tatsuo Shibata[2] ([1]*Col Life Sci, Ritsumeikan Univ*, [2]*Riken BDR*, [3]*Grad Sch Life Sci, Tohoku Univ*)

It has been shown that the genitalia rotation in Drosophila embryo is caused by the collective migration of surrounding epithelial cells. Previously, two theoretical models have been proposed assuming different asymmetric properties: The first model considers a direction-dependent interfacial tension. The second model introduces cellular torque under a hypothetical torque gradient. We discuss differences in the simulation results for these two to get hints for identifying the underlying mechanical mechanism. We analyzed the distribution of the angles of cell boundaries undergoing cell rearrangements and the associated cell shapes. Comparison with the experimental results revealed the genitalia rotation is better described via the interfacial tension scenario.

3Pos269 生態・進化ダイナミクスにおける一般的な速度制限
General constraint on speeds in ecological and evolutionary dynamics

Kyosuke Adachi[1,2], Ryosuke Iritani[2,4], Ryusuke Hamazaki[2,3] ([1]*RIKEN BDR*, [2]*RIKEN iTHEMS*, [3]*RIKEN CPR*, [4]*Grad. Sch. Sci., Univ. Tokyo*)

In ecology and evolution, population dynamics often characterizes the underlying biological processes. For example, temporal oscillation of the prey-predator populations or irreversible extinction of some species can be described as nonlinear population dynamics. Discovering general relations in such nonlinear dynamics should be important to predict complex biological processes. Here, we propose a general relation that limits the speeds in population dynamics, including an evolutionary model with mutation, an epidemiological model, and an ecological model with competitive interactions. We also show that the obtained relation is regarded as an extension of Fisher's fundamental theorem of natural selection.
[1] Adachi, Iritani, and Hamazaki, Commun. Phys. 5, 129 (2022)

3Pos270 ヒト血中インスリンによるアミノ酸および脂質代謝制御機構のモデルベース同定
Model-based identification of the regulation of amino acid and lipid metabolism by insulin in human blood

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Insulin is the major anabolic hormone that regulates glucose metabolism. In addition to glucose metabolism, insulin also regulates other metabolism such as amino acids and lipids, but the mechanism of metabolic control at the human blood level is not well understood. In this study, we identified the regulatory mechanism of blood metabolite concentrations by insulin based on a mathematical model in the S-system format. We constructed the mathematical model using a data set that measured the effects of different doses and different time patterns of intake on blood metabolites and hormones. The model structure and parameters revealed differences in metabolic control mechanisms for amino acids and lipids.

3Pos271 ネットワーク解析に基づく乳がんのバイオマーカー予測
Biomarker prediction of breast cancer based on network analysis

Saito Torii (*Fac. Adv. Math. Sci., Meiji Univ.*)

Various biomarker panels have been used for breast cancer subtype classification and prognosis prediction. In this study, we proposed a set of genes useful for predicting basal-like type breast cancer based on the network analysis. Specifically, by targeting genes which forms PPI interaction network with PAM50 panel genes, we identified differential expression genes accompanied by cancerization using Reactome and The Human Protein Atlas. As a result, 14 genes were selected that are useful for predicting basal-like breast cancer. In this presentation, we will also discuss the results of centrality analysis for PPI interaction network by biomarker panel genes.

3Pos272 A general approach to chemical thermodynamics and constraints for growing systems

Yuki Sughiyama, **Atsushi Kamimura**, Dimitri Loutchko, Tetsuya J. Kobayashi (*IIS, The University of Tokyo*)

We consider a general thermodynamic framework of open chemical reaction networks (CRNs), in which autocatalytic chemical reactions are encapsulated in a finite volume and its size can change with the reactions. The thermodynamics of such open CRNs is essential for understanding biological and artificial cells by clarifying physical conditions and costs for their growing states. The framework provides the environmental conditions to determine if the system grows or not. We also identify thermodynamic constraints; one to restrict possible states of the CRNs and the other to further limit the region where a steady growing state can exist. The results are based solely on the second law of thermodynamics without assuming any specific thermodynamic potentials or kinetics.

3Pos273 動物の老化に伴う活動速度の指数減衰とトランスポゾン駆動老化仮説の検証
Exponential decline of *C. elegans* behavioral activity along with aging and experimental test of the transposon-driven aging hypothesis

Yukinobu Arata, Jurica Peter, Sako Yasushi (*RIKEN, CPR, Cell Info*)

During lifespan, animals change their morphology and behavior. Statistical laws and molecular mechanism governing such slow dynamics remain unknown. By our lifelong video-recorder, nemaLife-logger, we found that *C. elegans* behavioral activity declined exponentially along aging. We hypothesized that exponential aging is driven by some stochastic reaction with a slow rate as animal ages. The transposon-driven aging hypothesis claims that animals age by somatic genome disruption via transposon. By bioinformatics, we identified 140 active genes for transposon-mobility in the *C. elegans* genome. Here, we will introduce our experimental setting for knocking out the 140 active genes in *C. elegans* and recent statistical analyses of aging dynamics measured by nemaLife-logger.

3Pos274 Overpotential Estimation in Enzymatic Reactions of Mitochondrial Respiratory Chains

Nuning Anugrah Putri Namari[1], Kotaro Takeyasu[2,3], Junji Nakamura[3,4] ([1]*Graduate School of Science and Technology, University of Tsukuba*, [2]*Department of Materials Science, Faculty of Pure and Applied Sciences, University of Tsukuba*, [3]*Tsukuba Research Center for Energy Materials Science, University of Tsukuba*, [4]*Mitsui Chemicals, Inc.-Carbon Neutral Research Center, International Institute for Carbon-Neutral Energy Research, Kyushu University*)

The mechanism of heat generation in mitochondrial respiratory chain is still unestablished. In respiratory chains, redox reactions take place flowing electrons from complex I to IV which are finally used for oxygen reduction reaction (ORR). This process is similar to fuel cell, a device that uses ORR to convert chemical energy into electricity. In the fuel cell, heat is generated by overpotential, which is the additional voltage required to drive a reaction and mass transport. This study aims to prove that overpotential is the heat source in mitochondria. We estimated overpotentials at each complex using reported electrochemical voltammetry data of each reaction. The result showed that complex IV needs the highest overpotential owing to ORR which is converted to heat.

3Pos275 細胞内微小管の物理的性質
Probing physical properties of intracellular microtubules

Ryota Ori, Hirokazu Tanimoto (*Grad. Sch. Nanobioscience., Univ. Yokohama City*)

Microtubules are very important structures for cellular functions and their physical properties are of central importance for the functions. To understand the physical properties of intracellular microtubules, active measurement inside the cell is important, but it is rarely performed. We have developed a setup which enables us to directly apply calibrated forces to microtubules inside cells. We measured strain fields in microtubule's network and derived a scaling law. Moreover, we demonstrated that the applied external force induces buckling of single microtubule. In contrast to classical Euler buckling, higher-order modes became unstable in the induced buckling. We discuss the relation between the mechanics of single microtubules and of its network.

3Pos276 磁気刺激による細胞活動制御のための磁気レシーバー・磁気刺激システムの開発
Development of novel technique for magnetic activation of living-cell functions

Shunki Takaramoto[1], Hiromu Yawo[1], Yujiro Nagasaka[1], Hikaru Yoshioka[2], Masaki Sekino[2], Keiichi Inoue[1] ([1]*ISSP Univ. Tokyo*, [2]*Sch. Eng., Univ. Tokyo*)

Optogenetics is extremely useful technique for remote manipulation of cellular functions by using light stimuli. However, one of the serious problems is that optical stimulation is absorbed or scattered by biological tissues, then it is difficult to penetrate deep into the tissues. In order to overcome it, the remote-control method using magnetic fields is emerging as a non-invasive and deep stimulation method. We are now developing molecular tools for magnetic stimulation of cells, which is based on a combination of mechanosensitive channel and iron-binding protein such as ferritin. In the presentation, we will discuss the progress in the development of the molecular tools, and of a novel system to detect cell activity during magnetic stimulation.

3Pos277 (2SGA-3) Decoding single-cell transcriptomic phenotypes from cell images enabled by robotic data acquisition and deep learning

Jianshi Jin[1], Taisaku Ogawa[1], Nozomi Hojo[1], Kirill Kryukov[2], Kenji Shimizu[3], Tomokatsu Ikawa[4], Tadashi Imanishi[2], Taku Okazaki[3], Shiroguchi Katsuyuki[1] ([1]*BDR, RIKEN*, [2]*Dept. of Mol. Life Sci., Tokai Univ. Sch. of Med.*, [3]*Inst. for Quant. Biosci., Univ. of Tokyo*, [4]*Res. Inst. for Biomed. Sci., Tokyo Univ. of Sci.*)

Predicting marker-gene-defined phenotypes of cells from microscopy images by deep learning has had a great impact on biological studies and medical applications. Here, we developed a robot named ALPS (Automated Live-imaging and cell Picking System), and performed whole transcriptome analysis (RNA-seq) for microscopically observed single cells, *e.g.*, peripheral blood mononuclear cells. Using these datasets, we predicted the transcriptome-defined (unbiased) cell types or states of the same cell type from the label-free live cell images (dynamics) by deep learning. Furthermore, we found that the deep learning had the ability to predict RNA expression levels of individual genes, which opened a new window to challenge the image-based prediction of all genes.

3Pos278 Plunus Lanessiana から抽出した蛍光色素の解析と水素化アモルファスシリコン薄膜上での特性
Characterization of fluorescent pigment extracted from Plunus Lanessiana and the properties on hydrogenated amorphous silicon film

Kazunori Takada[1], Mao Izumi[1], Satomi Kimura[1], Koyu Akiyama[1], Hiroshi Masumoto[2], Yutaka Tsujiuchi[1,2] ([1]*Material Science and Engineering, Akita University*, [2]*Frontier Research Institute for Interdisciplinary Sciences, Tohoku University*)

Fluorescent property of pigment extracted from Plunus Lanessiana was characterized for investigating a high ultraviolet absorption and visible light emission molecule. At first the thin film contains the pigments on hydrogenated amorphous silicon (a-Si:H) was fabricated. Secondly the fluorescent spectrum change depend on electric field that is yielded on a-Si:H were analyzed for study the interaction of pigment and hydrogen rich subsurface of a-Si:H. Firstly it was found that the pigment emits turquoise color in high pH environment solution and revealed an isosbestic points. Secondly, the pigment on the solid state showed the function as a pH indicator that is useful for hydrogen generations.

3Pos279 センサシステム研究のための水素化アモルファスシリコンで増強された脂肪酸とクマリンの複合分子薄膜
Composite molecular film of fatty acid and coumarin for sensor system enhanced by hydrogenated amorphous silicon

Koyu Akiyama[1], Kazunori Takada[1], Hiroshi Masumoto[2], Yutaka Tsujiuchi[1,2] ([1]*Material Science and Engineering, Akita University*, [2]*Frontier Research Institute for Interdisciplinary Sciences, Tohoku University*)

The ionic state of composite molecular film of fatty acid and coumarin and fluorescent properties were characterized for detection of volatile gas molecule. And the organic molecular film on continuous laminated hydrogenated amorphous silicon (a-Si:H) film was characterized. The light absorption of 7-hydroxy-4-methylcoumarin (7C) or 4-hydroxymethylcoumarin (4C) and fatty acid was measured for determine the stabilized state on solid substrate. Further a composite Langmuir Blodgett film (LB film) of fatty acid and fluorescent molecule, stearic acid (SA) and 7C, on a-Si:H film was fabricated for investigate the molecular interaction of organic film and ammonia gas. Several absorption changes showed a response for gas sensor.

3Pos280 光退色後蛍光寿命回復法の開発と応用
Fluorescence Lifetime Recovery After Photobleaching (FLRAP): Concept and application

Ikumi Mori, Miyuki Sakaguchi, Shoichi Yamaguchi, Takuhiro Otosu (*Grad. Sch. Sci. Eng. Saitama Univ.*)

Fluorescence recovery after photobleaching (FRAP) has been widely used to analyze the molecular diffusion in vitro as well as in vivo and is now an indispensable tool in the field of bioscience. However, it is hard to analyze the diffusion of multiple species simultaneously. Here, we develop the methodology of Fluorescence Lifetime Recovery After Photobleaching (FLRAP) which analyze the recovery of both fluorescence intensity and fluorescence lifetime. This enables us to analyze the diffusion of multiple species based on the recovery of their intrinsic fluorescence lifetimes. We will report the concept as well as instrument for FLRAP, and its application on some biological systems.

3Pos281 光ファイバ型蛍光相関分光装置の開発と性能評価
Development of a fiber-optic based fluorescence correlation spectroscopy and its performance evaluation

Johtaro Yamamoto[1], Akira Sasaki[2] ([1]*Health & Med. Res. Inst., AIST*, [2]*Biomed. Res. Inst., AIST*)

Fiber-optic based fluorescence correlation spectroscopy (FB-FCS), which provides the measurement of molecular size and concentration, was developed. Pinhole adjustment is no longer needed in FB-FCS different from conventional FCS systems. Furthermore, FB-FCS is low cost and compact compared with conventional FCS. We performed some experiments to investigate the accuracy and sensitivity of FB-FCS. The molecular size and concentration were in good agreement with expected values. The fluorescence sensitivity of FB-FCS was lower than conventional FCS, however, FB-FCS had enough sensitivity to measure solutions of organic fluorescence dye. We expect that FB-FCS is widely used as a desktop FCS system in laboratories.

3Pos282 Measuring the heat flux of intracellular reactions using differential scanning calorimetry

Tasuku Sato[1], Akira Murakami[1], Kohki Okabe[1,2], Takashi Funatsu[1] ([1]*Graduate School of Pharmaceutical Sciences, The University of Tokyo*, [2]*PRESTO, JST*)

The intracellular temperature is spatiotemporally variable. However, the principle that drives this variation is elusive because the heat flux of living cells is unknown. Here, we experimentally quantified the heat flow in cells using differential scanning calorimetry (DSC). First, we established a method for DSC analysis of living cells and detected the heat generation. Next, when DSC of COS7 cells was performed using inhibitors of mitochondrial respiration, cellular heat production was suppressed, indicating that mitochondria serve as the major heat generator in cells. Furthermore, because metabolic-dependent heat generation was also observed in the cell extracts, this measurement will allow to investigate the heat flux originating from intracellular reactions.

3Pos283 Measurement of the physical properties in a cell with optical method

Yasuhiro Maeda[1], Sonja Tarama[2], Mitsusuke Tarama[2], Junichi Kaneshiro[1], Tatsuo Shibata[2], Tomonobu Watanabe[1]
([1]*Laboratory for Comprehensive Bioimaging , RIKEN BDR*, [2]*Laboratory for Physical Biology, RIKEN BDR*)

Measurement of the force induced to or generating in a cell are quite important for understanding cell dynamics. The deformation and the physical properties of a cell are needed to estimate the force in a cell. There are some methods to measure the deformation of a cell. But it is quite difficult to measure the physical properties in a cell or tissue not by using destructive manner. We are developing the new method to obtain the physical properties in a cell or tissue based on Brillouin scattering optical microscope and estimation method of the physical properties with non-destructive manner. We measure not only the cell but also the hydrogel with various properties as a model to find the relationship between the physical properties and Brillouin signal from a cell.

3Pos284 ゼブラフィッシュ心臓における細胞外マトリックスの弾性率の AFM 測定と細胞運命制御機構
AFM analysis of the stiffness of extracellular matrix of zebrafish heart and its contribution to cell fate determination

Sho Matsuki, Ryuta Watanabe, Yuuta Moriyama, Toshiyuki Mitsui (*Grad. Sch. Sci., Univ. Aogaku*)

How does living systems acquire evolutionary novelties? This has fascinated scientists for decades. Teleost, the most diversified species in vertebrates, have adapted to the aquatic environment by converting heart outflow tract into a more specialized organ, bulbus arteriosus. Recent studies have shown that teleost have acquired a gene during evolution, which encodes an extracellular matrix, *elastin b*, that converts the cells of the outflow tract from cardiac muscle to smooth muscle and forms a bulbus arteriosus. In this study, we investigated the stiffness of the extracellular matrix of a bulbus arteriosus in which *elastin b.* is expressed using an atomic force microscopy and evaluate the relationship between extracellular matrix stiffness and cell fate determination.

3Pos285 High-Speed AFM revealed dynamic behavior of antibody

Norito Kotani, Takashi Morii, Takao Okada (*Research Institute of Biomolecule Metrology Co.,Ltd.*)

High-Speed Atomic Force Microscope (HS-AFM) is a powerful imaging tool with both spatial and temporal resolution. HS-AFM can distinct dynamic behavior and nanoscopic scale structure of biomolecules.
Antibody IgG is one of the important proteins in immunity. We have observed dynamic behavior of IgG in solution using HS-AFM. IgG was observed as “Y” shaped structure clearly, and each of the two Fab regions were distinguished.
IgG has a flexibility structure between Fab and Fc region. On the HS-AFM movie, Fab regions swung by thermal fluctuation. The flexibility increases their affinity to antigens. We estimated mechanical aspects of IgG hinge regions.
HS-AFM movie could provide a new method to measure the flexibility of protein functions.

3Pos286 シロザケ椎骨の骨質解析
Assessment of Bone Quality in Chum Salmon Vertebrae

Shota Hironaka, Chihiro Kawamoto, Humiya Nakamura, Hiromi Kimura-Suda (*Graduate School of Science and Engineering, Chitose Institute of Science and Technology*)

Bones support the body and protect organs, and their shape and strength are affected by the living environment and age. Bone is an *organic-inorganic* hybrid *material* consisting principally of type I collagen and calcium phosphates. Bone quality, which is a material and structural property of bone, contributes to bone strength independently of bone mineral density. In this work, we assessed bone quality, including the mineral-to-matrix ratio, carbonate-to-phosphate ratio, crystallinity, and mineral maturity, in adult chum salmon using Fourier transform infrared (FTIR) spectroscopic imaging. The FTIR images of chum salmon vertebrae showed strong distributions of the PO_4^{3-} band around both the chordacentrum and the vertebral body endplate.

3Pos287 Application of a bench-top NMR instrument for omics studies of gut microbiota metabolites

Zihao Song[1], Yuki Ohnishi[1], Seiji Osada[2], Li Gan[1], Jiaxi Jiang[1], Zhiyan Hu[1], Hiroyuki Kumeta[1], Yasuhiro Kumaki[1], Kiminori Nakamura[1], Tokiyoshi Ayabe[1], Kazuo Yamauchi[3], Tomoyasu Aizawa[1] ([1]*Grad. Sch. Life Sci., Hokkaido Univ.*, [2]*Nakayama Co.,Ltd.*, [3]*IAS, OIST*)

Metabolomics has shown its potential of recognizing diseases and identifying biomarkers. Indeed, high-field nuclear magnetic resonance (NMR) represents one of the routinely used techniques for this study while further application for medical purposes or field research are restricted by its low accessibility. In this study, we applied low field, benchtop NMR (60 MHz) to characterize the alteration of metabolic profile of feces sample obtained from the DSS-induced ulcerative colitis model mice. Non-targeted multivariate analysis successfully discriminated the DSS-induced group from the healthy control and showed high comparability with high field NMR (800 MHz). In addition, the determination of the concentration of each metabolite was discussed using 60 MHz NMR spectra.

3Pos288 Research on metabolomics of human breast milk samples by benchtop NMR and high field NMR

Zhiyan Hu[1], Jiaxi Jiang[1], Li Gan[1], Zihao Song[1], Yuki Ohnishi[1], Seiji Osada[2], Hiroyuki Kumeta[1], Yasuhiro Kumaki[1], Kazuo Yamauchi[3], Tomoyasu Aizawa[1] ([1]*Grad. Sch. Life Sci., Hokkaido Univ.*, [2]*Nakayama Co.,Ltd.*, [3]*IAS, OIST*)

NMR spectroscopy has played an essential role in metabolomics for about fifty years. In addition to the traditional high field NMR, a new system called benchtop NMR, with low filed, has emerged. It has the advantages of being easier to use, less expensive and no cryogen.
In this research, some of the strengths and weaknesses of NMR-based metabolomics have been discussed. The main purpose is to explore more convenient and efficient methods to determine and quantify lactose and human breast milk from different aspects. We have tried different parameters of benchtop NMR to seek better conditions. Comparison between benchtop NMR and high field NMR (800MHz) of 2'-FL and 3-FL in huamn breast milk samples has been done.

3Pos289 大腸菌一遺伝子欠損株におけるラマンスペクトルとオミクスデータの対応
Correspondence between Raman spectra and omics data in *E. coli* single gene deletion strains

Genta Chiba[1], Ken-ichiro Kamei[2], Arisa Oda[2,3], Kunihiro Ohta[2,3], Yuichi Wakamoto[2,3] ([1]*Dept. Integ. Sci., Univ. Tokyo*, [2]*Grad. Sch. Art Sci., Univ. Tokyo*, [3]*UBI, Univ. Tokyo*)

Raman spectroscopy is a non-invasive, non-labeling technique that can comprehensively acquire intracellular molecular spectra and is attracting attention as a tool for tracking and predicting cellular state changes in real time. Although it is known that the Raman spectra of *E. coli* single gene deletion strains can predict their growth curve characteristics, how the differences are linked to the changes in molecular profiles are not well understood. To address this, we explored the correspondence between the Raman spectra and the transcriptome of *E. coli* single gene deletion strains and discuss the effect of local perturbations of gene deletion on changes in high-dimensional gene expression profiles of the whole cell.

3Pos290 アクチン繊維の QCM 測定における独特の周波数シフト
Unique frequency-shifts in QCM measurement on binding biomolecules having filamentous shape

Naoki Matsumoto[1], Honoka Kobayashi[2], Taiki Nishimura[1], Yuki Sakurai[1], Kaito Kobayashi[1], Kaho Yokomuro[1], Kazuya Soda[1], Ikuko Fujiwara[2], Hajime Honda[2] ([1]*Dept. of Bioeng. Nagaoka Univ. of Tech.*, [2]*Dept. of Matl. Sci. and Bioeng., Nagaoka Univ. of Tech.*)

The Quartz Crystal Microbalance method (QCM) can measure binding reactions as a shift in frequency by taking advantage of the crystal characteristic of oscillation. QCM exhibits negative-shifts in proportion to the mass of the substance bound on the QCM-electrode surface. On the other hand, positive-shifts are also observed based on the conditions of substances, such as appearance of the substitutes. To detect the mass and the appearance of the substitutes of the target substance separately by QCM, we have employed actin molecules, because they can take two forms, monomers and filaments. Our results show the positive-shifts in the frequency when actin filaments are bound to the QCM, confirming that the QCM candetect the shape of the material.

3Pos291 交流電場による細胞の回転運動を利用した，非標識に細胞の誘電特性を計測する電極デバイスの開発
Development of Simultaneous Electrorotation Device with Microwells for Non-Labeled Characterization of Cellular Dielectric Properties

Masato Suzuki[1], Mio Tsuruta[1], Shee Chean Fei[2], Seiichi Uchida[2], Tomoyuki Yasukawa[1] ([1]*Grad. Sch. Sci., Univ. Hyogo*, [2]*Grad. Sch. Info. Sci. Elect. Eng., Kyushu Univ.*)

Electrorotation (ROT) is one of the electrokinetic phenomena and has also been utilized to characterize the dielectric properties of single cells. However, a relatively long experimental period was required because several single cells must be repeatedly arranged at the center of quadrupole electrodes. We describe a unique ROT device for characterizing the dielectric properties of cells. The device consisted of two pairs of interdigitated array electrodes stacked orthogonally through an insulating layer with rectangular microwells patterns. We demonstrated that change in membrane capacitance was successively detected as a decrease in ROT rate during stimulation with an activator regent for cells.

3Pos292 RNA ポリメラーゼによる転写開始素過程の一分子解析
Probing processes in transcription initiation by *Escherichia coli* RNA polymerase using single-molecule methods

Shingo Fukuda, Toshio Ando (*WPI Nano Life Science Institute (WPI-NanoLSI), Kanazawa University*)

The key step of transcription initiation is formation of the open promotor complex (RP_O) where the RNA polymerase (RNAP) loads the promotor DNA into its active site and unwinds the ~13 base pairs of DNA. Here, we used single-molecule methodologies such as high-speed atomic force microscopy and total internal reflection fluorescence microscopy to interrogate the initiation processes. We show direct evidence of DNA wrapping around the RNAP surface in the RP_O. Real-time observations of transition from the closed complex to RP_O suggest a model of the transcriptional bubble formation and impacts of the DNA wrapping on the RP_O formation. Our results provide mechanisms of the transcription initiation, highlighting the dynamic actions of RNAP and DNA at single-molecule level.

3Pos293 水中測定におけるサブミクロン分解能赤外分析法（O-PTIR）の汎用性拡大に向けた検討
Expanding the versatility of sub-micron resolution infrared analysis method (O-PTIR) in underwater measurement

Naoki Baden (*Nihon Thermal Consulting, Co., Ltd.*)

Infrared analysis is widely used for chemical structure analysis of biological materials. However, the conventional microscopic FT-IR has a limited spatial resolution of about 3 to 10 micorons due to diffraction limit, which makes difficult to analyze smaller regions than that. Recently, optical photothermal infrared spectroscopy (O-PTIR), whose spatial resolution is sub-micron has been developed. O-PTIR uses a visible laser as a probe to detect infrared absorption through the photothermal phenomenon of samples induced by IR laser irradiation. O-PTIR has been applied to the analysis of cells and amyloid in water as well as dry environment. In order to expand the versatility of underwater measurement, we have tried to obtain basic data.

3Pos294 Importance of annexin V N-terminal for 2D crystal formation revealed by HS-AFM

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Annexin V is a member of a family of structurally homologous proteins sharing the ability to bind to negatively charged phospholipid membranes. This protein forms trimeric structures on negatively charged phospholipid bilayers, which assemble into a two-dimensional lattice (2D crystals) in the presence of Ca2+. Two 2D crystal forms of annexin V have been reported, which are six-fold (p6) and three-fold symmetry (p3). The p6 lattice also contains additional trimers in the gaps between the p6 axes, which are also referred to as non-p6 trimers because they do not participate in the formation of the p6 lattice. We here show that the annexin V N-terminal has a significant influence on 2D crystal formation using high-speed atomic force microscopy (HS-AFM) observations.

3Pos295 蛍光タンパク質型高感度温度センサーを用いた小胞体での微小な熱発生計測
Extremely sensitive measurement of thermogenesis in the endoplasmic reticulum using a FRET-based thermosensor with huge dynamic range

Shun-ichi Fukushima, Takeharu Nagai (*SANKEN, Univ. Osaka*)

Intracellular temperature is an important factor for biological processes. Even small temperature changes of as little as 1 °C can potentially induce changes in cellular conditions such as metabolic responses and signaling. To clearly capture when and where intracellular temperature changes at the subcellular level, we developed a genetically-encoded fluorescent thermosensor which can be localized to specific organelles such as endoplasmic reticulum (ER) and mitochondria with high temperature sensitivity (maximum 22%/°C in mitochondria and 37%/°C in ER). The ER-localized sensor successfully detected thermogenesis below 1°C caused by histamine-evoked calcium concentration change. This sensor can be a powerful tool to find new cellular thermogenetic event.

3Pos296 超広視野顕微鏡の安価版(SeMATERAS)の開発
Inexpensive development of ultra-wide-field microscope SeMATERAS

Masashi Ohmach, Hiromichi Wakebe, Yuichi Inoue (*SIGMA KOKI Co.,LTD.*)

Ultra-wide-field microscope is essential for understanding dynamics of a huge population of cells at sub-cellular resolution. Although the special system (called AMATERAS) is reported (Ichimura et al., 2021), such a microscope requires large cost and techniques to be developed. Here, we tried a new combination of the commercial components including 8K camera, and long focus objective lens. Our system has comparable to AMATERAS in spatial resolution (~2 μm) and temporal resolution (~0.1 s), but smaller field-of-view (~φ 6 mm) than AMATERAS. The new system, called SeMATERAS available from SigmaKoki, has several advantages such as ~1/10 cost of AMATERAS and flexibility to combine other units as fluorescence imaging and laser-induced activation of the target cells.

3Pos297 Protein Unfolding Dynamics during Translocation through a Solid-state Nanopore

Hirohito Yamazaki, Sotaro Uemura (*The University of Tokyo, Department of Biological Science*)

The protein folding/unfolding is one of the fundamental mechanisms that have yet been disclosed and relates with the protein function. Here, we report our investigation of unfolding protein dynamics during translocation through a solid-state nanopore for understanding of protein unfolding state. First, we demonstrated detection of model protein, cytochrome c, using 3 nm hourglass shaped pore. We saw two distinct populations of blockade events that represents electrical field induced folded/unfolded transition. On the other hand, when passing through conically like pore. we found abnormal cytochrome c translocation dynamics, which possibly represents specific protein conformational state. More detailed analysis will be provided in this presentation.

3Pos298 チラコイド膜中に存在する光化学系 II 超複合体の高速 AFM による可視化
Visualization of photosystem II super complex in thylakoid membrane by HS-AFM

Daisuke Yamamoto (*Fac. Sci., Fukuoka Univ.*)

Photosystem II (PSII) is a membrane protein that initiates photosynthetic reaction in the thylakoid membrane. PSII is associated with light-harvesting complex (LHCII) to form the so called PSII supercomplex. The details in the structure of PSII supercomplexes have been obtained. However, the structures and the dynamics of the complexes embedded in the thylakoid membrane is still to be elucidated. Here, we have applied HS-AFM to directly visualize PSII-supercomplexes in the thylakoid membrane. PSII dimers and the associated LHCII were visualized with a molecular resolution. Image processing further showed that the observed structure was in good agreement with that obtained by cryoEM. We will discuss the structural dynamics of the complex from the HS-AFM observations.

3Pos299 Nanoscale visualization of cell membrane exposed to non-thermal atmospheric pressure plasma

Han Gia Nguyen[1], Linhao Sun[2], Tatsuya Kitazaki[3], Shinya Kumagai[3], Shinji Watanabe[2] ([1]*Grad. Sch. Nano Life Sci., Univ. Kanazawa*, [2]*WPI NanoLSI, Univ. Kanazawa*, [3]*Univ. Meijo*)

Non-thermal atmospheric pressure plasma (NTAPP) has been used to promote gene transfer into cells. We have investigated how NTAPP affects living cell surface in a liquid environment at a nanometer resolution. Although scanning electron microscopy (SEM) provides us with a large-scan area and high-resolution images of the cell surface, it is still challenging to capture dynamic changes on the cell surface under NTAPP applications. In this study, we used scanning ion conductance microscopy (SICM) to visualize dynamic changes of the cell surface, adding SEM. The combination of SEM and SICM images allowed us to clarify a pore of 20 - 500 nm in diameter on the cell surface exposed by NTAPP. Further investigation will be presented in the poster.

3Pos300 ナノレベルの精度を持つ光電子相関顕微鏡の要素開発：無冷媒クライオスタットを用いたサンプルホルダーのサブミリケルビン安定化
Sub-milliKelvin stabilization of sample holders with closed-cycle cryostat for correlative light and electron microscopy with nm accuracy

Takuma Yorita, Michio Matsushita, Satoru Fujiyoshi (*Department of Physics,Tokyo Institute of Technology*)

For single molecule nanoscopy in cells, we are developing a cryogenic fluorescence microscopy with nanometer resolution. Fluorescence microscopy is noninvasive method and identify molecular species with the selective fluorescent labeling. We will correlate this nanoscope with cryogenic electron microscope. Here we show a sub-milliKelvin cryogenic sample holder refrigerated by a closed-cycle helium compressor. From a finite element method simulation, a radiation shield was important to cooling down the holder to several kelvin and the temperature stability. We constructed the holder equipped with two radiation shields. The temperature of the holder was refrigerated to 4.9961±0.00018K. The sub-milliKelvin fluctuation corresponds to the picometer-level image stability.

3Pos301 (2SBA-6) 細胞内の一分子を三次元でナノレベルの分解能で観察できる「クライオ三次元ナノスコピー」の開発
(2SBA-6) Cryo-3D Nanoscopy to localize three-dimensional position of individual fluorophore with nanometer precision in the cell

Kanta Naruse[1], Tsuyoshi Matsuda[1], Yuta Mizouchi[1], Takeshi Shimi[2], Hiroshi Kimura[2], Eiji Nakata[3], Takashi Morii[3], Michio Matsushita[1], Satoru Fujiyoshi[1] ([1]*Department of physics, Tokyo institute of technology*, [2]*Cell Biology Center, Institute of Innovative Research, Tokyo institute of technology*, [3]*Institute of Advanced Energy, Kyoto University*)

Biological phenomena are regulated by many biomolecules in the cell. In order to study them, it is needed to observe the individual molecules and three-dimensional network of them in the cell. For such purpose, we developed “cryo-3D nanoscopy” to determine three-dimensional position of individual fluorophore with nm precision in the cell. We have already achieved precision of 1 nm in lateral direction, but about 17 nm in axial direction. The z-localization precision was worse than the theoretical limit 1 nm. It is because of the blinking noise and the background noise. To improve the precision, we developed “cryo-3D nanoscopy” and achieved precision of 0.5 nm in lateral direction and 1.9 nm in axial direction. These are less than 2 times the theoretical limit.

3Pos302 SARS-CoV-2 スパイク（S）タンパク質の時空間追跡と ACE2 受容体および小さな細胞外小胞との相互作用
Spatiotemporal tracking of SARS-CoV-2 spike (S) protein and its interaction with ACE2 receptor and small extracellular vesicles

KeeSiang Lim[1], Goro Nishide[2], Takeshi Yoshida[4], Takahiro Watanabe-Nakayama[1], Akiko Kobayashi[3], Masaharu Hazawa[1,3], Rikinari Hanayama[1,4], Toshio Ando[1], Richard W. Wong[1,3] ([1]*Kanazawa University., WPI-Nano Life Science Institute*, [2]*Kanazawa University., Division of Nano Life Science in the Graduate School of Frontier Science Initiative, WISE Program for Nano-Precision Medicine, Science and Technology*, [3]*Kanazawa University., Cell-Bionomics Research Unit, Institute for Frontier Science Initiative (INFINITI)*, [4]*Kanazawa University., Department of Immunology, Graduate School of Medical Sciences.*)

Spike (S) protein is the key player of SARS-CoV-2 infection. Here, we use high-speed atomic force microscopy (HS-AFM) to study S protein structure, and its interaction with hACE2 and small extracellular vesicles (sEVs). Results indicated structural heterogeneity of S protein, and mobility of S protein stalk and receptor-binding domain (RBD). S protein bound with ACE2 in an all-RBD up conformation. S protein and S2 subunit showed two different docking mechanisms on sEVs. S-hACE2 interaction mediated S protein docking on sEVs. In contrast, S2 subunit docked on lipid layer and entered sEV using its fusion peptide, mimicking the viral entry scenario. Altogether, our study provides a platform for real-time assessment of various interventions to block SARS-CoV-2 entry.

3Pos303 細胞内一分子ナノスコピーのための近赤外蛍光標識技術の開発
Near-infrared fluorescent labeling technique for cryogenic single molecule nanoscopy in cell

Kazuki Kuramoto[1], Kei Muto[2], Ryuya Miyazaki[2], Junichiro Yamaguchi[2], Kanta Naruse[1], Naoki Kamiya[1], Hidekazu Aramaki[1], Michio Matsushita[1], Haruka Oda[3,4], Takeshi Shimi[3,4], Hiroshi Kimura[3,4], Satoru Fujiyoshi[1] ([1]*Department of Physics, Tokyo Institute of Technology*, [2]*Department of Applied Chemistry, Waseda University,*, [3]*Bioscience and Biotechnology, Tokyo Institute of Technology*, [4]*Cell Biology Center, Institute of Innovative Research, Tokyo Institute of Technology,*)

To understand biological phenomena, it is important to visualize biomolecules in cells. Under cryogenic condition, biomolecules in cells are immobilized at subnanometer level. Therefore, cryogenic fluorescent microscopy is a highly promising method to localize the intracellular biomolecules at nanometer resolution. In my project, I try to visualize the subcellular structure (nuclear pore complex) at nanometer resolution by the cryogenic fluorescence microscope. Therefore, I have studied near-infrared fluorescence labeling technique of nuclear pore complex in U2OS cell. Autofluorescence background is expected to be suppressed by using the near-infrared fluorophores.

3Pos304 局在化する高分散化表面修飾ナノダイヤモンドの開発とその細胞移行に関する研究
Research on the development of localized highly dispersed surface modified nanodiamond and their cellular uptake

Hirotaka Okita[1], Shingo Sotoma[1], Shunsuke Chuma[1,2], Madoka Suzuki[1], Yoshie Harada[1,3] ([1]*IPR., Osaka Univ.*, [2]*Grad. Sch. Sic., Osaka Univ.*, [3]*QIQB., Osaka Univ.*)

We mainly research on the significance of temperature in life phenomena by means of quantum sensing technology using fluorescent nanodiamonds (FNDs). We have developed highly water soluble surface-modified FNDs. These can be chemically modified and suppress nonspecific adsorption of biomolecules. In addition, it can be delivered into multiple cells while suppressing nonspecific adsorption, and is expected to be applied to wide field observation and omics analysis such as flow cytometry. Therefore, in this presentation, we will report on the characteristics of various surface-modified FNDs and their cellular uptake. We will also present the development of technology for producing FNDs showing stealth effect, high dispersity, and the ability for multicellular targeting.

3Pos305 (2SBA-5) High-resolution mapping of chromatin compaction and dynamics in live cells by label-free interference microscopy

Yi-Teng Hsiao, Chia-Ni Tsai, Fasih Bintang Ilhami, Chia-Lung Hsieh (*Institute of Atomic and Molecular Sciences (IAMS), Academia Sinica / Taiwan*)

We present a novel optical microscope technique to resolve the chromatin organization in the unlabeled live cell nuclei. A highly sensitive interference microscopy, coherent brightfield microscopy (COBRI), is used to directly record the dynamic scattering signal of chromatin at a high speed. The chromatin density and the level of chromatin compaction are estimated with sub-micrometer spatial resolutions by analyzing the temporal fluctuation of the scattering signal. The reconstructed chromatin density map is highly correlated to the fluorescence image of chromatin. In addition, the chromatin compaction changes by chemical drugs are successfully detected. Using our methods, we investigate the chromatin remodeling of local DNA damage induced by laser microirradiation.

3Pos306 A new technique for detecting single biomolecule fluctuations using surface distance-dependent spectral changes in the QD emission

Kaoru Okura, Hitoshi Tatsumi (*Department of Applied Bioscience, Kanazawa Inst. of Technol., Ishikawa, Japan*)

Single quantum dots (QDs) are often used in the field of single-molecule imaging. However, the spectral changes in single QD emission have not been studied well. We examined the effect of low-temperature plasma treatment of glass surface on the QD emission spectra, and observed changes in the QD emission spectrum, which was dependent on the distance between QD and glass surface. Single actin filaments were labeled with QDs and the fluctuations of the QD on the filament were examined which showed the QD spectral change reflecting the 20 nm distance changes. Our results suggest the local interaction between the QD and glass surface improves the spatial and temporal resolution of optical measurement of biomolecules labeled with QDs.

3Pos307 Gaussian Weighted Background Correction For Raman images with application to hydrogel samples

Jean-Emmanuel Clement (*Institute for Chemical Reaction Design and Discovery (ICReDD), Hokkaido University*)

In the chemometric workflow, restoring Raman data free from experimental variations is an essential part that contributes to reliable data analysis. In this contribution we propose an extension of the standard chemometric method for Raman data analsysis, adapted for single cell Raman images contaminated by spatial variations, such as subtrate heterogeneity, non-inhomogeneous illumination profile or others. This method is applied to preprocess single cell Raman images collected with complexe substrates such as hydrogels.

3Pos308 一分子イメージングを用いた生細胞内 RNA ポリメラーゼⅡの様々な転写サイクル段階におけるダイナミクス解析
RNA Polymerase II dynamics analysis at different stages of the transcription cycle in living cells using single-molecule imaging

Ryo Akita, Yuma Ito, Makio Tokunaga (*Sch. Life Sci. Tech., Tokyo Inst. Tech.*)

RNA Polymerase II (Pol II) transcription is a tightly regulated multistep process consisting of initiation, promoter pausing, and elongation. However, it is not clear what the characteristics of Pol II dynamics in these steps. To quantify the dynamics of Pol II in living cells, we generated U2OS cells expressing Halo-Tagged RPB1 (the largest subunit of Pol II). Using single-molecule microscopy, we observed Pol II at different transcription steps with inhibitors. Single-molecule tracking analysis revealed subdiffusion under promoter-pausing inhibitor, while simple diffusion was found under initiation inhibitor. The result gives us the clue to elucidate the relationship between the dynamics and the molecular function of each step in the transcription cycle.

3Pos309 A green color fluorescence lifetime-based biosensor for quantitative imaging of intracellular ATP in multicellular system

Cong Quang Vu[1], Taketoshi Kiya[2], Toshinori Fujie[3], Tetsuya Kitaguchi[4], Satoshi Arai[1] ([1]*Grad. Sch. NanoLS., Kanazawa Univ.*, [2]*Grad. Sch. of Nat. Sci. Tech., Kanazawa Univ.*, [3]*Sch. of Life Sci. and Tech., Tokyo Tech.*, [4]*Inst. of Inno. Res., Tokyo Tech.*)

Quantification of adenosine triphosphate (ATP) as the main cellular energy source will provide information on different cell states and types. Here, we developed a green color fluorescence lifetime-based biosensor, named qMaLioffG, by inserting an ATP-binding domain into a green fluorescent protein. Its fluorescence lifetime changed upon binding to ATP, enabling the quantitative imaging of ATP by fluorescence lifetime microscopy. Using qMaLioffG, we quantified ATP change in 3D spheroid HeLa cells to a drug treatment. Furthermore, we expressed qMaLioffG in *Drosophila* brain and observed ATP heterogeneity in different cell types between the mushroom body and optic lobes. Our qMaLioffG is a useful tool to investigate cellular metabolism.

3Pos310 膜受容体と脂質ドメインの共クラスター化を評価するための 3 色 SMLM 解析ワークフロー
Workflows of triple-color single-molecule localization microscopy analysis to assess co-clustering of membrane receptors and lipid domains

Masataka Yanagawa[1,2], Mitsuhiro Abe[1], Yasushi Sako[1] ([1]*Riken CPR*, [2]*JST PRESTO*)

Single-molecule localization microscopy (SMLM) is a useful super-resolution method to monitor the spatial organization of membrane components. To improve the throughput of the multicolor TIRF imaging, we have developed an automated imaging system with integrated control of five lasers, a dual-axis galvanometer, two cameras, and an inverted microscope. Here we introduce a semi-automated triple-color SMLM measurement and analysis workflows. As a model measurement, we analyzed the co-clustering of epidermal growth factor receptor (EGFR) and lipid probes (PH domains of PLCδ and evectin-2, which detect PIP_2 and PS, respectively). We will discuss the EGF stimulation-dependent changes in receptor-lipid interaction using Ripley's K function-based co-clustering analysis.

3Pos311 NIR-triggered vesicles to manipulate spatial and temporal dynamics of a neurotransmitter in skeletal muscle and Drosophila brain

Takeru Yamazaki[1], Satya Sarker[1], Taketoshi Kiya[2], Satoshi Arai[1] ([1]*Grad. Sch. NanoLS., Kanazawa Univ.*, [2]*Grad. Sch. of Nat. Sci. Tech., Kanazawa Univ*)

A photocaged methodology that provides rapid concentration changes of a bioactive molecule by light illumination allows the direct observation of the dynamic behavior of molecular and cellular functions. Yet, applicable compounds to be caged are still limited. Here, we proposed near infrared (NIR)-triggered vesicles that encapsulate and release a variety of hydrophilic biomolecules at a high concentration. By placing the vesicles nearby a targeted cell, the spatial distribution of acetylcholine as a representative neurotransmitter could be altered on the surface of a cell with NIR stimulation. In this study, we further demonstrated this system in Ca^{2+} imaging in cells of skeletal muscle and Drosophila brain.

3Pos312 (1SEP-3) Triple-color photothermal dye-based nanoheaters to generate multiple heat spots within a single cell

Md Monir Hossain, Takeru Yamazaki, Kayoko Nomura, Satoshi Arai (*Grad. Sch. NanoLS., Kanazawa Univ.*)

Nano-heating technology enables spatiotemporal temperature control for the investigation of thermal effects on the subcellular microenvironment. Here, we designed a photothermal dye-based nanoheater that allows to create the subcellular sized heat spot with concurrent fluorescent thermometry. Specifically, three different photothermal dyes were embedded into the polymeric particles, respectively. An individual nanoheater could be operated by a relevant near-infrared laser at 808, 855, and 980 nm. When three nanoheaters were applied to a live cell, we could achieve to produce multi-heat spots within a single cell at the same time. We further attempted to alter energy metabolism and muscle contractions locally by the combination of three nanoheaters and different lasers.

3Pos313 可逆的ターンオン型蛍光標識技術の開発とライブセル蛍光イメージングへの応用
Development of reversible turn-on fluorescent labeling technology and its application to live cell fluorescence imaging

Shigeyuki Namiki, Daisuke Asanuma, Hiroki Ishikawa, Shinkuro Kobayashi, Kenzo Hirose (*Department of Pharmacology, Graduate school of Medicine, The University of Tokyo*)

Fluorescent labeling technique of biomolecules with high specificity and sensitivity in living cells is required in life science research. We developed a turn-on fluorescent labeling technique named DeQODE system, consisting of DeQuenching of Organic Dye Emission (DeQODE) tag and a Quenched Organic Dye Emission (QODE) probe. The QODE probe is a non-fluorescent small organic molecule converted to fluorescence by binding to the DeQODE tag. The cells expressing a series of proteins fused with DeQODE tag showed fluorescence upon applying the QODE probe. Also, super-resolution imaging, single molecule tracking, and in vivo imaging were successfully achieved with DeQODE system, demonstrating that DeQODE system is a promising next-generation fluorescent labeling technology.

3Pos314 DNA で作るナノミウラ折り
Nano Miura fold fabricated with DNA

Daisuke Ishikawa, Masahiko Hara (*Sch. Mater. Chem. Tech., Tokyo Tech*)

Origami engineering based on the geometric folding and unfolding of chained and planar structures has a wide range of industrial applicability. In particular, the Miura fold is widely used on macroscales such as maps and solar panels for artificial satellites because it makes it possible to fold a flat large-area structure into small pieces. However, there are no reports that the reversible folding and unfolding origami technique has been applied to the nanoscale. This study aims to develop nano-origami to show that macro-scale folding technology can be used on a nanoscale, which influences the function and physical properties of materials.

3Pos315 相分離液滴をテンプレートとした DNA オリガミカプセルの構築
Construction of DNA origami capsules using phase-separated droplets as templates

Nagi Yamashita[1], Marcos Masukawa[2], Mayumi Chano[3], Yusuke Sato[4], Masahiro Takinoue[1,3] ([1]*Department of Life Science and Technology, School of Life Science and Technology, Tokyo Institute of Technology.*, [2]*Department of Chemistry, Johannes Gutenberg University Mainz.*, [3]*Department of Computer Science, School of Computing, Tokyo Institute of Technology.*, [4]*Department of Systems Design and Informatics, School of Computer Science and Systems Engineering, Kyushu Institute of Technology.*)

Functional microcapsules have attracted much attention because of their potential to construct molecular robots and artificial cells. The presence of DNA nanostructures on the surface of the microcapsule allows other functional molecules to be incorporated into the surface of the nanostructure through sequence-specific DNA hybridization. Therefore, DNA is a strong candidate as a component of functional microstructures. We developed a DNA microcapsule by self-assembling DNA origami nanostructures (DNA nanoplates) at the interface of a phase-separated droplet surface as a template. We believed that this method of constructing microcapsules using only the aqueous phase has the advantage for the use of DNA microcapsules in vitro and in vivo.

3Pos316 DNA ハイドロゲルの形成と変形の光制御
Photocontrol of DNA hydrogel formation and deformation

Yoshiaki Sano[1], Masahiro Takinoue[1,2] ([1]*Department of Life science and Technology, Tokyo Institute of Technology, Japan*, [2]*Department of Computer Science, Tokyo Institute of Technology, Japan*)

DNA hydrogels have attracted attention as multifunctional molecular systems such as artificial cells and molecular robots. To apply DNA hydrogels to such systems, DNA hydrogels with desired sizes and shapes need to be fabricated and to be remotely controlled. However, suitable methods have not been developed, yet. Here, we report a method for generating and controlling DNA hydrogels by irradiation of light. This method forms DNA hydrogels at the site of light irradiation, and DNA hydrogel can be controlled by the light irradiation time. This method would be applied to the formation and control of nano/micrometer-sized molecular robots.

3Pos317 電子線照射が微生物細胞に及ぼす影響
Effects of an electron beam irradiation on living bacterial cells

Junya Katai[1], Yuta Nagano[1], Kenshi Suzuki[2], Kazuki Yasuike[1], Ryoya Hayashi[1], Asahi Tanaka[3], Tetsuo Narumi[1], Masaki Shintani[1], Yosuke Tashiro[1], Wataru Inami[4], Yoshimasa Kawata[4], Fumihiro Sassa[5], Hiroyuki Futamata[6] ([1]*Dept. Appl. Chem. Biological Eng., Univ. Shizuoka*, [2]*Grad. Sch. Scie. Tech., Univ. Shizuoka*, [3]*Coop. Major. Med. Photo., Univ. Shizuoka.*, [4]*Res. Inst. Elect., Univ. Shizuoka*, [5]*Grad. Sch. Fac. Inf. Sci. Elect. Eng.,Unv. Kyushu*, [6]*Res. Inst. Green. Sci. Tech., Univ. Shizuoka*)

To develop an alternative method for managing microbial metabolisms, effects of an electron beam irradiation on living bacterial cells were investigated using a direct electron-beam excitation assisted microscope (D-EXA). *Escherichia coli* strain MG1655 cells grown in LB liquid medium were collected at middle exponential phase and were set on Si_3N_4 plate with 50 nm thickness. MG1655 cells were stained with SYTO9 and propidium iodide to distinguish live or death conditions. The cells elongated under some irradiating conditions, and DAPI stain showed that DNA replication was performed during the cell elongation. These results suggest that the beam irradiation change physiological conditions in the cells, suggesting the possibility of metabolic control.

3Pos318 サブテラヘルツ照射によるタンパク質および核酸の構造変化の溶液 NMR 解析
Structural changes of proteins and nucleic acids induced by sub-terahertz radiation investigated by using solution NMR spectroscopy

Yuji Tokunaga[1], Masahiko Imashimizu[2], Koh Takeuchi[1] ([1]*Grad. Sch. Pharm. Sci., UTokyo*, [2]*CMB, AIST*)

There are functionally relevant vibrational modes of proteins and nucleic acids in the terahertz (THz) frequency region. Irradiation of sub-THz electromagnetic waves on these molecules may perturb such dynamics to nonthermally modulate their physiological activity. We investigated THz-induced changes in structural features of several different biomolecules, including ubiquitin, lysozyme, and DNA fragments, by using NMR spectroscopy. We observed structural changes of these molecules upon irradiation, including changes in hydrogen-deuterium exchange rates of ubiquitin, and chemical shift perturbations around a hydrophobic cavity of lysozyme. We will discuss the mechanisms of these phenomena.

3Pos319 Medusavirus の局所構造解析によるウイルス粒子形成に伴う構造変化の可視化
Visualization of structural changes associated with virus particle formation by local structural analysis of Medusavirus

Ryoto Watanabe[1,2], Chihong Song[1,2,3], Kazuyoshi Murata[1,2,3], Masaharu Takemura[4] ([1]*National Institute for Physiological Sciences (NIPS)*, [2]*The Graduate University for Advanced Studies (SOKENDAI)*, [3]*The Exploratory Research Center on Life and Living Systems (ExCELLS)*, [4]*Tokyo University of Science*)

Medusavirus, a giant virus with a diameter of about 260 nm, was isolated from an Acanthamoeba host. Medusavirus particles showed four different types inside and outside the host cell, suggesting a process of viral particle formation. Cryo-EM single-particle analysis was performed for DNA-Empty and DNA-Full particles, which were particularly numerous, and were calculated at 21.5 Å and 19.5 Å resolution respectively. However, no significant difference in viral particle structure was observed at this resolution. Therefore, in this study, a block-based reconstruction method was used to analyze the local structure. As a result, the resolution was greatly improved and the details of the structural changes associated with the viral particle formation could be shown.

3Pos320 人工多細胞の自動生産に関する研究
Toward automated production of lipid-based multi-compartment assemblies

Ryo Shimizu[1], Richard James Archer[1], Gen Hayase[2], Satoshi Murata[1], Shin-Ichiro Nomura[1] ([1]*Grad. Sch. Eng., Univ. Tohoku/Japanese*, [2]*WPI-MANA*)

The research of artificial cells reconstructing the structures and functionalities of living cells have been actively studied in recent years. Artificial multicellular systems consisting of multiple cells specialized for different functions such as material production and movement are particularly attracting attention. The conditions for the generation of artificial multicellular systems are not clear, and it is essential to search for the conditions. Here we present a method for automated production of artificial multicellular systems to automatically search for the conditions. This method is based on the sponge method [ChemSysChem 2022], which can automate experimental operations such as soaking sponges by controlling a pipetting robot and robot arms from a computer.

3Pos321 表面微細構造上における付着珪藻の増殖挙動
The growth of marine benthic diatoms on micro patterned surfaces

Takayuki Murosaki[1], Taiki Kishigami[2], Yuji Hirai[3], Yasuyuki Nogata[4] ([1]*Department of Chemistry, Asahikawa Medical University*, [2]*Graduate School of of Science and Engineering, Chitose Institute of Science and Technology*, [3]*Department of Applied Chemistry and Bioscience, Faculty of Science and Engineering, Chitose Institute of Science and Technology*, [4]*Sustainable System Research Laboratory, Central Research Institute of Electric Power Industry*)

Marine benthic diatoms adhere strongly and growth on submerged structures by secreting viscous polysaccharides. Recently, micro-patterned surfaces inspired by the surface textures of marine organisms have attracted attention as fouling control materials. In this study, we prepared the several micro dimple arrayed surfaces, and investigated the growth behavior of marine benthic diatoms on each substrate.

The results found that in initial stage, diatom cells are adhered individually on small dimple (6μm) arrayed surfaces, compared to large dimple (22μm) and flat surfaces. Furthermore, the surface coverage on small dimple was higher compared to other surfaces in final stage. These results indicated that initial cell distribution might be affect the diatom cell growth.

3Pos322 Magnetic induced assembly of anisotropic structures for reversible lipid compartment deformations

Richard Archer, Shinichiro M. Nomura (*Tohoku University, Department of Robotics*)

The artificial mimicry of the dynamic molecular motility of life is a monumental challenge which could take us closer towards synthetic bio-inspired micro-machines. Biomimetic attempts to replicate the complex molecular machinery of cells presents many challenges such as high environmental sensitivity, poor long term stability and inhibitive costs.
Here we present the attempt of using magnetic anisotropic silica as a stable robust material which can self-assemble under magnetic fields into larger macroscopic structures to induce deformation in lipid compartments. Induced assembly of structures can quickly reach over 20 μm in length and is fully reversible. Our aim is to use this work to create inducible macroscale deformations for applications in soft robotics.

3Pos323 超撥水表面上の水滴の跳ね返り挙動に関する理論的考察
Theoretical Consideration on Bouncing Behavior of Water Droplet on Superhydrophobic Surface

Hiroyuki Mayama (*Department of Chemistry, Asahikawa Medical University*)

Fog droplets adhere to superhydrophobic surfaces such as lotus leaf and termite wings, but, raindrops bounce. Thus, it is observed that smaller water droplets adhere to superhydrophobic surfaces and larger water droplets bounce. To understand such different behavior, the energy of a bouncing droplet is discussed in terms of such as kinetic energy, adhesion energy and dissipation energy due to viscosity. As a result, we found the reason that the kinetic energy to bounce becomes larger than the sum of dissipation energy and adhesion energy in larger-sized droplets. Furthermore, the effect of surface morphology of superhydrophobic surfaces on the bouncing behavior was discussed.

3Pos324 Self-assembly of DNA origami blocks into two-dimensional crystalline structures with designed geometries

Yuki Suzuki[1], Ibuki Kawamata[2] ([1]*Grad. Sch. Eng., Mie Univ.*, [2]*Grad. Sch. Eng., Tohoku Univ.*)

The DNA origami technique is used to construct custom-shaped nanostructures that can be used as components of two-dimensional crystalline structures with user-defined structural patterns. Here, we designed a DNA origami block with self-shape-complementary ruggedness. DNA origami blocks were electrostatically adsorbed onto a fluidic lipid bilayer membrane. A subsequent change in ionic conditions induced the self-assembly of the blocks into lattices with prescribed geometries based on a self-complementary shape fit. Time-lapse atomic force microscopy images revealed dynamic events involved in the self-assembly process, including edge reorganization, and defect splitting, diffusion, and filling, which provide a glimpse into how the lattice structures are self-improved.

名字（Family Name）のアルファベット順にソートしています。すべて，オンラインで入力されたデータのまま，表示しています。演題番号の末尾が 00 または 99 は，シンポジウムのオーガナイザーによる開会挨拶等を示しています。

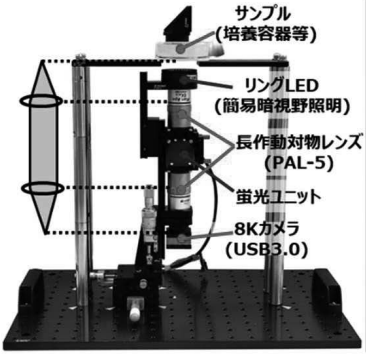
第 60 回日本生物物理学会年会　バイオフィジックスセミナー

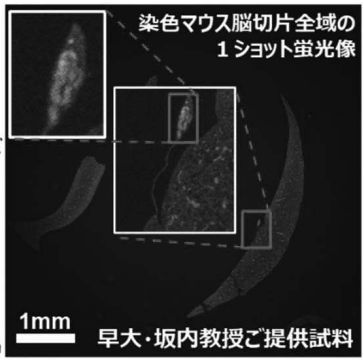
コアユニット製品で広がる光学システム

発表日: 9 月 28 日(水)　11:50 – 12:40
会場　：A 会場(函館アリーナ, 武道館)

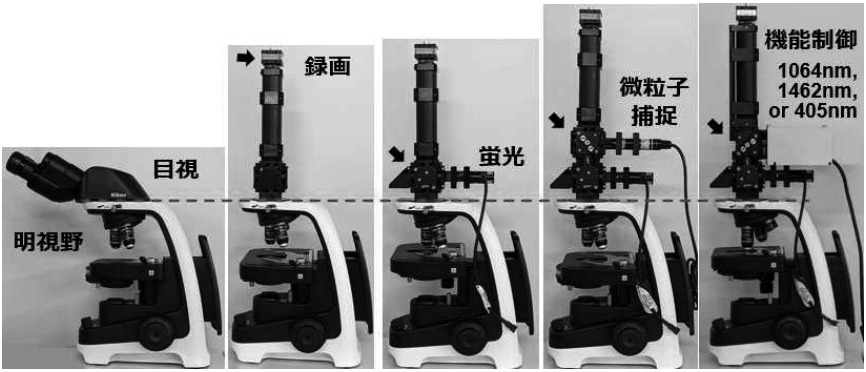
生物物理学会員が生物物理のために設計した光学製品をご紹介します。

「超広視野観察をあなたの研究室でも」分部寛道(シグマ光機)





「ここまで機能拡張できる教育用顕微鏡」井上裕一(シグマ光機)



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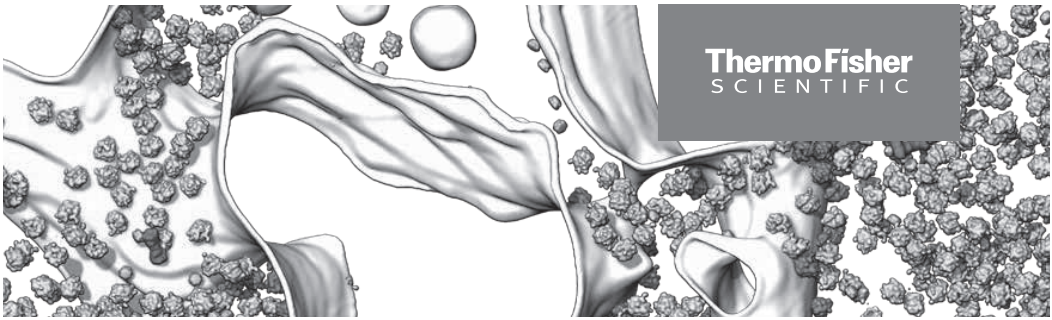

クライオ電子線トモグラフィーの細胞生物学への応用展開

Structural understanding of cellular mechanisms by cryo electron tomography

甲斐 翼, Alexander Rigort（Tsubasa Kai, Alexander Rigort）
サーモフィッシャーサイエンティフィック（Thermo Fisher Scientific）

日 時：9 月 28 日（水）11:50-12:40
会 場：B 会場(函館アリーナ、武道館)

細胞やオルガネラ、タンパク質複合体の三次元微細構造の解析は、生体内で起こる事象を理解するうえで重要な役割を担っている。細胞内でのタンパク質の局在状態やオルガネラとの相関、タンパク質複合体の細胞内での状態を分子レベルで詳細に三次元観察することができれば、これまで明らかでなかったタンパク質の細胞内での機能環境を知る手がかりを得ることができる。 生体三次元構造解析法の一つとして、試料を液体窒素温度で観察するクライオ電子顕微鏡がある。クライオ電子顕微鏡を用いたアプリケーションの一つであるクライオトモグラフィー法は、細胞内のオルガネラや微細構造の詳細な三次元観察を可能とする革新的な手法である。急速凍結によりアモルファス状の氷に包埋した細胞試料はその自然に近い状態を保ったまま、クライオ電子顕微鏡観察に用いることができる。クライオトモグラフィー法を用いることで、自然状態に近い細胞内の様子を数 nm～数百 nm スケールの高分解能で三次元観察を実現できる。さらには、クライオトモグラフィーのための凍結薄片試料作製を行うクライオFIB-SEM を用いることで、クライオ生体三次元構造解析をより大きなスケールへ拡大できる。本セミナーでは、クライオトモグラフィー法及びクライオ FIB-SEM を用いた最新アプリケーション事例を紹介する。

thermo scientific

第６０回日本生物物理学会年会

浜松ホトニクス株式会社
BP セミナー１

日時：2022 年 9 月 28 日（水） 11：50 ～ 12：40

会場：C 会場（函館アリーナ、武道館）

ご案内

本セミナーは、11:50～12:20までの予定です。（12:20以降、会場はフリースペースとなります。）
お弁当・お茶につきましては、セミナー後に配布させていただきます。
弊社ではCOVID-19を考慮して、セミナー時間と食事時間を分けさせていただきます。

演題 CMOS カメラを用いた 次世代ハイコンテント解析システムへの展望

演者 柳川　正隆 先生

国立研究開発法人　理化学研究所　開拓研究本部　佐甲細胞情報研究室

セミナー内容

ウェルプレートにおける蛍光顕微鏡計測・画像解析ワークフローを自動化したハイコンテント解析(HCA)システムは、細胞生物学・薬理学・創薬において広く利用されている。当研究室は大阪大学・上田昌宏教授らと共に、細胞内1分子自動観察システム「AiSIS」を開発し、1分子計測のハイスループット化を推進してきた。

現在、講演者はAiSISをモジュール化し、多色1分子計測と、発光計測を自動化した次世代ハイコンテント解析システムを開発中である(図1)。本開発にあたり、近年、急速に進化しているCMOSカメラを採用することで、EMCCDと比較して低コストで多色1分子計測・広視野発光イメージングができるようになってきた。

本セミナーでは、浜松ホトニクス株式会社のImagEM X2・ORCA-Fusion BT・ORCA-Questを用いた、蛍光1分子計測・発光計測を比較する。また、GPCR・RTK・イオンチャネル等の膜受容体を起点とした細胞内シグナル伝達研究への応用例を紹介したい。

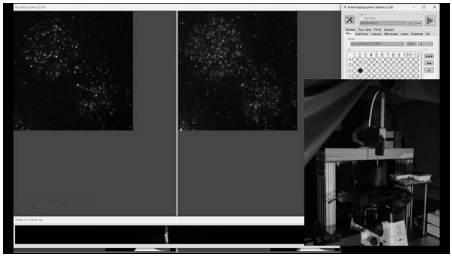

図１：開発中の次世代HCAシステムのキャプチャ

左ポート：ORCA-Fusion BT×２台（４色１分子計測）
右ポート：ORCA-Quest×1台（2色発光計測）

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第60回 日本生物物理学会年会

株式会社リバネス
ランチョンセミナー

日時：9月28日(水) 11:50-12:40

会場：G会場(函館市民会館 小ホール)

特別トークセッション

「研究者として生きる道はアカデミアだけではない」

未知のことを解明する、不可能だったことを可能にする、社会の課題を解決する、人類の知識に資する研究のあり方はどんどん多様化してきています。近年は、研究成果を社会実装する一つの形として、研究開発型ベンチャーという道が存在感を増してきています。

本ランチョンセミナーでは、**研究開発型ベンチャーとして研究成果の社会実装に奮闘する数名の研究者に登壇**いただき、ベンチャーを立ち上げた/ジョインした理由や想い、自らの手で研究を社会実装するベンチャーの実際などを、トークセッション形式でお話しします。研究者であり続けるキャリアを考えている学生・若手研究者の皆さんは奮ってご参加ください。

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JEOL - Leica 合同ランチョンセミナー

“損傷を低減した観察を可能にするクライオテクノロジー”

開催日時： 9 月 29 日（木） 11:30 - 12:20　　場所： A 会場

口演 1 ： 「最新クライオ FIB-SEM システムのご紹介」

日本電子株式会社 （JEOL）

松島 英輝（EP 事業ユニット EP アプリケーション部）

FIB-SEM は集束イオンビーム装置(FIB)と走査電子顕微鏡(SEM)を備えた複合装置で、高い位置精度での試料作製が可能で、半導体業界を中心に故障解析等で広く使用されている。近年、クライオステージを装着し凍結した生物試料の加工観察も可能となった。本講演では装置のクライオ化に伴う改良点や搬送機構、酵母菌を用いたクライオ FIB-SEM 技法を紹介する。

口演 2 ： 「CLEM のための、新型クライオ共焦点レーザー顕微鏡システム CORAL Cryo と、高圧凍結装置新機能 CORAL Life の紹介」

ライカ マイクロシステムズ株式会社 （Leica Microsystems）

伊藤 喜子（ライフサイエンスリサーチ事業部ナノテクノロジー）

CLEM は、常温からクライオまで広く活用されている。各種クライオ電顕法では、クライオ光顕が有用でありターゲット座標を活用することでワークフローの歩留まりを改善する。最新共焦点顕微鏡をクライオ化した CORAL Cryo を紹介する。CORAL Life は、高圧凍結装置の Live Cell システムである。細胞のダイナミックなイベントを光顕から電顕の高分解能解析を目指し前処理のアプローチでライカの CLEM ソリューションを紹介する。

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第60回日本生物物理学会

中山商事株式会社
バイオフィジックスセミナー

日時：9月29日（木）　11:30-12:20
会場：C会場（函館アリーナ、武道館）

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また、北海道大学 相沢先生より、本製品をご利用いただいている研究内容について、ご講演いただきます。

演題1	「卓上型NMR Spinsolveのラインアップと性能等について」 長田 誠司　中山商事株式会社　海外事業部　海外事業課

卓上型NMR Spinsolveは、生物・物理・化学の分野において、様々なご用途でご利用いただいており、多くのラインアップがございます。また、サンプル中の溶媒ピークを軽減できるSolvent Suppression機能やサンプルの反応過程を追跡可能なリアクションモニタリング等のオプションもご用意しております。これらについて、ご紹介させていただきます。

演題2	「高性能卓上型NMR装置の生物系研究への応用」 相沢 智康 先生　北海道大学 大学院先端生命科学研究院

近年、卓上NMR装置の高性能化が急激に進んでいる。特に、安定性の高い永久磁石による均一性の高い磁場が実現され、水などの溶媒消去も効率的に行えるようになったことから、海外では尿や血液、食品等の生物系試料への応用の報告も増えてきている。冷媒の供給が一切不要で、装置の維持管理が極めて容易という卓上NMR装置の特徴から、将来的には医療診断や農林水産物・食品分野等への幅広い応用も期待される。我々のグループでは、高度な溶媒消去が可能な装置であるSpinsolve ULTRAを用いて、卓上NMR装置の生物系への応用研究、特にNMRメタボローム解析への応用の検討を進めてきた。本講演では、我々の最近の研究成果について紹介する。

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Nakayama

Refeyn Japan BP セミナー

2022 年 9 月 29 日(木) 11:30 -12:20
H 会場（函館市民会館 大会議室）

Invited Lecture

Understanding biomolecular behaviour with mass photometry

Cathryn Langley, Ph.D.

Product Manager, Refeyn Ltd.

※発表者は日本の海外からの渡航者の受け入れ状況によって変更する場合があります

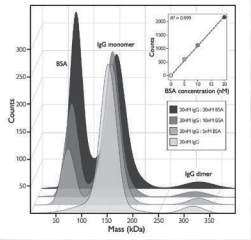
What is the impact of changing physiological conditions or genetic modification on biomolecular interactions, and what are the consequences of those changes on biological function? What are the compositions of those functional species? Which complex forms, is it stable and how strong are those interactions?

These represent fundamental questions at the heart of biochemical research and in this presentation, we will introduce mass photometry as an innovative technique that helps address them.

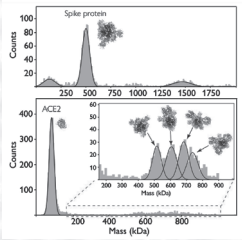
It complements the biophysical analysis toolkit, delivering a rapid, accurate mass measurement of single molecules in solution, in their native state without the need for labels. Mass photometry covers a wide mass range, has high mass resolution, and can be used to study proteins, nucleic acids and other particles. In a one assay format, It can be harnessed in numerous applications, including:

- Confirm if a desired complex has formed and is stable;
- Characterise the stoichiometry of complexes;
- Verify the composition of functional species;
- Track complex, multi-step processes;
- Calculate binding affinities;
- Identify the oligomeric states present in a sample;
- Detect aggregate formation;
- Determine the fill status of gene delivery vehicles;
- Assess sample purity.

Mass Photometry を用いたアプリケーション事例



20 nM IgG 存在下における、BSA のタイトレーション結果



新型コロナウイルス（SARS-CoV2）スパイク蛋白質の分子量分布（上）と、ACE2 との相互作用による複合体分布（下）

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気液界面を用いた細胞ハンドリング技術のご紹介

Introduction of Gas-liquid Interface-based Cell Handling Technology

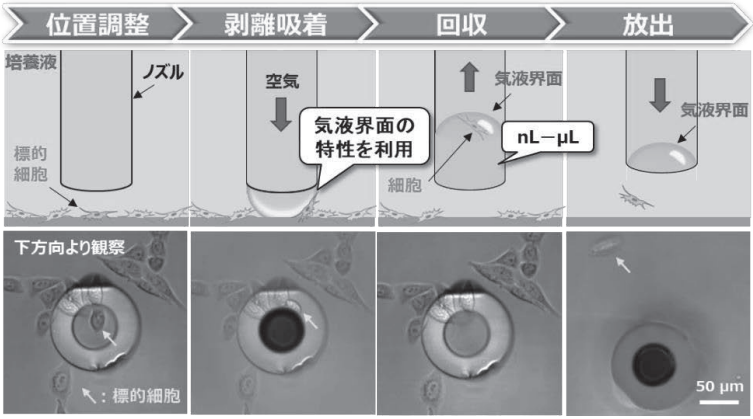
森山　真樹(Masaki Moriyama)
株式会社ニコン(Nikon Corporation)

日時:9 月 30 日(金)12:00-12:50
会場:C 会場(函館アリーナ、武道館)
発表言語:日本語

高精度に細胞をハンドリングする技術は細胞解析や自動培養の技術発展とともに精力的に開発されてきた。培養容器から細胞回収する際は液体吸引による液流を用いた細胞操作が一般的であるが、液流を用いるのではなく、気液界面の特性に注目した細胞ハンドリング技術を開発した。

気泡などの気液界面は界面により物体に力を加える、また表面張力により物体を界面に吸着させるという特性を有する。細胞を培養した液中にノズルを入れ、空気を供給することでノズル先端に気泡を形成し、気液界面により細胞を操作するシステムを構築した。本システムにより、気液界面で細胞に力を加えて細胞を剥離させることや、細胞を表面張力で界面に吸着させて自由に操作可能である。気液界面に吸着させた細胞は気液界面をノズル内に取込むことにより容易に回収でき、標的細胞以外の混入を抑制しながら低液量で標的細胞を回収することができる。また、気液界面は細胞に力を加えることできるため、メカノバイオロジー分野への応用に向けた基礎技術開発を進めている。

本セミナーでは、気液界面を用いた細胞ハンドリング技術の原理詳細からアプリケーション事例を紹介する。



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