

生物物理

S E I B U T S U B U T S U R I

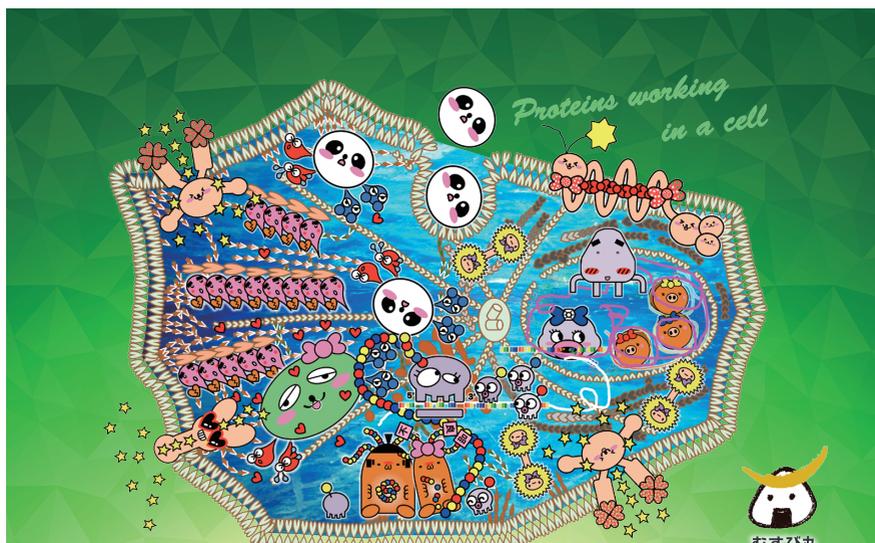
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Vol.61

第59回年会予稿集

主催 一般社団法人 日本生物物理学会



Proteins working in a cell

むすび丸

第59回 日本生物物理学会年会

Create New Biophysics. 10 years since 3.11.

会期	2021年11月25日(木)・27日(土)
会場	仙台国際センター オンライン開催
年会長	高橋 聡(東北大学多元物質科学研究所)



The Biophysical Society
of Japan

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

第 59 回日本生物物理学会年会

The 59th Annual Meeting of the Biophysical Society of Japan

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開催概要／General Information

The 59th Annual Meeting of the Biophysical Society of Japan
第59回日本生物物理学会年会（2021年度）

会期／Period

2021年11月25日（木）－27日（土）
25 (Thu.) – 27 (Sat.), November, 2021

会場／Venue

オンライン開催
Online Conference

年会長・実行委員長／Chair of the Organizing Committee

高橋 聡（東北大学多元物質科学研究所）
Satoshi Takahashi (Tohoku University)

年会ウェブサイト／Website of the Annual Meeting

<https://www2.aeplan.co.jp/bsj2021>

予稿本文／Proceedings

※下記サイトからpdf版の予稿集をダウンロードいただけます。

※You can download the abstracts in the pdf format in the following site.

<https://www2.aeplan.co.jp/bsj2021/program/index.html>

ID: 59ambsj Password: webtohoku2021

※年会Confitサイトからも予稿本文の閲覧や検索が可能です。

※You can read and search the abstracts from the Confit site also.

※会期後は日本生物物理学会にデータが移行されますので、学会ウェブサイトよりご覧ください。

※The abstract data will be transferred to the society web site after the annual meeting.

年会長挨拶



第59回年会 年会長・実行委員長
高橋 聡
(東北大学多元物質科学研究所)

日本生物物理学会の第59回年会を、2021年11月25日から27日までオンラインにて開催します。「生物物理学」は、生物が示すさまざまな活動を、物理、化学、生物学、情報科学などを基礎とした幅広い研究者の共同作業により解明する学問です。ヘテロな研究者の集まりである日本生物物理学会にとって、最新の研究成果を発表し議論する年会はもっとも大切なイベントと言えます。多くの皆様に年会への参加を呼びかけたいと思います。

第59回年会は、東北大学と山形大学の学会員を中心とした年会実行委員会により運営します。我々は、本年会を仙台市において現地開催すべく準備を進めてきましたが、新型コロナウイルスの感染状況を考慮し、現地開催にはリスクが大きすぎると判断しました。この判断について、ご理解をいただけますと幸いです。

本年会では、オンライン開催だからこそ可能な工夫により、活発な議論を促すとともに、多くの参加者が時間を共有した一体感を得られる運営を目指します。一般演題はビデオ撮影された口頭発表としますが、リアルタイムでの質疑応答の時間を持ちます。シンポジウムも基本的にリアルタイムにて実施しますが、学会期間中はオンデマンド聴講も可能にします。また、SNSによる参加者の横の繋がりを促す取り組みを行います。さらには、オンライン懇親会を開催し、若手奨励賞受賞者の発表などを楽しみながら、参加者が交流する時間を持ちたいと考えています。

オンライン開催とはなりますが、年会の場で多くの皆様とお会いすることを心から楽しみにしています。通常の年会と同じようにテンションを上げ、存分にサイエンスと交流を楽しむ場として第59回年会にご参加ください。

第59回日本生物物理学会年会実行委員会 Organizing Committee

年会長・実行委員長

高橋 聡 (東北大学)

Chair

Satoshi Takahashi (Tohoku University)

会計・会場

○中林 孝和 (東北大学)

Accounting/Venue

○Takakazu Nakabayashi (Tohoku University)

プログラム

○田中 良和 (東北大学)
梅津 光央 (東北大学)
鎌形 清人 (東北大学)
羽鳥 晋由 (山形大学)
藤原 孝彰 (東北大学)
眞壁 幸樹 (山形大学)
横山 武司 (東北大学)

Program

○Yoshikazu Tanaka (Tohoku University)
Mitsuo Umetsu (Tohoku University)
Kiyoto Kamagata (Tohoku University)
Kuniyuki Hatori (Yamagata University)
Takaaki Fujiwara (Tohoku University)
Koki Makabe (Yamagata University)
Takeshi Yokoyama (Tohoku University)

Confit監修

○稲葉 謙次 (東北大学)

Confit supervise

○Kenji Inaba (Tohoku University)

懇親会

○南後 恵理子 (東北大学)
眞壁 幸樹 (山形大学)
中村 修一 (東北大学)
西 羽美 (東北大学)
鎌形 清人 (東北大学)

Banquet

○Eriko Nango (Tohoku University)
Koki Makabe (Yamagata University)
Shuichi Nakamura (Tohoku University)
Hafumi Nishi (Tohoku University)
Kiyoto Kamagata (Tohoku University)

oViceデザイン

○西 羽美 (東北大学)
鎌形 清人 (東北大学)

oVice design

○Hafumi Nishi (Tohoku University)
Kiyoto Kamagata (Tohoku University)

SNS

○松井 敏高 (東北大学)
吉留 崇 (東北大学)
横山 武司 (東北大学)

SNS

○Toshitaka Matsui (Tohoku University)
Takashi Yoshidome (Tohoku University)
Takeshi Yokoyama (Tohoku University)

高校生・高専生向けワークショップ

○鳥谷部祥一 (東北大学)
柴田 穰 (東北大学)
羽鳥 晋由 (山形大学)
最上 譲二 (東北大学)
元池 育子 (東北大学)

Workshop for High School Students

○Shoichi Toyabe (Tohoku University)
Yutaka Shibata (Tohoku University)
Kuniyuki Hatori (Yamagata University)
George Mogami (Tohoku University)
Ikuko Motoike (Tohoku University)

高校生・高専生発表

○盛田 伸一 (東北大学)

参加登録サイト監修

○城田 松之 (東北大学)

最上 譲二 (東北大学)

学生アルバイト手配

○権田 幸祐 (東北大学)

柴田 穰 (東北大学)

閉会式

○森本 展行 (東北大学)

最上 譲二 (東北大学)

渡部 聡 (東北大学)

実行委員

今井 正幸 (東北大学)

小井川 浩之 (東北大学)

大場 哲彦 (東北大学)

木下 賢吾 (東北大学)

佐々木 一夫 (東北大学)

野村 M 慎一郎 (東北大学)

宮田 英威 (東北大学)

Webサイトデザイン

林 久美子 (東北大学)

Hight School Students Presentation

○Shin-ichi Morita (Tohoku University)

Registration site supervise

○Matsuyuki Shiota (Tohoku University)

George Mogami (Tohoku University)

Arrangement of part timers

○Kohsuke Gonda (Tohoku University)

Yutaka Shibata (Tohoku University)

Closing Session

○Nobuyuki Morimoto (Tohoku University)

George Mogami (Tohoku University)

Satoshi Watanabe (Tohoku University)

Members

Masayuki Imai (Tohoku University)

Hiroyuki Oikawa (Tohoku University)

Tetsuhiko Ohba (Tohoku University)

Kengo Kinoshita (Tohoku University)

Kazuo Sasaki (Tohoku University)

Shin-ichiro M. Nomura (Tohoku University)

Hidetake Miyata (Tohoku University)

Website design

Kumiko Hayashi (Tohoku University)

■ 2021年11月23日（火）・祝

	8	9	10	11	12	13
Ch01						
oVice		談話スペース				

■ 2021年11月24日（水）

	8	9	10	11	12	13
Ch01			第59回日本生物物理学会サテライトイベント アジア地区PDB50周年記念シンポジウム ～アジア地区構造生物学の最先端とProtein Data Bank 50年の歩み～			
oVice		談話スペース				

14	15	16	17	18	19	20
<日本語開催> 高校生・高専生向け 生物物理ワークショップ ～生物？物理？二刀流で生命の謎に迫る！～						
談話スペース						

14	15	16	17	18	19	20
談話スペース			会議室			

■ 2021年11月25日（木）

	8	9	10	11	12	13
Ch01		第17回 若手奨励賞招待講演			第10回BPPB論文 賞 受賞講演	
Ch02		1S1 Japan-US symposium on cytoskeletal motor proteins and their associated proteins (Kumiko Hayashi, Shinsuke Niwa)			BPセミナー－1 DKSHジャパン	
Ch03		1S2 ケミカルAIを創る分子システム工学の黎明 (豊田 太郎、浜田 省吾)			<日本語開催> キャリア支援説明会	
Ch04		1S3 実験と理論の共同による 生命金属動態研究の最前線 (重田 育照、富舎 武彦)				
Ch05		1S4 生体分子の構造的・機能的ダイナミクス： 1分子計測と分子シミュレーションの交流 (古田 忠臣、鎌形 清人)				
Ch06		1S5 1細胞解析が切り開く新しい細胞観 (谷口 雄一、黒田 真也)				
Ch07		1S6 GPCR研究における新たなコンセプトと 創薬への示唆 (片山 耕大、寿野 良二)				
Ch08						
Ch09						
Ch10						
Ch11						
Ch12						
Ch13						
Ch14						
Ch15						
Ch16						
oVice		談話スペース			展示ブース	

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1G01 タンパク質：設計 I、 一般 I		1S7 インドー日本交流シンポジウム： 生物物理の多彩な挑戦 (坂内 美幸、永井 健)				
1G02 タンパク質：構造 I		1S8 水のダイナミクスと生物機能：再考 (今清水 正彦、村上 洋)				
1G03 タンパク質：計算 I		1S9 温度感覚研究の新潮流 ー温度を測る、制御する、感知機構とその意義を探る (内田 邦敏、藤原 祐一郎)				
1G04 タンパク質：計測 I		1S10 生命の起源とプロトセル研究における新たな進歩 (Tony Z. Jia、車 愈激)				
1G05 核酸 I		1S11 原子レベルの動的構造解析が拓く 生体分子機能の理解 (宮下 治、南後 恵理子)				
1G06 ヘム蛋白質・膜蛋白質・ 核酸結合蛋白質： 構造 I、機能と反応場 I		1S12 生物物理・ソフトマター物理と医学の接点を探る (藤崎 弘土、好村 滋行)				
1G07 筋肉・分子モーター I		1S13 シンギュラリティ細胞が生み出す 多様な生命現象へのアプローチ (坂内 博子、若林 憲一)				
1G08 細胞生物：膜		1S14 勾配検知の情報生物物理学 (石島 秋彦、岡田 康志)				
1G09 細胞生物 I、骨格 I						
1G10 生体膜・人工膜 I						
1G11 ロドプシン： 光制御 I、性質・機 能 I						
1G12 ゲノム生物学 I						
1G13 ゲノム生物学 II						
1G14 数理生物学・非平衡・ 生体リズム I						
1G15 計測 I						
1G16 バイオエンジニアリング						
談話スペース					会議室	

■ 2021年11月26日（金）

	8	9	10	11	12	13
Ch01		2S1 高分解能クライオ電子顕微鏡の進展と共同利用 (中村 春木、吉川 雅英、村田 武士)			<日本語開催> 第8回会員総会 シンポジウム	
Ch02		2S2 生物物理学的手法を駆使した 細胞内プロセスにおけるタンパク質間相互作用の理解 (武藤 梨沙、小柴 琢己)			BPセミナー2 日本蛋白質構造 データバンク	
Ch03		2S3 多様な光受容体とオプトジェネティクスの最前線 (徳富 哲、角田 聡)			<日本語開催> BPセミナー3 サーモフィッシャー サイエンティフィック	
Ch04		2S4 ゲノムDNAの生物物理学 ～ゲノムモタリテの理解へ向けて～ (瀧ノ上 正浩、高田 彰二、前島 一博)				
Ch05		2S5 統合的多階層アプローチによるシアロバクテリア 生物時計システムの新展開 (秋山 修志、上久保 裕生)				
Ch06		2S6 蛋白質系の分子シミュレーションの サンプリング手法の発展 (光武 亜代理、奥村 久士)				
Ch07		2S7 生体膜機能の人工制御化に有用な新アプローチ と生物物理応用 (中瀬 生彦、矢野 義明)				
Ch08						
Ch09						
Ch10						
Ch11						
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Ch14						
Ch15						
Ch16						
oVice		談話スペース			展示ブース	

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2G01A タンパク質： 設計 II、一般 II				2G01B タンパク質：一般 IV				オンライン懇親会					
2G02A タンパク質： 構造 II				2G02B 水・水和・電解質									
2G03A タンパク質： 計算 II				2G03B タンパク質：計算 III									
2G04A タンパク質： 一般 III				2G04B タンパク質：計測 II									
2G05A 核酸 II				2G05B タンパク質：一般 V									
2G06A ヘム蛋白質・膜蛋白質・核酸結合蛋白質：構造 I、機能と反応場 II、動態 I				2G06B ヘム蛋白質・膜蛋白質・核酸結合蛋白質：構造 III、動態 II									
2G07A 筋肉・分子モーター II				2G07B 筋肉・分子モーター III									
2G08A 細胞生物 II、骨格 II				2G08B 細胞生物：分子モーター									
2G09A 神経回路				2G09B 神経回路、化学受容・行動									
2G10A 生体膜・人工膜 II				2G10B 生体膜・人工膜 III									
2G11A 光合成I、光応答タンパク質：DNA I				2G11B 光合成 II、光応答タンパク質：DNA II									
2G12A ロドプシン： 性質・機能 II、構造 I				2G12B ロドプシン：光制御 II、性質・機能 III、構造 II									
2G13A 生命の起源、生態				2G13B 分子遺伝、ゲノム生物学III									
2G14A 数理生物学・非平衡・生体リズム II				2G14B 数理生物学・非平衡・生体リズム III									
2G15A 計測 II				2G15B 計測 IV									
2G16A 計測 III				2G16B 計測 V									
談話スペース										オンライン懇親会 展示ブース			

■ 2021年11月27日（土）

	8	9	10	11	12	13
Ch01		351 オーストラリアー日本交流シンポジウム (片山 耕大, Matthew AB Baker)			<日本語開催> 男女共同参画・若手支援委員 会企画シンポジウム	
Ch02		352 パラメトリックな翻訳調節機構 (岡部 弘基, 原田 慶恵)			<日本語開催> 科学研究費 助成事業について	
Ch03		353 タンパク質の水和とその凍結現象 -細胞凍結や食品冷凍保存への応用- (山本 直樹, 中川 洋)			<日本語開催> BPセミナー 4 シグマ光機 (株)	
Ch04		354 統合的アプローチによる タンパク質の大規模タイナミクスの探索 (齋尾 智英, 井上 倫太郎)				
Ch05		355 ライプセルイメージングと融合した 機能的オミクス解析の新潮流 (白崎 善隆, 城口 克之)				
Ch06		356 ヘプタド-膜生物物理学：膜結合抗園ヘプタド およびアミロイドヘプタドの最新生物物理研究 (川村 出, 相沢 智康)				
Ch07						
Ch08						
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oVice		談話スペース			展示ブース	

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3G01 タンパク質： 一般 VI				閉会式									
3G02 タンパク質： 構造 III													
3G03 タンパク質： 計算 IV													
3G04 タンパク質： 一般 VII													
3G05 核酸 III													
3G06 筋肉・ 分子モーター IV													
3G07 筋肉・ 分子モーター V													
3G08 細胞生物： 計測・イメージング													
3G09 細胞生物 III													
3G10 生体膜・ 人工膜 IV													
3G11 光応答タンパク質：細胞													
3G12 ゲノム生物学 IV													
3G13 計測 VI													
3G14 計測 VII													
談話スペース				会議室									

一般口頭発表表座長表

	11月25日 (木) 13:30-15:30	11月26日 (金) 13:30-15:40
Ch01	1G01 タンパク質：設計I、一般I	2G01A タンパク質：設計II、一般II
	谷中 冴子 (分子研)、加藤 晃一 (分子研)	古賀 信康 (分子研)、濡木 理 (東大)
Ch02	1G02 タンパク質：構造I	2G02A タンパク質：構造II
	岩崎 憲治 (筑波大)、村田 武士 (千葉大)	杉田 有治 (理研)、吉川 雅英 (東大)
Ch03	1G03 タンパク質：計算I	2G03A タンパク質：計算II
	菊地 武司 (立命大)、寺田 透 (東大)	高野 光則 (早大)、河野 秀俊 (量子研)
Ch04	1G04 タンパク質：計測I	2G04A タンパク質：一般III
	茶谷 絵理 (神戸大)、乙須 拓洋 (埼玉大)	池口 雅道 (創価大)、中迫 雅由 (慶應大)
Ch05	1G05 核酸I	2G05A 核酸II
	姚 閔 (北大)、皆川 慶嘉 (東大)	瀧ノ上 正浩 (東工大)、寺川 剛 (京大)
Ch06	1G06 ヘム蛋白質・膜蛋白質・核酸結合蛋白質：構造I、 機能と反応場I	2G06A ヘム蛋白質・膜蛋白質・核酸結合蛋白質：構造II、 機能と反応場II、動態I
	木村 哲就 (神戸大)、池口 満徳 (横浜市大)	横田 浩章 (光産業創成大院大)、村本 和優 (兵庫県大)
Ch07	1G07 筋肉・分子モーター I	2G07A 筋肉・分子モーター II
	富重 道雄 (青学大)、矢島 潤一郎 (東大)	西坂 崇之 (学習院大)、飯野 亮太 (分子研)
Ch08	1G08 細胞生物：膜	2G08A 細胞生物 II、骨格II
	太田 善浩 (東農大)、松浦 友亮 (東工大)	鈴木 健一 (岐阜大)、小松 英幸 (九工大)
Ch09	1G09 細胞生物 I、骨格I	2G09A 神経回路
	樋口 秀男 (東大)、楠見 明弘 (沖縄科技大)	細川 千絵 (大阪市大)、工藤 卓 (関学大)
Ch10	1G10 生体膜・人工膜I	2G10A 生体膜・人工膜II
	松木 均 (徳島大)、高橋 浩 (群馬大)	森垣 憲一 (神戸大)、中野 実 (富山大)
Ch11	1G11 ロドプシン：光制御I、性質・機能I	2G11A 光合成I、光応答タンパク質：DNA I
	須藤 雄気 (岡山大)、今元 泰 (京大)	藤井 律子 (大阪市大)、栗栖 源嗣 (阪大)
Ch12	1G12 ゲノム生物学I	2G12A ロドプシン：性質・機能II、構造I
	高田 彰二 (京大)、高橋 卓也 (立命大)	片山 耕大 (名工大)、永田 崇 (東大)
Ch13	1G13 ゲノム生物学II	2G13A 生命の起源、生態
	太田 元規 (名大)、佐々木 貴規 (明大)	今井 正幸 (東北大)、市橋 伯一 (東大)
Ch14	1G14 数理生物学・非平衡・生体リズムI	2G14A 数理生物学・非平衡・生体リズムII
	佐甲 靖志 (理研)、亀尾 佳貴 (京大)	安田 賢二 (早大)、野口 博司 (東大)
Ch15	1G15 計測I	2G15A 計測II
	原田 慶恵 (阪大)、永井 健治 (阪大)	小松崎 民樹 (北大)、酒井 誠 (岡山理大)
Ch16	1G16 バイオエンジニアリング	2G16A 計測III
	角五 彰 (北大)、船津 高志 (東大)	古寺 哲幸 (金沢大)、内橋 貴之 (名大)

	11月26日(金) 16:00-18:40	11月27日(土) 13:30-15:40
Ch01	2G01B タンパク質：一般IV 津本 浩平(東大)、徳楽 清孝(室蘭工大)	3G01 タンパク質：一般VI 後藤 祐児(阪大)、出村 誠(北大)
Ch02	2G02B 水・水和・電解質 白神 慧一郎(京大)、笠原 浩太(立命大)	3G02 タンパク質：構造III 田中 元雅(理研)、新井 宗仁(東大)
Ch03	2G03B タンパク質：計算III 梅澤 公二(信州大)、宮下 尚之(近大)	3G03 タンパク質：計算IV 清水 伸隆(高工ネ研)、奥村 久士(分子研)
Ch04	2G04B タンパク質：計測II 重田 育照(筑波大)、川野 竜司(東農大)	3G04 タンパク質：一般VII 堀谷 正樹(佐賀大)、黒田 裕(東農大)
Ch05	2G05B タンパク質：一般V 亀田 倫史(産総研)、本間 道夫(名大)	3G05 核酸III 富樫 祐一(立命大)、片平 正人(京大)
Ch06	2G06B ヘム蛋白質・膜蛋白質・核酸結合蛋白質：構造III、動態II 光武 亜代理(明大)、柴田 幹大(金沢大)	3G06 筋肉・分子モーターIV 野地 博行(東大)、福岡 創(阪大)
Ch07	2G07B 筋肉・分子モーターⅢ 岩城 光宏(理研)、鳥澤 嵩征(遺伝研)	3G07 筋肉・分子モーターV 上田 太郎(早大)、宮田 真人(大阪市大)
Ch08	2G08B 細胞生物：分子モーター 岩楯 好昭(山口大)、今田 勝巳(阪大)	3G08 細胞生物：計測・イメージング 岡嶋 孝治(北大)、山下 隼人(阪大)
Ch09	2G09B 神経回路、化学受容・行動 村山 能宏(東農大)、権田 幸祐(東北大)	3G09 細胞生物 III 澤井 哲(東大)、三井 敏之(青学大)
Ch10	2G10B 生体膜・人工膜Ⅲ 山崎 昌一(静岡大)、松尾 光一(広島大)	3G10 生体膜・人工膜IV 井出 徹(岡山大)、岩本 真幸(福井大)
Ch11	2G11B 光合成II、光応答タンパク質：DNA II 三野 広幸(名大)、久富 修(阪大)	3G11 光応答タンパク質：細胞 上久保 裕生(奈良先端大)、寺嶋 正秀(京大)
Ch12	2G12B ロドプシン：光制御II、性質・機能III、構造II 菊川 峰志(北大)、古谷 祐詞(名工大)	3G12 ゲノム生物学IV 白井 剛(長浜バイオ大)、藤原 慶(慶應大)
Ch13	2G13B 分子遺伝、ゲノム生物学III 田端 和仁(東大)、土方 敦司(長浜バイオ大)	3G13 計測VI 相沢 智康(北大)、真壁 幸樹(山形大)
Ch14	2G14B 数理生物学・非平衡・生体リズムIII 笹井 理生(名大)、望月 敦史(京大)	3G14 計測VII 永山 國昭(N-EMラボラトリーズ)、昆 隆英(阪大)
Ch15	2G15B 計測IV 前島 一博(遺伝研)、徳永 万喜洋(東農大)	
Ch16	2G16B 計測V 岡 浩太郎(慶大)、小嶋 寛明(情報通信研究機構)	

参加者へのご案内

1. 参加方法

◇年会への参加方法

本年会ウェブサイト：

<https://www2.aeplan.co.jp/bsj2021/index.html>

から、Confitにログインしてください。ログインには、11月16日ごろにメールにて送付されるIDとパスワードが必要です。Confitにてプログラムや要旨の閲覧が可能です。また、シンポジウム、一般口頭演題、サテライトシンポジウム、企業展示や懇親会など、すべての企画やイベントへのリンクも掲示されています。Confitへのログインは、11月17日（水）から可能です。

◇シンポジウム・一般口頭発表への参加方法

Confit内で、参加するシンポジウムや一般口頭発表を選択してください。シンポジウムや一般口頭発表はZoomを使って開催します。Zoomに参加する際には「Name (Affiliation)」をログイン名として英語にて表記下さい。オーガナイザーから許可がない限り、ご自身のマイクおよびカメラはオフにして下さい。

一般口頭発表では、Zoomを用いて演題発表者により提出された発表動画（8分）を視聴したのちに、リアルタイムの質疑（3分）を持ちます。質問のある方は、挙手ボタンにより質問の意思を表示し、座長の指示により質疑をお願いします。ぜひ活発な議論をお願いいたします。

発表に参加できなかった場合は、Confitの演題サイトにて発表動画を視聴できるほか、チャット機能を使って質問することも可能です。発表者は、年会中は毎日コメントを確認し、質問に対応するようお願いいたします。発表動画の視聴とチャットによる質疑は、12月10日（金）まで可能です。

◇oViceの談話スペースの利用

年会参加者同士にて個別の議論を行いたい場合は、oViceの談話スペースをご利用ください。oViceへのリンクもConfitに掲示します。oViceの談話スペース内では、近くにいる参加者と音声と映像を使って会話が可能です。画像を共有しながら議論することも可能です。参加登録を行った年会参加者のみがoViceスペースに入室できます。

oViceの基本的な使用方法について、以下の動画をご覧ください：

<https://www.youtube.com/watch?v=C8r02gYDA50&t=1s>

oViceの談話スペースは、11月23日以降27日まで、全日（24時間）使用可能です。

◇oViceスペースの「会議室」の利用

同窓会などを企画したい方、ある話題についてオンライン飲み会形式で話し合う場を持ちたい方、支部会や若手の会などで集まりたいなどの希望がある方は、oViceスペース内に用意する「会議室」をぜひご利用ください。50人程度が集まることを想定した会議室と20人程度が集まることを想定した会議室を、複数用意します。会議室は予約制で、11月23日、24日の17時以降、25日の19時以降、27日の16時以降に利用できます。

会議室の予約情報（主催者名、イベント名、目的など）を、Google Calenderにて公開します。年会参加者が気軽に立ち寄れる開かれた集まりを歓迎します。サイエンスの話し合いが主目的でも、

親睦を目的とした話し合いが主目的でも、どちらでも歓迎します。一方で、守秘性がある集まりなどでの使用はお避けください。

会議室の予約は、11月17日以降にConfit内に掲示したGoogle formを用いてお願いします。申し込みが多い場合には、会議室の数を増やす予定です。

◇企業展示

協賛企業の展示スペースを、学会ウェブサイトとoViceスペースの両方に用意します。学会ウェブサイトでは、製品カタログのダウンロードや動画視聴などが常時可能です。oViceスペースでは、昼休み時間や懇親会の時間に、担当の方と直接話をする事が可能です。年会の開催にご協力いただいた企業の皆様の展示ブースを、ぜひご訪問ください。

◇懇親会

オンライン懇親会を、11月26日（金）19時-21時の予定で開催します。参加費は無料です。懇親会の最初に、若手奨励賞授賞式をZoomを用いて30分程度行います。続いてoViceスペースにて懇親会を開催します。今回、宮城の地酒とおつまみの懇親会セットを年会ウェブサイトにてご紹介しています（注文締め切り11月12日まで）。同じお酒とおつまみを片手にどうぞご歓談ください。

◇閉会式

オンライン閉会式を、11月27日（土）の15時40分からZoomを使って開催します。閉会式において、学生発表賞の受賞者の発表を行います。ぜひ閉会式へのご参加をお願いいたします。

◇サテライトシンポジウムへの参加

学会参加登録をされた方は、11月24日に開催されるサテライトシンポジウムへの参加が可能です。Confitに掲示したリンクからお進みください。

◇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、バイオフィジックスセミナー、高校生・高専生向けワークショップなどの企画は日本語で実施します。

2. 配布物など

◇参加登録IDとパスワード

参加登録が完了された方は、日本生物物理学会会員・非会員共に、オンライン参加用IDとパスワードが11月16日ごろにメールで送られます。これらは、Confitにログインするために必要です。

注意1) 参加登録は年会参加登録費（参加費）の振込後に完了します。振込がない場合、登録は無効となります。

注意2) 日本生物物理学会会員であっても、年会会費を納めていない場合、オンライン参加用ID、パスワードが送付されません。

注意3) 非会員のシンポジウム招待講演者は、参加登録費が免除されます。

◇プログラム集冊子/予稿集PDF版

プログラム集冊子は日本生物物理学会会員および事前登録が完了した非会員に、11月2日ご

ろに送付します。なお予稿本文はプログラム集冊子には掲載されません。

予稿集PDF版は10月26日以降に年会ウェブサイトからダウンロード可能です。予稿本文は、Confitからも閲覧可能です。

予稿集PDF版：

<https://www.2.aeplan.co.jp/bsj2021/program.html>

ダウンロードID: 59ambsj

Password: webtohoku2021

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ェ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。

◇参加証

本年会は、オンライン開催のため参加証は発行しません。

◇領収書の発行

参加費の領収書が必要な場合は、年会事務局までご連絡下さい。

3. SNSの利用について

第59回年会では、参加者の交流を促進するために、SNSの利用を積極的に推奨します。そのために、年会開始前に、ぜひご自身やご自身の研究室の発表のポイントや面白さなどの宣伝を、年会のハッシュタグ（#59bsj2021）と発表番号とともにSNSに投稿するようお願いいたします。ご自身による発信がなされていると、他の参加者による引用が容易になります。そのほか、所属グループの発表情報、面白かった発表の紹介、お勤めのセッションやシンポジウムの感想、受賞の報告やお祝い、出展製品の情報なども、積極的に発信してください。通常の年会では立ち話の中で行っていた情報交換を、本年会ではSNSにより補完できたらと願っています。

一方で、ご自身の発表（あるいはその一部）がSNSで拡散されることを望まない発表者は、発表時にその旨を明示してください。参加者の皆さんは、SNSによる情報発信に関する発表者の意思を尊重することをお願いします。

4. 禁止事項

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。

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。ただし実行委員会は、理事会・組織委員会等の承認を得て、記録用として録画を行う場合があります。

一部のシンポジウムでは、個人の利用に限定したスクリーンショットの撮影等をオーガナイザーが許可する場合がありますが、許可の内容や適用範囲をよくご確認ください。

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。

共催／協賛（敬称略）

PDB50周年記念事業

学術変革領域研究(A)「分子サイバネティクス」

学術変革領域研究(A)「DNAの物性から理解するゲノムモダリティ」

学術変革領域研究(B)「パラメトリク翻訳」

新学術領域研究「高速分子動画」

新学術領域研究「生命金属科学」

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「発動分子科学」

AMED「創薬等ライフサイエンス研究支援基盤事業(BINDS)」

JST さきがけ「生命機能メカニズム解明のための光操作技術」

第59回日本生物物理学会年会

年会長 高橋 聡

Greeting



The 59th Annual Meeting of the Biophysics Society of Japan
Chair of the Organizing Committee

Satoshi Takahashi, Ph.D.

(Tohoku University)

The 59th annual meeting of the Biophysical Society of Japan (BSJ) will be organized as an on-line event from Nov. 25th to Nov. 27th, 2021. The progress in biophysics requires a close collaboration of researchers based on the multiple scientific fields. The annual meeting is an invaluable chance where the heterogeneous researchers discuss their latest progress, and hence is the most important event for the members of BSJ. I would like to strongly invite you to participate in the event.

The 59th annual meeting will be organized by the Executive Committee (EC) composed of the local society members mainly based in Tohoku and Yamagata Universities. We once sought to have the meeting to be held as a face-to-face event, but now judged that we should have the event in the on-line format due to the spread of COVID-19. We would greatly appreciate your understanding on this decision.

The EC plans to organize the 59th annual meeting to stimulate active discussions and to create a sense of unity among the participants of the event. All General Presentation will be video recorded talks; however, we plan to have the real-time discussion session in the meeting schedule. The invited talks will be given as the real-time on-line talks, which will also be accessible as the on-demand lectures during the annual meeting. We will encourage the use of SNSs so that the participants can interact through multiple media. We also plan to have an on-line meeting banquet to celebrate awardees of the Early Career Award in Biophysics and to promote the networking among the participants.

Let us enjoy science and biophysics by attending the 59th annual meeting of the Biophysical Society of Japan!!

■ 23(Tue.) November, 2021

	8	9	10	11	12	13
Ch01						
oVice		Conversation Lounge				

■ 24(Wed.) November, 2021

	8	9	10	11	12	13
Ch01			PDB 50th Anniversary Symposium in Asia 50 years of the Protein Data Bank and the Frontier of Structural Biology in Asia			
oVice		Conversation Lounge				

14	15	16	17	18	19	20
Japanese Session Biophysics workshop for high school and technical college students						
Conversation Lounge						

14	15	16	17	18	19	20
Conversation Lounge			Meeting Rooms			

■ 25 (Thu.) November, 2021

	8	9	10	11	12	13
Ch01		The 17th Early Career Award in Biophysics Candidate Presentation				
Ch02		151 Japan-US symposium on cytoskeletal motor proteins and their associated proteins (Kumiko Hayashi, Shinsuke Niwa)			BP Seminar 1 DKSH Japan	
Ch03		152 Dawn of Molecular System Engineering for Chemical AI (Taro Toyota, Shogo Hamada)			Japanese Session Career Support Events	
Ch04		153 Recent progress in biometal sciences: synergy between theory and experiments (Yasuteru Shigeta, Takehiko Tosha)			The 10th Award Seminar of Outstanding Biophysics and Physicobiology Paper	
Ch05		154 Structural and Functional Dynamics of Biomolecules: Interplay between Single Molecule Measurement and Molecular Simulation (Tadaomi Furuta, Kyoto Kamagata)				
Ch06		155 New perspectives on cells provided by single cell analyses (Yuichi Taniguchi, Shinya Kuroda)				
Ch07		156 New concepts in GPCR research and implications for drug discovery (Kota Katayam, Ryoji Suno)				
Ch08						
Ch09						
Ch10						
Ch11						
Ch12						
Ch13						
Ch14						
Ch15						
Ch16						
oVice		Conversation Lounge			Exhibition Booths	

14		15		16		17		18		19		20	
1G01 Protein: Design I, General I				1S7 India-Japan joint symposium: Various challenges on biophysical research (Miyuki Sakaguchi, Ken H. Nagai)									
1G02 Protein: Structure I				1S8 Water dynamics and biological functions: Revisit (Masahiko Imashimizu, Hiroshi Murakami)									
1G03 Protein: Simulation I				1S9 Trends in the research field of thermosensation (Kunitoshi Uchida, Yuichiro Fujiwara)									
1G04 Protein: Measurement I				1S10 Recent Advances in Origins of Life and Protocell Research (Tony Z. Ja, Yutetsu Kuruma)									
1G05 Nucleic Acids I										1S11 Toward understanding biological functions: atomic-level characterization of structures and dynamics of biomolecules (Osamu Miyashita, Eriko Nango)			
				1S12 Bridging biophysics/soft-matter physics and medical science (Hiroshi Fujisaki, Shigeyuki Komura)									
1G07 Muscle & Molecular motor I				1S13 Approaches to diverse biological phenomena produced by singularity cells (Hiroko Bannai, Ken-ichi Wakabayashi)									
1G08 Membrane				1S14 Information biophysics of gradient sensing in organisms (Akihiko Ishijima, Yasushi Okada)									
1G09 Cell biology I, Cytoskeleton I													
1G10 Biological & Artificial membrane I				1G06 Heme-, Membrane- & Nucleic acid binding-protein: Structure I, Function and environment I									
				1G11 Rhodopsins: Optical control I, Characteristics and function I									
1G12 Genome biology I													
1G13 Genome biology II													
1G14 Mathematical biology, Nonequilibrium state & Biological rhythm I													
1G15 Measurements I													
1G16 Bioengineering													
										Meeting Rooms			

■ 26 (Fri.) November, 2021

	8	9	10	11	12	13
Ch01		2S1 Technical Development and Sharing of High-Resolution Cryo-Electron Microscopes (Haruki Nakamura, Masahide Kikkawa, Takeshi Murata)			Japanese Session General Assembly Symposium	
Ch02		2S2 Biophysical basis for understanding the protein-protein interaction involved in essential cellular process (Risa Mutoh, Takumi Koshiba)			BP Seminar 2 Protein Data Bank Japan	
Ch03		2S3 A variety of photoreceptors and the frontiers of optogenetics (Satoru Tokutomi, Satoshi P Tsunoda)			Japanese Session BP Seminar 3 Thermo Fischer Scientific	
Ch04		2S4 Biophysics on Genome DNA - Toward Understanding of Genome Modality - (Masahiro Takinoue, Shoji Takada, Kazuhiro Maeshima)				
Ch05		2S5 An Integrated Multi-scale Approach for Studying Cyanobacterial Circadian Clock System (Shuji Akiyama, Hisashi Okumura)				
Ch06		2S6 Advances in enhanced sampling methods for molecular simulations of protein systems (Ayori Mitsutake, Hisashi Okumura)				
Ch07		2S7 New artificial approaches and biophysical communications to control function of biological membranes (Ikuhiko Nakase, Yoshiaki Yano)				
Ch08						
Ch09						
Ch10						
Ch11						
Ch12						
Ch13						
Ch14						
Ch15						
Ch16						
oVice		Conversation Lounge			Exhibition Booths	

14		15		16		17		18		19		20	
2G01A Protein: Design II, General II				2G01B Protein: General IV						On-line Banquet			
2G02A Protein: Structure II				2G02B Water, Hydration & Electrolyte									
2G03A Protein: Simulation II				2G03B Protein: Simulation III									
2G04A Protein: General III				2G04B Protein: Measurement II									
2G05A Nucleic Acids II				2G05B Protein: General V									
2G06A Heme-, Membrane- & Nucleic acid binding-protein: Structure II, Function and environment II, Dynamics I				2G06B Heme-, Membrane- & Nucleic acid binding-protein: Structure III, Dynamics II									
2G07A Muscle & Molecular motor II				2G07B Muscle & Molecular motor III									
2G08A Cell biology II, Cytoskeleton II				2G08B Molecular motor									
2G09A Neural circuit				2G09B Neural circuit, Chemoreception & Behavior									
2G10A Biological & Artificial membrane IV				2G10B Biological & Artificial membrane III									
2G11A Photosynthesis I, Light sensitive proteins: DNA I				2G11B Photosynthesis II, Light sensitive proteins DNA II									
2G12A Rhodopsins: Characteristics and function II, Structure I				2G12B Rhodopsins: Characteristics and function II, structure I									
2G13A Origin of life/Ecology				2G13B Molecular genetics, Genome biology III									
2G14A Mathematical biology, Nonequilibrium state & Biological rhythm II				2G14B Mathematical biology, Nonequilibrium state & Biological rhythm III									
2G15A Measurements II				2G15B Measurements IV									
2G16A Measurements III				2G16B Measurements V									
Conversation Lounge										On-line Banquet Exhibition Booths			

■ 27 (Sat.) November, 2021

	8	9	10	11	12	13
Ch01		3S1 ASB-BSJ Joint Symposium (Kota Katayam, Matthew AB Baker)			Japanese Session Gender Equality and Young Researchers Support Symposium	
Ch02		3S2 Parametric biology based on translation rate regulatory mechanism (Kohki Okabe, Yoshie Harada)			Japanese Session KAKENHI Guide Meeting	
Ch03		3S3 Protein hydration and its freezing phenomena -toward the application for cell freezing and frozen food storage- (Naoki Yamamoto, Hiroshi Nakagawa)			Japanese Session BP Seminar 4 Sigmakoki	
Ch04		3S4 Probing large-scale dynamics in protein through integrative approaches (Tomohide Saio, Rintaro Inoue)				
Ch05		3S5 Peptide-Membrane Biophysics: Current Biophysical Studies of Membrane-bound Antimicrobial Peptides and Amyloid Peptides (Izuru Kawamura, Tomoyasu Aizawa)				
Ch06		3S6 New Trends in Functional Omics Analysis Integrated with Live Cell Imaging (Yoshitaka Shirasaki, Katsuyuki Shiroguchi)				
Ch07						
Ch08						
Ch09						
Ch10						
Ch11						
Ch12						
Ch13						
Ch14						
oVice		Conversation Lounge			Exhibition Booths	

14		15		16		17		18		19		20	
3G01 Protein: General VI				Closing Ceremony									
3G02 Protein: Structure III													
3G03 Protein: Simulation IV													
3G04 Protein: General VII													
3G05 Nucleic acids III													
3G06 Muscle & Molecular motor IV													
3G07 Muscle & Molecular motor V													
3G08 Cell biology: Measurements, Imaging													
3G09 Cell biology III													
3G10 Biological & Artificial membrane													
3G11 Light sensitive proteins: Cell													
3G12 Genome biology IV													
3G13 Measurements VI													
3G14 Measurements VII													
Conversation Lounge				Meeting Rooms									

List of Oral Presentation Chairs

	25(Thu.) November, 2021 13:30-15:30	26(Fri.) November, 2021 13:30-15:40
Ch01	1G01 Protein: Design I, General I	2G01A Protein: Design II, General II
	Saeko Yanaka, Koichi Kato	Nobuyasu Koga, Osamu Nureki
Ch02	1G02 Protein: Structure I	2G02A Protein: Structure II
	Kenji Iwasaki, Takeshi Murata	Yuji Sugita, Masahide Kikkawa
Ch03	1G03 Protein: Simulation I	2G03A Protein: Simulation II
	Takeshi Kikuchi, Tohru Terada	Mitsunori Takano, Hidetoshi Kono
Ch04	1G04 Protein: Measurement I	2G04A Protein: General III
	Eri Chatani, Takuhiro Otsu	Masamichi Ikeguchi, Masayoshi Nakasako
Ch05	1G05 Nucleic acids I	2G05A Nucleic acids II
	Min Yao, Yoshihiro Minagawa	Masahiro Takinoue, Tsuyoshi Terakawa
Ch06	1G06 Heme-, Membrane- & Nucleic acid binding-protein: Structure I, Function and environment I	2G06A Heme-, Membrane- & Nucleic acid binding-protein: Structure II, Function and environment II, Dynamics I)
	Tetsunari Kimura, Mitsunori Ikeguchi	Hiroaki Yokota, Kazumasa Muramoto
Ch07	1G07 Muscle & Molecular motor I	2G07A Muscle & Molecular motor II
	Michio Tomishige, Junichiro Yajima	Takayuki Nishizaka, Ryota Iino
Ch08	1G08 Membrane	2G08A Cell biology II, Cytoskeleton II
	Yoshihiro Ohta, Tomoaki Matsuura	Kenichi Suzuki, Hideyuki Komatsu
Ch09	1G09 Cell biology I, Cytoskeleton I	2G09A Neural circuit
	Hideo Higuchi, Akihiro Kusumi	Chie Hosokawa, Suguru Kudoh
Ch10	1G10 Biological & Artificial membrane I	2G10A Biological & Artificial membrane II
	Hitoshi Matsuki, Hiroshi Takahashi	Kenichi Morigaki, Minoru Nakano
Ch11	1G11 Rhodopsins: Optical control I, Characteristics and Function I	2G11A Photosynthesis I, Light sensitive proteins: DNA I
	Yuki Sudo, Yasushi Imamoto	Ritsuko Fujii, Genji Kurisu
Ch12	1G12 Genome biology I	2G12A Rhodopsins: Characteristics and Function II, Structure I
	Shoji Takada, Takuya Takahashi	Kota Katayama, Takashi Nagata
Ch13	1G13 Genome biology II	2G13A Origin of life/Ecology
	Motonori Ota, Takanori Sasaki	Masayuki Imai, Norikazu Ichihashi
Ch14	1G14 Mathematical biology, Nonequilibrium state & Biological rhythm I	2G14A Mathematical biology, Nonequilibrium state & Biological rhythm II
	Yasushi Sako, Yoshitaka Kameo	Kenji Yasuda, Hiroshi Noguchi
Ch15	1G15 Measurements I	2G15A Measurements II
	Yoshie Harada, Takeharu Nagai	Tamiki Komatsuzaki, Makoto Sakai
Ch16	1G16 Bioengineering	2G16A Measurements III
	Akira Kakugo, Takashi Funatsu	Noriyuki Kodera, Takayuki Uchihashi

	26(Fri.) November, 2021 16:00-18:40	27(Sat.) November, 2021 13:30-15:40
Ch01	2G01B Protein: General IV	3G01 Protein: general VI
	Kouhei Tsumoto, Kiyotaka Tokuraku	Yuji Goto, Makoto Demura
Ch02	2G02B Water, Hydration & Electrolyte	3G02 Protein: structure III
	Keiichiro Shiraga, Kota Kasahara	Motomasa Tanaka, Munehito Arai
Ch03	2G03B Protein: Simulation III	3G03 Protein: simulation IV
	Koji Umezawa, Naoyuki Miyashita	Nobutaka Shimizu, Hisashi Okumura
Ch04	2G04B Protein: Measurement II	3G04 Protein: General VII
	Yasuteru Shigeta, Ryuji Kawano	Masaki Horitani, Yutaka Kuroda
Ch05	2G05B Protein: General V	3G05 Nucleic acids III
	Tomoshi Kameda, Michio Homma	Yuichi Togashi, Masato Katahira
Ch06	2G06B Heme-, Membrane- & Nucleic acid binding-protein: Structure III, Dynamics II	3G06 Muscle & Molecular motor IV
	Ayori Mitsutake, Mikihiko Shibata	Hiroyuki Noji, Hajime Fukuoka
Ch07	2G07B Muscle & Molecular motor III	3G07 Muscle & Molecular motor V
	Mitsuhiro Iwaki, Takayuki Torisawa	Taro Ueda, Makoto Miyata
Ch08	2G08B Molecular motor	3G08 Cell biology: Measurements, Imaging
	Yoshiaki Iwadate, Katsumi Imada	Takaharu Okajima, Hayato Yamashita
Ch09	2G09B Neural circuit, Chemoreception & Behavior	3G09 Cell biology III
	Yoshihiro Murayama, Kohsuke Gonda	Satoshi Sawai, Toshiyuki Mitsui
Ch10	2G10B Biological & Artificial membrane III	3G10 Biological & Artificial membrane IV
	Masahito Yamazaki, Koichi Matsuo	Toru Ide, Masayuki Iwamoto
Ch11	2G11B Photosynthesis II, Light sensitive proteins: DNA II	3G11 Light sensitive proteins: Cell
	Hiroyuki Mino, Osamu Hisatomi	Hironari Kamikubo, Masahide Terazima
Ch12	2G12B Rhodopsins: Optical control II, Characteristics and Function III, Structure II	3G12 Genome biology IV
	Takashi Kikukawa, Yuji Furutani	Tsuyoshi Shirai, Kei Fujiwara
Ch13	2G13B Molecular genetics, Genome biology III	3G13 Measurements VI
	Kazuhiro Tabata, Atsushi Hijikata	Tomoyasu Aizawa, Koki Makabe
Ch14	2G14B Mathematical biology, Nonequilibrium state & Biological rhythm III	3G14 Measurements VII
	Masaki Sasai, Atsushi Mochizuki	Kuniaki Nagayama, Takahide Kon
Ch15	2G15B Measurements IV	
	Kazuhiro Maeshima, Makio Tokunaga	
Ch16	2G16B Measurements V	
	Kotaro Oka, Hiroaki Kojima	

Information for Participants

1. How to participate

◇ Overview

Log in to Confit from the link on the Annual Meeting website:

<https://www2.aeplan.co.jp/bsj2021/english/index.html>

Login ID and password are required, which are emailed to the registered participants at around Nov. 16th. The meeting program and abstracts are available in Confit. Links to all the symposia, general presentations and other events can be found in Confit. You can log in to Confit from Nov. 17th.

◇ Symposia and general presentations

Find a Zoom link of the symposium you want to attend in Confit and enter the room. Please indicate your name and affiliation in the format “Name (affiliation)”. Turn off your microphone and camera unless the organizers give you a permission.

The general oral presentations will also be held by using Zoom. The pre-recorded oral presentation (8 min) will be broadcasted followed by a question time to the presenter (3min). If you have questions or comments, please use “raise hand” function of Zoom and follow directions of the session chairs.

You can also watch presentation movies in Confit and ask questions using its chat function. We ask presenters to check comments daily during the annual meeting. You can view the presentation movies and use the chat function of Confit by Dec. 10th.

◇ Use of the oVice space

Please use the oVice space to meet and discuss with your colleagues during the meeting. The link to the oVice space is also shown in Confit. Please learn the usage of Confit by watching the following movie:

<https://www.youtube.com/watch?v=rJiR2XVmrig&t=58s>

You can use the oVice space from Nov. 23rd to 27th freely.

◇ Use of “Meeting Room” in the oVice space

If you are planning to have an alumni reunion, or if you want to organize an on-line discussion and drinking event, please consider using “Meeting Room” in the oVice space. We will prepare two-types of rooms designed for 20 or 50 participants. Upon the reservation, you can use the rooms after 17pm of Nov. 23rd and 24th, after 19pm of 25th, and after 16pm of 27th.

Once reserved, we will open the reservation information including organizers’

names, event name and purpose using Google Calender. We welcome event proposals open to participants of the annual meeting. Proposals with purely scientific purposes or for the promotion of exchange among participants are both welcomed. Please refrain from using the rooms for confidential discussions.

You can reserve the rooms after Nov. 17th using Google forms prepared in the Confit site. We might increase the # of the meeting rooms if there are many proposals.

◇ **Exhibitions of the meeting sponsors**

We will prepare an exhibition information page for the sponsors of the annual meeting in the meeting web site. Sponsors' information such as product catalogues and promotion videos can be accessible from the page. In addition, we will prepare sponsors' booths in the oVice space. You can meet the sales persons of the sponsors during the lunch times and during the on-line banquet.

◇ **On-line banquet**

We will have an on-line banquet from 19:00 to 21:00 of Nov. 26th. Participation fee is free. At the start of the banquet, we will have an award ceremony for Early Career Award in Biophysics and for Early Career Presentation Award using Zoom (30 min). We will then move to the oVice space. Together with the conversations with other participants, enjoy a set of local foods and sakes that can be ordered at a discount price from the meeting web site. The deadline of the ordering is Nov. 12th.

◇ **Closing ceremony**

We will have an on-line closing ceremony from 15:40 to 16:00 of Nov. 27th using Zoom. We will announce the awardees of Student Presentation Award for this years meeting in the ceremony.

◇ **Satellite symposium**

All the registered participants of the annual meeting are welcomed to attend the satellite symposium. The link to the satellite is posted in Confit.

◇ **Language**

The official language of the meeting is English. However, Japanese will be used in some of the special events. The events that will use Japanese are indicated in the schedule and in the program.

2. Items to be distributed

◇ **Participation ID and password**

We will email on-line participation ID and password required to enter Confit

to the registered participants at around Nov. 16th.

Attention 1: Registration is valid only after the payment of the registration fee.

Attention 2: If you have not paid this year's annual fee of the society, the participation ID and password will not be emailed to you.

Attention 3: Invited speakers of the symposium will be exempt from the registration fee if he/she is not the member of the society.

◇ **Program booklet / The pdf version of full abstracts**

A program booklet will be sent to the BSJ members and the non-members with the advanced registration at around Nov. 2nd. The abstracts will not be included in the printed booklet.

The pdf version of the full program and abstracts will be available in the meeting web site from Oct. 26th. Abstracts can also be accessible from Confit.

The pdf version of program and abstracts:
<https://www2.aeplan.co.jp/bsj2021/english/program/index.html>
Download ID: 59ambsj
Password: webtohoku2021

The full program and abstracts will be released without password protection in the web site of the Biophysical Society of Japan and in the "Seibutsu Butsuri" site of the J-STAGE web site after the meeting.

◇ **Participation certificate**

We will not issue a participation certificate, since this is the on-line meeting.

◇ **Receipt**

If you need a receipt for your participation fee, please contact the Annual Meeting Secretariat.

3. Usage of SNS

The organizing committee of the 59th annual meeting encourages the use of social media to promote communication among the participants of the meeting. We ask all the presenters who are using some of the social media to post his/her presentation information as well as that of his/her group members. Please use the annual meeting hashtag #59bsj2021 and the presentation number when posting. This will facilitate citations of your presentation by other participants. We further encourage you to share presentation information of your group members, highlights from other presentations, and award information, suggest sessions to attend, and connect with your fellows, as well as our sponsors and exhibitors.

If a presenter does not wish to have his/her research shared via social media,

please make an announcement before and during his/her presentation. We strongly encourage compliance with speaker requests regarding social media sharing.

4. Prohibited matters

Passwords and URLs sent to the registered participants should NOT be shared with non-registered people.

Photography and recording by any devices including camera, video, mobile phone and PC (screenshots) is NOT allowed during the online meeting. The organization committee might record symposia with the approval of the society board.

In some symposia, organizers might allow the audience to capture the presentation for the better understanding of only himself or herself. Please follow the rules explained by the organizers of each symposium.

第 8 回会員総会シンポジウム：構造予測開闢

オーガナイザー：日本生物物理学会 理事会

日 時：11 月 26 日（金）12:00 ～ 13:00

演 者：森脇由隆（東大院・農），小杉 貴洋（分子研）

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：時は令和，ついにアミノ酸配列だけで構造がわかる時代が来た。まず世に現れたのは，AlphaFold2 であった。そしてそれを追うように RoseTTAFold が現れた。この二つは，深層学習という根本をともに持つ兄弟のようなものである。ある日，弟である RoseTTAFold は兄に向かって言った「おまえは遅い。出来ることが同じならば，早く出来る私の方が優れている。」と。AlphaFold2 も黙ってはいなかった。「私は生まれたときより 16 倍も速くなっている。それより私は構造予測データを 35 万件も公開している。皆に愛されているのは私の方だ。」。この端から見ればよく似た兄弟の諍いは始まったばかり。とはいえ我々科学者はこの兄弟の与える影響があまりにも大きく，見過ごすわけにもいかない。そしてあわよくばこの二人を使い倒してやろうと考えている。しかしながら我々は，この兄弟の違いや得意なこと，何が出来て出来ないのかなど，わからないことも多い。そこで，今回のシンポジウムでは，この兄弟のことをもっと知るための機会を設けたいと考えている。

一般社団法人日本生物物理学会 第10回 Biophysics and Physicobiology 論文賞受賞講演会
The 10th 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：11月25日（木）12:10～13:00 / Nov. 25 Thu.

場所：オンライン開催 / Online

形式：講演会 / Lecture

第10回 Biophysics and Physicobiology 論文賞受賞者

木下正弘

Masahiro Kinoshita

千葉大学大学院理学研究院

Graduate School of Science, Chiba University

蛋白質の折り畳みおよび変性における水の並進配置エントロピーの役割：ブドウ球菌ヌクレアーゼの変異体の熱安定性に関する一理論研究

Roles of translational, configurational entropy of water in protein folding and denaturation: a theoretical study on thermal stability of staphylococcal nuclease mutants

In general, the structures formed by the biological self-assembly processes are collapsed by the application of high pressures, and the power of forming the structures becomes considerably weaker at low temperatures. In a series of papers [1-4], we have shown that the solute-water many-body correlation component of the translational, configurational entropy of water universally plays critical roles as the driving force in all of these processes. Our theory, where this physical factor is emphasized, is capable of elucidating the pressure [2] and cold [3] denaturation of a protein. Our hybrid of the angle-dependent integral equation theory applied to a molecular model for water and the morphometric approach has been a powerful theoretical method. The Asakura-Oosawa theory, which takes account of only the solute-water pair correlation component, cannot reproduce the pressure and temperature effects described above [4]. In the awarded paper, we investigated the thermal stability of the wild type and nine mutants of staphylococcal nuclease. The thermal stability is correlated not with the number of intramolecular hydrogen bonds, intramolecular electrostatic energy, and area of exposed hydrophobic surface of the protein in the folded state but with the water-entropy gain upon protein folding related to the packing efficiency, core volume, or number of van der Waals contacts of the protein in the folded state.

References: [1] M. Kinoshita, *Biophys. Rev.* 5, 283 (2013); [2] M. Inoue, T. Hayashi, S. Hikiri, M. Ikeguchi, and M. Kinoshita, *J. Chem. Phys.* 152, 065103 (2020); [3] M. Inoue, T. Hayashi, S. Hikiri, M. Ikeguchi, and M. Kinoshita, *J. Mol. Liq.* 317, 114129 (2020); [4] H. Oshima and M. Kinoshita, *J. Chem. Phys.* 142, 145103 (2015).

1 日目 (11 月 25 日 (木)) / Day 1 (Nov. 25 Thu.)

9:00~11:30

1YA 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

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 17th year, we received 38 highly qualified applications. After the first round of competitive screening based on submitted documents, the applicants were selected as the young invited speakers. In this symposium, each speaker will make 10-minute presentation followed by 3-minute discussion as the second round of screening. Up to five awardees of the Early Career Award in Biophysics will be selected. 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 石綿 整 [3-14-1342](#)

1YA0900 ナノスケール量子計測を用いたラベルフリー脂質二重層相転移計測

Label-free phase change detection of lipid bilayers using nanoscale diamond magnetometry

○石綿 整^{1,2}, 渡邊 宙志^{1,3}, 花島 慎弥⁴, 岩崎 孝之², 波多野 睦子² (1 さきがけ JST, ² 東工大 工学院, ³ 慶應大学 量子コンピューティングセンター, ⁴ 大阪大学 理学部 化学科)

Hitoshi Ishiwata^{1,2}, Hiroshi C. Watanabe^{1,3}, Shinya Hanashima⁴, Takayuki Iwasaki², Mutsuko Hatano²
(¹PRESTO JST, ²School of Engineering, Tokyo Institute of Technology, ³Quantum Computing Center, Keio University, ⁴Department of Chemistry, Graduate School of Science, Osaka University)

9:15 小林 和弘 [2-01-1515](#)

1YA0915 ヒト PTH1 受容体における内因性リガンド認識メカニズムとそのダイナミクス

Endogenous ligand recognition and structural transition of a human PTH receptor

○小林 和弘¹, 川上 耕季², 草木 迫 司¹, 郷野 弘剛¹, 富田 篤弘¹, 志甫 谷 渉¹, 小林 幹¹,

山下 恵太郎³, 西澤 知宏⁴, 加藤 英明^{1,5}, 井上 飛鳥², 瀧木 理¹ (1 東京大学理学系研究科生物化学専攻, ² 東北大学 薬学系研究科, ³ MRC 研究所, ⁴ 横浜市立大学生命医科学研究科, ⁵ 東京大学総合文化研究科)

Kazuhiro Kobayashi¹, Kouki Kawakami², Tsukasa Kusakizako¹, Hirotake Gono¹, Atsuhiko Tomita¹, Wataru Shihoya¹, Kan Kobayashi¹, Keitaro Yamashita³, Tomohiro Nishizawa⁴, Hideaki Kato^{1,5}, Asuka Inoue², Osamu Nureki¹ (¹Department of Biological Sciences Graduate School of Science The University of Tokyo, ²Graduate School of Pharmaceutical Sciences, Tohoku University, ³MRC Laboratory of Molecular Biology, ⁴Graduate School of Medical Life Science, Yokohaya City University, ⁵Komaba Institute for Science, The University of Tokyo)

- 9:30 坂本 遼太 [2-08-1415](#)
 1YA0930 アクティブな界面摩擦と流体抵抗の幾何学的バランスが決めるアクトミオシン液滴の自発運動
 Geometric trade-off between interfacial active friction and passive fluid drag determines the motility of actomyosin droplets
 ○坂本 遼太¹, イズリ ジャン², 島本 勇太³, 宮崎 牧人^{4,5,6,7}, 前多 裕介¹ (¹九大・院理,²ミネソタ大・物理,³遺伝研,⁴京大・白眉,⁵京大・物理,⁶キュリー一研,⁷JST PRESTO)
Ryota Sakamoto¹, Ziane Izri², Yuta Shimamoto³, Makito Miyazaki^{4,5,6,7}, Yusuke Maeda¹ (¹Grad. Sch. Sci., Kyushu Univ., ²Sch. Phys. Astro., Univ. Minnesota, ³Nat. Inst. Genetics, ⁴Hakubi Ctr., Kyoto Univ., ⁵Dept. Phys., Kyoto Univ., ⁶Inst. Curie, ⁷PRESTO, JST)
- 9:45 塩見 晃史 [2-15-1736](#)
 1YA0945 (3S6-2) 微小電気穿孔法を用いた細胞膜の機械特性と遺伝子発現の統合解析
 (3S6-2) A combined analysis of membrane-mechanical phenotyping and transcriptomics using nanoelectroporation
 ○塩見 晃史, 金子 泰洗ボール, 西川 香里, 新宅 博文 (理研・開拓・白眉)
Akifumi Shiomi, Taikopaul Kaneko, Kaori Nishikawa, Hirofumi Shintaku (*Hakubi, CPR, RIKEN*)
- 10:00 杉田 昌岳 [2-03-1712](#)
 1YA1000 分子動力学シミュレーションに基づいた環状ペプチドの膜透過率の大規模予測
 Large-scale membrane permeability prediction of cyclic peptides crossing a lipid bilayer based on molecular dynamics simulations
 ○杉田 昌岳, 杉山 聡, 藤江 拓哉, 吉川 寧, 柳澤 溪甫, 大上 雅史, 秋山 泰 (東工大・情理)
Masatake Sugita, Satoshi Sugiyama, Takuya Fujie, Yasushi Yoshikawa, Keisuke Yanagisawa, Masahito Ohue, Yutaka Akiyama (*Dept. Comput. Sci., Tokyo Inst. Tech.*)
- 10:15 杉浦 一徳 [1-15-1406](#)
 1YA1015 生体機能多重測定のための最短吸収・発光波長を持つ蛍光タンパク質の開発
 Development of a violet fluorescent protein with the shortest absorption/emission wavelengths for multiplex bioimaging
 ○杉浦 一徳, 永井 健治 (大阪大学・産業科学研究所)
Kazunori Sugiura, Takeharu Nagai (*Osaka Univ., SANKEN*)
- 10:30 杉山 博紀 [2-10-1736](#)
 1YA1030 流れ環境下で生じる非対称脂質膜が引き起こす細胞サイズのリポソームへの分子濃縮
 Abiotic molecular transport against a concentration gradient caused by flow-induced membrane asymmetry of cell-sized liposomes
 ○杉山 博紀¹, 大崎 寿久^{2,3}, 竹内 昌治^{2,4}, 豊田 太郎^{5,6} (¹自然科学研究機構・ExCELLS, ²東大・生産研, ³神奈川産技研, ⁴東大院・情理, ⁵東大院・総合, ⁶生物普遍性連携研究機構)
Hironori Sugiyama¹, Toshihisa Osaki^{2,3}, Shoji Takeuchi^{2,4}, Taro Toyota^{5,6} (¹ExCELLS, NIBB, ²IIS, UTokyo, ³KISTEC, ⁴Grad. Sch. Info Sci. Tech., UTokyo, ⁵Grad. Sch. Arts and Sci., UTokyo, ⁶UBI, UTokyo)

- 10:45 丹澤 豪人 [3-05-1342](#)
1YA1045 構造レベルでの RRF と tRNA によるリボソームリサイクリングの解明
Structural basis for ribosome recycling by RRF and tRNA
○丹澤 豪人^{1,2}, Zhou Dejian³, Lin Jinzhong³, Matthieu G. Gagnon^{2,4} (¹ 阪大・蛋白研, ² テキサス州立大・医・微生物学/免疫学, ³ 復旦大・中山医院・生命科学, ⁴ テキサス州立大・医・シーラー構造生物学/生物物理学センター)
Takehito Tanzawa^{1,2}, Dejian Zhou³, Jinzhong Lin³, Gagnon Matthieu G.^{2,4} (*1Inst., for Protein Res., Osaka Univ., 2Dept. of Microbiol. & Immunol., Univ. of Texas Med. Branch, 3Schl. of Life Sci., Zhongshan Hospital, Fudan Univ., 4Sealy Center for Struct. & Biophys., Univ. of Texas Med. Branch*)
- 11:00 富田 篤弘 [1-02-1406](#)
1YA1100 クライオ電子顕微鏡単粒子解析と分子動力学シミュレーションを用いた ATP13A2 のポリアミン輸送機構の解明
Cryo-EM structures and MD simulations of ATP13A2 reveal transport mechanism of polyamines
○富田 篤弘¹, 大保 貴嗣², 西澤 知宏³, 濡木 理¹ (¹ 東大・院理学, ² 旭川医大・医学, ³ 横浜市大・院生命医科学)
Atsuhiko Tomita¹, Takashi Daiho², Tomohiro Nishizawa³, Osamu Nreki¹ (*1Grad. Sch. Sci., Univ. Tokyo, 2Dept. of Med., Asahikawa Medical Univ., 3Grad. Sch. Sci., Yokohama City Univ.*)
- 11:15 渡邊 千穂 [2-10-1724](#)
1YA1115 細胞サイズのミクロな膜閉じ込めによる相分離と分子拡散の制御
Phase separation and molecular diffusion modulated by cell-size micrometric membrane confinement
○渡邊 千穂^{1,2}, 柳澤 実穂² (¹ 広大院・統合生命科学, ² 東大院・総合文化・先進)
Chiho Watanabe^{1,2}, Miho Yanagisawa² (*1Hiroshima Univ., 2Univ. Tokyo*)

9:00~11:30 Ch02

1S1 Japan-US symposium on cytoskeletal motor proteins and their associated proteins

オーガナイザー : Hayashi Kumiko (Tohoku Univ.), Niwa Shinsuke (Tohoku Univ.)

Organizers: Kumiko Hayashi (Tohoku Univ.), Shinsuke Niwa (Tohoku Univ.)

Speakers in this symposium are recognized internationally as experts in the field of cytoskeletal motor proteins such as kinesin and dynein, 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 the intracellular transport and motor proteins, as well as interesting applications of existing single-molecule techniques.

Opening Remarks

- [1S1-1](#) (1-07-1418) Dissociation mechanism of IF₁ from mitochondrial ATP synthase revealed by single-molecule analysis and manipulation
Ryohei Kobayashi, Hiroshi Ueno, Hiroyuki Noji (*Appl. Chem., Grad. Sch. Eng., Univ. Tokyo*)
- [1S1-2](#) Engineering biomolecular motors
Zev Bryant (*Department of Bioengineering, Stanford University*)
- [1S1-3](#) (3-07-1342) Engineering of hybrid kinesin-1 dimer with synthetic linker by tuning the neck linker length
Jakia Jannat Keya¹, Akasit Visootsat¹, Akihiro Otomo¹, Sanghun Han², Kazushi Kinbara², Ryota Iino¹
(¹*Institute for Molecular Science, National Institutes of Natural Sciences*, ²*School of Life Science and Technology, Tokyo Institute of Technology*)
- [1S1-4](#) Deciphering the function of activating adaptors in the motor-driven transport of mitochondria and autophagosomes
Erika Holzbaur (*University of Pennsylvania Perelman School of Medicine*)
- [1S1-5](#) A rogue kinesin that destroys microtubules in cells
Kristen Verhey^{1,2}, Yang Yue¹, Lynne Blasius¹, Breane Budaitis¹ (¹*Department of Cell & Developmental Biology, University of Michigan Medical School*, ²*Department of Biophysics, University of Michigan*)
- [1S1-6](#) Analyses of KIF1A-associated neuronal disorder by genetics and single molecule assays
Shinsuke Niwa (*FRIS, Tohoku Univ.*)
- [1S1-7](#) In Vitro Reconstitution of Kinesin-1 Activation
Kyoko Chiba (*FRIS, Tohoku Univ.*)

オーガナイザー：豊田 太郎（東京大学），浜田 省吾（東北大学）

Organizers: Taro Toyota (The Univ. of Tokyo), Shogo Hamada (Tohoku Univ.)

C. Elegance has a brain consisting of 302 cells, which controls all the behaviors of the organism. The neurons in its brain are classified into three levels, and they are connected by about 6000 synapses. On what principle do these "wet" information processing systems operate? At least, such systems must be constructed by the power of chemistry. A new methodology of "how to assemble individual molecules and molecular devices into complex functional systems" is attracting attention as "molecular systems engineering". In Grant-in-Aids for transformational research "Molecular Cybernetics" (2020-2024), we will investigate principles of the molecular systems engineering. Specifically, designed molecules that function as sensors, processors, and actuators will be assembled in a micrometer-sized compartment (artificial cell) such as a liposome. The resulting artificial cells can then be further combined with each other to construct higher-order functional systems. In this symposium, we will discuss the design principles and practice of such artificial cells and other issues related to the construction of chemical artificial intelligence (AI).

[1S2-1](#) Molecular pattern recognition in DNA-based artificial neural networks
Lulu Qian (*Caltech*)

[1S2-2](#) Computer designed organisms
Josh Bongard (*Dept. Computer Sci., Univ. of Vermont*)

[1S2-3](#) 化学反応ネットワークと連携したベシクルの再生産
Reproduction of vesicle coupled with chemical reaction network
○今井 正幸¹, 栗栖 実¹, わるで びーたー² (¹ 東北大・物理, ² チューリッヒ工科大・物質)
Masayuki Imai¹, Minoru Kurisu¹, Peter Walde² (¹ *Dep. Phys., Tohoku Univ.*, ² *Dep. Materials, ETH Zurich*)

[1S2-4](#) Mesoscale DNA-based machines powered by artificial metabolism
Shogo Hamada (*Dept. of Robotics, Tohoku Univ.*)

[1S2-5](#) ケミカル AI 構築に向けた修飾アデニンの光環化付加反応による人工核酸の光制御
Photoregulation of Artificial Nucleic Acid via Photo-Cycloaddition of Modified Adenine Residues for Chemical AI
○村山 恵司¹, 山野 雄平², 浅沼 浩之¹ (¹ 名大・院工学, ² 東北大・多元研)
Keiji Murayama¹, Yuuhei Yamano², Hiroyuki Asanuma¹ (¹ *Grad. Sch. Eng., Nagoya Univ.*, ² *IMRAM, Tohoku Univ.*)

おわりに

Closing Remarks

オーガナイザー：重田 育照（筑波大学），當舎 武彦（理化学研究所）

Organizers: Yasuteru Shigeta (Univ. of Tsukuba), Takehiko Tosha (RIKEN)

Various metallic and semi-metallic elements, which are present in very small amounts in living organisms (defined as biometals), are essential for all living organisms. Their functions range from signal transduction and electron transfer to enzymatic reactions for the production and metabolism of substances. It is mystery that these trace amounts of biometals are programmed into life besides the central dogma. In this symposium, the latest researches on biological reactions and structures involving biometals and their kinetic analysis will be presented from both theoretical and experimental approaches.

- [1S3-1](#) 銅・亜鉛スーパーオキシドディスムターゼの成熟化におけるシステイン残基の役割
A dual role of cysteine residues in the maturation of prokaryotic Cu/Zn-superoxide dismutase
○古川 良明（慶應・理工）
Yoshiaki Furukawa (*Dept. Chem., Keio Univ.*)
- [1S3-2](#) 時間分解分光法を用いたヘム ABC トランスポーター BhuUV-T における輸送過程の速度論的解析
Kinetic analysis of the transport in heme ABC transporter; BhuUV-T, by time-resolved spectroscopy
○木村 哲就（神戸大・院理）
Tetsunari Kimura (*Grad. Sch. Sci., Kobe Univ.*)
- [1S3-3](#) Computational study of the structural–function relationship of heme proteins
Yu Takano¹, Hiroko X. Kondo², Yusuke Kanematsu³ (¹*Grad. Sch. Info. Sci., Hiroshima City Univ.*, ²*Fac. Eng., Kitami Inst. Tech.*, ³*Grad. Sch. Adv. Sci. Eng., Hiroshima Univ.*)
- [1S3-4](#) SR-Ca²⁺-ATPase における E1/E2 転移の反応座標の解析
Analysis of reaction pathway in E1/E2 transition of SR-Ca²⁺-ATPase
○小林 千草¹, 松永 康佑², Jung Jaewoon^{1,3}, 杉田 有治^{1,3,4} (¹理研・R-CCS, ²埼玉大・院理工, ³理研・CPR, ⁴理研・BDR)
Chigusa Kobayashi¹, Yasuhiro Matsunaga², Jaewoon Jung^{1,3}, Yuji Sugita^{1,3,4} (¹*RIKEN, R-CCS*, ²*Grad. Sch. Sci. Eng., Saitama Univ.*, ³*RIKEN, CPR*, ⁴*RIKEN, BDR*)
- [1S3-5](#) Design of staphylococcal two-component pore forming toxin to change pore formation property
Nouran Ghanem^{1,2}, Takashi Matsui^{1,3}, Jun Kaneko⁴, Tomomi Uchikubo-Kamo², Mikako Shirouzu², Tsubasa Hashimoto¹, Tomohisa Ogawa^{1,4}, Tomoaki Matsuura⁵, Po-Ssu Huang⁶, Takeshi Yokoyama^{1,2}, **Yoshikazu Tanaka**¹ (¹*Graduate School of Life Sciences, Tohoku University*, ²*Laboratory for Protein Functional and Structural Biology, RIKEN Center for Biosystems Dynamics Research*, ³*School of Science, Kitasato University*, ⁴*Graduate School of Agricultural Science, Tohoku University*, ⁵*Earth-Life Science Institute, Tokyo Institute of Technology*, ⁶*Department of Bioengineering, Stanford University*)
- [1S3-6](#) 放射光顕微システムによる細胞内小分子イメージングと医学応用の試み
Visualization of intracellular small molecules using synchrotron radiation and its trials for medical application
○志村 まり（国立国際医療研究センター）
Mari Shimura (*Nat. Cent. for Global Health and Med.*)

9:00~11:30 Ch05

1S4 共催：新学術領域「発動分子科学」

生体分子の構造的・機能的ダイナミクス：1分子計測と分子シミュレーションの交流
Structural and Functional Dynamics of Biomolecules: Interplay between Single Molecule
Measurement and Molecular Simulation

オーガナイザー：古田 忠臣（東京工業大学）、鎌形 清人（東北大学）

Organizers: Tadaomi Furuta (Tokyo Tech), Kiyoto Kamagata (Tohoku Univ.)

Currently, the qualitative and quantitative developments of experimental and computational methods have made it possible to directly observe important structural and functional dynamics of various biomolecules. Recently, there have been many reports that lead to further understandings of biological phenomena by integrating information obtained from these experiments and simulations. In view of this situation, the theme of this symposium is at the stage where it should be promoted further. Therefore, in this symposium, several researchers on the experimental side, simulation side, and integrated researches will present the latest research results and general remarks, which would be clues leading to profound understandings of biological phenomena.

- [1S4-1](#) 高速 AFM による一分子動態イメージングデータと分子シミュレーション
High-speed-AFM imaging of single-molecule dynamics and molecular simulation
○内橋 貴之^{1,2} (¹名古屋大学大学院理学研究科,²自然科学研究機構 生命創成探究センター)
Takayuki Uchihashi^{1,2} (¹Graduate School of Science, Nagoya University, ²ExCELLS, NINS)
- [1S4-2](#) 高速原子間力顕微鏡データと分子シミュレーションのデータ同化による動的構造解析
Dynamic structure analysis by data assimilation combining high-speed atomic force microscopy
data and molecular simulations
○湖上 壮太郎¹, 松永康佑², 高田 彰二¹ (¹京大院・理,²埼玉大・工)
Sotaro Fuchigami¹, Yasuhiro Matsunaga², Shoji Takada¹ (¹Grad. Sch. of Science, Kyoto Univ., ²Fac. of
Engin., Saitama Univ.)
- [1S4-3](#) 分子モーターの化学力学共役モデルのベイズ推定
Bayesian inference of the chemomechanical coupling model of molecular motors
○岡崎 圭一（分子研）
Kei-ichi Okazaki (Inst. for Mol. Sci.)
- [1S4-4](#) DNA 上や相分離複合体内でのタンパク質ダイナミクスの単分子計測と分子動力学解析
Single molecule and molecular dynamics characterization of protein action along DNA and in
liquid droplets
○鎌形 清人（東北大・多元研）
Kiyoto Kamagata (IMRAM, Tohoku Univ.)
- [1S4-5](#) 光子相関計測で解き明かす生体分子のマイクロ秒構造・機能ダイナミクス
Microsecond Structural and Functional Dynamics of Biomolecules Revealed by Photon
Correlation Measurements
○石井 邦彦（理研・田原分子分光）
Kunihiko Ishii (Mol. Spectrosc. Lab., RIKEN)
- [1S4-6](#) 生物分子モーターの再デザインと計測
Re-designing and measuring biomolecular motors
○古田 健也（情報通研、未来 ICT）
Ken'ya Furuta (Advanced ICT, NICT)

- [1S4-7](#) 一分子計測からたんぱく質のエネルギー地形の階層性を抽出する
Capturing hierarchical features in protein energy landscape from single molecule time series
○小松崎 民樹^{1,2} (¹北大・電子研,²北大・化学反応創成研究拠点)
Tamiki Komatsuzaki^{1,2} (¹*RIES, Hokkaido Univ.*, ²*WPI-ICReDD, Hokkaido Univ.*)

9:00~11:30 Ch06

1S5 1 細胞解析が切り開く新しい細胞観

New perspectives on cells provided by single cell analyses

オーガナイザー：谷口 雄一（京都大学）、黒田 真也（東京大学）

Organizers: Yuichi Taniguchi (Kyoto Univ.), Shinya Kuroda (The Univ. of Tokyo)

Single cell biology is a growing field to quantitatively understand the nature of individual cells that inherently have large heterogeneity. This growth is supported by progresses in a variety of single-cell approaches such as DNA/RNA sequencing, optical imaging, mass spectroscopy, high-throughput measurement, theory and informatics. In this symposium, we invite several single-cell biology scientists who conduct cutting-edge research using different approaches, aiming at discussing what single cell biology will bring towards understanding of life phenomena.

はじめに

Opening Remarks

- [1S5-1](#) Large-scale transcriptome analysis at single cell level
Piero Carninci (*RIKEN Center for Integrative Medical Sciences*)

- [1S5-2](#) 機械学習によるシングルセル・ダイナミクスからの生物学的原理の解読
Deciphering Biological Principles from Single-cell Dynamics by Machine Learning
○小林 徹也（東大・生産研）
J. Tetsuya Kobayashi (*IIS, UTokyo*)

- [1S5-3](#) ネットワーク化計測によるプール型細胞解析
Networked measurement for pooled cell analysis
○太田 禎生^{1,2} (¹東大・先端研,²シンクサイト株式会社)
Sadao Ota^{1,2} (¹*RCAST, Univ. Tokyo*, ²*Thinkcyte Inc*)

- [1S5-4](#) 情報理論解析による細胞間のばらつきを活かした正確な応答制御機構の解明
Information analysis reveals that cell-to-cell variability can improve the accuracy of the control of biological responses
○和田 卓巳¹, 廣中 謙一², 黒田 真也^{2,3} (¹京大・iPS細胞研究所,²東京大・理学系,³東京大・新領域創成科学)
Takumi Wada¹, Ken-ichi Hironaka², Shinya Kuroda^{2,3} (¹*Center for iPS Research and Application, Kyoto Univ.*, ²*Grad. Sch. Sci., Univ. Tokyo*, ³*Grad. Sch. Front. Sci., Univ. Tokyo*)

- [1S5-5](#) 一細胞プロテオーム解析を目指した三次元一分子イメージングによるバイオ分析法の開発
3D single-molecule imaging-based bioanalyses towards single-cell proteomics
○金 水縁^{1,2}, Kamarulzaman Latiefa^{1,3}, 谷口 雄一^{1,2,3} (¹理研・BDR,²京大・iCeMS,³阪大・院生命機能研)
Sooyeon Kim^{1,2}, Latiefa Kamarulzaman^{1,3}, Yuichi Taniguchi^{1,2,3} (¹*RIKEN, BDR*, ²*iCeMS, Kyoto Univ.*, ³*Grad. Sch. Front. Biosci., Osaka Univ.*)

おわりに

Closing Remarks

オーガナイザー：片山 耕大 (名古屋工業大学), 寿野 良二 (関西医科大学)

Organizers: Kota Katayama (Nagoya Inst. of Tech.), Ryoji Suno (Kansai Medical Univ.)

The recent trend in the field of structural studies of G-protein-coupled receptors (GPCRs) using cryo-electron microscopy (Cryo-EM) and 3D reconstruction techniques supported by biophysical, computational and advanced biochemistry have facilitated GPCRs research towards drug discovery. These techniques contributed significantly to our understanding about GPCRs functions, ligand recognition, pharmacological targets in biomedicine. This symposium will highlight the latest developments in GPCR structure/function, ligand discovery and design, intracellular signalling pathways and their impact on modern drug discovery.

はじめに

Opening Remarks

[1S6-1](#)

ヒトプロスタグランジン受容体 EP3-G タンパク質複合体の構造解析

Structural insights into the human Prostaglandin E2 receptor EP3- Gi signaling complex

○寿野 良二 (関西医大・医)

Ryoji Suno (*Dept. Med., Kansai Med. Univ.*)

[1S6-2](#)

Back and forth between purified and cellular systems for GPCR biology

Asuka Inoue (*Grad. Sch. Pharm., Tohoku Univ.*)

[1S6-3](#)

Spatiotemporal Determinants and Allosteric Communication Modulate the Ligand Bias in GPCRs

Nagarajan Vaidehi (*Chair, Department of Computational & Quantitative Medicine, Beckman Research Institute of the City of Hope, Duarte, CA*)

[1S6-4*](#)

(2-06-1515) 分子シミュレーションによるオレキシン 2 受容体-G タンパク質複合体の動的性質の研究

(2-06-1515) Dynamics of Orexin2 Receptor and G-protein Complex with Molecular Dynamics Simulations

○横井 駿, 光武 亜代理 (明治大学 理工学研究科 物理学専攻)

Shun Yokoi, Ayori Mitsutake (*Department of Physics, School of Science and Technology, Meiji University*)

[1S6-5](#)

配位ケモジェネティクスによる GPCR 型グルタミン酸受容体の活性制御

Coordination chemogenetics for direct activation of GPCR-type glutamate receptors in brain tissue

○清中 茂樹 (名大・院工)

Shigeki Kiyonaka (*Grad. Sch. Eng., Nagoya Univ.*)

[1S6-6*](#) (2-01-1451) アデノシン A_{2A} 受容体の不活性型構造を安定化するための all- α 融合パートナータンパク質のゼロからの合理デザイン
(2-01-1451) De novo design of an alpha-helical fusion partner protein to stabilize adenosine A_{2A} receptor in the inactive state
○三本 齊也^{1,2}, 菅谷 幹奈³, 風間 一輝³, 中野 僚介³, 小杉 貴洋^{1,2,4}, 村田 武士³, 古賀 信康^{1,2,4}
(¹総研大・物理学, ²分子研, ³千葉大・理, ⁴自然科学・生命創成)
Masaya Mitsumoto^{1,2}, Kanna Sugaya³, Kazuki Kazama³, Ryosuke Nakano³, Takahiro Kosugi^{1,2,4}, Takeshi Murata³, Nobuyasu Koga^{1,2,4} (¹SOKENDAI, ²IMS, NINS, ³Grad. Sch. of Sci. and Eng., Chiba Univ., ⁴ExCELLS, NINS)

[1S6-7](#) Conformational dynamics upon ligand binding in muscarinic acetylcholine receptor revealed by FTIR spectroscopy
Kota Katayama^{1,2} (¹Grad. Sch. Eng., Nagoya Inst. Tech., ²PRESTO, JST)

おわりに
Closing Remarks

16:00~18:30 Ch01

1S7 インドー日本交流シンポジウム：生物物理の多彩な挑戦
India-Japan joint symposium: Various challenges on biophysical research

オーガナイザー：坂口 美幸（埼玉大学）、永井 健（北陸先端科学技術大学院大学）
Organizers: Miyuki Sakaguchi (Saitama Univ.), Ken H. Nagai (JAIST)

To promote the exchange between the Indian Biophysical Society (IBS) and the Biophysical Society of Japan (BSJ), this joint symposium focusing on energetic young scientists was planned. Four up-and-coming researchers are nominated by IBS, and they will give talks in a wide range of fields like protein function during embryogenesis, super-resolution imaging with DNA, morphogenesis in an active-polar gel, and the physical basis on self-reproducing catalytic RNAs. From BSJ, three leading researchers in related fields will also give talks. In the symposium, we will share the problems at the forefront, and exchange cutting-edge technologies and knowledge.

はじめに
Opening Remarks

[1S7-1](#) Secondary-probe based DNA-PAINT super-resolution imaging for unlimited multiplexing
Mahipal Ganji (*Department of Biochemistry, Indian Institute of Science, Bangalore, India*)

[1S7-2](#) 1 分子イメージングで迫るヒト染色体の動的組織化
Single molecule imaging unveils the dynamic organization of the human chromosomes
○日比野 佳代¹, 境 祐二², 鐘巻 将人¹, 前島 一博¹ (¹ 遺伝研・総研大, ² 東京大学)
Kayo Hibino¹, Yuji Sakai², Masato Kanemaki¹, Kazuhiro Maeshima¹ (¹Natl. Inst. Genet. & SOKENDAI, ²Univ. Tokyo)

[1S7-3](#) BAR domain protein function in plasma membrane remodeling during embryogenesis
Richa Rikhy (*Biology, IISER, Pune, India*)

- [1S7-4](#) 上皮集団遊走におけるメカノケミカルフィードバック
 Mechanochemical feedbacks in collective cell migration of epithelial cells
 ○平島 剛志^{1,2}, 日野 直也^{2,4}, Boocock Daniel⁴, 松田 道行^{2,3}, Hannezo Edouard⁴ (¹京大・白眉,²京大・生命,³京大・医,⁴IST Austria)
Tsuyoshi Hirashima^{1,2}, Naoya Hino^{2,4}, Daniel Boocock⁴, Michiyuki Matsuda^{2,3}, Edouard Hannezo⁴
 (¹*The Hakubi Center, Kyoto Univ.*, ²*Grad Sch Biostudies, Kyoto Univ.*, ³*Grad Sch Med, Kyoto Univ.*, ⁴*IST Austria*)
- [1S7-5](#) Dynamics of active-polar gels on curved surfaces
Vijay Kumar Krishnamurthy¹, Siddharth Jha², Swapnil Kole², Sriram Ramaswamy² (¹*International Centre for Theoretical Sciences, Bengaluru*, ²*Indian Institute of Science, Bengaluru*)
- [1S7-6](#) Compositional identity and robustness of autocatalytic RNA reaction networks in coacervate protocells
Shashi Thutupalli^{1,2} (¹*National Centre for Biological Sciences, Tata Institute for Fundamental Research*, ²*International Centre for Theoretical Sciences, Tata Institute for Fundamental Research*)
- [1S7-7](#) *C. elegans* の集団運動
 Collective motion of *C. elegans*
 ○北井 健¹, 伊藤 浩史², 杉 拓磨³ (¹北陸先端科学技術大学院大学,²九州大学,³広島大学)
Ken H. Nagai¹, Hiroshi Ito², Takuma Sugi³ (¹*JAIST*, ²*Kyushu University*, ³*Hiroshima University*)
- おわりに
 Closing Remarks

16:00~18:30 Ch02

1S8 水のダイナミクスと生物機能：再考

Water dynamics and biological functions: Revisit

オーガナイザー：今清水 正彦（産業総合研究所），村上 洋（量子科学技術研究開発機構）

Organizers: Masahiko Imashimizu (AIST), Hiroshi Murakami (QST)

Extensive studies of hydration water dynamics show that they occur from the picosecond to nanosecond timescales. We, however, consider from recent studies that much slower dynamics of water may play critical roles in expressing biological functions. Such studies include findings of glass-like water in a model of cells and glassy behaviors of cytoplasm, and of nonthermal effects on slow biomolecular dynamics and reactions by the externally applied alternating electromagnetic field with terahertz frequency. In this symposium, we will attempt to discuss new directions that connect the physicochemical studies of hydration to biological functions through water relaxation processes in a wide temporal range.

- [1S8-1](#) Nonthermal Excitation Effects Mediated by Sub-Terahertz Radiation on Biomolecular Hydration Dynamics and Reactions
Masahiko Imashimizu¹, Yuji Tokunaga¹, Masahito Tanaka², Jun-ichi Sugiyama³ (¹*CMB, AIST*, ²*NMRI, AIST*, ³*NMRI, AIST*)
- [1S8-2](#) 荷電フィラメント周りの協同的水分子運動 -マイクロ波誘電緩和とラマン OH 伸縮/ベンディング分光-
 Collective water behavior around charged filaments by microwave dielectric relaxation and Raman OH-stretching/bending bands spectroscopy
 ○鈴木 誠（東北大・多元研）
Makoto Suzuki (*IMRAM, Tohoku Univ.*)

- [1S8-3*](#) (2-02-1624) 水和水の OH 伸縮振動バンドに基づく生体保護作用を持つ小分子の水素結合強化作用の評価
(2-02-1624) Hydrogen bond strengthening effect of stabilizing osmolytes investigated by OH stretching band of hydration water
○松村 郁希¹, 四方 俊幸², 小川 雄一¹, 鈴木 哲仁¹, 近藤 直¹, 白神 慧一郎¹ (¹京都大・院農学研究科, ²東京農工大・院農学研究科)
Fumiki Matsumura¹, Toshiyuki Shikata², Yuichi Ogawa¹, Tetsuhito Suzuki¹, Naoshi Kondo¹, Keiichiro Shiraga¹ (¹Grad. Sch. Agri., Kyoto Univ., ²Grad. Sch. Agri., Tokyo Univ. of Agriculture and Technology)
- [1S8-4](#) 高圧力下誘電分光測定による全濃度範囲におけるグリセロール水溶液の過冷却水のダイナミクスに関する研究
High-pressure dielectric study of dynamics of supercooled water in whole concentration range glycerol-water mixtures
○佐々木 海渡 (東海大・理物)
Kaito Sasaki (Dept. Phys. Sch. Sci., Tokai Univ.)
- [1S8-5](#) The role of water for biomolecular dynamics; slaving versus plasticization
Jan Swenson¹, Silvina Cerveny^{1,2} (¹Chalmers University of Technology, ²Donostia International Physics Center)
- [1S8-6](#) Hydration shells of biomolecules: dynamics and biochemical function
Damien Laage^{1,2,3,4} (¹Ecole Normale Supérieure, ²CNRS, ³PSL Univ., ⁴Sorbonne Univ.)
- [1S8-7](#) 低含水率媒質中の水和水の室温ガラス状態
Glass-like state of hydration water in aqueous mediums with low water contents at room temperature
○村上 洋 (量研・量子生命)
Hiroshi Murakami (Inst. Quantum life Sci., QST)

16:00~18:30 Ch03

1S9 温度感覚研究の新潮流 - 温度を測る、制御する、感知機構とその意義を探る -
Trends in the research field of thermo-sensation

オーガナイザー：内田 邦敏 (静岡県大学), 藤原 祐一郎 (香川大学)

Organizers: Kunitoshi Uchida (Univ. of Shizuoka), Yuichiro Fujiwara (Kagawa Univ.)

Since TRPV1 channel, the world's first mammalian thermo-receptor, was uncovered in 1997, several thermo-receptors have been elucidated, and the biological meaning of thermo-sensation are becoming clearer. In this symposium, we will introduce the recent works aimed to evaluate the measurement and manipulation techniques of temperature in living matter, and to elucidate the gating mechanisms of thermo-receptors by temperature changes and physiological roles of thermo-sensation. We will also discuss the biological significances and future perspectives of thermo-sensation.

- [1S9-1](#) 蛍光性タンパク質温度センサーを用いた生体内温度分布の可視化とその意義の解明
Visualization and understanding of subcellular thermodynamics using fluorescent protein-based thermosensors
○坂口 怜子^{1,2} (¹産業医科大学・医学部, ²京都大・院工)
Reiko Sakaguchi^{1,2} (¹Univ of Occupational and Environmental Health, ²Grad Sch Engineering, Kyoto Univ.)

- [1S9-2](#) Single-molecule dynamics of TRPV1 channel upon activation with different stimuli
Hirofumi Shimizu (*Div. Int. Physiol. Univ. Fukui. Fac. Med. Sci.*)
- [1S9-3](#) 電位依存性 H⁺チャネルの温度感受性ゲーティングの構造基盤
 Structural Basis for Temperature-Sensitive Gating of Voltage-Gated H⁺ Channels
 ○藤原 祐一郎 (香川大・院医)
Yuichiro Fujiwara (*Grad. Sch. Med., Kagawa Univ.*)
- [1S9-4](#) 温度感受性チャネル TRPM5 の温度依存的活性化及び不活性化
 Temperature-dependent activation and inactivation of TRPM5 channel
 ○内田 邦敏 (静科大・食品栄養・環境生命)
Kunitoshi Uchida (*Dept. Environ. Life Sci., Sch. Food Nutr. Sci., Univ. Shizuoka.*)
- [1S9-5](#) 両生類の生態的な棲み分けに起因した温度感覚の進化的変化とその分子機構
 The evolutionary tuning of thermal perception related to habitat selection in frogs
 ○齋藤 茂^{1,2,3}, 齋藤 くれあ^{1,2}, 井川 武⁴, 小巻 翔平⁵, 富永 真琴^{1,2,3} (¹生理研・細胞生理, ²生命創成探究センター・温度生物, ³総研大・生理科学, ⁴広島大・両生研, ⁵いわて東北メディカル・メガバンク)
Shigeru Saito^{1,2,3}, Claire Saito^{1,2}, Takeshi Igawa⁴, Shohei Komaki⁵, Makoto Tominaga^{1,2,3} (¹*Dep. Cell Signaling, Natl. Inst. Physiol. Sci.*, ²*Thermal Biol., ExCELLS*, ³*Dept. Physiol. Sci., SOKENDAI*, ⁴*Amphibian Res. Center, Hiroshima Univ.*, ⁵*Iwate Tohoku Med. Megabank Org.*)
- [1S9-6](#) てんかん原性域の局所発熱は TRPV4 活性化を介して病態悪化を引き起こす
 Temperature elevation in epileptogenic foci exacerbates the disease through TRPV4 activation
 ○柴崎 貢志 (長崎県立大院・人間健康科学・細胞生化学)
Koji Shibasaki (*Lab. Neurochem., Univ. Nagasaki*)

16:00~18:30 Ch04

1S10 生命の起源とプロトセル研究における新たな進歩
 Recent Advances in Origins of Life and Protocell Research

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

One of the major questions in ancient and modern science is the question of our own creation. How did life emerge on Earth? What were the structures and functions of the first cells? Recent technological advances in biophysics, especially in Japan, are now allowing researchers in a variety of fields such as synthetic biology, evolutionary biology, and biochemistry to finally begin to answer these questions. This symposium highlights recent advances in Origins of Life and Protocell research by biophysicists from Japan and around the world. We hope to inspire other biophysicists, especially young researchers, to also consider studying these very difficult (but important) unanswered questions.

- [1S10-1](#) Assembly of Primitive Liquid Crystal Peptide/DNA Coacervates
Tony Z Jia^{1,2}, Tommaso P Fraccia³ (¹*Earth-Life Science Institute, Tokyo Institute of Technology*, ²*Blue Marble Space Institute of Science*, ³*Institut Pierre-Gilles de Gennes, Chimie Biologie et Innovation, ESPCI Paris*)

- [1S10-2](#) 相分離を介して原始細胞モデル液滴を形成する核酸スキャフォールド
Nucleic acid scaffolds that undergo phase separation into liquid droplets serving as primitive cell models
○富田 峻介¹, 三村 真大^{1,2}, 新海 陽一³, 栗田 僚二^{1,2} (¹産総研・健康医工, ²筑波大院・数理物質, ³産総研・バイオメディカル)
Shunsuke Tomita¹, Masahiro Mimura^{1,2}, Yoichi Shinkai³, Ryoji Kurita^{1,2} (¹*Health Med. Inst., AIST*, ²*Grad. Sch. of Pure and Appl. Sci., Univ. Tsukuba*, ³*Biomed. Res. Inst., AIST*)
- [1S10-3*](#) (2-13-1427) アミノ酸配列と連携した原始生体膜の成長
(2-13-1427) Growth of Primitive Cell Membrane Coupled with Amino Acid Sequence
○馬場 晶子¹, オルソン ウルフ², 今井 正幸¹ (¹東北大・院理学, ² Lund 大・院理学)
Akiko Baba¹, Ulf Olsson², Masayuki Imai¹ (¹*Grad. Sch. Sci., Univ. Tohoku*, ²*Grad. Sch. Sci., Univ. Lund*)
- [1S10-4](#) 高分子混雑した細胞モデル中の分子挙動決定因子としての細胞サイズ
Cell size as a key determinant of molecular behaviors in macromolecular crowding artificial cells
○渡邊 千穂^{1,2}, 柳澤 実穂² (¹ 広大院・統合生命科学, ² 東大院・総合文化・先進)
Chiho Watanabe^{1,2}, Miho Yanagisawa² (¹*Hiroshima Univ.*, ²*Univ. Tokyo*)
- [1S10-5](#) Multiple fusion barriers for fatty acid protocells
Anna Wang¹, Tetsuya Yomo², Lauren Lowe¹, Daniel WK Loo¹, Yaam Deckel¹ (¹*School of Chemistry and the Australian Centre for Astrobiology, UNSW Sydney, Australia*, ²*Institute of Biology and Information Science, Biomedical Synthetic Biology Research Center, School of Life Sciences, East China Normal University, Shanghai, China*)
- [1S10-6](#) 人工細胞における細胞内構造形成の不安定性
Understanding the instability of intracellular organization in synthetic cells
○前多 裕介 (九大・物理)
Yusuke Maeda (*Kyushu Univ., Dept. Phys.*)
- [1S10-7*](#) (2-13-1451) 多相液滴のコアを用いた人工細胞内転写反応場の構築
(2-13-1451) Development of a transcription field in the artificial cell by the core of multiphase droplets
○友原 貫志, 皆川 慶嘉, 野地 博行 (東大院・工 応用化学)
Kanji Tomohara, Yoshihiro Minagawa, Hiroyuki Noji (*Dept. Appl. Chem., Grad. Sch. Eng., Univ. Tokyo*)

16:00~18:30 Ch05

1S11 共催：新学術領域研究「高速分子動画」

原子レベルの動的構造解析が拓く生体分子機能の理解

Toward understanding biological functions: atomic-level characterization of structures and dynamics of biomolecules

オーガナイザー：宮下 治（理化学研究所），南後 恵理子（東北大学）

Organizers: Osamu Miyashita (RIKEN), Eriko Nango (Tohoku Univ.)

Information on the structures and dynamics of biological molecules plays a critical role in understanding their functional mechanisms and possible medicinal applications. Time-resolved serial femtosecond crystallography (TR-SFX) using X-ray free electron laser (XFEL) is a state-of-art technique that can provide 3D structures of the molecules following the time-development of reactions. Furthermore, integrative analyses combining TR-SFX data with other approaches could provide more detailed information on dynamic structures and energetics. This symposium will focus on recent updates on TR-SFX experiments and applications, as well as recent developments of other experimental techniques and computational approaches, aiming to advance our understanding of biomolecular functions through integrative research.

[1S11-1](#) X-ray free electron lasers reveal the molecular mechanism for water oxidation in photosystem II
Michi Suga, Yoshiaki Nakajima, Hongjie Li, Jian-Ren Shen (*Okayama Univ.*)

[1S11-2](#) Involvement of conserved amino acids in ion transport pathways of multidrug and toxic compound extrusion (MATE) transporter
Keiko Shinoda¹, Hisashi Kawasaki¹, Satoshi Murakami², Sagar Raturi³, Asha V. Nair³, Himansha Singh³, Boyan Bai³, Hendrik W. van Veen³ (¹*AgTECH, GSALS, UTokyo*, ²*Sch. of Life Sci. and Tech., Tokyo Inst. of Tech.*, ³*Dept. of Pharmacology, Univ. of Cambridge*)

[1S11-3](#) ギャップ結合タンパク質のナノディスクにおける構造
Structures of gap junction proteins in nanodiscs
○大嶋 篤典^{1,2} (¹名大・細胞セ, ²名大・創薬)
Atsunori Oshima^{1,2} (¹*CeSPI, Nagoya Univ.*, ²*Grad. Sch. Pharm. Sci.*)

[1S11-4](#) Molecular mechanisms involved in the regulation of the Circadian Clock
Florence Tama^{1,2,3} (¹*RIKEN Center for Computational Science*, ²*Department of Physics, Nagoya University*, ³*Institute of Transformative Bio-Molecules*)

[1S11-5](#) XFEL analyses of molecular mechanism and structure in DNA photolyase photoreduction
Yoshitaka Bessho^{1,2} (¹*Academia Sinica, IBC*, ²*RIKEN SPring-8 Center*)

[1S11-6](#) 蛋白質結合解離ダイナミクスの分子動画
Molecular movie of protein association/dissociation dynamics
○北尾 彰朗（東工大・生命理工）
Akio Kitao (*Sch. Life Sci. Tech., Tokyo Tech.*)

オーガナイザー：藤崎 弘士（日本医科大学），好村 滋行（東京都立大学）

Organizers: Hiroshi Fujisaki (Nippon Medical School), Shigeyuki Komura (Tokyo Metro. Univ.)

Research towards tailor-made and precision medicine is accelerating, and this requires mathematical and physical approaches in addition to empirical medical traditions. Medical physics has been established as a field that links medicine and physics, and recently, AI has been used for pathological imaging diagnosis and particle therapy. On the other hand, biological phenomena have various hierarchies, starting from the molecular level to cells, organs, individuals, and populations, and with the advancement of computers, highly precise simulations of these phenomena are now becoming possible. In this symposium, we will explore the possibility of medical applications, including therapeutic methods, from the standpoint of biophysics and soft matter physics. The main purpose of this symposium is to have a lively discussion among medical scientists, biophysicists, and physicists about the awareness of problems in the field of medicine and how to deal with them in theory and calculations.

はじめに

Opening Remarks

[1S12-1](#) Biophysics of Infectious Diseases: How are the carriers of abnormal hemoglobin protected from severe malaria?

Motomu Tanaka^{1,2} (¹Heidelberg University, Institute of Physical Chemistry, ²Kyoto University, Center for Integrative Medicine and Physics)

[1S12-2](#) 形成外科学 とメカノバイオロジー —物理的的刺激が創傷治癒や組織再生に与える役割—
Plastic Surgery and Mechanobiology —The Role of Mechanical Forces on Wound Healing,
Tissue Repair and Regeneration—

○小川 令（日本医科大学形成外科）

Rei Ogawa (*Department of Plastic, Reconstructive and Aesthetic Surgery, Nippon Medical School*)

[1S12-3](#) 計算流体力学を用いた心血管系疾患に対する患者固有解析

Patient-specific analyses by computational fluid dynamics for cardiovascular diseases

○水藤 寛（東北大・AIMR）

Hiroshi Suito (*AIMR, Tohoku Univ.*)

[1S12-4](#) 質量分析イメージングの病理学応用

Pathology application of mass spectrometry imaging

○鶴山 竜昭^{1,2} (¹京都大学医学部, ²放射線影響研究所)

Tatsuaki Tsuruyama^{1,2} (¹Kyoto University, graduate school of medicine, ²Radiation effect Research Foundation)

[1S12-5](#) 光トモグラフィーと生物物理

Optical tomography and biophysics

○町田 学（浜松医科大学）

Manabu Machida (*Hamamatsu University School of Medicine*)

16:00~18:30 Ch07

1S13 共催：新学術領域「シンギュラリティ生物学」
シンギュラリティ細胞が生み出す多様な生命現象へのアプローチ
Approaches to diverse biological phenomena produced by singularity cells

オーガナイザー：坂内 博子（早稲田大学），若林 憲一（東京工業大学）

Organizers: Hiroko Bannai (Waseda Univ.), Ken-ichi Wakabayashi (Tokyo Tech)

In multicellular systems, there are many phenomena that result in dramatic changes in morphology and dynamics caused by a small number of cells. In this symposium, we will introduce challenging research to find rare cells, i.e. "singularity cells", which are the driving force of dramatic changes in diverse biological phenomena such as algal behavior, stem cell differentiation, organogenesis, and neurological diseases. Elucidating the mechanism by which "singularity cells" significantly change the entire system requires new perspectives and methodologies. By sharing this approach with members, we aim to spread a new methodology of biophysics and a new academic field "Singularity Biology".

[1S13-1](#) はじめに：「シンギュラリティ生物学」とは？

Introduction: What is "Singularity Biology"?

○坂内 博子（早大・理工学術院）

Hiroko Bannai (Waseda Univ., Fac. Sci. Eng.)

[1S13-2](#) あまのじゃく細胞から紐解く緑藻クラミドモナス走光性の生理的意義

Significance of phototaxis in the unicellular green alga *Chlamydomonas reinhardtii* revealed by "perverse" cells

○若林 憲一^{1,2} (¹東工大・化生研,²東工大・生命理工)

Ken-ichi Wakabayashi^{1,2} (¹CLS, Tokyo Tech, ²LST, Tokyo Tech)

[1S13-3](#) シンギュラリティ細胞の脱分化による幹細胞集団維持機構の解明

Homeostasis of stem cell populations maintained by rare de-differentiating subsets

○中西 未央（Chiba Univ.）

Mio Nakanishi (Grad. Sch. Med.)

[1S13-4](#) Self-patterning of brain organoids

Kent Imaizumi (Department of Physiology, Keio University School of Medicine)

[1S13-5](#) 免疫応答を介したアルツハイマー病発症への寄与の解明

Involvement in the development of Alzheimer's disease through activation of systemic immune response

○伊藤 美菜子, 金子 竜晟（九大・生医研）

Minako Ito, Ryusei Kaneko (Med. Inst. Bioreg., Kyusyu Univ.)

[1S13-6](#) 社会性アメーバの時空間自己組織化過程におけるシンギュラリティ ~AMATERAS1.0 で実現した定量トランススケール解析~

Quantitative trans-scale analysis of a singularity in spatiotemporal self-organization of social amoeba by using AMATERAS1.0

○垣塚 太志¹, 原 佑介², 市村 垂生¹, 永井 健治^{1,3}, 堀川 一樹² (¹阪大・先導,²徳大・先端研究推進センター,³阪大・産研)

Taishi Kakizuka¹, Yusuke Hara², Taro Ichimura¹, Takeharu Nagai^{1,3}, Kazuki Horikawa² (¹OTLI, Osaka Univ., ²Adv. Res. Prom. Cen., Tokushima Univ., ³SANKEN, Osaka Univ.)

おわりに

Closing Remarks

16:00~18:30 Ch08

1S14 共催：新学術領域「情報物理学でひもとく生命の秩序と設計原理」
勾配検知の情報生物物理学
Information biophysics of gradient sensing in organisms

オーガナイザー：石島 秋彦（大阪大学），岡田 康志（理化学研究所/東京大学）

Organizers: Akihiko Ishijima (Osaka Univ.), Yasushi Okada (RIKEN/The Univ. of Tokyo)

Biological sensory systems, such as chemotaxis, phototaxis, gradient sensing and so on, are functions that are widely available in the biological world. For example, bacterial chemotaxis is one of the most well-studied areas from both theoretical and experimental perspectives. Various methods have been used in experiments, including genetics, biochemistry, and imaging. Theories have been discussed from various perspectives such as Ising model, information theory, and efficiency. In this symposium, we would like to gather theoretical and experimental researches to promote mutual integration from the viewpoint of information biophysics.

- [1S14-1](#) ケモフォレシス・エンジン：ATPase 駆動型カーゴ輸送の理論
Chemophoresis Engine: Theory of ATPase-driven Cargo Transport
○菅原 武志¹, 金子 邦彦^{1,2} (¹東大・生物普遍性, ²東大・総合文化)
Takeshi Sugawara¹, Kunihiko Kaneko^{1,2} (¹UBI, Univ. Tokyo, ²Grad. Sch. Arts Sci., Univ. Tokyo)
- [1S14-2](#) サルモネラのべん毛運動と走化性
Flagellar motility and chemotaxis in *Salmonella*
○森本 雄祐^{1,2} (¹九工大・院情報工, ²JST・さきがけ)
Yusuke V. Morimoto^{1,2} (¹Fac. Comp. Sci. and Sys. Eng., Kyushu Inst. Tech., ²PRESTO, JST)
- [1S14-3](#) Near-critical tuning of conformational spread revealed by single-cell FRET in bacterial chemoreceptor arrays
Johannes M. Keegstra¹, Fotios Avgidis¹, Yuval Mullah¹, John S. Parkinson², Thomas Shimizu¹
(¹AMOLF Institute, Amsterdam, The Netherlands, ²Department of Biology, University of Utah, Salt Lake City, USA)
- [1S14-4](#) Subpopulation of chemotactic cells with extremely high sensitivity
Satomi Matsuoka^{1,2,3}, Masahiro Ueda^{1,2} (¹Grad. Sch. Frontier Biosciences, Osaka Univ., ²RIKEN, BDR, ³PRESTO, JST)
- [1S14-5](#) 初期胚組織はモルフォゲン勾配のノイズを感知し修復する能力を備えている
Embryonic cell community senses and eliminates the noise of morphogen gradient
○穠枝 佑紀（阪大・微研・生体統御）
Yuki Akieda (*Hom. Reg., RIMD, Osaka Univ.*)
- [1S14-6](#) ゼブラフィッシュ胚におけるモルフォゲン分布の制御
Spatiotemporal regulation of morphogen distribution in zebrafish embryo
○猪股 秀彦, 浜田 裕貴, 金村 節子（理研・BDR）
Hidehiko Inomata, Hiroki Hamada, Setsuko Kanamura (*BDR., Riken*)

9:00~11:30 Ch01

2S1 共催：AMED「創薬等ライフサイエンス研究支援基盤事業(BINDS)」
高分解能クライオ電子顕微鏡の進展と共同利用
Technical Development and Sharing of High-Resolution Cryo-Electron Microscopes

オーガナイザー：中村 春木 (大阪大学), 吉川 雅英 (東京大学), 村田 武士 (千葉大学)

Organizers: Haruki Nakamura (Osaka Univ.), Masahide Kikkawa (The Univ. of Tokyo), Takeshi Murata (Chiba Univ.)

Since 2017, high-end cryo-electron microscopes (EMs) have been installed with equipment grants by the BINDS (Basis for Supporting Innovative Drug Discovery and Life Science Research) project. In addition, eight more cryo-EMs are being installed in 2021 at several laboratories in Japan. These new shared cryo-EM facilities enable higher-resolution and higher-throughput structural analysis, together with the recent technological progresses, including the development of new grids and methods for online remote cryo-EM operation. In this symposium, the symposists will review the results of single particle analysis, tomography, and micro-ED by cryo-EMs. We will also review the issues to be overcome by technical development and by the next BINDS program that is expected to start in 2022.

[2S1-1](#) クライオ電子顕微鏡によるクロススケール構造解析

Cross-scale structural studies by cryo-electron microscopy

○吉川 雅英 (東京大学)

Masahide Kikkawa (*The University of Tokyo*)

[2S1-2](#) 高速データ収集と原子分解能を両立したクライオ電子顕微鏡撮影法と酸化修飾グラフェングリッド
High throughput atomic resolution cryoEM analysis by multi-hole imaging and epoxidized graphene grid

○難波 啓一 (阪大・院生命機能)

Keichi Namba (*Grad. Sch. Frontier Biosci., Osaka Univ., RIKEN BDR & SPRING-8*)

[2S1-3](#) Cryo-EM ネットワークと産学連携

Industry-academia collaboration with the cryo-EM network

○千田 俊哉¹, 村田 武士², 岩崎 憲治³ (¹高エネ機構・物構研・構造生物, ²千葉大・院理学, ³筑波大・生存ダイナミクス)

Toshiya Senda¹, Takeshi Murata², Kenji Iwasaki³ (¹SBRC, IMSS, KEK, ²Grad. Sch. Sci, Chiba Univ., ³TARA, Univ. Tsukuba)

[2S1-4](#) COVID-19 等の感染症に対する治療薬・ワクチン開発を目指した BSL3 クライオ電子顕微鏡を軸とする北大創薬拠点

BSL3 Cryo-EM facility of Hokkaido Univ. Drug Discovery Base for the Development of Therapeutics and Vaccines against COVID-19

○前仲 勝実 (北大・院薬)

Katsumi Maenaka (*Facult. Pharm.Sci., Hokkaido Univ.*)

[2S1-5](#) 東北大学の最新クライオ電子顕微鏡の活用と共同利用について

New 300kV Cryo EM of Tohoku University: application and public utilization

○小柴 生造^{1,2,3}, 木下 賢吾^{1,2,4}, 山本 雅之^{1,2,3} (¹ 東北大・未来型医療創成センター, ² 東北大・東北メディカル・メガバンク機構, ³ 東北大・院医, ⁴ 東北大・院情報)

Seizo Koshiba^{1,2,3}, Kengo Kinoshita^{1,2,4}, Masayuki Yamamoto^{1,2,3} (¹INGEM, Tohoku Univ., ²ToMMO, Tohoku Univ., ³Grad. Sch. Med., Tohoku Univ., ⁴Grad. Sch. Info., Tohoku Univ)

[2S1-6](#) 九州・西日本エリアにおける創薬支援を目指したクライオ電顕ネットワーク
Cryo-EM network aiming to support drug discovery in the Kyushu / West Japan area
○真柳 浩太 (九大・生体防御医学研究所)
Kouta Mayanagi (*Medical Institute of Bioregulation, Kyushu Univ.*)

おわりに
Closing Remarks
中村 春木 (阪大)
Haruki Nakamura (*Osaka Univ.*)

9:00~11:30 Ch02

2S2 生物物理学的手法を駆使した細胞内プロセスにおけるタンパク質間相互作用の理解
Biophysical basis for understanding the protein-protein interaction involved in essential cellular process

オーガナイザー：武藤 梨沙 (福岡大学), 小柴 琢己 (福岡大学)
Organizers: Risa Mutoh (*Fukuoka Univ.*), **Takumi Koshiba** (*Fukuoka Univ.*)

Protein-protein interactions are essential biological reactions occurring at inter- and intra-cellular levels. The analysis of their mechanism is generally required in order link to understand their various cellular functions. Recent biophysical methodologies provide us useful tools for investigating protein-protein interactions, especially in live cells. In this symposium, we invite domestic young investigators and discuss on new techniques (e.g. IP-MS, lipid mixing assay, bioluminescence) that explore a new study of protein-protein interaction and membrane protein complexes involved in essential cellular processes.

はじめに
Opening Remarks

[2S2-1](#) 質量分析法によるミトコンドリアタンパク質複合体の解析
Mass spectrometry-based methods for analysing the mitochondrial interactome in mammalian cells
○小柴 琢己 (福岡大・理学・化学)
Takumi Koshiba (*Dep. Sci., Chem., Fukuoka Univ.*)

[2S2-2](#) ミトコンドリア膜融合反応の試験管内再構成
In vitro reconstitution of mitochondrial membrane fusion
○伴 匡人¹, 石原 直忠² (¹久留米大・分子生命科学,²阪大・理・生物科学)
Tadato Ban¹, Naotada Ishihara² (¹*Inst. of Life Sci., Kurume Univ.*, ²*Dept. of Biol. Sci., Grad. Sch. of Sci., Osaka Univ.*)

[2S2-3](#) 熱力学的解離速度分析法を用いた光化学系I三量体間の結合エネルギーの解析
Investigation on the thermodynamic dissociation kinetics of Photosystem I trimer to determine the binding strengths of each protomer
○河合 寿子¹, 金 恩哲² (¹山形大・理学部,²基生研)
Hisako Kawai¹, Eunuchul Kim² (¹*Fac. Sci., Univ. Yamagata*, ²*NIBB*)

[2S2-4](#) (1-15-1330) 細胞膜中の TRPV1・TRPV4 チャネルの 1 分子動態の比較解析
(1-15-1330) Comparative analysis of single-molecule dynamics of TRPV1 and TRPV4 channels in living cells
○柳川 正隆^{1,2}, 桑島 佑太郎^{1,3}, 阿部 充宏¹, 廣島 通夫^{1,4}, 上田 昌宏^{4,5}, 有田 誠^{3,6,7}, 佐甲 靖志¹
(¹ 理研 CPR, ² 科学技術振興機構, ³ 慶應大・院薬, ⁴ 理研 BDR, ⁵ 阪大・院生命機能, ⁶ 理研 IMS, ⁷ 横浜市大・院生命医科学)
Masataka Yanagawa^{1,2}, Yutaro Kuwashima^{1,3}, Mitsuhiro Abe¹, Michio Hiroshima^{1,4}, Masahiro Ueda^{4,5}, Makoto Arita^{3,6,7}, Yasushi Sako¹ (¹*Riken CPR*, ²*JST, PRESTO*, ³*Faculty Pharm., Keio Univ.*, ⁴*Riken BDR*, ⁵*Grad. Sch. Front. Biosci., Osaka University*, ⁶*Riken IMS*, ⁷*Grad. Sch. Med. Life Sci., Yokohama City Univ.*)

[2S2-5](#) マルチ機能性光受容膜タンパク質・ロドプシンによる生命機能の光制御
Optical control of biological activities with multi-functional photoreactive membrane protein rhodopsin
○須藤 雄気 (岡山大・院医歯薬)
Yuki Sudo (*Grad. Sch. Med. Dent. Pharm. Sci., Okayama Univ.*)

[2S2-6](#) (1-02-1506) Cryo-EM analysis provides new mechanistic insight into ATP binding to Ca²⁺-ATPase SERCA2b
Yuxia Zhang¹, Satoshi Watanabe¹, Akihisa Tsutsumi², Hiroshi Kadokura¹, Masahide Kikkawa², Kenji Inaba¹ (¹*Institute of Multidisciplinary Research for Advanced Materials, Tohoku University*, ²*Graduate School of Medicine, The University of Tokyo*)

[2S2-7](#) Rhythmic ATP release from the cyanobacterial circadian clock protein KaiC revealed by real-time monitoring of bioluminescence
Risa Mutoh¹, Takahiro Iida¹, Kiyoshi Onai² (¹*Fac. Sci., Fukuoka Univ.*, ²*Grad. Sch. Agr., Kyoto Univ.*)

おわりに
Closing Remarks

9:00~11:30 Ch03

2S3 共催：JST さきがけ「生命機能メカニズム解明のための光操作技術」
多様な光受容体とオプトジェネティクスの最前線
A variety of photoreceptors and the frontiers of optogenetics

オーガナイザー：徳富 哲 (大阪府立大学), 角田 聡 (名古屋工業大学)
Organizers: Satoru Tokutomi (Osaka Prefect. Univ.), Satoshi P Tsunoda (Nagoya Inst. Tech.)

Lives have acquired a variety of photoreceptors which absorb light in the UV to far red region during the evolution, such as many different types of rhodopsin, blue-light receptors, cryptochrome and phototropin, and red-far red-light reversible phytochromes. Researchers have adapted and utilized them for photobiological studies including optogenetics. The present Symposium introduces some leading results which includes channel rhodopsin in the trendy neuroscience, a novel function of mouse cryptochrome in circadian rhythm, use of a light-inactivated rhodopsin, peropsin, for vision restoration, photoregulation of protein kinase by phototropin, application of phytochrome-PIF and cryptochrome-CIB for optogenetics, and color tuning of cyanobacteriochrome.

はじめに

Opening Remarks

徳富 哲^{1,2,3} (¹JST さきがけ, ²大阪府大, ³東北大・植物園)

Satoru Tokutomi^{1,2,3} (¹*PRESTO, JST*, ²*Osaka Pref. Univ.*, ³*Bot. Garden, Tohoku Univ.*)

- [2S3-1](#) 海馬台からの経路選択的な情報送出：投射先を光同定した大規模活動計測による解析
Projection-identified large-scale recording reveals pathway-specific information outflow from the subiculum
○北西 卓磨^{1,2} (¹大阪市立大・院医, ²科学技術振興機構・さきがけ)
Takuma Kitanishi^{1,2} (¹Grad. Sch. Med., Osaka City Univ., ²PRESTO, JST)
- [2S3-2](#) 概日光受容の新規メカニズムと光遺伝学への応用
Mechanism of circadian photoreception and its application for optogenetics.
○平野 有沙, 高橋 徹, 櫻井 武 (筑波大・医学医療系)
Arisa Hirano, Tohru Takahashi, Takeshi Sakurai (*Faculty of Medicine, University of Tsukuba*)
- [2S3-3](#) 視覚再生に向けた暗活性・光不活性化 GPCR 型光遺伝学ツールの開発
Development of a dark-active, light-inactivated GPCR-based optogenetic tool for vision restoration
○永田 崇^{1,2} (¹東大・物性研究所, ²JST・さきがけ)
Takashi Nagata^{1,2} (¹Inst. Solid State Phys., Univ. Tokyo, ²JST, PRESTO)
- [2S3-4](#) Development of photoinactivatable protein kinases to manipulate plant cell growth
Hiromasa Shikata^{1,2} (¹Dev. Plant Environmental Responses, NIBB, ²PRESTO, JST)
- [2S3-5](#) 培養細胞、分裂酵母、線虫における細胞内シグナル伝達系の光操作
Optical control of cell signaling in cultured cells, fission yeast, and worms
○青木 一洋^{1,2} (¹自然科学研究機構・基生研, ²自然科学研究機構・生命創成探究センター)
Kazuhiro Aoki^{1,2} (¹NIBB, NINS, ²ExCELLS, NINS)
- [2S3-6](#) 多様なシアノバクテリオクロム光受容体の発見と改変
Discovery and engineering of diverse cyanobacteriochrome photoreceptors
○成川 礼 (都立大・院理学)
Rei Narikawa (*Grad. Scho. Biol. Sci., Tokyo Metro. Univ.*)

9:00~11:30 Ch04

2S4 共催：学術変革領域(A)「DNAの物性から理解するゲノムモダリティ」
ゲノム DNA の生物物理学～ゲノムモダリティの理解へ向けて～
Biophysics on Genome DNA - Toward Understanding of Genome Modality -

オーガナイザー：瀧ノ上 正浩 (東京工業大学), 高田 彰二 (京都大学), 前島 一博 (国立遺伝学研究所)
Organizers: Masahiro Takinoue (Tokyo Tech), Shoji Takada (Kyoto Univ.), Kazuhiro Maeshima (NIG)

The current trends in genome research, from genome sequencing to genome editing, have revolved based on the understanding of the informational aspects of genome, such as the replication and recombination of base sequences, and epigenetic regulation by histone modifications. However, the physical properties of genomic DNA as a polymer have not been fully elucidated yet, although it is an important property underlying all the phenomena caused on the genome. In this symposium, we will introduce a research area “Genome Modalities”, which aims to reveal the true nature of genomes through understanding the physical properties of DNA, and discuss this issue with researchers inside and outside this area.

はじめに
Opening Remarks

- [2S4-1](#) コヒーシンのリング構造とゲノム機能
Opening cohesin's ring structure is essential for genome functions
○西山 朋子 (名古屋大学・院理・生命理学)
Tomoko Nishiyama (*Grad. Sch. Sci., Nagoya Univ.*)
- [2S4-2](#) ゲノムフォールディングを制御する SMC タンパク質の構造・機能のシミュレーション研究
Computational approach to structures and dynamic functions of SMC proteins that organize genome folding
○高田 彰二 (京大・理)
Shoji Takada (*Kyoto Univ. Grad. Sch. Sci.*)
- [2S4-3](#) 一分子ヌクレオソームイメージングによって明らかにする生細胞のクロマチン環境とその外的影響
Chromatin behavior in living cells revealed by single-nucleosome imaging
○前島 一博^{1,2} (¹国立遺伝学研究所, ²総合研究大学院大学)
Kazuhiro Maeshima^{1,2} (¹*National Institute of Genetics, ²SOKENDAI*)
- [2S4-4](#) DNA 液滴の液-液相分離：ナノ～メソスケールの DNA 物性のゲノムモダリティ
Liquid-liquid phase separation of DNA liquid: Genome modality of DNA physics in nano-mesoscopic scale
○瀧ノ上 正浩^{1,2} (¹東工大・情報工学系, ²東工大・生命理工学系)
Masahiro Takinoue^{1,2} (¹*Dept. Computer Sci., Tokyo Tech, ²Dept. Life Sci. Tech., Tokyo Tech*)
- [2S4-5](#) 精子クロマチンの操作と測定
Manipulation and measurement of sperm chromatin
○岡田 由紀 (東大・定量研)
Yuki Okada (*IQB, Univ. Tokyo*)

おわりに

Closing Remarks

9:00～11:30 Ch05

2S5 統合的多階層アプローチによるシアノバクテリア生物時計システムの新展開
An Integrated Multi-scale Approach for Studying Cyanobacterial Circadian Clock System

オーガナイザー：秋山 修志 (分子科学研究所), 上久保 裕生 (奈良先端科学技術大学院大学)

Organizers: Shuji Akiyama (CIMoS), Hironari Kamikubo (NAIST)

Circadian rhythms are self-sustained oscillations with a period of approximately 24 h, enabling organisms to adapt to daily alterations in the environment. So far, many studies have investigated the time-measuring mechanism in the circadian clocks from bacteria to mammals. However, it remains unknown how the period is implemented in clock oscillators and kept unaffected against temperature changes (temperature compensation). In this symposium, we will focus especially on cyanobacterial circadian clock as a model system and address these questions using a multidisciplinary approach including, biophysics, structural biology, chronobiology, molecular biology, and protein engineering.

はじめに

Opening Remarks

- [2S5-1](#) シアノバクテリアの時計タンパク質 KaiC の 2 つの ATPase ドメインによる概日時計の機械式時計モデル
Mechanical clock model for cyanobacterial circadian clock, based on the activities of two ATPase domains in KaiC
○三輪 (伊藤) 久美子, 近藤 孝男 (名古屋大・院理)
Kumiko Ito-Miwa, Takao Kondo (*Grad. Sch. Sci., Univ. Nagoya*)
- [2S5-2](#) KaiABC 振動子における温度補償性と 1 分子レベルのフィードバックループ
Temperature compensation and single-molecular feedback loops in the KaiABC oscillator
○笹井 理生 (名古屋大学)
Masaki Sasai (*Nagoya University*)
- [2S5-3](#) 連続滴定小角 X 線散乱測定を用いたリン酸化/脱リン酸化 KaiC アンサンブルに対する KaiA の滴定挙動解析
Binding behavior of KaiA for phosphorylated/dephosphorylated KaiC ensemble using continuous titration small-angle X-ray scattering
○上久保 裕生^{1,2,3}, 山崎 洋一² (1 奈良先端大・デジタルグリーンイノベーションセンター,² 奈良先端大・物質創成,³ 物構研・高エネ機構)
Hironari Kamikubo^{1,2,3}, Yoichi Yamazaki² (¹*CDG, NAIST*, ²*MS, NAIST*, ³*IMSS, KEK*)
- [2S5-4](#) Exploring ancient origin of circadian oscillation through KaiC evolution
Atsushi Mukaiyama^{1,2}, Yoshihiko Furuike^{1,2}, Shuji Akiyama^{1,2} (¹*IMS, CIMoS*, ²*SOKENDAI*)
- [2S5-5](#) シアノバクテリア時計タンパク質 KaiC の根幹を成すアロステリック制御
Core Allosteric Regulation in Cyanobacterial Circadian Clock Protein KaiC
○古池 美彦^{1,2}, 向山 厚^{1,2}, 欧陽 東彦¹, 三輪 久美子³, シモン ダミアン^{1,2}, 山下 栄樹⁴, 近藤 孝男³ (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 名古屋大学大学院・理学研究科,⁴ 大阪大学・蛋白質研究所)
Yoshihiko Furuike^{1,2}, Atsushi Mukaiyama^{1,2}, Dongyan Ouyang¹, Kumiko Ito-Miwa³, Simon Damien^{1,2}, Eiki Yamashita⁴, Takao Kondo³ (¹*Research Center of Integrative Molecular Systems (CIMoS), Institute for Molecular Science*, ²*SOKENDAI (The Graduate University for Advanced Studies)*, ³*Graduate School of Science, Nagoya University*, ⁴*Institute for Protein Research, Osaka University*)

9:00~11:30 Ch06

2S6 蛋白質系の分子シミュレーションのサンプリング手法の発展

Advances in enhanced sampling methods for molecular simulations of protein systems

オーガナイザー：光武 亜代理 (明治大学), 奥村 久士 (生命創成探究センター)

Organizers: Ayori Mitsutake (Meiji Univ.), Hisashi Okumura (ExCELLS)

In recent years, it has become possible to perform molecular simulations on time scales of the order of milliseconds using special-purpose system and massive parallel computers. However, sampling methods that is about 10 to 100 times more efficient than ordinary molecular simulations are still important to investigate binding simulations and longer simulations. Since about 25 years ago, various sampling methods have been energetically introduced and developed into protein systems in Japan. Currently, many enhanced sampling methods are widely introduced in protein softwares such as AMBER, CHARMM, GENESIS, GEMB, GROMACS, NAMD, and myPresto. In this symposium, researchers who have originally developed sampling methods and applied to protein systems will give their talks.

趣旨説明

Opening Remarks

- [2S6-1](#) (2-01-1712) Extensive Sampling of Spike protein down, one-up, one-open, and two-up-like Conformations and Transitions in SARS-Cov-2
Hisham Dokainish¹, Suyong Re⁴, Chigusa Kobayashi², Takaharu Mori¹, Jaewoon Jung^{1,2}, Yuji Sugita^{1,2,3} (¹Theoretical Molecular Science Laboratory, Riken, ²Computational Biophysics Research Team, RIKEN, ³Laboratory for Biomolecular Function Simulation, RIKEN, ⁴Center for Drug Design Research, National Institutes of Biomedical Innovation)
- [2S6-2*](#) (2-03-1327) An estimation method for the diffusion coefficient using MD simulations with the basic cell containing only one protein as solute
Tomoya Iwashita¹, Masaaki Nagao¹, Akira Yoshimori², Masahide Terazima³, Ryo Akiyama¹ (¹Department of Chemistry, Graduate School of Science, Kyushu University, ²Department of Physics, Niigata University, ³Department of Chemistry, Graduate School of Science, Kyoto University)
- [2S6-3](#) Oligomer formation of proteins studied by generalized-ensemble algorithms
Satoru G. Itoh^{1,2,3} (¹IMS, ²ExCELLS, ³SOKEKENDAI)
- [2S6-4](#) 大規模タンパク質系への適用を目指した構造サンプリング法の開発
Enhanced sampling methods targeting at large proteins
○森次 圭 (横浜市大院・生命医科学)
Kei Moritsugu (*Grad. Sch. Med. Life Sci., Yokohama City Univ.*)
- [2S6-5](#) マルチドメインタンパク質のリガンド結合による構造変化の分子機構
Molecular mechanisms underlying ligand-induced conformational changes in multi-domain proteins
○杉田 有治^{1,2,3} (¹理研・開拓研究本部, ²理研・計算科学研究センター, ³理研・生命機能科学研究センター)
Yuji Sugita^{1,2,3} (¹RIKEN CPR, ²RIKEN R-CCS, ³RIKEN BDR)
- [2S6-6](#) 膜に埋もれたヒトエンドセリン受容体に結合するボセンタンの結合メカニズム：スライドするフライ・キャストイングと配向選択メカニズム
Sliding fly-casting and directional-selection mechanisms of bosentan binding to human endothelin receptor embedded in membrane
○肥後 順一 (兵庫県立大学情報科学研究科)
Junichi Higo (*Graduate School of Information Science, University of Hyogo*)
- [2S6-7](#) 生体分子シミュレーションのための拡張アンサンブル法
Generalized-ensemble algorithms for biomolecular simulations
○岡本 祐幸 (名大・院理)
Yuko Okamoto (*Graduate School of Science, Nagoya Univ.*)

オーガナイザー：中瀬 生彦（大阪府立大学），矢野 義明（武庫川女子大学）

Organizers: Ikuhiko Nakase (Osaka Prefect. Univ.), Yoshiaki Yano (Mukogawa Women's Univ.)

Biological membranes have a complex supermolecular bilayer structure composed of diverse biomolecules such as lipids, proteins, and sugars. It is well known that biomembranes contain receptor proteins to detect changes in external environments, and their ligand molecules are available for controlling cell functions. Moreover, alternative approaches are possible to artificially perturb function of biomembranes by e.g., changing their shape, permeability, and domain structures following molecular interactions with lipids. New approaches using hybrid/designed molecules, model membranes, ultrafast spectroscopy, and chemistry on/in cells, will be introduced to discuss complex membrane functions with biophysical communications and their usefulness for molecular sensing and controlling cell functions.

はじめに

Opening Remarks

- [2S7-1](#) (1-10-1442) Local membrane curvature influences lipid signaling
Marcel Hoerning¹, Torsten Bullmann², Tatsuo Shibata³ (¹*Institute of Biomaterials and Biomolecular Systems, University of Stuttgart, 70569 Stuttgart, Germany*, ²*Carl-Ludwig-Institute for Physiology, University of Leipzig, 04103 Leipzig, Germany*, ³*Laboratory for Physical Biology, RIKEN Center for Biosystems Dynamics Research, Kobe 650-0047, Japan*)
- [2S7-2](#) Chemical tools for manipulating signaling proteins and lipids on organelle membranes
Shinya Tsukiji (*Grad. Sch. Eng., Nagoya Inst. Tech.*)
- [2S7-3](#) A common oligomer identified using 2D IR spectroscopy in mammals that contract type 2 diabetes
Martin Zanni (*University of Wisconsin-Madison*)
- [2S7-4](#) 膜貫通ペプチドを用いたナノポアの新規設計
 De novo design of nanopore using transmembrane peptides
 ○川野 竜司（東京農工大学・院生命工学）
Ryuji Kawano (*Department of Biotechnology and Life Science, Tokyo University of Agriculture and Technology*)
- [2S7-5](#) 生体膜機能の理解に向けた脂質－膜タンパク質相互作用解析
 Interaction analysis between membrane proteins and lipids to understand biological membranes
 ○松森 信明（九大・院理）
Nobuaki Matsumori (*Grad. Sch. Sci., Kyushu Univ.*)
- [2S7-6](#) スマートシャペロン高分子による脂質膜の刺激応答性小胞・シート転移
 Stimuli-responsive vesicle/sheet transformation of lipid membranes mediated by smart chaperone polymers
 ○丸山 厚（東工大・生命理工）
Atsushi Maruyama (*School of Life Sci. & Tech., Tokyo Inst. of Tech.*)

[2S7-7](#) 弱毒化カチオン性両親媒性ペプチド存在下のIgGによる液滴形成と効率的細胞内移行
Liquid droplet formation and facile cytosolic translocation of IgG in the presence of attenuated cationic amphiphilic lytic peptides
○二木 史朗 (京大・化研)
Shiroh Futaki (*Inst. Chem. Res., Kyoto Univ.*)

おわりに
Closing Remarks

3日目 (11月27日(土)) / Day 3 (Nov. 27 Sat.)

9:00~11:30 Ch02
3S1 オーストラリアー日本交流シンポジウム
ASB-BSJ Joint Symposium

オーガナイザー：片山 耕大 (名古屋工業大学), Matthew AB Baker (Univ. of New South Wales)
Organizers: Kota Katayama (Nagoya Inst. of Tech.), **Matthew AB Baker** (Univ. of New South Wales)

This symposium aims at highlighting the current main stream topics in protein science and biophysics and also searching for the collaboration and development in research filed of biophysics in the Japan-Australia region. The symposium includes three up-and-coming young researchers related to biophysics from the ASB and BSJ sides. With the rapid progress of science and technology in recent years, through this constructive discussion, we wish to keep the scientific activity, and to give a large impact to the community.

はじめに
Opening Remarks

[3S1-1](#) Cyclodextrins increase membrane tension and are universal activators of mechanosensitive channels
Charles David Cox (*Victor Chang Cardiac Research Institute, Sydney*)

[3S1-2](#) Understanding the interaction of phenolic acids with phospholipid bilayers
Sheik Imamul Hossain¹, **Evelyne Deplazes**^{1,2} (¹*School of Life Sciences, University of Technology Sydney, Australia*, ²*School of Chemistry and Molecular Biosciences, University of Queensland, Australia*)

[3S1-3](#) Structural analyses on pathogenic RNA viruses
Yukihiko Sugita^{1,2} (¹*InFront, Kyoto Univ.*, ²*Hakubi Center, Kyoto Univ.*)

[3S1-4](#) 酵母複製とプリオン伝送の多スケール運動・空間モデル
A multi-scale kinetic and spatial model of yeast replication and prion transmission
○Hall Damien (金沢大学 WPI-NANO-LSI)
Damien Hall (*Kanazawa University WPI-NANO-LSI*)

[3S1-5](#) 合成小分子を利用した細胞内タンパク質の光操作
Chemo-optogenetic manipulation of protein functions in living cells using synthetic small molecules
○吉井 達之 (京都大学 iPS 細胞研究所)
Tatsuyuki Yoshii (*CiRA, Kyoto Univ.*)

おわりに
Closing Remarks

9:00~11:30 Ch02

3S2 共催：学術変革領域研究(B)「パラメトリック翻訳」
パラメトリックな翻訳調節機構
Parametric biology based on translation rate regulatory mechanism

オーガナイザー：岡部 弘基（東京大学），原田 慶恵（大阪大学）

Organizers: Kohki Okabe (The Univ. of Tokyo), Yoshie Harada (Osaka Univ.)

Translation is not just a linear bridge between mRNA and protein, but is highly variable and characterized by a wide dynamic range (1,000 times that of transcription), local control within the cell, and reactions that consume up to 50% of the energy in the cell. This raises the possibility that translation is not controlled by 0 or 1 on/off control, but is subtly controlled by "rate variation" within a continuous reaction. Currently, we are beginning to create a translation parametric biology that focuses on the concept of "variable translation rate. This will elucidate its role in the flexible functional control of life.

[3S2-1](#) A specific eIF4A paralog facilitates LARP1-mediated translation repression during mTORC1 inhibition
Shintaro Iwasaki (*RIKEN Cluster for Pioneering Research*)

[3S2-2](#) 人工神経回路組織における神経回路とタンパク質合成制御
Organoids-on-a-chip models for understanding neuronal circuits and underlying protein synthesis regulations
○池内 与志穂^{1,2,3} (¹東大・生産研, ²東大・院工・化生, ³東大・Beyond AI 研究機構)
Yoshiho Ikeuchi^{1,2,3} (¹IIS, Univ. Tokyo, ²Chem. Bio., Eng., Univ. Tokyo, ³Inst. AI and Beyond, Univ. Tokyo)

[3S2-3](#) 生理的体温変化による体内時計のパラメトリック制御
Parametric entrainment of the circadian clock by body temperature change
○三宅 崇仁, 井ノ上 雄一, 土居 雅夫 (京都大学・院薬)
Takahito Miyake, Yuich Inoue, Masao Doi (*Grad. Sch. Pharm. Sci., Kyoto Univ.*)

[3S2-4](#) Fluorescent nanodiamonds for thermal biology
Shingo Sotoma¹, Yoshie Harada^{1,2} (¹IPR, Osaka Univ., ²QIQB, Osaka Univ.)

[3S2-5](#) 細胞内温度シグナリングによる翻訳調節機構
Intracellular thermal signaling facilitates translation control
○岡部 弘基^{1,2} (¹東京大学大学院薬学系研究科, ²JST さきがけ)
Kohki Okabe^{1,2} (¹Grad. Sch. Pharm. Sci., Univ. Tokyo, ²PRESTO, JST)

9:00~11:30 Ch03

3S3 タンパク質の水とその凍結現象 -細胞凍結や食品冷凍保存への応用-
Protein hydration and its freezing phenomena -toward the application for cell freezing and frozen food storage-

オーガナイザー：山本 直樹（自治医科大学），中川 洋（日本原子力研究開発機構）

Organizers: Naoki Yamamoto (Jichi Medical Univ.), Hiroshi Nakagawa (J-PARC)

Protein hydration water is crucial for the activation of the dynamics related to the protein functional expression. We introduce recent progress on the understanding of the interplay between hydration water and protein in terms of the freezing of hydration water. Recent experimental results obtained by broadband dielectric spectroscopy and neutron scattering on proteins and tissues will be reported. Furthermore, present recent progress in the understanding the cell-freezing and food frozen storage will be represented. Especially, polymeric cryoprotectants, which have low toxicity and high protection capability, will be introduced and its physicochemical property will be discussed.

はじめに

Opening Remarks

[3S3-1](#) 誘電緩和分光法で観測する水和角質層中の水と氷

Water and ices in hydrated stratum corneum observed via dielectric relaxation spectroscopy

○中西 真大（福岡工業大・工学部）

Masahiro Nakanishi (*Fac. Eng., Fukuoka Inst. Tech.*)

[3S3-2](#) 中性子散乱を用いて明らかとなった水和水の熱活性がタンパク質ダイナミクスに与える影響

Effect of hydration and its thermal energy on protein dynamics monitored by neutron scattering

○山本 直樹（自治医大・医）

Naoki Yamamoto (*Sch. Med., Jichi Med. Univ.*)

[3S3-3](#) 生体分子と水の凍結・融解・ガラス転移

Freezing, Thawing and Glass Transition of Biomolecules and Water

○中川 洋（日本原子力研究開発機構）

Hiroshi Nakagawa (*Japan Atomic Energy Agency*)

[3S3-4](#) Polyampholytes for low-temperature preservation of cells and proteins

Robin Rajan, Kazuaki Matsumura (*Japan Advanced Institute of Science and Technology*)

おわりに

Closing Remarks

オーガナイザー：齋尾 智英 (徳島大学), 井上 倫太郎 (京都大学)

Organizers: Tomohide Saio (Tokushima Univ.), Rintaro Inoue (Kyoto Univ.)

Large scale dynamics” (LS-dynamics) such as domain-domain correlation motion, often drives protein activity, but the scarcity of the information regarding them impedes the understanding of the mechanism. In other words, the LS-dynamics of protein is still a frontier in protein science. Everyone recognizes that, although state-of-the-art techniques provide the knowledge of various aspects of LS-dynamics, only a single method could not adequately cover the ranges of length and time scales required for the LS-dynamics. Hence, agenda are how to integrate their results and build the full picture of LS-dynamics. In this symposium, young scientists from variety of scientific fields, solution scattering, NMR, cryo-EM, and computation, will lead to discuss about the integration of their methods aiming to unveil the biologically significant LS-dynamics.

はじめに

Opening Remarks

[3S4-1](#) KEK クライオ電顕施設の運用と現状について

Operation and recent activities of the cryo-EM facility in KEK

○安達 成彦 (高エネ機構・物構研・構造生物)

Naruhiko Adachi (*SBRC, IMSS, KEK*)

[3S4-2](#) X線小角散乱データと粗視化分子動力学計算に基づく生体分子の構造ダイナミクスの解明

Modeling structural dynamics of biomolecules using small angle X-ray scattering data and coarse-grained molecular dynamics simulations

○清水 将裕, 奥田 綾, 守島 健, 柚木 康弘, 佐藤 信浩, 井上 倫太郎, 裏出 令子, 杉山 正明 (京大・複合研)

Masahiro Shimizu, Aya Okuda, Ken Morishima, Yasuhiro Yunoki, Nobuhiro Sato, Rintaro Inoue, Reiko Urade, Masaaki Sugiyama (*KURNS, Kyoto Univ.*)

[3S4-3](#) NMR と EPR を組み合わせたマルチドメインタンパク質の大規模ダイナミクスの探索

Large-scale conformational distribution of a multi-domain protein enzyme investigated by NMR and EPR

○齋尾 智英 (徳島大・先端酵素)

Tomohide Saio (*Inst. of Adv. Med. Sci.*)

[3S4-4](#) X線/中性子散乱と MD シミュレーションを用いた統合的アプローチによる IDP の動的構造と機能の理解

Integrated approach using X-ray/Neutron scattering and MD simulation for understanding dynamic structure and function of IDP

○小田 隆^{1,2} (¹立教大学理学部生命理学科, ²横浜市立大学大学院生命医科学研究科)

Takashi Oda^{1,2} (¹*Department of Life Science, Rikkyo University,*, ²*Graduate School of Medical Life Science, Yokohama City University*)

[3S4-5](#) ストレス刺激により誘起される ATP 枯渇および低 pH 条件における MAPK p38 α の頑強な酵素活性を担う機能的構造平衡の解明
Functional equilibrium underlying the robust kinase activity of MAPK p38 α under the stress-associated ATP-depleted, low pH condition
○徳永 裕二¹, 竹内 恒¹, 高橋 栄夫², 嶋田 一夫³ (¹産総研・細胞分子工学,²横浜市・生命医科学,³理研・鶴見)
Yuji Tokunaga¹, Koh Takeuchi¹, Hideo Takahashi², Ichio Shimada³ (¹*CMB, AIST*, ²*Grad. Sch. Med. Life Sci., Yokohama City Univ.*, ³*Tsurumi Inst., Riken*)

おわりに
Closing Remarks

9:00~11:30 Ch05

3S5 ペプチド-膜生物物理学：膜結合抗菌ペプチドおよびアミロイドペプチドの最新生物物理研究
Peptide-Membrane Biophysics: Current Biophysical Studies of Membrane-bound Antimicrobial Peptides and Amyloid Peptides

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 Natl. Univ.), Tomoyasu Aizawa (Hokkaido Univ.)

In the biophysical research field, the structure and dynamics of peptide and lipid molecules within complex biomolecular assemblies have been investigated for many years with a special focus on membrane-interaction of antimicrobial peptides (AMPs) and kinetics of amyloid fibril formation. In this symposium, current research topics on "peptide-membrane biophysics" by imaging, NMR, and computational methods will be presented. Additionally, advanced over-expression technology and deep learning for molecular design of AMPs will be presented.

はじめに
Opening Remarks

[3S5-1](#) 遺伝子組換え抗菌ペプチド生産と NMR 解析への応用
Application of novel overexpression systems of recombinant antimicrobial peptides for NMR analysis
○相沢 智康（北大・院生命科学）
Tomoyasu Aizawa (*Grad. Sch. Life Sci., Hokkaido Univ.*)

[3S5-2](#) AI で設計した膜貫通ペプチドの分子動力学計算による選択と理解
Using molecular dynamics simulations to prioritize and understand AI-generated cell penetrating peptides
○津田 宏治（東大・新領域）
Koji Tsuda (*Grad. Sch. Frontier Sci., Univ. Tokyo*)

[3S5-3](#) 単一巨大リポソーム法や単一細胞実験から解明された抗菌ペプチドの作用機構
Modes of Action of Antimicrobial Peptides (AMPs) revealed by the Single Giant Unilamellar Vesicle (GUV) Method and Single Cell experiments
○山崎 昌一^{1,2,3} (¹静大・電研,²静大・創造院・統合バイオ,³静大・院理)
Masahito Yamazaki^{1,2,3} (¹*Res. Inst. Ele., Shizuoka Univ.*, ²*Grad. Sch. Sci. Tech., Shizuoka Univ.*, ³*Grad. Sch. Sci., Shizuoka Univ.*)

[3S5-4*](#) (2-10-1351) 放射光円二色性・直線二色性・蛍光異方性により明確化された生体膜に誘起されたマガイニン 2 β 凝集体の特徴
(2-10-1351) Membrane-Induced β -Aggregates of Magainin 2 Characterized by Circular Dichroism, Linear Dichroism, and Fluorescence Anisotropy
○熊代 宗弘¹, 末永 翔磨¹, 松尾 光一² (¹ 広大・院理学, ² 広大・放射光)
Munehiro Kumashiro¹, Shoma Suenaga¹, Koishi Matsuo² (¹*Grad. Sch. Sci., Hiroshima Univ.*, ²*HiSOR, Hiroshima Univ.*)

[3S5-5](#) Conformational plasticity defines cell permeabilization activity of cyclic peptides
Koh Takeuchi^{1,2} (¹*CMB, AIST*, ²*Grad. Sch. Pharm. Sci., The Univ. of Tokyo*)

[3S5-6](#) アミロイド β ペプチドの凝集と解離の分子動力学シミュレーション
Molecular Dynamics Simulations for Aggregation and Disaggregation of Amyloid- β Peptides
○奥村 久士^{1,2,3} (¹ 生命創成探究センター, ² 分子科学研究所, ³ 総研大)
Hisashi Okumura^{1,2,3} (¹*Exploratory Research Center on Life and Living Systems*, ²*Institute for Molecular Science*, ³*SOKENDAI*)

[3S5-7](#) 膜環境におけるアミロイド β の分子集合
Molecular assembly of amyloid- β in membrane environments
○矢木 真穂^{1,2} (¹ 自然科学研究機構・生命創成探究セ, ² 自然科学研究機構・分子研)
Maho Yagi-Utsumi^{1,2} (¹*ExCELLS, NINS*, ²*IMS, NINS*)

9:00~11:30 Ch06

3S6 ライブセルイメージングと融合した機能的オミクス解析の新潮流
New Trends in Functional Omics Analysis Integrated with Live Cell Imaging

オーガナイザー：白崎 善隆（東京大学），城口 克之（理化学研究所）

Organizers: Yoshitaka Shirasaki (The Univ. of Tokyo), Katsuyuki Shiroguchi (RIKEN)

Cells change their function from time to time based on the alteration of their gene expression. Live cell imaging is an excellent technique for tracking the cellular functions, though it has limited targets. On the other hand, omics analyses such as high-throughput sequencing and mass spectrometry have advantages for comprehensiveness on gene expression analysis, although they cannot obtain time-series information due to disruptive manipulations. In this symposium, we will focus on advanced single-cell technologies that bridge the gap between time-series and comprehensive information on dynamic cellular functions, and will discuss the future prospects of this field.

はじめに

Opening Remarks

[3S6-1](#) SCOPE-seq: Scalable Technology for Linking Live Cell Imaging and Single-Cell RNA-seq
Peter Sims (Columbia University)

[3S6-2](#) (2-15-1736) 微小電気穿孔法を用いた細胞膜の機械特性と遺伝子発現の統合解析
(2-15-1736) A combined analysis of membrane-mechanical phenotyping and transcriptomics using nanoelectroporation
○塩見 晃史, 金子 泰洗ポール, 西川 香里, 新宅 博文（理研・開拓・白眉）
Akifumi Shiomi, Taikopaul Kaneko, Kaori Nishikawa, Hirofumi Shintaku (*Hakubi, CPR, RIKEN*)

- [3S6-3](#) 免疫細胞の活性化の瞬間を視て採って調べる
Analysis of Gene Expression at the Moment of Immune Cell Activation by Live Cell Imaging & Harvesting
○白崎 善隆 (東京大学・院薬)
Yoshitaka Shirasaki (*Grad.Sch.Pharm., Univ. Tokyo*)
- [3S6-4](#) 超高速流体制御が拓くオンチップ細胞操作・計測
On-chip cell manipulation and analysis opened up by ultra-high-speed flow control
○佐久間 臣耶 (九大・機械工学部門)
Shinya Sakuma (*Dept. of Mechanical Engineering, Kyushu University*)
- [3S6-5](#) 1細胞メタボローム・プロテオーム解析への挑戦
Challenge to single-cell metabolome and proteome analyses
○和泉 自泰¹, 中谷 航太¹, 秦 康祐¹, 山村 昌平², 松本 雅記³, 馬場 健史¹ (¹九州大学生体防御医学研究所, ²産業技術総合研究所健康医工学研究部門, ³新潟大学大学院医歯学総合研究科)
Yoshihiro Izumi¹, Kohta Nakatani¹, Kosuke Hata¹, Shohei Yamamura², Masaki Matsumoto³, Takeshi Bamba¹ (¹*Medical Institute of Bioregulation, Kyushu University*, ²*Health and Medical Research Institute, National Institute of Advanced Industrial Science and Technology*, ³*Graduate School of Medical and Dental Sciences, Niigata University*)
- [3S6-6](#) Decoding single-cell transcriptomic states from cell images enabled by robotic data acquisition and deep learning
Jianshi Jin, Katsuyuki Shiroguchi (*BDR, RIKEN*)

おわりに

Closing Remarks

1 日目 (11 月 25 日 (木)) / Day 1 (Nov. 25 Thu.)

13:30~15:30 Ch01

1G01 タンパク質：設計Ⅰ、一般Ⅰ

Protein: Design I, General I

座長：谷中 冴子 (分子科学研究所), 加藤 晃一 (分子科学研究所)

Session Chairs: Sacko Yanaka (IMS), Koichi Kato (IMS)

- [1-01-1330](#) SARS-CoV-2 変異株に有効な中和抗体の理論的設計
Theoretical design of neutralizing antibodies that are effective for SARS-CoV-2 variants
○青山 莉奈¹, 松本 彩里¹, 林 勇樹¹, 新井 宗仁^{1,2} (¹東大・総合文化・生命環境, ²東大・理・物理)
- Rina Aoyama¹**, Sairi Matsumoto¹, Yuuki Hayashi¹, Munchito Arai^{1,2} (¹*Dept. Life Sci., Univ. Tokyo*, ²*Dept. Phys., Univ. Tokyo*)
- [1-01-1342](#) Relationship between designability of proteins and frustration : A lattice model study
Kazuma Toko, George Chikenji (*Dept. of App. Phys., Nagoya Univ.*)
- [1-01-1354](#) アルカン合成酵素の高活性化変異体の合理的設計
Rational design of highly active mutants of an alkane-producing enzyme
○磯田 正覚¹, 林 勇樹^{1,2}, 新井 宗仁^{1,2,3} (¹東大・教養・統合自然, ²東大・総合文化・生命環境, ³東大・理・物理)
- Masaaki Isoda¹**, Yuuki Hayashi^{1,2}, Munchito Arai^{1,2,3} (¹*Dept. Integ. Sci., Univ. Tokyo*, ²*Dept. Life Sci., Univ. Tokyo*, ³*Dept. Physics, Univ. Tokyo*)
- [1-01-1406](#) 緑色蛍光蛋白質由来赤色蛍光蛋白質の開発
Engineering of a coral green fluorescent protein into red
○今村 博臣¹, 大坪 史歩², 西田 水穂¹, 竹川 宜宏², 今田 勝巳² (¹京大・院・生命科学, ²阪大・院理・高分子科学)
- Hiromi Imamura¹**, Shiho Otsubo², Mizuho Nishida¹, Norihiro Takekawa², Katsumi Imada² (¹*Grad. Sch. Biost., Kyoto Univ.*, ²*Dept. Macromol. Sci., Grad. Sch. Sci., Osaka Univ.*)
- [1-01-1418](#) 緑色蛍光蛋白質 AzamiGreen 由来赤色蛍光蛋白質の結晶構造解析に基づく赤色蛍光団形成の構造基盤
Structural basis of red chromophore formation based on crystal structures of artificial red fluorescent proteins derived from AzamiGreen
○大坪 史歩¹, 今村 博臣², 竹川 宜宏¹, 今田 勝巳¹ (¹阪大・院理・高分子科学, ²京大・院・生命科学)
- Shiho Otsubo¹**, Hiromi Imamura², Norihiro Takekawa¹, Katsumi Imada¹ (¹*Dept. Macromol. Sci., Grad. Sch. Sci., Osaka Univ.*, ²*Grad. Sch. Biost., Kyoto Univ.*)
- [1-01-1430](#) The register shift rules for $\beta\alpha\beta$ -motifs for de novo protein design: A database analysis and all-atom calculations
Senji Mishima, George Chikenji, Hiroto Murata (*Dept. of App. Phys., Nagoya Univ.*)
- [1-01-1442](#) The Effect of Molecular Weight on the Formation of Fibroin Precursor and Nanofiber
Kok Sim Chan¹, Kento Yonezawa², Takehiro Sato³, Yoichi Yamazaki¹, Sachiko Toma-Fukai¹, Hironari Kamikubo^{1,2,4} (¹*Division 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.*, ⁴*Institute of Materials Structure Science, High Energy Accelerator Research Organization (KEK)*)

- [1-01-1454](#) ペリプラズム結合蛋白質 AcfC と協働するコレラ菌定化性受容体 Mlp8 のリガンド認識機構
Ligand recognition mechanism of Mlp8, a chemoreceptor protein of *Vibrio cholera*, with AcfC, a periplasmic binding protein
○敷中 柚輝¹, 高橋 洋平¹, 都築 侑果¹, 竹川 宜宏¹, 西山 宗一郎², 田島 寛隆³, 川岸 郁朗³, 今田 勝巳¹ (¹ 阪大・院理・高分子科学, ² 新潟薬大・応用生命, ³ 法政大・生命科学)
Yuzuki Yabunaka¹, Yohei Takahashi¹, Yuka Tsuzuki¹, Norihiro Takekawa¹, So-ichiro Nishiyama², Hirotaaka Tajima³, Ikuro Kawagishi³, Katsumi Imada¹ (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.*)
- [1-01-1506](#) 光誘導可能な液滴への閉じ込めによる多酵素反応の活性化
Facilitating a two-step enzymatic reaction by trapping two enzymes in light-inducible droplets
○大窪 理仁¹, 林 勇樹¹, 新井 宗仁^{1,2} (¹ 東大・院総合文化研究科, ² 東大・院理学系研究科)
Rihito Okubo¹, Yuuki Hayashi¹, Munchito Arai^{1,2} (¹*Dept. Life Sci., Univ. Tokyo*, ²*Dept. Phys., Univ. Tokyo*)
- [1-01-1518](#) Analysis of differences in the number of β -sheet structures that have different β -strand's connections and orientations
Takumi Nishina, George Chikenji (*Dept. of App. Phys., Nagoya univ*)

13:30~15:30 Ch02

1G02 タンパク質：構造 I
Protein: Structure I

座長：岩崎 憲治 (筑波大学), 村田 武士 (千葉大学)

Session Chairs: Kenji Iwasaki (Univ. of Tsukuba), Takeshi Murata (Chiba Univ.)

- [1-02-1330](#) Structural analysis of monomeric photosystem II at 2.78 Å resolution using Cryo-electron microscopy
Huaxin Yu^{1,2}, Tasuku Hamaguchi³, Yoshiki Nakajima¹, Keisuke Kawakami³, Fusamichi Akita^{1,4}, Koji Yonekura^{3,5,6}, Jian-Ren Shen¹ (¹*Research Institute for Interdisciplinary Science and Graduate School of Natural Science and Technology, Okayama University*, ²*Department of Picobiology, Graduate School of Life Science, University of Hyogo*, ³*Biostructural Mechanism Laboratory, RIKEN SPring-8 Center*, ⁴*Japan Science and Technology Agency, PRESTO*, ⁵*Institute of Multidisciplinary Research for Advanced Materials, Tohoku University*, ⁶*Advanced Electron Microscope Development Unit, RIKEN-JEOL Collaboration Center, RIKEN Baton Zone Program*)
- [1-02-1342](#) High-resolution single-particle cryo-EM analyses with a CFE electron beam
Tasuku Hamaguchi¹, Keisuke Kawakami¹, Saori Maki-Yonekura¹, Koji Yonekura^{1,2} (¹*RIKEN SPring-8 Center*, ²*IMRAM, Tohoku Univ.*)
- [1-02-1354](#) Cryo-EM Structure of K⁺-Bound hERG Channel Complexed with the Blocker Astemizole
Tatsuki Asai¹, Naruhiko Adachi², Toshio Moriya², Hideyuki Oki³, Takamitsu Maru³, Masato Kawasaki², Kano Suzuki¹, Sisi Chen¹, Ryohei Ishii⁴, Kazuko Yonemori⁵, Shigeru Igaki⁵, Satoshi Yasuda^{1,6}, Satoshi Ogasawara^{1,6}, Toshiya Senda², Takeshi Murata^{1,6} (¹*Grad. Sch. Sci., Univ. Chiba*, ²*Tsukuba, KEK*, ³*Axelead Drug Discovery Partners, Inc.*, ⁴*Daiichi Sankyo RD Novare Co., Ltd.*, ⁵*Takeda Pharmaceutical Co., Ltd.*, ⁶*Molecular Chirality Research Center, Univ. Chiba*)
- [1-02-1406](#) クライオ電子顕微鏡単粒子解析と分子動力学シミュレーションを用いた ATP13A2 のポリアミン輸送機構の解明
Cryo-EM structures and MD simulations of ATP13A2 reveal transport mechanism of polyamines
○富田 篤弘¹, 大保 貴嗣², 西澤 知宏³, 瀧木 理¹ (¹ 東大・院理学, ² 旭川医大・医学, ³ 横浜市大・院生命医科学)
Atsuhiko Tomita¹, Takashi Daiho², Tomohiro Nishizawa³, Osamu Nreki¹ (¹*Grad. Sch. Sci., Univ. Tokyo*, ²*Dept. of Med., Asahikawa Medical Univ.*, ³*Grad. Sch. Sci., Yokohama City Univ.*)

- [1-02-1418](#) 鉄硫黄クラスターの構造と酵素活性の相関解析による tRNA 硫黄修飾機構の解明
Reaction mechanism of tRNA thiolation revealed by correlation analysis between the structure of Fe-S clusters and the enzymatic activity
○石坂 優人¹, 陳 明皓², 奈良井 峻¹, 堀谷 正樹³, 田中 良和^{2,4}, 姚 閔^{1,2} (¹ 北大・院生命, ² 北大・院先端生命, ³ 佐賀大・農, ⁴ 東北大・院生命)
Masato Ishizaka¹, Minghao Chen², Shun Narai¹, Masaki Horitani³, Yoshikazu Tanaka^{2,4}, Min Yao^{1,2} (¹*Grad. Sch. Life Sci., Hokkaido Univ.*, ²*Fac. Adv. Life Sci., Hokkaido Univ.*, ³*Fac. Agri., Saga Univ.*, ⁴*Grad. Sch. Life Sci., Tohoku. Univ.*)
- [1-02-1430](#) Overexpression of stable isotope-labeled cecropin P1 by using calmodulin-fusion protein system and structure analysis by NMR
Hao Gu¹, Takasumi Kato¹, Hiroyuki Kumeta¹, Hiroaki Ishida², Yasuhiro Kumaki¹, Takashi Tsukamoto¹, Takashi Kikukawa¹, Makoto Demura¹, Hans J. Vogel², Tomoyasu Aizawa¹ (¹*Graduate School of Life Science, Hokkaido University*, ²*Department of Biological Sciences, University of Calgary*)
- [1-02-1442](#) Structurer of a pentameric complex of MotA, a bacterial flagellar stator protein, from *Aquifex aeolicus* by single particle cryo-EM
Tatsuro Nishikino¹, Norihiro Takekawa², Jun-ichi Kishikawa¹, Mika Hirose¹, Michio Homma³, Takayuki Kato¹, Katsumi Imada² (¹*IPR., Osaka Univ.*, ²*Dept. of Macromol. Sci., Grad. Sch. of Sci., Osaka Univ.*, ³*Div. Biol. Sci. Grad. Sch. Sci., Nagoya Univ*)
- [1-02-1454](#) 蛍光寿命測定による脂質二重膜結合状態における α -Synuclein の立体構造解析
Structural analysis of α -Synuclein in the lipid bilayer bound state by fluorescence lifetime measurements
○笹田 航, 松原 亮介, 藤井 宏一, 木村 哲就 (神戸大・院理・化学)
Ko Sasada, Ryosuke Matsubara, Koichi Fujii, Tetsunari Kimura (*Grad. Sch. Sci., Kobe Univ*)
- [1-02-1506](#) (2S2-6) Cryo-EM analysis provides new mechanistic insight into ATP binding to Ca²⁺-ATPase SERCA2b
Yuxia Zhang¹, Satoshi Watanabe¹, Akihisa Tsutsumi², Hiroshi Kadokura¹, Masahide Kikkawa², Kenji Inaba¹ (¹*Institute of Multidisciplinary Research for Advanced Materials, Tohoku University*, ²*Graduate School of Medicine, The University of Tokyo*)
- [1-02-1518](#) CW-ESR 分光法によるヌクレオチド結合型 ABC トランスポーターの構造解析
Structural analyses of ABC transporters in nucleotide bound states investigated by CW-ESR spectroscopy
○仲 絢香¹, 小堀 康博^{1,2}, 鏑木 基成¹, 基成 宜嗣³, 杉本 宏⁴, 木村 哲就¹ (¹ 神戸大・院理, ² 神戸大・分子フォト, ³ 兵庫県大・院生命理学, ⁴ 理研・SPRING-8)
Ayaka Naka¹, Yasuhiro Kobori^{1,2}, Motonari Tsubaki¹, Yoshitsugu Shiro³, Hiroshi Sugimoto⁴, Tetsunari Kimura¹ (¹*Grad. Sch. Sci., Kobe Univ.*, ²*Mol. Photo. Res. Cent., Kobe Univ.*, ³*Grad. Sch. Sci., Univ. Hyogo*, ⁴*SPRING-8, RIKEN*)

13:30~15:30 Ch03
1G03 タンパク質：計算 I
Protein: Simulation I

座長：菊地 武司 (立命館大学), 寺田 透 (東京大学)

Session Chairs: Takeshi Kikuchi (Ritsumeikan Univ.), Terada Tohru (Univ. of Tokyo)

- [1-03-1330](#) Implementation of residue level coarse-grained models in GENESIS
Cheng Tan¹, Jaewoon Jung^{1,2}, Chigusa Kobayashi¹, 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*)

- [1-03-1342](#) 粗視化シミュレーションと SAXS データに基づくヘテロクロマチンタンパク HP1 α の構造モデリング
Structural modeling of the heterochromatin protein 1 alpha (HP1 α) based on coarse-grained MD simulations and SAXS data
○根上 樹¹, 古川 亜矢子², 米澤 健人³, 安達 成彦³, 千田 俊哉³, 清水 伸隆³, 西村 善文^{2,4}, 寺田 透¹ (¹東大・院農,²横浜市大・生命,³高エネ機構・物構研,⁴広島大・統合生命)
Tatsuki Negami¹, Ayako Furukawa², Kento Yonezawa³, Naruhiko Adachi³, Toshiya Senda³, Nobutaka Shimizu³, Yoshifumi Nishimura^{2,4}, Tohru Terada¹ (¹Grad. Sch. Agr. Life Sci., Univ. Tokyo, ²Grad. Sch. Med. Life Sci., Yokohama city Univ., ³IMSS, KEK, ⁴Grad. Sch. Integ. Sci. Life, Hiroshima Univ.)
- [1-03-1354](#) 深層学習を用いたタンパク質オーダーパラメータの時系列データの予測研究
Application of a deep-learning model for the prediction of the time course of an order parameter of a protein
○佐藤 連太, 吉留 崇 (東北大・院工)
Renta Sato, Takashi Yoshidome (*Dept. of Appl. Phys., Tohoku Univ.*)
- [1-03-1406](#) Dynamic Residue Interaction Network Analysis of Secondary Mutations in Protease that Promote Drug Resistance in HIV-1
Ayaka Ojima, Mohini Yadav, Norifumi Yamamoto (*Chiba Tech*)
- [1-03-1418](#) Coarse-grained simulations of multiple intermediates along conformational transition pathways of multi-domain proteins
Ai Shinobu¹, Chigusa Kobayashi², Yasuhiro Matsunaga³, Yuji Sugita^{1,2,4} (¹RIKEN, BDR, ²RIKEN, R-CCS, ³Saitama Univ., Grad. Sch. Sci. Eng., ⁴RIKEN, CPR)
- [1-03-1430](#) Application of ColDock to docking of cryptic pockets
Ryunosuke Kiuchi, Kazuhiro Takemura, Akio Kitao (*School of Life Science and Technology, Tokyo Institute of Technology*)
- [1-03-1442](#) 自由エネルギー不等式に基づく Checkpoint kinase1-リガンド系の相対的結合自由エネルギーの推定
Estimation of relative binding free energy based on a free energy inequality for the Checkpoint kinase1-ligand system
○芝原 慶太, 菊地 武司 (立命大・生命科学・生情)
Keita Shibahara, Takeshi Kikuchi (*Dept. Biosci., Col. Life Sci., Ritsumeikan Univ.*)
- [1-03-1454](#) 自由エネルギー不等式に基づく Cyclin Dependent Kinase2 ーリガンド系の相対的結合自由エネルギーの推定
Estimation of relative binding free energy based on a free energy for the cyclin dependent kinase2 – ligand system
○新 大樹, 菊地 武司 (立命大・生命科学・生情)
Daiki Atarashi, Takeshi Kikuchi (*Dept. Biosci., Col. Life Sci., Ritsumeikan Univ.*)
- [1-03-1506](#) ドッキング構造予測のリランキングに向けた蛋白質—ペプチド間相互作用の網羅的解析
Comprehensive analysis of protein-peptide interactions for reranking of docking predictions
○佐藤 圭一朗¹, 笠原 浩太², 高橋 卓也² (¹立命大・院生命,²立命大・生命)
Keiichiro Sato¹, Kota Kasahara², Takuya Takahashi² (¹Grad. Sci. Life Sci., Ritsumeikan Univ., ²Coll. Life. Sci., Ritsumeikan Univ.)
- [1-03-1518](#) The physical-based criterion for distinguishing superfolds and non-superfolds: the case of pure parallel beta-sheets
Hiroyo Murata, George Chikenji (*Dept. of Appl. Phys., Grad. Sch. of Eng., Nagoya. Univ.*)

座長：茶谷 絵理（神戸大学），乙須 拓洋（埼玉大学）

Session Chairs: Eri Chatani (Kobe Univ.), Takuhiro Otsu (Saitama Univ.)

- [1-04-1330](#) ヌクレオソームから H2A-H2B 量体が脱離する際の自由エネルギープロファイル
Free energy profile of H2A-H2B dimer dissociation from nucleosome
○石田 恒, 河野 秀俊（量子科学技術研究開発機構 量子生命・医学部門 量子生命科学研究所）
Hisashi Ishida, Hidetoshi Kono (*Quantum Life Science, National Institutes for Quantum and Radiological Science and Technology*)
- [1-04-1342](#) 低温条件下での微小管構造動態解析：溶液温度に依存した構造変化における非等方性とヒステリシス
Structural dynamics of native microtubules on cooling: anisotropic and hysteretic structural changes depending on temperature
○上村 慎治¹, 八木 俊樹², 近藤 裕祐², Estévez-Gallego Juan³, Lucena-Agell Daniel³, Díaz J. Fernando³, 岩本 裕之⁴（¹中大・理工・生命科学, ²県広大・生物資源・生命環境学科, ³El Centro de Investigaciones Biológicas Margarita Salas, CSIC, ⁴Res. & Util. Div., JASRI, SPring-8）
Shinji Kamimura¹, Toshiki Yagi², Yusuke Kondo², Juan Estévez-Gallego³, Daniel Lucena-Agell³, J. Fernando Díaz³, Hiroyuki Iwamoto⁴ (*¹Dept. Biol. Sci., Fac. Sci. & Eng., Chuo Univ., ²Dept. Life & Env. Sci., Fac. Bioresource Sci., Pref. Univ. Hiroshima, ³El Centro de Investigaciones Biológicas Margarita Salas, CSIC, ⁴Res. & Util. Div., JASRI, SPring-8*)
- [1-04-1354](#) ファージレセプター結合蛋白質と宿主レセプターの相互作用解析
Interaction analysis of the phage receptor binding protein and the host receptor
○金丸 周司¹, 竹村 和浩¹, Aleksandar Zdravković²（¹東工大・生命, ²東工大・IIR）
Shuji Kanamaru¹, Kazuhiro Takemura¹, Zdravković Aleksandar² (*¹Dep. of Life Sci. and Tech., Tokyo Inst. of Tech., ²Inst. of Innov. Res., Tokyo Inst. of Tech.*)
- [1-04-1406](#) 静電相互作用の計算コストを抑えた新規自由エネルギー摂動法の開発
Development of a new free-energy perturbation method for reducing the computational cost of electrostatic interactions
○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 Oshima¹, Yuji Sugita^{1,2,3} (*¹RIKEN BDR, ²RIKEN R-CCS, ³RIKEN CPR*)
- [1-04-1418](#) 微小管末端標識と高速 AFM による可視化
Visualization of microtubule ends by high-speed AFM
樋口 雄希¹, 古寺 哲幸², 林 郁子¹（¹横浜市大・生命医, ²金沢大・ナノ生命科学）
Yuuki Higuchi¹, Noriyuki Kodera², **Ikuko Hayashi**¹ (*¹Yokohama City Univ., ²Kanazawa Univ.*)
- [1-04-1430](#) Heparin-Induced Tau Oligomer Formation by Dynamic Light Scattering
Analysis of Heparin-Induced Tau Oligomer Formation by Dynamic Light Scattering
Ayumi Masui¹, Keisuke Yuzu¹, Keiichi Yamaguchi², Yuji Goto², Yasushi Kawata³, Eri Chatani¹ (*¹Grad. Sch. Sci., Kobe Univ., ²Glob. Ctr. for Med. Engin. and Info., Osaka Univ., ³Grad. Sch. Engin., Tottori Univ.*)
- [1-04-1442](#) 放射光 X 線溶液散乱測定における連続濃度変調型 μ 流路自動サンプリングシステムの性能評価
Evaluation of continuous concentration-modulated μ -fluidic auto sampling system for synchrotron SAXS measurements
○米澤 健人^{1,3}, 林 有吾², 山崎 洋一², 清水 伸隆³, 上久保 裕生^{1,2,3}（¹奈良先端大・デジタルグリーンイノベーションセンター, ²奈良先端大・物質, ³高エネ機構・物構研）
Kento Yonezawa^{1,3}, Yugo Hayashi², Yoichi Yamazaki², Nobutaka Shimizu³, Hironari Kamikubo^{1,2,3} (*¹NAIST, CDG, ²NAIST, MS, ³KEK, IMSS*)

- [1-04-1454](#) ホモロガスヘテロオリゴマーの構造的特性解析
Structural characterization of homologous hetero-oligomers
○伊藤 滉太¹, 塩生 くらら², 杉本 泰伸¹, 小池 亮太郎¹, 太田 元規¹ (¹名大・院・情報, ²長浜バイオ・バイオサイエンス)
Kota Ito¹, Clara Shionyu², Yasunobu Sugimoto¹, Ryotaro Koike¹, Motonori Ota¹ (¹*Grad. Sch. of Info. Sci., Nagoya Univ.*, ²*Faculty of Bioscience, Nagahama Institute of Bio-Science and Technology*)
- [1-04-1506](#) 溶解性成業ペプチド (SCP) タグによって会合させた BPTI 蛋白質の物性と免疫原性の解析
Biophysical and immunogenic properties of a Bovine Pancreatic Trypsin Inhibitor oligomerized using a Solubility Controlling Peptide tag
○黒田 裕¹, Rahman Nafsoon^{1,2}, Kabir M. Golam³, Islam M, Mohammad^{1,3} (¹東京農工大学・工・生命工, ²Department of Biochemistry and Molecular Biology, Jagannath University, Dhaka, Bangladesh, ³Department of Biochemistry and Molecular Biology, Chittagong University, Chittagong, Bangladesh)
Yutaka Kuroda¹, Nafsoon Rahman^{1,2}, M. Golam Kabir³, M, Mohammad Islam^{1,3} (¹*Graduate School Engineering, Tokyo University of Agriculture and Technology*, ²*Department of Biochemistry and Molecular Biology, Jagannath University, Dhaka, Bangladesh*, ³*Department of Biochemistry and Molecular Biology, Chittagong University, Chittagong, Bangladesh*)
- [1-04-1518](#) 天然変性タンパク質 p53 液滴内への分子取込と 1 分子ダイナミクス観測
Characterization of molecular uptake and single-molecule dynamics in liquid droplets of p53
○岩城 奈那子^{1,2}, 上林 さおり¹, パネルジー トリシット^{1,2}, 千葉 梨佳^{1,3}, 木村 美智子^{1,3}, 小井川 浩之^{1,2,3}, 高橋 聡^{1,2,3}, 鎌形 清人^{1,2,3} (¹東北大・多元研, ²東北大・院理化, ³東北大・院生命)
Nanako Iwaki^{1,2}, Saori Kanbayashi¹, Trishit Banerjee^{1,2}, Rika Chiba^{1,3}, Michiko Kimura^{1,3}, Hiroyuki Oikawa^{1,2,3}, Satoshi Takahashi^{1,2,3}, Kiyoto Kamagata^{1,2,3} (¹*IMRAM, Tohoku Univ.*, ²*Dep. Chem., Grad. Sch. Sci., Tohoku Univ.*, ³*Grad. Sch. Life Sci., Tohoku Univ.*)

13:30~15:06 Ch05
1G05 核酸 I
Nucleic acids I

座長：姚 閔 (北海道大学), 皆川 慶嘉 (東京大学)

Session Chairs: Min Yao (Hokkaido Univ.), Yoshihiro Minagawa (The Univ. of Tokyo)

- [1-05-1330](#) Roles of loop extrusion process in transcription dynamics of target genes of superenhancers
Tetsuya Yamamoto^{1,2}, Takahiro Sakaue³, Helmut Schiessel⁴ (¹*Institute for Reaction Design and Discovery, Hokkaido University*, ²*JST PRESTO*, ³*Department of Physical Sciences, Aoyama-Gakuin University*, ⁴*Cluster of Excellence Physics of Life, TU Dresden*)
- [1-05-1342](#) 粗視化分子シミュレーションによる SMC-kleisin 複合体の構造変化と DNA 結合状態の解明
Coarse-grained Molecular Simulation to Reveal Conformational Change and DNA binding of Bacterial SMC-kleisin Complex
○山内 仁喬, 高田 彰二 (京大・理・生物物理)
Masataka Yamauchi, Shoji Takada (*Dept. of Biophysics, Grad. of Sci., Kyoto Univ.*)
- [1-05-1354](#) 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
Generation of Phase Separated Droplet Induced by Soret Effect and DNA Enrichment by Optical Tweezers
○小林 美加, 皆川 慶嘉, 野地 博行 (東大・工)
Mika Kobayashi, Yoshihiro Minagawa, Hiroyuki Noji (*Grad. Sch. of Eng., Univ. Tokyo*)
- [1-05-1406](#) Elucidation of nucleosome sliding mechanism in all-atom detail via MD simulations
Syed Hashim Shah, Giovanni Brandani, Shoji Takada (*Department of Biophysics, Graduate School of Science, Kyoto University*)

- [1-05-1418](#) 拡散的ループ形成によるクロマチン相分離
Chromatin phase separation induced by diffusive loop formation
○藤城 新, 笹井 理生 (名古屋大・院応用物理)
Shin Fujishiro, Masaki Sasai (*Dept. Appl. Phys., Nagoya Univ.*)
- [1-05-1430](#) 多価相互作用を持つタンパク質の相分離をシミュレーションするためのメソスケール化学量論相互作用モデル
Mesoscale stoichiometric interaction model for simulating phase-separation of multivalent proteins
○村田 隆, 新稲 亮, 高田 彰二 (京都大学・理学研究科)
Yutaka Murata, Toru Niina, Shoji Takada (*Grad. Sch. Sci., Univ. Kyoto*)
- [1-05-1442](#) 3D DNA nanostructure-based string-like structure for the construction of chromatin-like heterogeneous system
Hong Xuan Chai, Masahiro Takinoue (*Tokyo Institute of Technology*)
- [1-05-1454](#) Formation of liquid-liquid phase separation droplets based on artificial RNA nanostructures
Minzhi Fan¹, Masahiro Takinoue¹, Hirohide Saito² (¹*Tokyo Institute of Technology*, ²*Kyoto University*)

13:30~15:30 Ch06

1G06 ヘム蛋白質・膜蛋白質・核酸結合蛋白質：構造I、機能と反応場I

Heme-, Membrane- & Nucleic acid binding-protein: Structure I, Function and environment I

座長：木村 哲就 (神戸大学), 池口 満徳 (横浜市立大学)

Session Chairs: Tetsunari Kimura (Kobe Univ.), Mitsunori Ikeguchi (Yokohama City Univ.)

- [1-06-1330](#) 鎖長の異なるパーフルオロアルキル基を有する部分フッ素化リン脂質群に再構成したバクテリロロドプシンの機能と構造安定性に関する比較研究
Comparison of functionality and structural stability of bR in partially fluorinated DMPC vesicles with varied perfluoroalkyl chain lengths
橋本 麻美¹, 村井 裕佳¹, 森田 康平¹, 菊川 峰志², 高木 俊之³, 高橋 浩¹, 横山 泰範⁴, 網井 秀樹^{1,5},
○園山 正史^{1,5,6} (¹群馬大・院理工,²北大・先端生命,³産総研,⁴名大・院工,⁵群馬大・未来先端,⁶群馬大・食健康セ)
Mami Hashimoto¹, Yuka Murai¹, Kohei Morita¹, Takashi Kikukawa², Toshiyuki Takagi³,
Hiroshi Takahashi¹, Yasunori Yokoyama⁴, Hideki Amii^{1,5}, **Masashi Sonoyama**^{1,5,6} (¹*Grad. Sch. Sci. Tech., Gunma Univ.*, ²*Fac. Adv. Life Sci., Hokkaido Univ.*, ³*AIST*, ⁴*Grad. Sch. Eng., Nagoya Univ.*, ⁵*GIAR, Gunma Univ.*, ⁶*GUCFW, Gunma Univ.*)
- [1-06-1342](#) ABC トランスポーター MsbA の ATPase 活性に対する機能場の影響
Effect of lipid environments on the ATPase activity of ABC transporter MsbA
○大谷 理紗子¹, 林 史夫², 園山 正史^{1,3,4} (¹群馬大・院理工,²群馬大・機器分析セ,³群馬大・未来先端,⁴群馬大・食健康セ)
Risako Otani¹, Fumio Hayashi², Masashi Sonoyama^{1,3,4} (¹*Grad. Sch. Sci. Tech., Gunma Univ.*, ²*Ctr. Inst. Anal. Gunma Univ.*, ³*GIAR, Gunma Univ.*, ⁴*GUCFW, Gunma Univ.*)
- [1-06-1354](#) ナノディスクに埋め込まれた BamA によって補助される外膜タンパク質のアセンブリ
Assembly of outer membrane proteins assisted by BamA embedded into the nanodisc
○青木 英莉子¹, 藤原 和夫², 池口 雅道² (¹創価大・糖鎖研,²創価大・生命理学)
Eriko Aoki¹, Kazuo Fujiwara², Masamichi Ikeguchi² (¹*GalSIC, Soka Univ.*, ²*Dept. of Biosci., Soka Univ.*)
- [1-06-1406](#) ナノディスクに再構成した鉄還元膜タンパク質 101F6 における電子移動反応の解析
Spectroscopic analysis of electron transfer reaction in iron-reducing membrane protein 101F6 reconstituted into nanodiscs
○山口 葵¹, Abosharaf Hamed A², 鏑木 基成¹, 木村 哲就¹ (¹神戸大・院理・化,²タンタ大)
Aoi Yamaguchi¹, Hamed A Abosharaf², Motonari Tsubaki¹, Tetsunari Kimura¹ (¹*Dept. of Chem., Grad Sch. of Sci., Kobe Univ.*, ²*Tanta Univ.*)

- [1-06-1418](#) Pressure and temperature phase diagram for liquid–liquid phase separation of the rna-binding protein fused in sarcoma
Shujie Li (*Grad. Sch. Phar., Ritsumei Univ.*)
- [1-06-1430](#) ウシ心筋シトクロム酸化酵素の第二のシトクロム c 結合構造
 Second cytochrome c binding structure of the bovine heart cytochrome c oxidase
 伊藤 (新澤) 恭子¹, 青江 新平², 島田 悟¹, 馬場 淳平¹, 藤本 光輝², 島田 敦広¹, 山下 栄樹³, 吉川 信也¹, 月原 富武^{1,3}, ○村本 和優¹ (¹ 兵庫県立大・院理, ² 兵庫県立大・理, ³ 阪大・蛋白質) Kyoko Shinzawa-Itoh¹, Shinpei Aoe², Satoru Shimada¹, Junpei Baba¹, Kouki Fujimoto², Atsuhiko Shimada¹, Eiki Yamashita³, Shinya Yoshikawa¹, Tomitake Tsukihara^{1,3}, **Kazumasa Muramoto**¹ (¹*Grad. Sch. Sci., Univ. Hyogo*, ²*Sch. Sci., Univ. Hyogo*, ³*Inst. Protein Res., Osaka Univ.*)
- [1-06-1442](#) 全長カーゴ受容体 ERGIC-53 と補助因子 MCFD2 との複合体の相関構造解析
 Correlative structural analysis of a full-length cargo receptor ERGIC-53 in complex with its partner MCFD2
 ○渡部 聡¹, 木瀬 孔明², 米澤 健人³, 清水 伸隆³, 濡木 理², 稲葉 謙次¹ (¹ 東北大・多元研, ² 東京大・院理, ³ 高エネ機構・物構研)
Satoshi Watanabe¹, Yoshiaki Kise², Kento Yonezawa³, Nobutaka Shimizu³, Osamu Nureki², Kenji Inaba¹ (¹*IMRAM, Tohoku Univ.*, ²*Grad. Sch. Sci., Univ. Tokyo*, ³*KEK, IMSS*)
- [1-06-1454](#) ヌクレオソーム DNA 解離の配列依存性
 Sequence dependence of nucleosomal DNA unwrapping
 ○角南 智子, 河野 秀俊 (量研・量子生命・生体分子シミュレーション)
Tomoko Sunami, Hidetoshi Kono (*MMS, iQLS, QST*)
- [1-06-1506](#) Catalytic enhancement of NSD2 following oncogenic mutations E1099K and T1150A is caused by increase in the autoinhibitory loop dynamics
Amarjeet Kumar¹, Ko Sato², Shun Sakuraba¹, Kazuhiko Ogata², Toru Sengoku², Hidetoshi Kono¹ (¹*Mole. Mod. Simu. Grp., Inst. Quant. Life Sci., QST*, ²*Dept. Biochem., YCU Grad. Sch. Med.*)
- [1-06-1518](#) DNA bending enhances the dissociation of tetrameric p53's core domains
Duy Tran, Akio Kitao (*Sch. Life Sci. Tech, TokyoTech*)

13:30~15:30 Ch07

1G07 筋肉・分子モーター I

Muscle & Molecular motor I

座長：富重 道雄 (青山学院大学), 矢島 潤一郎 (東京大学)

Session Chairs: Michio Tomishige (Aoyama Gakuin Univ.), Junichiro Yajima (The Univ. of Tokyo)

- [1-07-1330](#) 細胞分裂に関わるキネシン 5 の頭部間協調におけるネックリンカーの役割の高速一分子観察
 High-speed single molecule studies of the role of neck linker on the head-head coordination of kinesin 5
 ○石指 剣太郎 (青山学院大学大学院理工学研究科)
Kentaro Ishizashi (*Grad. Sch. Sci. Eng., Aoyama Gakuin Univ.*)
- [1-07-1342](#) 尾部ドメインによるキネシン 1 の運動制御の高速一分子観察
 Regulation of kinesin-1 motility by tail domain as studied by high-speed single molecule observation
 ○新野 素生¹, 橋爪 涼¹, 松崎 興平², 富重 道雄² (¹ 青山学院大学大学院 理工学研究科, ² 青山学院大学 理工学部 物理・数理学科)
Motoki Niino¹, Ryo Hashizume¹, Kohei Matsuzaki², Michio Tomishige² (¹*Grad. Sch. Sci. Eng., Aoyama Gakuin Univ.*, ²*Dept. Math. Phys., Col. Sci. Eng., Aoyama Gakuin Univ.*)

- [1-07-1354](#) キネシン 1 のネックリンカーの構造変化に伴う熱力学的変化の測定
Measurement of thermodynamic changes associated with conformational changes in the neck linker of kinesin-1
○田中 明美^{1,2}, 帆足 拓未¹, 富重 道雄¹ (¹ 青山学院大学理工学部, ² 東京大学大学院工学系研究科)
Akemi Tanaka^{1,2}, Takumi Hoashi¹, Michio Tomoshige¹ (¹College of Sci. and Eng., Aoyama Gakuin Univ., ²School of Eng., The Univ. of Tokyo)
- [1-07-1406](#) マイナスキネシン Kinesin-14 モーターコアの微小管プラス端方向への運動性の実証
Plus-end directionality is present in the catalytic core of kinesin-14 minus-end directed motors
○山岸 雅彦, 矢島 潤一郎 (東京大学・総合文化)
Masahiko Yamagishi, Junichiro Yajima (Dept. Life Sci., Grad. Arts& Sci., Univ. Tokyo)
- [1-07-1418](#) (1S1-1) 1 分子回転観察と操作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 IF₁ の解離機構
(1S1-1) Dissociation mechanism of IF₁ from mitochondrial ATP synthase revealed by single-molecule analysis and manipulation
○小林 稜平, 上野 博史, 野地 博行 (東大・院工・応化)
Ryohei Kobayashi, Hiroshi Ueno, Hiroyuki Noji (Appl. Chem., Grad. Sch. Eng., Univ. Tokyo)
- [1-07-1430](#) Direct Observation of Stepping Rotation of V-ATPase Reveals Rigid and Non-integer Coupling between V_o and V_i Motors
Akihiro Otomo^{1,2}, Tatsuya Iida², Hiroshi Ueno³, Takeshi Murata⁴, Ryota Iino^{1,2} (¹Institute for Molecular Science, ²SOKENDAI, ³Grad. Sch. Eng., The Univ. of Tokyo, ⁴Grad. Sch. Sci., Chiba Univ.)
- [1-07-1442](#) Effect of hinge mutations on F₁-ATPase energetics
Natsumi Sato¹, Yohei Nakayama¹, Takashi Yoshidome¹, Eiro Muneyuki², Shoichi Toyabe¹ (¹Grad. Eng., Tohoku Univ., ²Sch. Sci. Eng., Chuo Univ.)
- [1-07-1454](#) エンジニアリング的アプローチによる F₁-ATPase 制御因子 IF₁ の分子認識機構の解明
Elucidation of molecular recognition mechanism of IF₁, a regulator of F₁-ATPase, studied by an engineering approach
○畑崎 優一郎, 渡邊 亮, 小林 稜平, 上野 博史, 野地 博行 (東大・院工・応化)
Yuichiro Hatasaki, Ryo Watanabe, Ryohei Kobayashi, Hiroshi Ueno, Hiroyuki Noji (Appl. Chem., Grad. Sch. Eng., Univ. Tokyo)
- [1-07-1506](#) Simultaneous measurement for the stator-incorporation and the flagellar motor rotation
Tomohiro Teshima, Yumiko Uchida, Yong-Suk Che, Akihiko Ishijima, Hajime Hukuoka (Grad. Sch. Frontier Biosci. Osaka Univ)
- [1-07-1518](#) 極べん毛モーターと周べん毛モーターの回転方向制御の協同性の違い
Difference in cooperativity of the rotational control between the motors of polar and peritrichous flagella
○田島 寛隆^{1,2}, 西川 正俊^{1,3}, 三浦 勇輝³, 曾和 義幸^{1,2,3}, 川岸 郁朗^{1,2,3} (¹法政大・生命・生命機能, ²法政大・ナノテクセンター, ³法政大・院理工・生命機能)
Hirotaaka Tajima^{1,2}, Masatoshi Nishikawa^{1,3}, Yuki Miura³, Yoshiyuki Sowa^{1,2,3}, Ikuro Kawagishi^{1,2,3} (¹Dept. Front. Biosci., Hosei Univ., ²Res. Cent. Micro-Nano Tech., Hosei Univ., ³Grad. Sch. Eng., Hosei Univ.)

座長：太田 善浩（東京農工大学），松浦 友亮（東京工業大学）

Session Chairs: Yoshihiro Ohta (Tokyo Univ. of Agric. and Tech.), Tomoaki Matsuura (Tokyo Tech)

- [1-08-1330](#) ウニにおける H⁺/K⁺イオンポンプ活性は胚の細胞骨格分布極性を高めて原腸形成を促進させる
Sea urchin H⁺/K⁺ ion pump enhances cytoskeletal polarity to drive gastrulation
○渡辺 開智¹, 安井 優平¹, 黒瀬 友太², 坂本 尚昭¹, 粟津 暁紀¹ (¹ 広島大・院統合生命, ² 広島大・院理)
- Kaichi Watanabe¹**, Yuhei Yasui¹, Yuta Kurose², Naoaki Sakamoto¹, Akinori Awadu¹ (¹ *Grad. Sch. Int., Univ. Hiroshima*, ² *Grad. Sch. Sci., Univ. Hiroshima*)
- [1-08-1342](#) Membrane progress and backtracking at the critical condition of engulfment in macrophages
Dan Horonushi¹, Sota Suzuki², Kenji Yasuda^{1,2,3} (¹ *Dept. Pure & Appl. Phys., Grad. Sch. Adv. Sci. & Eng., Waseda Univ.*, ² *Dept. Phys., Sch. Adv. Sci. & Eng., Waseda Univ.*, ³ *Org. Univ. Res. Initiatives, Waseda Univ.*)
- [1-08-1354](#) 合成ポリペプチドの設計によるコンプレックスコアセルベートの物性制御
Control of Complex Coacervate Physical Properties by Design of Synthetic Polypeptides
○天見 雄大, 岸村 顕広, 森 健, 片山 佳樹, オン ガブリエル, ケーシー ビップラブ (九州大・院システム生命科学府)
- Yudai Amami**, Akihiro Kishimura, Takeshi Mori, Yoshiki Katayama, Gabrielle Ong, Biplab KC (*Grad. Sch. Systems Life Sciences, Univ. Kyushu*)
- [1-08-1406](#) デザインされたブロック共重合体型合成ポリペプチドからなる複合コアセルベートへのタンパク質取り込みと液滴内相分離挙動
Sequestration of proteins into complex coacervates of designed synthetic polypeptides and phase separation behavior inside the droplet
○岸村 顕広^{1,2,3}, KC Biplab¹, Gabrielle Anjani Ong¹, 天見 雄大¹, 森 健^{1,3}, 片山 佳樹^{1,2,3,4} (¹ 九州大学大学院工学研究院応用化学部門, ² 九州大学分子システム化学センター, ³ 九州大学未来化学創成センター, ⁴ 九州大学先端医療オープンイノベーションセンター)
- Akihiro Kishimura^{1,2,3}**, Biplab KC¹, Ong Gabrielle Anjani¹, Yudai Amami¹, Takeshi Mori^{1,3}, Yoshiki Katayama^{1,2,3,4} (¹ *Department of Applied Chemistry, Faculty of Engineering, Kyushu University*, ² *Center for Molecular Systems, Kyushu University*, ³ *Center for Future Chemistry, Kyushu University*, ⁴ *Center for Advanced Medical Open Innovation, Kyushu University*)
- [1-08-1418](#) 陰圧条件下における金魚ケラトサイト細胞シートの細胞間接着の増強
Cell-cell adhesion increase under the negative pressure conditions in fish keratocytes cell-sheets
○大久保 成貴, 辰巳 仁史 (金沢工業大学大学院 工学研究科 バイオ・化学専攻)
- Shigeki Ookubo**, Hitoshi Tatsumi (*Department of Applied Bioscience, Kanazawa Inst. of Technol., Ishikawa, Japan*)
- [1-08-1430](#) 圧力がミトコンドリア内膜の透過性に及ぼす影響
Effects of pressure on the permeability of the inner mitochondrial membrane
○尾家 佳樹, 太田 善浩 (東京農工大 院・工・生命)
- Yoshiki Oie**, Yoshihiro Ohta (*Dept. of Life Sci. & Biotech., Grad. Sch. Eng., Tokyo Univ. of Agric. & Tech*)
- [1-08-1442](#) 細菌の運動性、物性および病原性に与える外膜成分の影響
Effect of the outer membrane components on the bacterial motility, physical property, and pathogenicity
○阿部 圭吾¹, 中村 修一¹, 小泉 信夫² (¹ 東北大・院工学, ² 国立感染研究所・細菌第一部)
- Keigo Abe¹**, Shuichi Nakamura¹, Nobuo Koizumi² (¹ *Grad. Sch. Eng., Univ. Tohoku*, ² *Department of Bacteriology I, National Institute of Infectious Disease*)

- [1-08-1454](#) 細胞膜上の糖タンパク質の立体斥力とウイルス感染抑制効果
Cell membrane glycoproteins facilitate steric repulsive forces to modulate viral infections
○貝塚 芳久 (国立研究開発法人 物質・材料研究機構)
Yoshihisa Kaizuka (*National Institute for Materials Science*)
- [1-08-1506](#) 化学固定は膜タンパク質を凝集することによって細胞表面にナノスケールのクラスターを形成する
Chemical fixation creates nanoscale clusters on the cell surface by aggregating membrane proteins
○市川 壮彦¹, Dong Wang^{1,2}, 宮澤 佳甫^{1,3}, 宮田 一輝¹, 大島 正伸^{1,2}, 福岡 剛士^{1,3} (¹金沢大・ナノ研, ²金沢大・がん研, ³金沢大・フロンティア工)
Takehiko Ichikawa¹, Wang Dong^{1,2}, Keisuke Miyazawa^{1,3}, Kazuki Miyata¹, Masanobu Oshima^{1,2}, Takeshi Fukuma^{1,3} (¹*Kanazawa Univ.*, ²*NanoLSI*, ²*Kanazawa Univ.*, *Can. Res. Inst.*, ³*Kanazawa Univ.*, *Frontier Eng.*)
- [1-08-1518](#) ミトコンドリア電子伝達系のプロトンポンプ活性に及ぼす細胞サイズの影響
Effects of cell size on the activity of the proton pumps in mitochondrial electron transfer chain
○菅沼 芳樹, 柏木 広子, 三浦 正人, 太田 善浩 (農工大・院工)
Yoshiki Suganuma, Hiroko Kashiwagi, Masato Miura, Yoshihiro Ohta (*Grad. Sch. Eng., Univ. Noko*)

13:30~15:30 Ch09

1G09 細胞生物 I、骨格 I

Cell biology I, Cytoskeleton I

座長：樋口 秀男 (東京大学), 楠見 明弘 (沖縄科学技術大学院大学)

Session Chairs: Hideo Higuchi (The Univ. of Tokyo), Akihiro Kusumi (OIST)

- [1-09-1330](#) アミロイドβ凝集体による神経細胞遊走の抑制
Inhibition of neuronal cell migration by Amyloid-β aggregation
○北村 嶺大, 倉賀野 正弘, 近井 優作, 徳樂 清孝 (室蘭工業大学大学院)
Ryota Kitamura, Masahiro Kuragano, Yusaku Chikai, Kiyotaka Tokuraku (*Muroran Institute of Technology*)
- [1-09-1342](#) Emergence of coordinated migration behavior of isolated single macrophages in confined geometries of microstructures
Souta Suzuki¹, Dan Horonushi², Kenji Yasuda^{1,2,3} (¹*Dept. Phys., Sch. Adv. Sci. & Eng., Waseda Univ.*, ²*Dept. Pure & Appl. Phys., Grad. Sch. Adv. Sci. & Eng., Waseda Univ.*, ³*Org. Univ. Res. Initiatives, Waseda Univ.*)
- [1-09-1354](#) Synaptic anchorage of AMPA receptors mediated by their direct binding to PDZ proteins and dynamic interactions with TARPγ-2
Yuri L Nemoto^{1,2}, Rinshi S Kasai³, Hiroko Hijikata^{1,2}, Taka A Tsunoyama¹, Kazuma Naito², Nao Hiramoto-Yamaki², Takahiro K Fujiwara², Akihiro Kusumi^{1,2,3} (¹*Membrane Cooperativity Unit, OIST*, ²*WPI-iCeMS, Kyoto University*, ³*Institute for Frontier Life and Medical Sciences, Kyoto University*)
- [1-09-1406](#) High hydrostatic pressure regulate TGF-β signaling pathway in human chondrocytes
Masatoshi Morimatsu¹, Xinxuan Li¹, Masayoshi Nishiyama², Keiji Naruse¹ (¹*Grad. Sch. Med. Dent. Pharma., Okayama Univ.*, ²*Dept. Physics., Kindai Univ.*)
- [1-09-1418](#) ヒト原腸形成の自己組織化に向けて：iPS細胞の2Dパターン培養
Toward the self-organization of the human gastrulation: 2D pattern culture of iPS cells
○竹内 千尋 (長岡技術科学大学 大学院 工学研究科 生物機能工学専攻)
Chihiro Takeuchi (*Department of Bioengineering, Graduate School of Engineering, Nagaoka University of Technology*)

- [1-09-1430](#) 試験管内再構成による星状体微小管とアクチン繊維網の相互作用の解析
In vitro reconstitution of microtubule aster interaction with the actin network
○山本 昌平¹, Gaillard Jérémie¹, Guerin Christophe¹, Prioux Magali¹, Vianay Benoit^{1,2},
Blanchoin Laurent^{1,2}, Théry Manuel^{1,2} (¹ フランス原子力庁グルノーブル, ² サン・ルイ病院)
Shohei Yamamoto¹, Jérémie Gaillard¹, Christophe Guerin¹, Magali Prioux¹, Benoit Vianay^{1,2},
Laurent Blanchoin^{1,2}, Manuel Théry^{1,2} (¹CEA Grenoble, *CytoMorpho Lab*, ²Hôpital Saint Louis,
CytoMorpho Lab)
- [1-09-1442](#) ファロイジン-アクチンとサイトカラシン B-アクチンの相互作用の等温滴定熱測定
Isothermal titration calorimetry of phalloidin-actin and cytochalasin B-actin interactions
○呉 尚論, 清中 大陸, 小松 英幸 (九州工業大学・生命化学情報工学科)
Shouron Kure, Riku Kiyonaka, Hideyuki Komatsu (*Dept. of Bioscience and Bioinformatics, Kyushu
Inst. Tech.*)
- [1-09-1454](#) 微小管-微小管安定化因子相互作用の等温滴定熱測定
Isothermal titration calorimetry of microtubule-microtubule stabilizing factor interactions
○清中 大陸, 鹿嶋 純太, 小松 英幸 (九州工大・情報工・生命化学情報)
Riku Kiyonaka, Junta Kashima, Hideyuki Komatsu (*Dept. of Bioscience and Bioinformatics, Kyushu
Inst. Tech.*)
- [1-09-1506](#) 葉緑体運動に必要な CHUP1 によるアクチンの核形成
Actin nucleation promoted by CHUP1 required for chloroplast movement
○山崎 陽祐¹, 孔 三根², 貴嶋 紗久³, 和田 正三⁴, 上田 太郎¹ (¹早大 物理, ²公州大 生物, ³産総研
バイオメディカル, ⁴九大 生物)
Yosuke Yamazaki¹, Sam-Geun Kong², Saku Kijima³, Masamitsu Wada⁴, Taro QP Uyeda¹ (¹Dep. Phys.,
Waseda Univ., ²Dep. Biol. Sci., Kongju Natl. Univ., ³Biomed. Res. Inst., AIST, ⁴Dep. Biol., Kyushu Univ.)
- [1-09-1518](#) The amplitude of twisting and bending fluctuations of actin filaments decreased by mechanical stress
Kaoru Okura, Hitoshi Tatsumi (*Department of Applied Bioscience, Kanazawa Inst. of Technol.,
Ishikawa, Japan*)

13:30~15:30 Ch10
1G10 生体膜・人工膜 I
Biological & Artificial membrane I

座長：松木 均 (徳島大学), 高橋 浩 (群馬大学)

Session Chairs: Hitoshi Matsuki (Tokushima Univ.), Hiroshi Takahashi (Gunma Univ.)

- [1-10-1330](#) 気液界面における人工肺サーファクタント膜への負電荷微粒子の影響
Effect of negatively charged particles on a model lung surfactant monolayer at the air-water interface
○日比野 政裕¹, 伊藤 夏希² (¹ 室蘭工大・院環境創生, ² 室蘭工大・応理)
Masahiro Hibino¹, Natsuki Ito² (¹Div. Sustain. Environ. Eng., *Muroran Inst. Tech.*, ²Dept. Appl. Sci.,
Muroran Inst. Tech.)
- [1-10-1342](#) パターン化モデル膜とナノ空間を用いたドーパミン受容体の再構成と機能解析
Functional reconstitution of dopamine D2 receptor into a supported model membrane in a nanometric confinement
○杉町 純音¹, 永井 りか¹, 鈴木 健一³, 林 文夫⁴, 笠井 倫志³, 森垣 憲一^{1,2} (¹ 神戸大・農学研究科,
² 神戸大・バイオシグナル総合研究センター, ³ 岐阜大・糖鎖生命科学コア研究所, ⁴ 神戸大・理学研究科)
Ayane Sugimachi¹, Rurika Nagai¹, Kenichi Suzuki³, Fumio Hayashi⁴, Rinshi Kasai³,
Kenichi Morigaki^{1,2} (¹Grad. Sch. Agr. Sci., Univ. Kobe, ²Biosignal Research Center, Univ. Kobe, ³Glyco-
core Research (iGCORE) Inst., Univ. Gifu, ⁴Grad. Sch. Sci., Univ. Kobe)

- [1-10-1354](#) B型肝炎ウイルスのエンベロープのモデリングとシミュレーション
Hepatitis B virus envelope: modeling and simulation
○浦野 諒, 篠田 渉 (名大・院工)
Ryo Urano, Wataru Shinoda (*Grad. Sch. Eng., Nagoya Univ.*)
- [1-10-1406](#) 筋小胞体 Ca ポンプ M2 ヘリックスの Ca 輸送における役割
Role of M2 helix of sarcoplasmic reticulum Ca pump in Ca transport
○大保 貴嗣 (旭川医大・生化学)
Takashi Daiho (*Asahikawa Med. Univ.*)
- [1-10-1418](#) リポソーム再構成系を用いた細菌べん毛モーターの MS リング構築メカニズムの解析
Investigation of the flagellar MS-ring construction mechanism using liposome reconstitution system
○梶野 洗樹¹, 寺島 浩行², 本間 道夫¹, 小嶋 誠司¹ (¹名古屋大・院生命理学, ²長崎大・熱帯医学)
- Hiroyuki Kajino¹, Hiroyuki Terashima², Michio Homma¹, Seiji Kojima¹** (¹*Grad. Sch. Sci., Univ. Nagoya*, ²*Trop. Med. Inst., Univ. Nagasaki*)
- [1-10-1430](#) 両親媒性ペプチドから成るナノディスクを用いたロドプシンのパターン化モデル生体膜への再構成
Reconstitution of rhodopsin into a patterned model membrane using nanodisc formed from amphiphilic peptides
○杭田 美子¹, 林 文夫², 森垣 憲一^{1,3} (¹神戸大・農, ²神戸大・理学, ³神戸大・バイオシグナル総合研究センター)
- Fuko Kueda¹, Fumio Hayashi², Kenichi Morigaki^{1,3}** (¹*Grad. Sch. Agri., Univ. Kobe*, ²*Grad. Sch. Sci., Univ. Kobe*, ³*Biosignal Research Center, Univ. Kobe*)
- [1-10-1442](#) (2S7-1) Local membrane curvature influences lipid signaling
Marcel Hoerning¹, Torsten Bullmann², Tatsuo Shibata³ (¹*Institute of Biomaterials and Biomolecular Systems, University of Stuttgart, 70569 Stuttgart, Germany*, ²*Carl-Ludwig-Institute for Physiology, University of Leipzig, 04103 Leipzig, Germany*, ³*Laboratory for Physical Biology, RIKEN Center for Biosystems Dynamics Research, Kobe 650-0047, Japan*)
- [1-10-1454](#) 脂質スクランブリングペプチドによる細胞貪食誘導
Induction of phagocytosis by phospholipid scrambling peptides
○中尾 裕之, 木村 優介, 池田 恵介, 中野 実 (富山大・院薬)
Hiroyuki Nakao, Yusuke Kimura, Keisuke Ikeda, Minoru Nakano (*Fac. Pharm. Sci., Univ. Toyama*)
- [1-10-1506](#) Bt 菌 Cry46Ab トキシンの小孔形成とその殺蚊活性
Channel-pores formation of *Bacillus thuringiensis* Cry46Ab toxin and its mosquitocidal activity
○宮崎 美登香, 早川 徹, 井出 徹 (岡山大学・大学院ヘルスシステム統合科学研究科)
Midoka Miyazaki, Tohru Hayakawa, Toru Ide (*Grad Schl Interdiscip Sci Engrn Health Syst*)
- [1-10-1518](#) 四量体型ナトリウムチャンネルにおける二価カチオンによる活性阻害機構の創出
The generation of the divalent cation blocking on tetrameric sodium channel
○入江 克雅^{1,2}, 織田 祥徳³, 大嶋 篤典^{2,3} (¹和医大・薬, ²名大・細胞生理学研究センター, ³名大院・創薬)
Katsumasa Irie^{1,2}, Yoshinori Oda³, Atsunori Oshima^{2,3} (¹*Sch. Pharm., Wakayama. Med. Univ.*, ²*CeSPI, Nagoya Univ.*, ³*Grad. Sch. Pharm. Sci., Nagoya Univ.*)

座長：須藤 雄気 (岡山大学), 今元 泰 (京都大学)

Session Chairs: Yuki Sudo (Okayama Univ.), Yasushi Imamoto (Univ.)

- [1-11-1330](#) プロトンポンプ型ロドプシンを用いたアポトーシスの光制御
Optical control of apoptotic cell death by light-driven proton pumps
○小島 慧一^{1,2}, 中尾 新², 須藤 雄気^{1,2} (¹ 岡山大・医歯薬学域, ² 岡山大・薬学部)
Keiichi Kojima^{1,2}, Shin Nakao², Yuki Sudo^{1,2} (¹Grad. Sch. of Med. Dent. & Pharm. Sci. Okayama Univ., ²Fac. of Pharm. Sci., Okayama Univ.)
- [1-11-1342](#) 1 残基変異による光サイクル型脊椎動物ロドプシンの創製
Construction of photocyclic vertebrate rhodopsin by a single mutation
○酒井 佳寿美¹, 七田 芳則², 今元 泰¹, 山下 高廣¹ (¹ 京大・院理, ² 立命館・総合科学技術研究機構)
Kazumi Sakai¹, Yoshinori Shichida², Yasushi Imamoto¹, Takahiro Yamashita¹ (¹Grad. Sch. Sci., Kyoto Univ., ²Research organization for Sci. and Tech.)
- [1-11-1354](#) 赤色光感受性非視覚オプシンの解析
Characterization of red-sensitive non-visual opsin
○山下 高廣¹, 藤井 研吾¹, 藤藪 千尋¹, 酒井 佳寿美¹, 志賀 靖弘² (¹ 京大・院理, ² 東京薬大・院生命)
Takahiro Yamashita¹, Kengo Fujii¹, Chihiro Fujiyabu¹, Kazumi Sakai¹, Yasuhiro Shiga² (¹Grad. Sch. Sci., Kyoto Univ., ²Sch. Life. Sci., Tokyo Univ. of Pharm. and Life Sci.)
- [1-11-1406](#) 無脊椎動物ロドプシンの光構造変化
Light-induced conformational change of invertebrate rhodopsin
○今元 泰 (京大・院理)
Yasushi Imamoto (Grad. Sch. Sci., Kyoto Univ.)
- [1-11-1418](#) 藍色光にตอบสนองカルシウム透過性が高いチャンネルロドプシンの光遺伝学応用へ向けた取り組み
Calcium selectivity and optogenetics application of a deep blue absorbing channelrhodopsin
○角田 聡, 田代 凜太郎, 細島 頌子, 神取 秀樹 (名古屋工業大学生命応用化学専攻)
Satoshi Tsunoda, Rintaro Tashiro, Shoko Hososhima, Hideki Kandori (Nagoya Institute of Technology)
- [1-11-1430](#) 南極の好冷菌 *Hymenobacter nivis* P3^T 由来プロテオロドプシンの生理学的役割と光化学的特性
Physiological role and photochemical property of the cryophilic *Hymenobacter nivis* P3^T proteorhodopsin discovered in Antarctica
○近藤 香織¹, 大竹 峻平¹, 寺島 美亜², 小島 久弥², 福井 学², 出村 誠³, 菊川 峰志³, 塚本 卓³ (¹ 北海道大学・生命科学院, ² 北海道大学・低温科学研究所, ³ 北海道大学・先端生命科学研究院)
Kaori Kondo¹, Ryohei Ohtake¹, Mia Terashima², Hisaya Kojima², Manabu Fukui², Makoto Demura³, Takashi Kikukawa³, Takashi Tsukamoto³ (¹Graduate school of Life Science, Hokkaido University, ²Institute of Low Temperature Science, Hokkaido University, ³Faculty of Advanced Life Science, Hokkaido University)
- [1-11-1442](#) A *Geminigera cryophila* Anion Channelrhodopsin Shows Significantly Slow Photocycle
Hina Kurane¹, Makoto Demura², Takashi Kikukawa², Takashi Tsukamoto² (¹Graduate School of Life Science, Hokkaido University, ²Faculty of Advanced Life Science)
- [1-11-1454](#) クリプト藻由来の光受容陽イオンチャンネルのキネティクス
Kinetic evaluation of light-gated cation channels from cryptophyte
○細島 頌子, 重村 竣太, 神取 秀樹, 角田 聡 (名古屋工業大学 大学院工学研究科 生命・応用化学専攻)
Shoko Hososhima, Shunta Shigemura, Hideki Kandori, Satoshi Tsunoda (Life Science and Applied Chemistry, Nagoya Institute of Technology)

座長：高田 彰二（京都大学），高橋 卓也（立命館大学）

Session Chairs: Shoji Takada (Kyoto Univ.), Takuya Takahashi (Ritsumeikan Univ.)

- [1-12-1330](#) GroE 基質タンパク質によく見られる構造モチーフ
Small structural patterns common in chaperonin GroE substrate proteins
南 慎太郎¹, 丹羽 達也², 上村 英里², 小池 亮太郎¹, 田口 英樹², 〇太田 元規¹ (¹名大・情報,²東工大・科創研)
Shintaro Minami¹, Tatsuya Niwa², Eri Uemura², Ryotaro Koike¹, Hideki Taguchi², **Motonori Ota**¹
(¹Grad. Sch. Info., Nagoya Univ., ²IIR, Tokyo Tech.)
- [1-12-1342](#) Disentangling the Effects of Histone Post-Translational Modifications on Nucleosome Packing and Chromatin Structure
Justin Chan, Hidetoshi Kono (*Molecular Modeling and Simulation Group, Institute for Quantum and Life Science (iQLS), QST*)
- [1-12-1354](#) A meta-inference approach to modeling the 3d structure of chromatin from Hi-C data
Giovanni Bruno Brandani, Chenyang Gu, Shoji Takada (*Dept Biophysics, Div Biology, Grad School Science, Kyoto University*)
- [1-12-1406](#) Comparative Scoring Power Assessments of Protein-Ligand Docking Scoring Functions by Considering Protein Functional Groups
Yovita Ardiyani¹, Hafumi Nishi^{1,2,3}, Kengo Kinoshita^{1,3} (¹Grad. Sch. Info. Sci., Tohoku Univ., ²Fac. Core Res., Ochanomizu Univ., ³ToMMo, Tohoku Univ.)
- [1-12-1418](#) ヒトタンパク質データセットを利用した天然変性領域の長さタンパク質の機能の関係
Relationship between Length of Intrinsically Disordered Regions and Protein Function
〇谷本 悠, 小池 亮太郎, 太田 元規 (名大・院情報学)
Haruka Tanimoto, Ryotaro Koike, Motonori Ota (*Grad. Sch. Info., Nagoya Univ.*)
- [1-12-1430](#) 慢性歯周炎における血液組織の遺伝子発現データのメタ解析
Meta-analysis for gene expression data of blood tissue in chronic periodontitis
〇小泉 秀斗, 佐々木 貴規 (明治大・院先端数理)
Hideto Koizumi, Takanori Sasaki (*Fac. Adv. Math. Sci., Univ. Meiji*)
- [1-12-1442](#) 仮想系共役サンプリング法の開発と応用
Development and Application of the virtual-system coupled canonical sampling method
〇笠原 浩太¹, 謝 祺琳², 酒井 佑介², 中野 雄太², 肥後 淳一³, 高橋 卓也¹ (¹立命館大・生命,²立命館大・院・生命,³立命館大・総研機構)
Kota Kasahara¹, Qilin Xie², Yusuke Sakai², Yuta Nakano², Junichi Higo³, Takuya Takahashi¹ (¹Coll. Life Sci., Ritsumeikan Univ., ²Grad. Sch. Life. Sci., Ritsumeikan Univ., ³Res. Org. Sci. Tech., Ritsumeikan Univ.)

座長：太田 元規 (名古屋大学), 佐々木 貴規 (明治大学)
Session Chairs: Motonori Ota (Nagoya Univ.), Takanori Sasaki (Meiji Univ.)

- [1-13-1330](#) 結合蛋白質 CARMIL や twinfilin がキャップ蛋白質の構造ゆらぎに与える影響を弾性ネットワークモデルにより解析する
Elastic network model analysis shows distinct flexibilities of capping protein bound to CARMIL or twinfilin
○小池 亮太郎, 太田 元規 (名大・情報)
Ryotaro Koike, Motonori Ota (*Grad. Sch. Info., Nagoya Univ.*)
- [1-13-1342](#) RNA-seq 発現解析・パスウェイ解析による、腫瘍選択的抗 CD137 アゴニスト抗体 STA551 の癌微小環境および正常組織への効果
RNA-seq based expression analysis of the extracellular ATP dependent tumor-selective response of the STA551 antibody targeting CD137
○目次 正一¹, 高桑 和也¹, 堀川 小百合¹, 内川 亮¹, 谷口 健治¹, 濱田 孝樹¹, 成田 義規², 櫻井 実香¹ (¹ 中外製薬株式会社, ²Chugai Pharmabody Research Pte. Ltd)
Shoichi Metsugi¹, Kazuya Takakuwa¹, Sayuri Horikawa¹, Ryo Uchikawa¹, Kenji Taniguchi¹, Koki Hamada¹, Yoshinori Narita², Mika Sakurai¹ (¹Chugai Pharmaceutical Co. Ltd., ²Chugai Pharmabody Research Pte. Ltd)
- [1-13-1354](#) 精製因子によるゲノム転写翻訳系の再構成とその網羅的解析
Reconstitution of the *E.coli* genome transcription and translation system with its purified elements
○松井 ゆきの¹, 丹羽 達也², 田口 英樹², 土居 信英¹, 藤原 慶¹ (¹慶大・理工,²東工大・細胞センター)
Yukino Matsui¹, Tatsuya Niwa², Hideki Taguchi², Nobuhide Doi¹, Kei Fujiwara¹ (¹Dept. Biosci. Info., Keio Univ., ²Cell Biol. Center IIR, Tokyo Tech.)
- [1-13-1406](#) 核スペckルの構造形成・動態のシミュレーション
Simulations of structural dynamics of nuclear speckle
○若尾 真吾, 藤井 雅史, 粟津 暁紀 (広島大・院統合生命科学)
Shingo Wakao, Masashi Fuji, Akinori Awazu (*Graduate School of Integrated Sciences for Life, Hiroshima University*)
- [1-13-1418](#) 転写因子 PC4 の天然変性領域とテグメントタンパク質 VP16 の結合メカニズムの計算科学的検討
Simulation study of binding mechanism between intrinsically disordered region of transcription factor PC4 and tegument protein VP16
○謝 祺琳¹, 中野 雄太¹, 酒井 佑介¹, 笠原 浩太², 肥後 順一³, 高橋 卓也² (¹立命館大・院・生命,²立命館大・生命,³立命館大・総研機構)
Qilin Xie¹, Yuta Nakano¹, Yusuke Sakai¹, Kota Kasahara², Junichi Higo³, Takuya Takahashi² (¹Grad. Sch. Life Sci., Ritsumeikan Univ., ²Coll. Life Sci., Ritsumeikan Univ., ³Res. Org. Sci. Tech., Ritsumeikan Univ.)
- [1-13-1430](#) 出芽酵母の胞子形成関連遺伝子群の各時間クラスへの非階層的クラスタリング
Non-hierarchical clustering of sporulation related genes of budding yeast to each temporal class
○谷 葵衣, 佐々木 貴規 (明治大・院・先端数理)
Aoi Tani, Takanori Sasaki (*Fac. Adv. Math. Sci., Meiji Univ.*)

- [1-13-1442](#) UV_C 照射によるゲノム変異導入は効果的な方法か？
Is the introduction of genomic mutations by UV_C irradiation an effective method?
○井原 邦夫^{1,2}, 松尾 佳祐², 上坂 一馬¹ (¹名古屋大学 遺伝子実験施設, ²名古屋大学 理学部生命理学科)
Kunio Ihara^{1,2}, Keisuke Matsuo², Kazuma Uesaka¹ (¹Nagoya University, Center for Gene Research, ²Nagoya University, Faculty of Science)
- [1-13-1454](#) トランスクリプトーム解析による表現型多型の考察
Transcriptome data analysis for phenotype polymorphism
今田 実子, ○粟津 暁紀 (広大統合生命)
Miko Imada, **Akinori Awazu** (Dept. Math. and Life Sci., Hiroshima Univ.)

13:30~15:30 Ch14

1G14 数理生物学・非平衡・生体リズム I

Mathematical biology, Nonequilibrium state & Biological rhythm I

座長：佐甲 靖志 (理化学研究所), 亀尾 佳貴 (京都大学)

Session Chairs: Yasushi Sako (RIKEN), Yoshitaka Kameo (Kyoto Univ.)

- [1-14-1330](#) A log-periodic based model of cell-group repair and failure—cancer
Hiroshi Yoshida (Math Dept. Kyushu Univ.)
- [1-14-1342](#) Emergent slower synchronous beating behavior in spontaneous beating cardiomyocyte clusters
Yoshitsune Hondo, Kazufumi Sakamoto, Kenji Yasuda (Dept. Pure & Appl. Phys., Grad. Sch. Adv. Sci. & Eng., Waseda Univ.)
- [1-14-1354](#) Can overdrive suppression explain the synchronized beating behavior of spontaneous beating cardiomyocyte clusters?
Kazufumi Sakamoto, Yoshitsune Hondo, Kenji Yasuda (Dept. Pure & Appl. Phys., Grad. Sch. Adv. Sci. & Eng., Waseda Univ.)
- [1-14-1406](#) Stochastic modeling of the effect of vaccination strategies on the spread of a COVID-19-type virus
Yuki Matsuzawa¹, Shiho Ando¹, Mc Gahan Patricia¹, Hiromichi Tsurui², Hall Damien³, Yutaka Kuroda¹ (¹Department of Biotechnology and Life Sciences, Tokyo University of Agriculture and Technology, ²Department of Immunological Diagnosis, Juntendo University School of Medicine, ³W.P.I. Nano Life Science Institute. Kanazawa University)
- [1-14-1418](#) 曲率誘導タンパク質の反応拡散波による管状膜の変形
Deformation of tubular membranes with excitable reaction-diffusion waves of curvature-inducing proteins
○爲本 尚樹, 野口 博司 (東大・物性研)
Naoki Tamemoto, Hiroshi Noguchi (ISSP, Univ. Tokyo)
- [1-14-1430](#) 自己駆動粒子の確率的な走化性
Stochastic Chemotaxis Demonstrated by a Self-Propelled Particle
○末松 J. 信彦¹, 池田 幸太¹, 小田切 健太² (¹明大・院先端数理, ²専修大・情報ネットワーク)
J. Nobuhiko Suematsu¹, Kota Ikeda¹, Kenta Odagiri² (¹Grad. Sch. Adv. Math. Sci., Meiji Univ., ²Dep. Net. and Info., Senshu Univ.)
- [1-14-1442](#) 繊維状粒子凝集の CA タイプ解析
CA-type formal analysis of fibrous assembly of particles
○今野 卓 (福井大学医学部生物数学)
Takashi Konno (Biomath., Med., Uni. Fukui)
- [1-14-1454](#) Establishment of quantitative mechanical measurements for intracellular structures
Ryota Ori, Hirokazu Tanimoto (Grad. Sch. Nanobioscience., Univ. Yokohama City)

- [1-14-1506](#) 力学刺激に応じた非石灰化・石灰化線維軟骨の分布を有する腱・靭帯附着部形成の数理モデリング
Mathematical modeling of enthesis formation with mechano-dependent distribution of uncalcified and calcified fibrocartilage
○福田 晃子¹, 亀尾 佳貴^{1,2}, 安達 泰治^{1,2} (¹京大・院生命科学,²京大・ウイルス再生研)
Akiko Fukuda¹, Yoshitaka Kameo^{1,2}, Taiji Adachi^{1,2} (¹*Grad. Sch. Biostudies, Kyoto Univ.*, ²*Inst. Front. Life Med. Sci., Kyoto Univ.*)
- [1-14-1518](#) クサカゲロウの翅の規範とした表面に微細構造を持つフィルムの電場計算
Electric field calculations of a film with surface fine structure inspired by a wing of green lacewing
○桂嶋 優呂¹, 高橋 玲央奈², 吉田 一也¹ (¹山形大・院理工学,²青学大・院理工学)
Yuro Katsurashima¹, Leona Takahashi², Kazunari Yoshida¹ (¹*Grad.Sch.Sci., Univ.Yamagata*, ²*Grad.Sch.Sci., Yniv.Ymagata*)

13:30~15:30 Ch15
1G15 計測 I
Measurements I

座長：原田 慶恵 (大阪大学), 永井 健治 (大阪大学)
Session Chairs: Yoshie Harada (Osaka Univ.), Takeharu Nagai (Osaka Univ.)

- [1-15-1330](#) (2S2-4) 細胞膜中の TRPV1・TRPV4 チャンネルの 1 分子動態の比較解析
(2S2-4) Comparative analysis of single-molecule dynamics of TRPV1 and TRPV4 channels in living cells
○柳川 正隆^{1,2}, 桑島 佑太郎^{1,3}, 阿部 充宏¹, 廣島 通夫^{1,4}, 上田 昌宏^{4,5}, 有田 誠^{3,6,7}, 佐甲 靖志¹
(¹理研 CPR, ²科学技術振興機構, ³慶應大・院薬, ⁴理研 BDR, ⁵阪大・院生命機能, ⁶理研 IMS, ⁷横浜市大・院生命医学)
Masataka Yanagawa^{1,2}, Yutaro Kuwashima^{1,3}, Mitsuhiro Abe¹, Michio Hiroshima^{1,4}, Masahiro Ueda^{4,5}, Makoto Arita^{3,6,7}, Yasushi Sako¹ (¹*Riken CPR*, ²*JST, PRESTO*, ³*Faculty Pharm., Keio Univ.*, ⁴*Riken BDR*, ⁵*Grad. Sch. Front. Biosci., Osaka University*, ⁶*Riken IMS*, ⁷*Grad. Sch. Med. Life Sci., Yokohama City Univ.*)
- [1-15-1342](#) G タンパク質共役型受容体オリゴマーと G タンパク質の結合能に関する生細胞一分子解析
Live-cell single-molecule analysis on the binding affinity of G protein-coupled receptor oligomers with G protein
○西口 知輝¹, 吉村 英智², 笠井 倫志³, 藤原 敬宏⁴, 小澤 岳昌² (¹新潟大・院医歯学,²東京大・院理学,³岐阜大・糖鎖生命コア研究所,⁴京都大・物質-細胞統合システム拠点)
Tomoki Nishiguchi¹, Hideaki Yoshimura², Rinshi S. Kasai³, Takahiro K. Fujiwara⁴, Takeaki Ozawa² (¹*Grad. Sch. Med. Dent. Sci., Niigata Univ.*, ²*Grad. Sch. Sci., Univ. Tokyo*, ³*iGCORE, Gifu Univ.*, ⁴*iCeMS, Kyoto Univ.*)
- [1-15-1354](#) 0.1 °C の温度上昇をオルガネラレベルで可視化する：蛍光タンパク質を用いた高感度温度プローブの開発
A highly sensitive thermosensor using fluorescent proteins to capture temperature change of 0.1 °C at the organelle level
○福島 俊一, 永井 健治 (大阪大・産研)
Shun-ichi Fukushima, Takeharu Nagai (*SANKEN, Osaka Univ.*)
- [1-15-1406](#) 生体機能多重測定のための最短吸収・発光波長を持つ蛍光タンパク質の開発
Development of a violet fluorescent protein with the shortest absorption/emission wavelengths for multiplex bioimaging
○杉浦 一徳, 永井 健治 (大阪大学・産業科学研究所)
Kazunori Sugiura, Takeharu Nagai (*Osaka Univ., SANKEN*)
- [1-15-1418](#) High throughput genotype-phenotype linkage by Raman microscopy
Yuki Yoshida, Reiko Okura, Kenichiro F. Kamei, Yuichi Wakamoto (*Grad. Sch. Arts Sci., Univ. Tokyo*)

- [1-15-1430](#) カルマン smoother を用いたノイズに対して頑健な細胞牽引力測定
Kalman smoother traction force microscopy for robust force inference
○松田 青創¹, 難波 利典², 石原 秀至² (¹ 東京大学前期教養学部理科一類, ² 東京大学大学院総合文化研究科)
Aozora Matsuda¹, Toshinori Namba², Shuji Ishihara² (*1Junior Division Science 1 of College of Art and Science, The University of Tokyo, 2Graduate school of Arts and Sciences, The University of Tokyo*)
- [1-15-1442](#) Development of iSCAT Microscopy and Improvement of the Images with Deep Learning
Satori Kawashi¹, Yasushi Okada^{1,2,3} (*1Univ. of Tokyo, Grad. Sch. of Sci., Dept. of Phys., 2RIKEN, BDR, Lab. for Cell Polarity Regulation, 3Univ. of Tokyo, Grad. Sch. of Med., Dept. of Med. Sci.*)
- [1-15-1454](#) 熱揺らぎ一定モード原子間力顕微鏡の開発
Development of constant thermal fluctuation mode atomic force microscopy
○山本 大輔 (福岡大・理)
Daisuke Yamamoto (*Fac. Sci., Fukuoka Univ.*)
- [1-15-1506](#) Development of Damage-free Imaging Cell Sorter Exploiting Alginate Capsules
Toshinosuke Akimoto, Kenji Yasuda (*Dept. Pure & Appl. Phys., Grad. Sch. Adv. Sci. & Eng., Waseda Univ.*)
- [1-15-1518](#) A programmable DNA origami nanospring that reports dynamics of single integrin traction forces in living cells
Hitomi Matsubara^{1,2}, Hiroki Fukunaga^{1,2}, Takahiro Saitoh¹, Keigo Ikezaki³, Mitsuhiro Iwaki^{2,4} (*1Grad. FBS., Univ. Osaka, 2BDR, RIKEN, 3Grad. Pys. Sci., Univ. Tokyo, 4IFReC., Univ. Osaka*)

13:30~15:30 Ch16

1G16 バイオエンジニアリング
Bioengineering

座長：角五 彰 (北海道大学), 船津 高志 (東京大学)

Session Chairs: Akira Kakugo (Hokkaido Univ.), Takashi Funatsu (The Univ. of Tokyo)

- [1-16-1330*](#) Analyzing a printable actuator composed of an engineered kinesins by a computer simulation
Yurino Aoyama¹, Yuichi Hiratsuka², Takahiro Nitta³ (*1Grad. Appl. Math. Phys. Div. , Gifu University, 2Sch. Materials Sci. ,JAIST, 3Appl. Phys. Course, Faculty of Eng., Gifu University*)
- [1-16-1342*](#) 自動振動を利用した羽ばたきロボットの開発
The development of insect-like flapping robot using self-excited vibration
○藤森 嵩人¹, 若本 稜生², 増田 容一² (¹ 大阪大学理学部生物科学科, ² 大阪大学工学研究科機械工学専攻)
Takahito Fujimori¹, Ryo Wakamoto², Youichi Masuda² (*1Undergraduate of School of Science of Biology ,Osaka university, 2Department of Mechanical Engineering,Osaka University*)
- [1-16-1354*](#) DNA コンピューティングを用いた分子ロボットの自動制御
Automated control of molecular robots using DNA computing
○西山 晃平¹, 松本 大輝², ケヤ ジャナット ジャキア³, 川又 生吹², 野村 M. 慎一郎², 角五 彰^{1,3} (¹ 北大院・総化, ² 北大院・工, ³ 北大院・理)
Kohei Nishiyama¹, Daiki Matsumoto², Jakia Jannat Keya³, Ibuki Kawamata², Shin-ichiro M. Nomura², Akira Kakugo^{1,3} (*1Grad. Sch. of Chem. Sci. and Eng., Hokkaido Univ., 2Grad. Sch. of Eng., Tohoku Univ., 3Grad. Sch. of Sci., Hokkaido Univ.*)
- [1-16-1406*](#) 蛍光増大能を指標とした新規蛍光 RNA アプタマー創出法の開発
An efficient method to obtain fluorogenic RNA aptamers based on ability to activate fluorescence
○伊藤 敬佑, 飯塚 怜, 上村 想太郎 (東京大・理学系研究科・生物科学専攻)
Keisuke Ito, Ryo Iizuka, Sotaro Uemura (*Dept. Biol. Sci., Grad. Sch. Sci., The Univ. Tokyo*)

- [1-16-1418*](#) On-chip 無細胞クローニングに向けた 1 分子環状 DNA からの増幅
Amplification from single molecular circular DNA for on-chip cell-free cloning
○東 耕平¹, 皆川 慶嘉¹, 末次 正幸², 野地 博行¹ (¹東京大・院応用化学,²立教大・生命理学)
Kohei Higashi¹, Yoshihiro Minagawa¹, Masayuki Su'tsugu², Hiroyuki Noji¹ (¹*Dept. Appl. Chem., Grad. Sch. Eng., Univ. Tokyo*, ²*Dept. Life Sci., Coll. Sci., Rikkyo Univ.*)
- [1-16-1430*](#) 水性二相系液滴を利用した DNA マイクロカプセルの設計
Design of DNA microcapsules using aqueous two-phase system droplets
○瀬野 真由美, マスカワ マルコス, 瀧ノ上 正浩 (東京工業大学 情報理工学院 情報工学系)
Mayumi Chano, Marcos Masukawa, Masahiro Takinoue (*Department of Computer Science, School of Computing, Tokyo Institute of Technology*)
- [1-16-1442](#) 負のポアソン比をもつ 3 次元 DNA ナノ構造体の設計
Design of 3D DNA nanostructures with negative Poisson's ratio
○山下 和諠¹, 瀧ノ上 正浩² (¹東京工業大学 生命理工学院 生命理工学系,²東京工業大学 情報理工学院 情報工学系)
Nagi Yamashita¹, Masahiro Takinoue² (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*)
- [1-16-1454](#) 低温条件下で DNA 状態機械が効率的に動作するための状態配列長の短縮
Reduction of the length of state sequences for efficient operation of a DNA state machine under low temperature conditions
○小宮 健 (海洋研究開発機構)
Ken Komiya (*JAMSTEC*)
- [1-16-1506](#) フェリチン 1 分子中の H, L サブユニットの割合制御と鉄ナノ粒子の結晶性の比較
Regulation of H/L subunit content in apoferritin and crystallinity of the iron core
金丸 朋子¹, 金丸 周司², ○吉村 英恭¹ (¹明大・理工,²東工大・生命理工)
Tomoko Kanamaru¹, Shuji Kanamaru², **Hideyuki Yoshimura**¹ (¹*Meiji Univ.*, ²*Tokyo Inst. Tech.*)
- [1-16-1518](#) Screening of agarolytic microbial cells with a deformability-based microfluidic microdroplet sorting device
Mikihisa Muta¹, Kai Saito¹, Ryo Iizuka¹, Wataru Kawakubo², Dong Hyun Yoon³, Tetsushi Sekiguchi³, Shuichi Shoji², Mei Ito⁴, Yuji Hatada⁴, Takashi Funatsu¹ (¹*Grad. Sch. of Pharm. Sci., The Univ. of Tokyo*, ²*Dept. of Nanosci. and Nanoeng., Waseda Univ.*, ³*Res. Org. for Nano & Life Innov., Waseda Univ.*, ⁴*Dept. of Life Sci. and Green Chem., Saitama Inst. of Technol.*)

2 日目 (11 月 26 日 (金)) / Day 2 (Nov. 26 Fri.)

13:15~15:27 Ch01
2G01A タンパク質：設計 II、一般 II
Protein: Design II, General II

座長：古賀 信康 (分子科学研究所), 濡木 理 (東京大学)
Session Chairs: Nobuyasu Koga (IMS), Osamu Nureki (The Univ. of Tokyo)

- [2-01-1315*](#) The potential of artificially designed α -helical peptide nanofibers
Minami Kurokawa¹, Mika Hirose², Akihiro Kawamoto², Atsuo Tamura¹ (¹*Grad. Sch. Sci., Univ. Kobe.*, ²*IPR, Osaka Univ.*)
- [2-01-1327*](#) SARS-CoV-2 スパイクタンパク質の受容体結合ドメインに対する中和抗体の合理的設計
Rational design of neutralizing antibodies against the receptor-binding domain of SARS-CoV-2 Spike protein
○松本 彩里¹, 林 勇樹¹, 新井 宗仁^{1,2} (¹東大・総合文化・生命環境,²東大・理・物理)
Sairi Matsumoto¹, Yuuki Hayashi¹, Munehito Arai^{1,2} (¹*Dept. Life Sci., Univ. Tokyo*, ²*Dept. Phys., Univ. Tokyo*)

- [2-01-1339*](#) 転写活性化に関する相互作用を標的としたペプチド阻害剤の合理的設計
Rational design of the peptide inhibitor targeting the interactions involved in transcriptional activation
○佐藤 那音¹, 季高 駿士¹, 林 勇樹¹, 新井 宗仁^{1,2} (¹東大・総合文化・生命環境, ²東大・理・物理)
Nao Sato¹, Shunji Suetaka¹, Yuuki Hayashi¹, Munchito Arai^{1,2} (¹*Dept. Life Sci., Univ. Tokyo*, ²*Dept. Phys., Univ. Tokyo*)
- [2-01-1351*](#) αヘリックスを介したタンパク質間相互作用の阻害に向けた合理的医薬品設計
Rational drug design to inhibit α-helix-mediated protein-protein interactions
○季高 駿士¹, 佐藤 那音¹, 本多 栄治², 高島 一², 岡 芳樹¹, 榎原 朋子¹, 竹原 大², 吉森 篤史³, 林 勇樹¹, 新井 宗仁^{1,4} (¹東大・総合文化・生命環境, ²PRISM BioLab, ³理論創薬研究所, ⁴東大・理・物理)
Shunji Suetaka¹, Nao Sato¹, Eiji Honda², Hajime Takashima², Yoshiki Oka¹, Tomoko Kuniyama¹, Dai Takehara², Atsushi Yoshimori³, Yuuki Hayashi¹, Munchito Arai^{1,4} (¹*Dept. Life Sci., Univ. Tokyo*, ²*PRISM BioLab Co., Ltd.*, ³*Inst. Theor. Med., Inc.*, ⁴*Dept. Phys., Univ. Tokyo*)
- [2-01-1403*](#) Magnet のタンパク質間相互作用を強化する変異体の合理的設計
Improving dimer affinity of Magnets photodimerizers by computational design
○吉村 匡隆¹, 青野 侑基¹, 林 勇樹¹, 佐藤 守俊^{1,2}, 新井 宗仁^{1,3} (¹東大・総合文化・生命環境, ²JST・CREST, ³東大・理・物理)
Masataka Yoshimura¹, Yuki Aono¹, Yuuki Hayashi¹, Moritoshi Sato^{1,2}, Munchito Arai^{1,3} (¹*Dept. Life Sci., Univ. Tokyo*, ²*CREST, JST*, ³*Dept. Phys., Univ. Tokyo*)
- [2-01-1415*](#) PD-1 受容体を標的とする免疫チェックポイント阻害タンパク質の合理的設計
Rational design of immune checkpoint inhibitory proteins targeting the PD-1 receptor
○島村 博太郎¹, 林 勇樹², 新井 宗仁^{1,2} (¹東大・理・物理, ²東大・総合文化・生命環境)
Hirotarō Shimamura¹, Yuuki Hayashi², Munchito Arai^{1,2} (¹*Dept. Phys., Univ. Tokyo*, ²*Dept. Life Sci., Univ. Tokyo*)
- [2-01-1427*](#) アレルギー性喘息を抑制する interleukin-33/ST2 阻害剤の合理的な設計
Rational design of an interleukin-33/ST2 inhibitor for suppressing allergic asthma
○寺西 美月¹, 佐野 美桜¹, 林 勇樹¹, 新井 宗仁^{1,2} (¹東大・総合文化・生命環境, ²東大・理・物理)
Mizuki Teranishi¹, Mio Sano¹, Yuuki Hayashi¹, Munchito Arai^{1,2} (¹*Dept. Life Sci., Univ. Tokyo*, ²*Dept. Phys., Univ. Tokyo*)
- [2-01-1439*](#) バンドル様相互作用面を用いない多様な回転対称複合体の設計
Toward design of diverse symmetric protein homo-oligomers using non-bundle-like interface
○海田 新悟¹, 小林 直也², 小杉 貴洋^{3,4,5,6}, 古賀 信康^{3,4,5} (¹総研大・物・構造, ²奈良先端大・物質創成, ³自然科学・生命創成, ⁴分子研・協奏, ⁵総研大, ⁶JST・さきかけ)
Shingo Kaida¹, Naoya Kobayashi², Takahiro Kosugi^{3,4,5,6}, Nobuyasu Koga^{3,4,5} (¹*Dept. Structural Molecular Sci., SOKENDAI*, ²*Div. Mat. Sci., Grad. Sch. Sci. Tech., NAIST*, ³*ExCELLS, NINS*, ⁴*CIMoS, IMS*, ⁵*SOKENDAI*, ⁶*JST, PRESTO*)
- [2-01-1451*](#) (1S6-6) アデノシン A_{2A} 受容体の不活性型構造を安定化するための all-α 融合パートナータンパク質のゼロからの合理デザイン
(1S6-6) De novo design of an alpha-helical fusion partner protein to stabilize adenosine A_{2A} receptor in the inactive state
○三本 斉也^{1,2}, 菅谷 幹奈³, 風間 一輝³, 中野 僚介³, 小杉 貴洋^{1,2,4}, 村田 武士³, 古賀 信康^{1,2,4} (¹総研大・物理科学, ²分子研, ³千葉大・理, ⁴自然科学・生命創成)
Masaya Mitsumoto^{1,2}, Kanna Sugaya³, Kazuki Kazama³, Ryosuke Nakano³, Takahiro Kosugi^{1,2,4}, Takeshi Murata³, Nobuyasu Koga^{1,2,4} (¹*SOKENDAI*, ²*IMS, NINS*, ³*Grad. Sch. of Sci. and Eng., Chiba Univ.*, ⁴*ExCELLS, NINS*)

[2-01-1503](#) 脂肪酸結合タンパク質 FABP3 と FABP7 におけるリガンド結合特性の比較
A comparative study of ligand-binding properties between fatty acid-binding proteins FABP3 and FABP7

○並木 葉月¹, 徳留 俊¹, 野村 舞¹, 林 史夫², 井上 裕介^{1,3}, 杉山 成⁴, 松岡 茂⁵, 村田 道雄⁶, 園山 正史^{1,3,7} (¹群馬大・院理工,²群馬大・機器分析セ,³群馬大・食健康セ,⁴高知大・理工,⁵大分大・院医,⁶阪大・院理,⁷群馬大・未来先端)

Hazuki Namiki¹, Shun Tokudome¹, Mai Nomura¹, Fumio Hayashi², Yusuke Inoue^{1,3}, Shigeru Sugiyama⁴, Shigeru Matsuoka⁵, Michio Murata⁶, Masashi Sonoyama^{1,3,7} (¹*Grad. Sch. Sci. Tech., Gunma Univ.*, ²*Ctr. Inst. Anal., Gunma Univ.*, ³*GUCFW, Gunma Univ.*, ⁴*Sch. Sci. Tech., Kochi Univ.*, ⁵*Grad. Sch. Med., Oita Univ.*, ⁶*Grad. Sch. Sci., Osaka Univ.*, ⁷*GIAR, Gunma Univ.*)

[2-01-1515](#) ヒト PTH1 受容体における内因性リガンド認識メカニズムとそのダイナミクス

Endogenous ligand recognition and structural transition of a human PTH receptor

○小林 和弘¹, 川上 耕季², 草木 迫司¹, 郷野 弘剛¹, 富田 篤弘¹, 志甫 谷 渉¹, 小林 幹¹, 山下 恵太郎³, 西澤 知宏⁴, 加藤 英明^{1,5}, 井上 飛鳥², 濡木 理¹ (¹東京大学理学系研究科生物化学専攻,²東北大学 薬学系研究科,³MRC 研究所,⁴横浜市立大学生命医科学研究科,⁵東京大学総合文化研究科)

Kazuhiro Kobayashi¹, Kouki Kawakami², Tsukasa Kusakizako¹, Hirotake Gono¹, Atsuhiro Tomita¹, Wataru Shihoya¹, Kan Kobayashi¹, Keitaro Yamashita³, Tomohiro Nishizawa⁴, Hideaki Kato^{1,5}, Asuka Inoue², Osamu Nureki¹ (¹*Department of Biological Sciences Graduate School of Science The University of Tokyo*, ²*Graduate School of Pharmaceutical Sciences, Tohoku University*, ³*MRC Laboratory of Molecular Biology*, ⁴*Graduate School of Medical Life Science, Yokohaya City University*, ⁵*Komaba Institute for Science, The University of Tokyo*)

16:00~18:24 Ch01

2G01B タンパク質：一般 IV

Protein: General IV

座長：津本 浩平 (東京大学), 徳樂 清孝 (室蘭工業大学)

Session Chairs: Kouhei Tsumoto (The Univ. of Tokyo), Kiyotaka Tokuraku (Muroran Inst. of Tech.)

[2-01-1600](#) Role of the domain 3 of the hemolytic lectin CEL-III in hemolytic activity and oligomerization
Shuichiro Goda^{1,2}, Keisuke Fukumoto¹, Yuta Yamawaki¹, Hideaki Unno¹, Tomomitsu Hatakeyama¹ (¹*Grad. Sch. Of Eng., Nagasaki Univ.*, ²*GalSIC, Soka Univ.*)

[2-01-1612](#) Mechanistic insights into Bedaquiline inhibition of the mycobacterial ATP synthase
Alexander Krahl¹, Peter J. Bond^{1,2} (¹*Bioinformatics Institute (BII), Agency for Science, Technology and Research (A*STAR)*, ²*Department of Biological Sciences, National University of Singapore*)

[2-01-1624](#) タンパク質の熱伝導度
Thermal conductivity of proteins

○倭 剛久 (名大・院理)

Takahisa Yamato (*Nagoya Univ.*)

[2-01-1636](#) フィンブリンのアクチンフィラメントに対する一方向性の協同的相互作用はフィラメントの短縮を引き起こす

Unidirectional cooperative interaction of fimbrin to actin filaments evokes the filament shortening
○綱淵 椋介¹, 細川 直輝¹, 倉賀野 正弘¹, 吉野 敦貴¹, 柴田 桂太郎², 上田 太郎³, 徳樂 清孝¹ (¹室蘭工業大学大学院,²徳島大学大学院医歯薬学研究所,³早稲田大学理工学術院)

Ryosuke Tsunabuchi¹, Naoki Hosokawa¹, Masahiro Kuragano¹, Atsuki Yoshino¹, Keitaro Shibata², Taro Q.P. Uyeda³, Kiyotaka Tokuraku¹ (¹*Muroran Institute of Technology*, ²*Graduate School of Medical Science, Tokushima University*, ³*Faculty of Science and Engineering, Waseda University*)

- [2-01-1648](#) マグネトソーム鎖の細胞内配置の制御に関わる MamY タンパク質の機能解析
Functional analyses of MamY protein involving in subcellular positioning of magnetosomes chain
○下茂 梨乃¹, 菊池 洋輔², 田岡 東^{2,3} (¹金沢大・院・自然科学, ²金沢大・理工, ³金沢大・ナノ研)
Rino Shimoshige¹, Yousuke Kikuchi², Azuma Taoka^{2,3} (¹*Grad. Sch. Nat. Sci. Tech. Kanazawa Univ.*, ²*Inst. Sci. Eng. Kanazawa Univ.*, ³*NanoLSI, Kanazawa Univ.*)
- [2-01-1700](#) バッファー成分が抗体製剤の不溶性異物形成に与える影響について
Impact of Buffer Component on the Formation of Visible Particles in Antibody Preparations
○和湯 千紘, 末友 裕行, 三谷 麻綺, 細川 俊仁 (協和キリン株式会社 バイオ生産技術研究所)
Chihiro Wayu, Hiroyuki Suetomo, Maki Mitani, Toshihito Hosokawa (*Bio Process Research and Development Laboratories, Kyowa Kirin Co., Ltd.*)
- [2-01-1712](#) (2S6-1) Extensive Sampling of Spike protein down, one-up, one-open, and two-up-like Conformations and Transitions in SARS-Cov-2
Hisham Dokainish¹, Suyong Re⁴, Chigusa Kobayashi², Takaharu Mori¹, Jaewoon Jung^{1,2}, Yuji Sugita^{1,2,3} (¹*Theoretical Molecular Science Laboratory, Riken*, ²*Computational Biophysics Research Team, RIKEN*, ³*Laboratory for Biomolecular Function Simulation, RIKEN*, ⁴*Center for Drug Design Research, National Institutes of Biomedical Innovation*)
- [2-01-1724](#) 繊毛虫テトラヒメナにおける内腕ダイニン発現系の開発および単頭分子種の運動特性
Development of an expression system in *Tetrahymena* inner arm dynein and motile properties of the single-headed subspecies
○枝松 正樹 (東大・院生命)
Masaki Edamatsu (*Dept. Life Sci., Grad. Sch. Arts Sci., Univ. Tokyo*)
- [2-01-1736](#) 発色団および非発色団解離基間の相互作用は、蛍光タンパク質の光学的性質において重要な役割を担う
Interplay of protonations at chromophore and non-chromophore sites plays a key role in the photo-properties of fluorescent proteins
○和沢 鉄一, 野間 涼平, 杉浦 一徳, 永井 健治 (阪大・産研)
Tetsuichi Wazawa, Ryohei Noma, Kazunori Sugiura, Takeharu Nagai (*SANKEN, Osaka Univ.*)
- [2-01-1748](#) Measurement on integrated forces of multiple kinesin motors through cross-linked microtubules with a glass microneedle
Naruaki Tsuji¹, Naritaka Kobayashi¹, Seiichiro Nakabayashi¹, Hiroshi Yoshikawa², Ryuzo Kawamura¹ (¹*Grad. Sch. Sci. Eng., Saitama Univ.*, ²*Grad. Sch. Eng., Osaka Univ.*)
- [2-01-1800](#) グルタミン酸脱水素酵素活性クレフト周辺での補酵素結合経路探索
Search for binding pathway of co-enzyme around the active-site cleft of glutamate dehydrogenase
○若林 大貴^{1,2}, 大出 真央^{1,2}, 加藤 貴之³, 中迫 雅由^{1,2} (¹慶應・理工, ²理研・RSC, ³阪大・蛋白研)
Taiki Wakabayashi^{1,2}, Mao Oide^{1,2}, Takayuki Kato³, Masayoshi Nakasako^{1,2} (¹*Dept. Phys., Keio Univ.*, ²*RSC, RIKEN*, ³*Protein Inst., Osaka Univ.*)
- [2-01-1812](#) Free energy landscape analysis of conformational transition of NtrC by chameleon model
Taisei Nagata, Masaki Sasai, Tomoki P. Terada (*Dept. Appl. Phys., Grad. Sch. Eng., Nagoya Univ.*)

座長：杉田 有治 (理化学研究所), 吉川 雅英 (東京大学)

Session Chairs: Yuji Sugita (RIKEN), Masahide Kikkawa (The Univ. of Tokyo)

[2-02-1315*](#) 繊毛虫ヨツヒメゾウリムシ由来アルギニンキナーゼの構造解析

Structural analysis of arginine kinase from the ciliate *Paramecium tetraurelia*

○横田 淳平¹, 大塚 夢斗¹, 児島 よしの¹, 矢野 大地², 宇田 幸司¹, 鈴木 知彦¹, 杉山 成¹ (¹ 高知大・理工, ² 中部大・応用生物)

Junpei Yokota¹, Yumeto Otsuka¹, Yoshino Kojima¹, Daichi Yano², Koji Uda¹, Tomohiko Suzuki¹, Shigeru Sugiyama¹ (¹*Fac. Sci. & Tec., Kochi Univ.*, ²*Dept. Environ. Biol., Chubu Univ.*)

[2-02-1327*](#) SSX1 に示唆される新規の DNA 結合ドメインのその溶液中構造解析

Structural analysis of the C-terminal region of SSX1 harboring a potential DNA-binding site

○高橋 花南¹, 古寺 哲幸², 宮ノ入 洋平³, 千田 美紀⁴, 加藤 広介⁵, 堀越 直樹⁶, 竹中 聡⁷, 岩崎 憲治⁸ (¹ 筑波大・院数理物質, ² 金沢大・ナノ生命研, ³ 阪大・蛋白研, ⁴ 高エネ研・構造生物学研究セ, ⁵ 筑波大・医学医療, ⁶ 東京大・定量研, ⁷ 大阪国際がんセ, ⁸ 筑波大・生存ダイナミクス研究セ)

Kanami Takahashi¹, Noriyuki Kodera², Yohei Miyanoiri³, Miki Senda⁴, Kosuke Kato⁵, Naoki Horikoshi⁶, Satoshi Takenaka⁷, Kenji Iwasaki⁸ (¹*Grad. Sch. Sci. and Tech., Univ. of Tsukuba*, ²*WPI-NanoLSI, Kanazawa Univ.*, ³*IPR, Osaka Univ.*, ⁴*SBRC, KEK*, ⁵*Grad. Sch. of Comprehensive Human Sciences, Univ. of Tsukuba*, ⁶*IQB, Univ. of Tokyo*, ⁷*Osaka International Cancer Inst. Hosp.*, ⁸*TARA, Univ. of Tsukuba*)

[2-02-1339*](#) 表面増強赤外分光法を用いた Heliorhodopsin の光誘起構造変化解析

Light-induced structural change of Heliorhodopsin analyzed by using SEIRA spectroscopy

○加藤 壯一郎¹, 唐 靜一¹, Binti Muhammad Jauhari Insyeeerah², 橋本 真典¹, 神取 秀樹^{1,3}, 古谷 祐詞^{1,3} (¹ 名古屋工業大学 大学院工学研究科, ² 名古屋工業大学 工学部, ³ 名古屋工業大学 オプトバイオ)

Soichiro Kato¹, Jingyi Tang¹, Insyeeerah Binti Muhammad Jauhari², Masanori Hashimoto¹, 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*)

[2-02-1351*](#) NMR によるシニヨリンとその変異体の立体構造解析

Structure analysis of chignolin and its mutant by NMR

○小 隼平¹, 今井 美咲², 竹内 恒², 丸山 豊³, 光武 亜代理¹ (¹ 明治大学, ² 産総研, ³ 理研)

Shumpei Koroku¹, Misaki Imai², Koh Takeuchi², Yutaka Maruyama³, Ayori Mitsutake¹ (¹*Meiji Univ.*, ²*AIST*, ³*RIKEN*)

[2-02-1403*](#) ヒト由来抗菌ペプチド LL-37 とその霊長類オルソログの大量発現系構築及び NMR 法を用いた構造・機能解析

Construction of an overexpression system for a human antimicrobial peptide LL-37 and its primate orthologs and elucidation by NMR

○柴垣 光希¹, 上田 和佳¹, 加納 康平², 谷 昊², 相沢 智康^{1,2,3} (¹ 北大・理学部生科, ² 北大・院生命, ³ 北大・院先端生命)

Mitsuki Shibagaki¹, Waka Ueda¹, Kohei Kano², Hao Gu², Tomoyasu Aizawa^{1,2,3} (¹*Sch. Sci., Hokkaido Univ.*, ²*Grad. Sch. Life Sci., Hokkaido Univ.*, ³*Fac. Adv. Life Sci., Hokkaido Univ.*)

[2-02-1415*](#) Cryo-EM structure analysis of Secretory Pathway Calcium/Manganese ATPase 1 (SPCA1)

Zhenghao Chen^{1,2}, Satoshi Watanabe^{1,2}, Hironori Hashida^{1,2}, Michio Inoue^{1,2}, Akihisa Tsutsumi³, Masahide Kikkawa³, Kenji Inaba^{1,2} (¹*Dept. of Struc. Biol., Grad. Sch. of Life Sci., Tohoku Univ.*, ²*IMRAM, Tohoku Univ.*, ³*Dept. of Cell Biol. and Ana., Grad. Sch. of Med, Univ. Tokyo*)

- [2-02-1427*](#) セイヨウイトスギ GRP (ジベレリン調節タンパク質) アレルゲンの立体構造解析と抗体結合部位予測
NMR Structural Analysis and Epitope Prediction of GRP (Gibberellin Regulated Protein) Allergen of European Cypress Pollen
○飯塚 友菜, 鄭 靖康, 久米田 博之, 熊木 康裕, 相沢 智康 (北大・院生命科学)
Tomona Iizuka, Jingkang Zheng, Hiroyuki Kumeta, Yasuhiro Kumaki, Tomoyasu Aizawa (*Grad. Sci. Life Sci., Hokkaido Univ.*)
- [2-02-1439](#) *Porphyromonas gingivalis* における主要 Mfa1 線毛バリエントである Mfa53 の構造
Structure of Mfa53, a major fimbriin variant of Mfa1 fimbriae, of *Porphyromonas gingivalis*
○小島 嶺¹, 柴田 敏史², 竹川 宜宏¹, 庄子 幹郎³, 今田 勝巳¹ (¹ 阪大・院理・高分子科学, ² 鳥取大・医, ³ 長崎大・院医歯薬)
- Rei Kojima**¹, Satoshi Shibata², Norihiro Takekawa¹, Mikio Shoji³, Katsumi Imada¹ (¹Dept. Macromol. Sci., Grad. Sch. Sci., Osaka Univ., ²Fac. Med., Tottori Univ., ³Grad. Sch. Biomed Sci., Nagasaki Univ.)
- [2-02-1451](#) Cryo-CLEM 法を用いた糸状仮足観察に関する研究
A study on the observation of Filopodia using the Cryo-CLEM method
○中深迫 美穂, 肥後 智也, 五味湖 由貴, 森本 雄祐, 安永 卓生 (九工大・情報工学府)
Miho Nakafukasako, Tomoya Higo, Yuki Gomibuchi, Yusuke V. Morimoto, Takuo Yasunaga (*Grad. Sch. Comp. Sci. Syst. Eng., KIT*)
- [2-02-1503](#) Cryo-EM flexible fitting refinement with automatic error fixing for de novo protein structure modeling
Takaharu Mori¹, Genki Terashi², Daisuke Matsuoka¹, Daisuke Kihara², Yuji Sugita^{1,3,4} (¹RIKEN CPR, ²Purdue Univ., ³RIKEN BDR, ⁴RIKEN R-CCS)

16:00~18:12 Ch02

2G02B 水・水和・電解質

Water, Hydration & Electrolyte

座長：白神 慧一郎 (京都大学), 笠原 浩太 (立命館大学)

Session Chairs: Keiichiro Shiraga (Kyoto Univ.), Kota Kasahara (Ritsumeikan Univ.)

- [2-02-1600*](#) マイクロ波および中赤外誘電分光法が示すグリセロールの保水様式：強い水素結合と弱い水素結合の共存
The water-holding mechanism of glycerol revealed by microwave and mid-infrared spectroscopy: coexistence of strong and weak hydrogen bonds
○森田 美穂¹, 四方 俊幸², 小川 雄一¹, 鈴木 哲仁¹, 近藤 直¹, 白神 慧一郎¹ (¹ 京大・院農学, ² 東京農工大・院農学)
- Miho Morita**¹, Toshiyuki Shikata², Yuichi Ogawa¹, Tetsuhito Suzuki¹, Naoshi Kondo¹, Keiichiro Shiraga¹ (¹Grad. Sch. Agriculture., Kyoto Univ., ²Grad. Sch. Agriculture., Tokyo Univ. of Agriculture and Tech.)
- [2-02-1612*](#) 機械学習による蛋白質の水和構造予測
Prediction of hydration structures of proteins by using machine learning
○佐藤 航地^{1,2}, 大出 真央^{1,2}, 中迫 雅由^{1,2} (¹ 慶應・理工, ² 理研・RSC)
Kochi Sato^{1,2}, Mao Oide^{1,2}, Masayoshi Nakasako^{1,2} (¹Dept. Phys., Keio Univ., ²RSC, RIKEN)

- [2-02-1624*](#) (1S8-3) 水和水の OH 伸縮振動バンドに基づく生体保護作用を持つ小分子の水素結合強化作用の評価
(1S8-3) Hydrogen bond strengthening effect of stabilizing osmolytes investigated by OH stretching band of hydration water
○松村 郁希¹, 四方 俊幸², 小川 雄一¹, 鈴木 哲仁¹, 近藤 直¹, 白神 慧一郎¹ (¹京都大・院農学研究科, ²東京農工大・院農学研究院)
Fumiki Matsumura¹, Toshiyuki Shikata², Yuichi Ogawa¹, Tetsuhito Suzuki¹, Naoshi Kondo¹, Keiichiro Shiraga¹ (¹Grad. Sch. Agri., Kyoto Univ., ²Grad. Sch. Agri., Tokyo Univ. of Agriculture and Technology)
- [2-02-1636](#) 深層学習と溶液理論のハイブリッドアプローチによるタンパク質水合分布予測
A hybrid approach of deep learning and solvation theory for predicting the hydration structures around proteins
○河間 光祐¹, 福島 悠朔¹, 吉留 崇¹, 池口 満徳^{2,3}, 大田 雅照³ (¹東北大院工, ²横浜市大生命医科学, ³理研)
Kosuke Kawama¹, Yusaku Fukushima¹, Takashi Yoshidome¹, Mitsunori Ikeguchi^{2,3}, Masateru Ohta³ (¹Dep. of Appl. Phys., Tohoku Univ., ²Grad. Sch. of Med. Life Sci., Yokohama City Univ., ³Riken)
- [2-02-1648](#) 深層学習による GIST の高速計算法の研究
A Fast Calculation Method for the Grid Inhomogeneous Solvation Theory via Deep Learning
○福島 悠朔, 吉留 崇 (東北大・院工)
Yusaku Fukushima, Takashi Yoshidome (Dept. of Appl. Phys., Tohoku Univ.)
- [2-02-1700](#) Analysis of urea effect for binding free energy of lysozyme-(GlcNac)₃
Simon Hikiri, Nobuyuki Matubayasi (Osaka Univ. Grad. Sch. Eng. Sci.)
- [2-02-1712](#) 分子動力学シミュレーションによるタンパク質の水和ダイナミクスと構造の相関解析
Analysis of relationship between the hydration dynamics and the structures of model proteins with MD simulations
○高橋 卓也¹, 藤澤 太公也², 延永 慎吾², 伊納 竜太郎¹, 中村 優似¹, 坂本 溪¹, 笠原 浩太¹ (¹立命館大・生命, ²立命館大・院・生命)
Takuya Takahashi¹, Takuya Fujisawa², Shingo Nobunaga², Ryutarou Inou¹, Yui Nakamura¹, Kei Sakamoto¹, Kouta Kasahara¹ (¹Coll. Life. Sci., Ritsumeikan Univ., ²Grad. Sch. Life Sci., Ritsumeikan Univ.)
- [2-02-1724](#) 蛋白質水合自由エネルギーの十分な精度および超高速での計算
Calculation of hydration free energy of a protein with sufficient accuracy and remarkably high speed
○川村 勝人¹, 宮本 俊輔¹, 林 智彦¹, 木下 正弘² (¹新潟大・工学, ²千葉大・院理工学)
Masato Kawamura¹, Syunsuke Miyamoto¹, Tomohiko Hayashi¹, Masahiro Kinoshita² (¹Grad. Sch. Eng., Niigata Univ., ²Grad. Sch. Sci., Chiba Univ.)
- [2-02-1736](#) 統計力学に基づくタンパク質-ペプチド複合体の天然構造予測法の開発
Theoretical study based on statistical mechanics for predicting native-like poses of a protein-peptide complex
○宮本 隼輔, 川村 勝人, 林 智彦 (新潟大・工学)
Shunsuke Miyamoto, Masato Kawamura, Tomohiko Hayashi (Grad. Sch. Eng., Niigata Univ.)
- [2-02-1748](#) 分子シミュレーションベースの機械学習アプローチによる水分子低温ダイナミクス
Simulation-based machine-learning approach for the low-temperature water dynamics
○水上 卓¹, グエン ヴェト クーン³, ダム ヒョウ チ² (¹北陸先端大・マテリアル, ²北陸先端大・知識, ³HPC システムズ)
Taku Mizukami¹, Nguyen Viet Cuong³, Dam Hieu Chi² (¹Materials Sci. JAIST, ²Knowledge Sci. JAIST, ³HPC systems Inc.)

- [2-02-1800](#) 蛋白質の機能的動きに沿った溶媒と自由エネルギー変化の評価法開発
Changes in solvation free energy along protein functional motion: analyses using restraint-free grid-based inhomogeneous solvation theory
○荳口 友隆^{1,2} (¹慶應大・理工,²理研・RSC)
Tomotaka Oroguchi^{1,2} (¹Facult. Sci. Tech., Keio Univ., ²RIKEN Spring-8 Center)

13:15~15:39 Ch03
2G03A タンパク質：計算 II
Protein: Simulation II

座長：高野 光則（早稲田大学），河野 秀俊（量子科学技術研究開発機構）
Session Chairs: Mitsunori Takano (Waseda Univ.), Hidetoshi Kono (QST)

- [2-03-1315*](#) HSP70 と HSP40 の複合体のダイナミクスと HSP70 の Lid ドメインの役割に関するシミュレーション研究
Simulation study of the dynamics of Heat Shock Protein (HSP) 70 and HSP40 complex and the role of the Lid domain in HSP70
○松倉 里紗¹, 福岡 綺羅², 宮下 尚之^{1,2} (¹近大・院生物理工,²近大・生物理工)
Lisa Matsukura¹, Kira Fukuoka², Naoyuki Miyashita^{1,2} (¹Grad. Sch. BOST., KINDAI University, ²Faculty of BOST., KINDAI University)
- [2-03-1327*](#) (2S6-2) An estimation method for the diffusion coefficient using MD simulations with the basic cell containing only one protein as solute
Tomoya Iwashita¹, Masaaki Nagao¹, Akira Yoshimori², Masahide Terazima³, Ryo Akiyama¹
(¹Department of Chemistry, Graduate School of Science, Kyushu University, ²Department of Physics, Niigata University, ³Department of Chemistry, Graduate School of Science, Kyoto University)
- [2-03-1339*](#) 18 残基チオエーテル結合環状ペプチドと humanPlexinB1 の複合体のシミュレーション
Simulation of complex of 18-residue thioether-bonded cyclic peptide and human PlexinB1
○野口 大輝, 光武 亜代理（明治大学大学院理工学研究科）
Daiki Noguchi, Ayori Mitsutake (*Graduate School of Meiji, University of Meiji*)
- [2-03-1351*](#) 統計力学モデルによるタンパク質のフォールディング反応機構の解析
Predicting mechanism and kinetics of protein folding reactions by an extended statistical mechanical model
○大岡 絃治¹, 新井 宗仁^{1,2} (¹東大・理・物理,²東大・総合文化・生命環境)
Koji Ooka¹, Munchito Arai^{1,2} (¹Dept. Phys., Univ. Tokyo, ²Dept. Life Sci., Univ. Tokyo)
- [2-03-1403*](#) 統計力学モデルへの厳密なコンタクト計算の導入によるタンパク質フォールディング経路予測の改善
Improving the statistical mechanical model of protein folding by accurate contact calculation
○劉 潤晶¹, 大岡 絃治², 新井 宗仁^{1,2,3} (¹東大・教養・統合自然,²東大・理・物理,³東大・総合文化・生命環境)
Runjing Liu¹, Koji Ooka², Munchito Arai^{1,2,3} (¹Dept. Integ. Sci., Univ. Tokyo, ²Dept. Phys., Univ. Tokyo, ³Dept. Life Sci., Univ. Tokyo)
- [2-03-1415*](#) 分子動力学計算による肝細胞増殖因子受容体 MET のアロステリック機構解析
Allosteric mechanism of hepatocyte growth factor receptor MET analyzed by molecular dynamics simulation
○難波 樹, 飯島 美来, 大貫 隼, 高野 光則（早大・先進理工・物理応物）
Tatsuki Namba, Mikuru Iijima, Jun Ohnuki, Mitsunori Takano (*Dept. of Pure & Appl. Phys., Grad. Sci. Adv. Sci. & Eng., Waseda Univ.*)

- [2-03-1427](#) 分子動力学シミュレーションによる繊維形成に関与する FUS-LC タンパク質の天然変性領域の特性評価
Characterization of the Intrinsically Disordered Region of FUS-LC protein involved in fibril formation with molecular dynamics simulations
○Chan-Yao-Chong Maud, 陳偉順, KUMAR Amarjeet, 桜庭 俊, 河野 秀俊 (量子科学技術研究開発機構 量子生命・医学部門、量子生命科学研究所 生体分子シミュレーショングループ)
Maud Chan-Yao-Chong, Justin Chan, Amarjeet Kumar, Shun Sakuraba, Hidetoshi Kono (*National Institutes for Quantum and Radiological Science and Technology; Quantum Life and Medicine Department, Quantum Life Science Institute; Biomolecule simulation group*)
- [2-03-1439](#) Quantum chemistry analysis of the high-resolution crystal structure of GFP in the A state
Hoang Anh Dao, Kazuki Takeda (*Kyoto University, Graduate School of Science*)
- [2-03-1451](#) 細胞スケール分子動力学シミュレーションのためのトラジェクトリ解析プログラムの開発
Development of Trajectory Analyzer for Cellular-Scale Molecular Dynamics Simulations
○優 乙石¹, 松岳 大輔², 杉田 有治² (¹前橋工科大・生命情報, ²理研・杉田理論分子研)
Isseki Yu¹, Daisuke Matsuoka², Yuji Sugita² (¹*Dep. Bioinformatics*, ²*Theoret. Mol. Sci. Lab.*)
- [2-03-1503](#) VAE による機械学習を用いた MSES 法の拡張
VAE-driven multiscale enhanced sampling
○森次 圭 (横浜市大院・生命医科学)
Kei Moritsugu (*Grad. Sch. Med. Life Sci., Yokohama City Univ.*)
- [2-03-1515](#) Unguided Binding MD of Protein-Protein Complexes by PPI-ColDock
Kazuhiro Takemura, Akio Kitao (*SLST, TokyoTech*)
- [2-03-1527](#) Molecular dynamics simulation of phosphorylated and unmodified intrinsically disordered region of TGIF-1 with its homeodomain
Yuta Nakano¹, Qilin Xie¹, Yusuke Sakai¹, Kota Kasahara², Toru Sengoku⁴, Junichi Higo³, Kazuhiro Ogata⁴, Takuya Takahashi² (¹*Grad. Sch. Life Sci., Ritsumeikan Univ.*, ²*Coll. Life. Sci., Ritsumeikan Univ.*, ³*Res. Org. Sci. Tech., Ritsumeikan Univ.*, ⁴*Grad. Sch. Med., Yokohama City Univ.*)

16:00~18:36 Ch03

2G03B タンパク質：計算 III

Protein: Simulation III

座長：梅澤 公二 (信州大学), 宮下 尚之 (近畿大学)

Session Chairs: Koji Umezawa (Shinshu Univ.), Naoyuki Miyashita (KINDAI Univ.)

- [2-03-1600](#) Analysis of interactions at protein-protein interfaces in protein structure database
Wataru Sagawa (*Dept. of Appl. Phys., Grad. Sch. Eng., Nagoya Univ.*)
- [2-03-1612](#) Tau 断片が C 末端領域を含むチューブリンヘテロ二量体の構造に及ぼす効果を分子動力学計算で解明する
Tau Segment Affecting Conformations of Tubulin Heterodimers Including C-Terminal Tails Revealed by Molecular Dynamics Simulation
○古田 尚之¹, 轟 拓磨¹, 梅澤 公二^{1,2} (¹信大・総合理工, ²信大・バイオメディカル研)
Naoyuki Furuta¹, Takuma Todoroki¹, Koji Umezawa^{1,2} (¹*Grad. Sch. Of Sci. & Tech., Shinshu Univ.*, ²*IBS, Shinshu Univ.*)
- [2-03-1624](#) Molecular dynamics simulation of loop capturing during cohesin-mediated DNA loop extrusion mechanism
Chenyang Gu, Shoji Takada, Tsuyoshi Terakawa, Giovanni Brandani (*Grad. Sch. Sci., Univ. Kyoto*)
- [2-03-1636](#) Conformations and distributions of Cryptdin-4, lipids, and water observed in membrane self-assembly molecular dynamics simulations
Takao Yoda (*Nagahama Institute of Bio-Science and Technology*)

- [2-03-1648](#) タンパク質フォールディングにおける動的協同性
Dynamic Cooperativity in Protein Folding
○鄭 誠虎 (理研・神戸)
Song-Ho Chong (*Kobe, Riken*)
- [2-03-1700](#) gmfit による単一および複数サブユニットの 3D 密度マップの重ね合わせの改良: ラプラシアン演算と CSS 探索の適用
An improvement of gmfit for single and multiple subunit fitting on 3D density map : Laplacian operator and CSS search
○川端 猛¹, 中村 春木², 栗栖 源嗣² (¹ 蛋白質研究奨励会, ² 大阪大・蛋白研)
Takeshi Kawabata¹, Haruki Nakamura², Genji Kurisu² (¹ *Protein Research Foundation*, ² *Inst. Prot. Res., Osaka Univ.*)
- [2-03-1712](#) 分子動力学シミュレーションに基づいた環状ペプチドの膜透過率の大規模予測
Large-scale membrane permeability prediction of cyclic peptides crossing a lipid bilayer based on molecular dynamics simulations
○杉田 昌岳, 杉山 聡, 藤江 拓哉, 吉川 寧, 柳澤 溪甫, 大上 雅史, 秋山 泰 (東工大・情理)
Masatake Sugita, Satoshi Sugiyama, Takuya Fujie, Yasushi Yoshikawa, Keisuke Yanagisawa, Masahito Ohue, Yutaka Akiyama (*Dept. Comput. Sci., Tokyo Inst. Tech.*)
- [2-03-1724](#) タンパク質における連続 3 残基 Loop-Closure 問題の解の個数に関するロボット工学的解析
Robotics-based Analysis of the Number of Solutions for Loop-Closure Problem of Three Consecutive Residues in a Protein
○有川 敬輔 (神奈川工大・工学部)
Keisuke Arikawa (*Fcl. Eng., Kanagawa Inst. of Tech.*)
- [2-03-1736](#) Verification of simulations using Virtual system coupled canonical molecular dynamics for the small protein inhibitor
Yusuke Sakai¹, Yuuta Nakano¹, Qilin Xie¹, Kota Kasahara², Junichi Higo³, Takuya Takahashi² (¹ *Grad. Sch. Life Sci., Ritsumeikan Univ.*, ² *Coll. Life. Sci., Ritsumeikan Univ.*, ³ *Res. Org. Sci. Tech., Ritsumeikan Univ.*)
- [2-03-1748](#) 粗視化分子シミュレーションで探る ABC トランスポーター ABCG2 の構造ダイナミクス
Structural dynamics of the ABC transporter ABCG2 explored by coarse-grained molecular simulations
平野 諒輔, 櫻井 実, ○古田 忠臣 (東工大・生命理工)
Ryosuke Hirano, Minoru Sakurai, **Tadaomi Furuta** (*Sch. Life Sci. Tech., Tokyo Tech*)
- [2-03-1800](#) 粗視化モデルによる転写因子 Nanog のオリゴマー化と相分離についてのシミュレーション研究
Coarse-grained molecular simulations on oligomerization and condensate formation of transcription factor Nanog
○水谷 淳生, 高田 彰二 (京都大・院理)
Azuki Mizutani, Shoji Takada (*Grad. Sch. Sci., Univ. Kyoto*)
- [2-03-1812](#) ヘリックス傾向の異なる 9 種類のペプチド周囲における水和ダイナミクスの分子動力学的研究
Molecular dynamics study of hydrated water dynamics around 9 peptides with different helix propensity
○延永 慎吾, 高橋 卓也, 笠原 浩太 (立命館大学・院・生命)
Shingo Nobunaga, Takuya Takahashi, Kota Kasahara (*Grad. Sch. Life Sci., Ritsumeikan Univ.*)
- [2-03-1824](#) ディープニューラルネットワークと分子動力学シミュレーションを用いた 3 次元反応座標上のタンパク質構造変化モーフィングプログラムの開発
Development of the Morphing Program for Protein Structural Changes on 3D Reaction Coordinates Using DNN and MD Simulations
○清岡 亮太¹, 松倉 里紗¹, 大多和 克紀¹, 福岡 綺羅², 宮下 尚之^{1,2} (¹ 近畿大・院生物理工, ² 近畿大・生物理工)
Ryota Kiyooka¹, Lisa Matsukura¹, Masaki Ottawa¹, Kira Fukuoka², Naoyuki Miyashita^{1,2} (¹ *Grad. Sch. BOST, KINDAI Univ.*, ² *BOST, KINDAI Univ.*)

座長：池口 雅道（創価大学），中迫 雅由（慶應義塾大学）

Session Chairs: Masamichi Ikeguchi (Soka Univ.), Masayoshi Nakasako (Keio Univ.)

[2-04-1315*](#) 抗体表面への正荷電残基変異導入による抗体の pH 非依存的な熱安定性獲得機構

The mechanism by which positive supercharging mutations confer pH-independent thermal stability of an antibody

○笠原 慶亮¹, 黒田 大祐^{1,2,3}, 河出 来時¹, 田部 亜季¹, 長門石 曉⁴, 津本 浩平^{1,2,3,4} (1 東大・院工学・バイオエネジ, 2 東大・院工学・医工 RS, 3 東大・院工学・化生, 4 東大・医科研)

Keisuke Kasahara¹, Daisuke Kuroda^{1,2,3}, Raiji Kawade¹, Aki Tanabe¹, Satoru Nagatoishi⁴, Kouhei Tsumoto^{1,2,3,4} (¹Dept. Bioeng., Grad. Sch. Eng., Univ. Tokyo, ²Med. Dev. Dev. Reg. Res Ctr., Grad. Sch. Eng., Univ. Tokyo, ³Dept. Chem. Biotech., Grad. Sch. Eng., Univ. Tokyo, ⁴Inst. Med. Sci., Univ. Tokyo)

[2-04-1327*](#) Dynamic residue interaction network analysis of the H274Y mutant in neuraminidase conferring drug resistance in influenza virus

Mohini Yadav¹, Manabu Igarashi^{2,3}, Norifumi Yamamoto¹ (¹Department of Applied Chemistry, Faculty of Engineering, Chiba Institute of Technology, ²Division of Global Epidemiology, Research Center for Zoonosis Control, Hokkaido University, ³International Collaboration Unit, Research Center for Zoonosis Control, Hokkaido University)

[2-04-1339*](#) Investigation of pore diameter conversion of β -barrel nanopore-forming protein by changing number of β -strands

Toshiyuki Tosaka, Koki Kamiya (*Grad. Sci. & Tech., Univ. Gunma*)

[2-04-1351*](#) インスリンの由来種に依存したアミロイド核形成メカニズム

Early aggregation kinetics upon the amyloid nucleation of bovine and human insulin

○柚 佳祐¹, 今村 比呂志², 野崎 拓郎¹, 藤井 悠生¹, 守島 健³, 奥田 綾³, 井上 倫太郎³, 杉山 正明³, 茶谷 絵理¹ (1 神戸大・院理, 2 立命館大・生命科学, 3 京大・複合研)

Keisuke Yuzu¹, Hiroshi Imamura², Takuro Nozaki¹, Yuki Fujii¹, Ken Morishima³, Aya Okuda³, Rintaro Inoue³, Masaaki Sugiyama³, Eri Chatani¹ (¹Grad. Sch. Sci., Kobe Univ., ²Coll. Life Sci., Ritsumeikan Univ., ³KURNS, Kyoto Univ.)

[2-04-1403*](#) チャネルロドプシン C1C2 の光中間状態におけるレチナル発色団の構造ダイナミクス
Structural Dynamics of the Retinal Chromophore in the Photo-Intermediate States of Channelrhodopsin C1C2

○柴田 桂成¹, 小田 和正², 西澤 知宏², 挾間 優治¹, 小野 稜平^{1,3}, 濡木 理², 井上 圭一¹, 秋山 英文¹ (1 東大物性研, 2 東大院理, 3 群大院理工)

Keisei Shibata¹, Kazumasa Oda², Tomohiro Nishizawa², Yuji Hazama¹, Ryohei Ono^{1,3}, Osamu Nureki², Keiichi Inoue¹, Hidefumi Akiyama¹ (¹ISSP, Univ. Tokyo, ²Sch. Sci., Univ. Tokyo, ³Sch. Sci. and Tech., Gunma Univ.)

[2-04-1415*](#) 線維前駆中間体の成長を防ぐ α B-クリスタリンのアミロイド線維化阻害: 安定な複合体の形成
Inhibition of amyloid fibrillation by α B-crystallin by preventing the growth of prefibrillar intermediates: Formation of a stable complex

○國尾 祐貴¹, 柚 佳祐¹, Hayashi Junna², Carver John A.², 茶谷 絵理¹ (1 神戸大・院理, 2 オーストラリア国立大・化研)

Yuki Kokuo¹, Keisuke Yuzu¹, Junna Hayashi², John A. Carver², Eri Chatani¹ (¹Grad. Sch. Sci., Kobe Univ., ²Res. Sch. Chem., The Austral. Natl. Univ.)

- [2-04-1427*](#) 大腸菌フェリチンの構造・機能に及ぼす正味電荷の効果
Effects of net charge on the structure and function of *Escherichia coli* ferritin
○桑田 巧¹, 佐藤 大輔², 柳田 侑樹¹, 藤原 和夫¹, 池口 雅道¹ (¹創価大・生命理学,²創価大・生命情報工学)
Takumi Kuwata¹, Daisuke Sato², Yuki Yanagida¹, Kazuo Fujiwara¹, Masamichi Ikeguchi¹ (¹*Dept. of Biosci., Soka Univ.*, ²*Dept. of Bioinfo., Soka Univ.*)
- [2-04-1439*](#) ラン藻でのアルカン合成に関わる2つの酵素の親和性を理論的に向上させる
Improving bioalkane production by computationally enhancing the affinity between two enzymes for cyanobacterial alkane synthesis
○岩屋 克尚¹, 林 勇樹², 新井 宗仁^{1,2} (¹東大・理・物理,²東大・総合文化・生命環境)
Katsuhisa Iwaya¹, Yuuki Hayashi², Munehito Arai^{1,2} (¹*Dept. Phys., Univ. Tokyo*, ²*Dept. Life Sci., Univ. Tokyo*)
- [2-04-1451*](#) アクチンとAβの相互作用特性はアクチンの重合状態に異なる
The interaction behavior between actin and Aβ differs depending on the polymerization state of actin
○黒滝 晋奈¹, Ragheed H. Yousif², 近井 優作¹, 島森 圭弥¹, 倉賀野 正弘¹, 徳樂 清孝¹ (¹室蘭工業大学,²アルファラヒデイ大学)
Yukina Kurotaki¹, Ragheed H. Yousif², Yusaku Chikai¹, Keiya Shimamori¹, Masahiro Kuragano¹, Kiyotaka Tokuraku¹ (¹*Muroran Institute of Technology*, ²*Al-Farahidi University*)
- [2-04-1503*](#) 酵素一分子の活性ゆらぎと進化能の関係
Correlation between the fluctuation of single enzyme activity and evolvability
○飯田 隆仁, 上野 博史, 野地 博行 (東京大・院応用科学)
Takahito Iida, Hiroshi Ueno, Hiroyuki Noji (*Grad. App. Chem., Univ. Tokyo*)
- [2-04-1515*](#) 新規スコアによる相分離関連 IDR の分類
Classification of Intrinsically Disordered Regions involved in Liquid-Liquid Phase Separation Using the Novel Score
○會田 勇斗^{1,2,3}, 原田 隆平², 重田 育照², 富井 健太郎¹ (¹産総研・人工知能,²筑波大・計セ,³筑波大院・生命地球・生物)
Hayato Aida^{1,2,3}, Ryuhei Harada², Yasuteru Shigeta², Kentaro Tomii¹ (¹*AIRC, AIST*, ²*CCS, Univ. of Tsukuba*, ³*Master's Program in Biol., Univ. of Tsukuba*.)
- [2-04-1527](#) 粒径に関する非加算性を取り入れた朝倉一大沢理論：生体高分子の壁面への吸着物性に関する検討
Asakura-Oosawa theory incorporating non-additivities of particle sizes: Study of adsorption properties of biopolymers on a wall
○天野 健一, 前林 正弘 (名城大・農)
Ken-ichi Amano, Masahiro Maebayashi (*Fac. Agric., Meijo Univ.*)

16:00~18:36 Ch04

2G04B タンパク質：計測Ⅱ

Protein: Measurement II

座長：重田 育照 (筑波大学), 川野 竜司 (東京農工大学)

Session Chairs: Yasuteru Shigeta (Univ. of Tsukuba), Ryuji Kawano (Tokyo Univ. of Agric. and Tech.)

- [2-04-1600*](#) ラマン分光法を用いた液-液相分離による液滴内のタンパク質濃度変化のラベルフリー観測
Label-free observation of protein concentration change in a droplet formed by liquid-liquid phase separation using Raman spectroscopy
○横澤 公平¹, 柴田 大輝¹, 梶本 真司^{1,2}, 中林 孝和¹ (¹東北大・院薬,²JST さきがけ)
Kohei Yokosawa¹, Daiki Shibata¹, Shinji Kajimoto^{1,2}, Takakazu Nakabayashi¹ (¹*Grad. Sch. Pharm. Sci., Tohoku Univ.*, ²*JST PRESTO*)

- [2-04-1612*](#) 静水圧印加時における in vitro Ras 活性測定系の確立
Establishment of in vitro system to measure Ras activity under hydrostatic pressure
○松田 瑛彦¹, 張 珉箕², 古川 克子², 牛田 多加志³, 上田 太郎¹ (¹早稲田大学 理工学術院 先進理工学研究科 物理学及応用物理専攻, ²東京大学大学院工学系研究科 バイオエンジニアリング専攻, ³東京大学大学院工学系研究科 機械工学専攻)
Teruhiko Matsuda¹, Minki Chang², Katsuko Furukawa², Takashi Ushida³, Taro Uyeda¹ (¹*Dept. Physics / Applied Physics, School of Advanced Science and Engineering, Waseda Univ.*, ²*Dept. Bio Eng. Faculty of Engineering, Univ of Tokyo*, ³*Dept. Mech Eng, Faculty of Engineering, Univ of Tokyo*)
- [2-04-1624*](#) 疾患関連タンパク質の液-液相分離とラマン分光法を用いたその定量
Liquid-liquid phase separation of disease-associated protein and its quantification using Raman spectroscopy
○村上 一輝¹, 梶本 真司¹, 柴田 大輝¹, 黒井 邦巧², 中林 孝和¹ (¹東北大・院薬, ²神戸学院大・院薬)
Kazuki Murakami¹, Shinji Kajimoto¹, Daiki Shibata¹, Kunisato Kuroi², Takakazu Nakabayashi¹ (¹*Grad. Sch. Pharm. Sci., Tohoku Univ.*, ²*Fac. Pharm. Sci., Kobe Gakuin Univ.*)
- [2-04-1636*](#) 自家蛍光寿命イメージングを用いた液-液相分離におけるタンパク質の構造変化のラベルフリー観測
Label-free observation of protein structural changes in liquid-liquid phase separation using autofluorescence lifetime imaging
○松浦 宇宙¹, 田原 進也¹, 梶本 真司^{1,2}, 中林 孝和¹ (¹東北大学薬学部, ²JST さきがけ)
Uchu Matsuura¹, Shinya Tahara¹, Shinji Kajimoto^{1,2}, Takakazu Nakabayashi¹ (¹*Faculty of Pharmaceutical Sciences, Tohoku University.*, ²*JST PRESTO, Japan.*)
- [2-04-1648*](#) ナノポア内における β ヘアピンペプチドの段階的なトランスロケーション過程の観測
Observing a stepwise translocation of β -hairpin peptides through a nanopore
○福田 美唯, 宇佐美 将誉, 川野 竜司 (東京農工大学大学院 工学府 生命工学専攻)
Miyu Fukuda, Masataka Usami, Ryuji Kawano (*Department of Biotechnology and Life Science, Tokyo University of Agriculture and Technology.*)
- [2-04-1700*](#) 異なるカチオン存在下でのウイルスロドプシン OLPVR I の時間分解光誘起赤外分光研究
Time-dependent light-induced ATR-FTIR study of viral rhodopsin OLPVRI in the presence of different cations
○青山 真子, 片山 耕大, 神取 秀樹 (名工大・院工)
Mako Aoyama, Kota Katayama, Hideki Kandori (*Grad. Sch. Eng., Nagoya Inst. Tech.*)
- [2-04-1712*](#) Amino acid side chain parameters on phase separation of protein
Akira Nomoto, Suguru Nishinami, Kentaro Shiraki (*Pure and Appl. Sci., Univ. Tsukuba*)
- [2-04-1724](#) 高速原子間力顕微鏡を用いたアミロイド β 線維に対するダイナミックフォースマッピング
Dynamic Force Mapping to Amyloid-Beta Fibrils Using High-Speed Atomic Force Microscopy
○宮島 将吾¹, 矢木 真穂², Ganser Christian², 内橋 貴之^{1,2}, 加藤 晃一² (¹名古屋大・院理学, ²ExCELLS)
Shogo Miyajima¹, Maho Yagi-Utsumi², Christian Ganser², Takayuki Uchihashi^{1,2}, Koichi Kato² (¹*Grad. Sch. Sci., Univ. Nagoya.*, ²*ExCELLS*)
- [2-04-1736](#) 糖ガラスに包埋されたタンパク質の構造と安定性
Structure and stability of proteins embedded in sugar glass
○平井 光博¹, 新井 栄揮², 岩瀬 裕希³, 中川 洋⁴, 清水 伸隆⁵ (¹群大・理工, ²量研機構, ³総研機構, ⁴原子力機構, ⁵高エネ研)
Mitsuhiro Hirai¹, Shigeki Arai², Hiroki Iwase³, Hiroshi Nakagawa⁴, Nobutaka Shimizu⁵ (¹*Grad. Sch. Sci. Tech. Gunma Univ.*, ²*QST*, ³*Cross*, ⁴*JAEA*, ⁵*KEK*)

[2-04-1748](#) VHH における CDR3-Framework region 間分子内相互作用に着目した Framework region 変異体の物理化学的解析

Physicochemical studies of mutations in framework regions of VHH focusing on intramolecular interactions with CDR3

○木下 清晶¹, 中木戸 誠^{1,2}, 黒田 大祐^{1,2}, カアベイロ ホセ³, 津本 浩平^{1,2,4} (¹東大・院工・バイオエンジニアリング,²東大・院工・化生,³九大・院薬,⁴東大・医科研)

Seisho Kinoshita¹, Makoto Nakakido^{1,2}, Daisuke Kuroda^{1,2}, Jose Caaveiro³, Kouhei Tsumoto^{1,2,4} (*Dept. of Bioeng., Sch. of Eng., Univ. of Tokyo, ²Dept. of Chem. Biotech., Sch. of Eng., Univ. of Tokyo, ³Grad. Sch. of Pharm. Sci., Kyushu Univ., ⁴Inst. of Med. Sci., Univ. of Tokyo*)

[2-04-1800](#) フィブロインの剪断応力解析

Shear Stress Analysis of Fibroin

○堤 健人¹, 大西 悟¹, 大代 宗弥¹, 米沢 健人³, 佐藤 健大³, 山崎 洋一¹, 藤間 祥子¹, 上久保 裕生^{1,2,4} (¹奈良先端大・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,³スパイバー (株),⁴高エネ機構・物構研)

Kento Tsutsumi¹, Satoru Onishi¹, Muneya Daidai¹, Kento Yonezawa³, Takehiro Satou³, Yoichi Yamazaki¹, Sachiko Toma¹, Hironari Kamikubo^{1,2,4} (*¹NAIST,MS, ²NAIST,CDG, ³Supiber inc., ⁴KEK,IMSS*)

[2-04-1812](#) 光誘起フォールディング反応および分子シャペロン SecB との相互作用カイネティクス

Kinetic analyses of photoinduced protein folding and interaction with molecular chaperone SecB

○中岡 育也¹, 中曽根 祐介¹, 太田 帆香², 川越 聡一郎^{2,3}, 石森 浩一郎², 齋尾 智英^{3,4}, 寺嶋 正秀¹ (¹京都大学大学院理学研究科,²北海道大学大学院総合化学院,³徳島大学大学院医科学教育部,⁴徳島大学先端酵素学研究所)

Ikuya Nakaoka¹, Yusuke Nakasone¹, Honoka Ota², Soichiro Kawagoe^{2,3}, Koichiro Ishimori², Tomohide Saio^{3,4}, Masahide Terazima¹ (*¹Graduate School of Science, Kyoto University, ²Hokkaido University Graduate School of Chemical Sciences and Engineering, ³Graduate School of Medical Sciences, Tokushima University Faculty of Medicine, ⁴Institute of Advanced Medical Sciences Tokushima University*)

[2-04-1824](#) MSDC-MD によるカルシウム結合タンパク質の自由エネルギー解析

Free-energy analysis of Calmodulin (calcium ion binding protein) using MSDC-MD

○下山 紘充, 重田 育照 (筑波大 CCS)

Hiroimitsu Shimoyama, Yasuteru Shigeta (*CCS, Univ. Tsukuba*)

13:15~15:39 Ch05

2G05A 核酸 II

Nucleic acids II

座長：瀧ノ上 正浩 (東京工業大学), 寺川 剛 (京都大学)

Session Chairs: Masahiro Takinoue (Tokyo Tech), Tsuyoshi Terakawa (Kyoto Univ.)

[2-05-1315*](#) 長鎖 DNA では発現活性が増大する。無細胞系発現系での検証

Longer DNA enhances the efficiency of cell free-gene expression

○西尾 天志¹, 吉川 祐子¹, 吉川 研一¹, 佐藤 慎一² (¹同志社大・生命医科,²京大・化研)

Takashi Nishio¹, Yuko Yoshikawa¹, Kenichi Yoshikawa¹, Shin-ichi Sato² (*¹Faculty of Life and Medical Sci., Doshisha Univ., ²Institute for Chem. Res., Kyoto Univ.*)

[2-05-1327*](#) DNA 演算とナノポア計測による癌特異的 microRNA 発現上昇・低下のパターン認識

Nanopore decoding for DNA-computed microRNA patterns involving over and under-expression

○滝口 創太郎, 川野 竜司 (東京農工大・院生命工学)

Sotaro Takiguchi, Ryuji Kawano (*Dep. of Biotech. and Life Sci., Tokyo Univ. of Agri. and Tech.*)

- [2-05-1339*](#) レーンスイッチメカニズム：DNA トランスロケースによるヌクレオソームリポジショニング
The lane switch mechanism: Nucleosome repositioning induced by a DNA translocase
○長江 文立津, ブランダーニ ジョバンニ, 高田 彰二, 寺川 剛 (京都大・院理学)
Fritz Nagae, Giovanni Brandani, Shoji Takada, Tsuyoshi Terakawa (*Grad. Sch. Sci, Kyoto Univ.*)
- [2-05-1351*](#) 真核生物の転写開始複合体における DNA 開裂過程の調査
Investigation of DNA opening process in eukaryotic transcription initiation complexes
○篠 元輝, 高田 彰二 (京大・理学・生物科学)
Genki Shino, Shoji Takada (*Div. of Bio. Sci., Grad. Sch. of Sci., Kyoto Univ.*)
- [2-05-1403*](#) DNA ハイブリダイゼーションのキネティックな制御
Kinetic control of DNA hybridization
○青柳 拓志¹, 小野 慎司¹, ビゴロッチェ シモーネ², 鳥谷部 祥一¹ (¹ 東北大・院工学, ²OIST)
Hiroyuki Aoyanagi¹, Shinji Ono¹, Simone Pigolotti², Shoichi Toyabe¹ (*¹Grad. Sch. Eng., Univ. Tohoku, ²OIST*)
- [2-05-1415*](#) DNA-polymer emulsions: self-assembly and purification of DNA structures
Marcos Masukawa¹, Fujio Yu¹, Yusuke Sato², Kanta Tsumoto³, Kenichi Yoshikawa⁴,
Masahiro Takinoue¹ (*¹Department of Computer Science, Tokyo Institute of Technology, ²Department of Applied Physics, Tohoku University, ³Graduate School of Engineering, Mie University, ⁴Faculty of Life and Medical Sciences, Doshisha University*)
- [2-05-1427*](#) Cancer diagnosis based on identifying miRNAs with DNA computing droplets
Jing Gong¹, Nozomi Tsumura², Yusuke Sato³, Masahiro Takinoue² (*¹School of Life Science and Technology, Tokyo Institute of Technology, ²School of Computing, Tokyo Institute of Technology, ³Frontier Research Institute for Interdisciplinary Sciences, Tohoku University*)
- [2-05-1439*](#) 分子ネットワークのボトムアップ構築のための RNP 分子集合体の設計と制御技術の研究
Development of design and control techniques of RNP molecular assemblies for bottom-up construction of molecular networks
○安海 一優¹, 野村 M. 慎一郎¹, 大野 博久², 齊藤 博英² (¹ 東北大・院工ロボティクス, ² 京大・iPS 細胞研究所)
Kazuya Ankaï¹, Shin-ichiro M. Nomura¹, Hirohisa Ohno², Hirohide Saito² (*¹Dept. Robotics, Tohoku Univ., ²CiRA, Kyoto Univ.*)
- [2-05-1451*](#) クライオ電子顕微鏡単粒子解析を用いたリボソームを標的としたアミノ配糖体抗菌薬の新規作用機序の解明
Elucidation of new action mechanism of aminoglycoside antibiotics on ribosomes using single particle cryo-electron microscopy
○伴野 詢太¹, 浅野 航佑¹, 鈴木 仁人², 横山 武司¹, 田中 良和¹ (¹ 東北大・院生命科学, ² 国立感染症研究所・薬剤耐性研究センター)
Junta Tomono¹, Kosuke Asano¹, Masato Suzuki², Takeshi Yokoyama¹, Yoshikazu Tanaka¹ (*¹Grad. Sch. Life Sci., Tohoku Univ., ²AMR Research Center, National Institute of Infectious Diseases*)
- [2-05-1503](#) 側方相分離が誘起するカプセル様 DNA ハイドロゲル表面のパターン形成
Lateral phase separation of DNA nanostructures that induces pattern formation on capsule-like DNA hydrogels
○佐藤 佑介^{1,2}, 瀧ノ上 正浩² (¹ 東北大・学際研, ² 東工大・情報理工)
Sato Yusuke^{1,2}, Masahiro Takinoue² (*¹FRIS, Tohoku Univ., ²Dept. Comput. Sci., TokyoTech*)
- [2-05-1515](#) Gold nanoparticle modification of DNA gel for remote control with radiofrequency magnetic field
Yoshiaki Sano (*Department of Life Science and Technology, School of Life Science and Technology, Tohoku Institute of Technology.*)
- [2-05-1527](#) DNA 反応拡散系によるパターン形成のカスケード化
DNA-based reaction-diffusion system for cascaded pattern formation
○安部 桂太¹, 村田 智¹, 川又 生吹^{1,2} (¹ 東北大・工学研究科, ² お茶の水女子大)
Keita Abe¹, Satoshi Murata¹, Ibuki Kawamata^{1,2} (*¹Grad. Sch. Eng., Univ. Tohoku, ²Univ. Ochanomizu*)

座長：亀田 倫史（産業技術総合研究所），本間 道夫（名古屋大学）

Session Chairs: Tomoshi Kameda (AIST), Michio Homma (Nagoya Univ.)

- [2-05-1600](#) アミノ酸のアロマフィリシティ・インデックス：芳香族表面に対するタンパク質の親和性の予測
Aromaphilicity index of amino acids: Prediction of protein binding affinity for aromatic surfaces
 ○平野 篤¹, 亀田 倫史² (¹産総研・ナノ材料, ²産総研・人工知能)
Atsushi Hirano¹, Tomoshi Kameda² (¹NMRI, AIST, ²AIRC, AIST)
- [2-05-1612](#) アミロイド凝集反応におけるダイナミクスと凝集形態に及ぼす超音波キャビテーション効果について
 Ultrasonic-cavitation effects on morphology and kinetics of amyloidogenic aggregation reaction
 ○戸田 元¹, 中島 吉太郎², 山口 圭一², 荻 博次¹, 後藤 祐晃² (¹大阪大学大学院 工学研究科, ²大阪大学 医工情報センター)
Hajime Toda¹, Kichitaro Nakajima², Keiichi Yamaguchi², Hirotsugu Ogi¹, Yuji Goto² (¹Grad. School Eng., Osaka Univ., ²Global Center for Med. Eng. Info., Osaka Univ.)
- [2-05-1624](#) Helix nucleation facilitated by the closed loop structure
Yuki Yanagida, Kiyomi Yoshida, Kazuo Fujiwara, Masamichi Ikeguchi (Dept. Biosci., Soka Univ.)
- [2-05-1636](#) Photocontrol of the small G-protein H-Ras GTPase activity using thiol reactive photochromic compounds incorporated into the HVR domain
Nahar Rufiat, Shinsaku Maruta (Department of Bioinformatics, Soka University, Japan)
- [2-05-1648](#) タンパク質のローカルな静電ポテンシャルを用いたプロトンの濃度勾配調節機能
 Regulation of proton concentration gradient by local electrostatic potential of proteins
 ○千葉 かおり (茨城高専・国際創造工学)
Kaori Chiba (Nat'l Inst. Tech, Ibaraki Col.)
- [2-05-1700](#) 海洋性ビブリオ菌極べん毛遺伝子のマスターレギュレーター FlaK の機能と生化学的性質
 Functional and biochemical characterization of FlaK, a master regulator for the polar flagellar genes of *Vibrio alginolyticus*
 ○小早川 友哉, 小嶋 誠司, 本間 道夫 (名古屋大・院生命理学)
Tomoya Kobayakawa, Seiji Kojima, Michio Homma (Grad. Sch. Sci., Univ. Nagoya)
- [2-05-1712](#) Molecular mechanism of glycolytic flux control intrinsic to human phosphoglycerate kinase
Hiromasa Yagi¹, Takuma Kasai¹, Elisa Rioual¹, Teppei Ikeya², Takanori Kigawa¹ (¹BDR, RIKEN, ²Grad. Sch. Sci., Tokyo Metropolitan Univ.)
- [2-05-1724](#) SARS-CoV-2 の RNA 依存性 RNA ポリメラーゼにおけるリジン残基による「バケツリレー」リガンド輸送
 "Bucket brigade" ligand transportation by lysine residues in RNA-dependent RNA polymerase of SARS-CoV-2
 ○谷本 勝一¹, 伊藤 暁^{1,2,3}, 奥村 久士^{1,2,3} (¹分子研, ²生命創成探求センター, ³総研大)
Shoichi Tanimoto¹, Satoru Itoh^{1,2,3}, Hisashi Okumura^{1,2,3} (¹IMS, ²ExCELLS, ³SOKENDAI)
- [2-05-1736](#) カメラオンモデルによるアデニル酸キナーゼの構造転移の研究
 A study on the conformational transition of adenylate kinase by the chameleon model
 ○吉田 樹生, 笹井 理生, 寺田 智樹 (名大・院工・応物)
Itsuki Yoshida, Masaki Sasai, Tomoki P. Terada (Dept. Appl. Phys., Grad. Sch. Eng., Nagoya Univ.)
- [2-05-1748](#) ローダミンファロイジン標識アクチンフィラメントにおける蛍光強度の時空間的ゆらぎ
 Spatiotemporal fluctuations in fluorescence intensity of rhodamine phalloidin-labeled actin filaments
 ○歳納 健太, 山崎 陽祐, 上田 太郎 (早稲田大学 理工学術院 先進理工学研究科 物理専攻)
Kenta Toshino, Yosuke Yamazaki, Taro Q.P. Uyeda (Dept. Physics, School of Advanced Science and Engineering, Waseda Univ.)

- [2-05-1800](#) コレステロールと γ 切断酵素の基質結合部位との相互作用
Interaction Between Cholesterol and Substrate Binding Sites of γ -secretase
○南 知香, 宮下 尚之 (近畿大・院生物理工)
Chika Minami, Naoyuki Miyashita (*Grad. Sch. BOST, KINDAI Univ.*)
- [2-05-1812](#) Expression and purification of the antimicrobial peptide cryptdin family in *Escherichia coli* by enhancing inclusion body formation
Yuchi Song, Shaonan Yan, Yi Wang, Wendian Yang, Weiming Geng, Tomoyasu Aizawa (*Grad. Sch. of Life Sci, Hokkaido Univ.*)
- [2-05-1824](#) Multiple bactericidal actions of cryptdin-4 and its reduced from via oxidative stress and membrane disruption
Yi Wang, Yuchi Song, Rina Hiramine, Tomoyasu Aizawa (*Grad. Sci. Life Sci., Hokkaido Univ.*)

13:15~15:27 Ch06

2G06A ヘム蛋白質・膜蛋白質・核酸結合蛋白質：構造 II、機能と反応場 II、動態 I
Heme-, Membrane- & Nucleic acid binding-protein: Structure II, Function and environment II, Dynamics I

座長：横田 浩章 (光産業創成大学院大学), 村本 和優 (兵庫県立大学)

Session Chairs: Hiroaki Yokota (The Grad. Sch. for the Creation of New Photonics Industries), Kazumasa Muramoto (Univ. of Hyogo)

- [2-06-1315*](#) リン脂質二重膜に再構成したアーキロドプシン-3(AR3)の四次構造と光サイクル
Quaternary structure and photocycle of archaerhodopsin-3 (AR3) reconstituted in phospholipid bilayer membrane
○菊地 莉緒¹, 林 史夫², 井上 圭一³, 園山 正史^{1,4,5} (1 群馬大・院理工, 2 群馬大・機器分析セ, 3 東大・物性研, 4 群馬大・未来先端, 5 群馬大・食健康セ)
Rio Kikuchi¹, Fumio Hayashi², Kiichi Inoue³, Masashi Sonoyama^{1,4,5} (*1 Grad. Sch. Sci. Tech., Gunma Univ., 2 Ctr. Inst. Anal. Gunma Univ., 3 ISSP, Univ. Tokyo, 4 GIAR, Gunma Univ., 5 GUCFW, Gunma Univ.*)
- [2-06-1327*](#) リン脂質二分子膜及び可溶化状態におけるプロテオロドプシンの多量体構造や光サイクルの比較研究
A comparative study of oligomeric states and photocycle of proteorhodopsin in phospholipid bilayer membranes and detergent micelles
○篠原 由佳¹, 山本 愛理¹, 林 史夫², 菊川 峰志³, 園山 正史^{1,4,5} (1 群馬大・院理工, 2 群馬大・機器分析セ, 3 北大・先端生命, 4 群馬大・未来先端, 5 群馬大・食健康セ)
Yuka Shinohara¹, Airi Yamamoto¹, Fumio Hayashi², Takashi Kikukawa³, 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.*)
- [2-06-1339*](#) Effect of acidity and salt concentration on functional properties of Na⁺ pump rhodopsin from *Indibacter alkaliphilus*
Shingo Yoshizawa¹, Takashi Kikukawa², Fumio Hayashi³, Masashi Sonoyama^{4,5} (*1 Grad. Sch. Sci. Tech., Gunma Univ., 2 Fac. Adv. Life Sci., Hokkaido Univ., 3 Inst. Anal. Cent., Gunma Univ., 4 GIAR, Gunma Univ., 5 GUCFW, Gunma Univ.*)
- [2-06-1351*](#) 擬環状エーテル型脂質の部分フッ素化が膜物性に及ぼす影響
Effects of partial fluorination of phospholipids bearing a single membrane-spanning chain on membrane properties
○嶋本 佳那子¹, 川原 るい¹, 土田 直之¹, 高木 俊之², 高橋 浩¹, 網井 秀樹^{1,3}, 園山 正史^{1,3,4} (1 群馬大・院理工, 2 産総研, 3 群馬大・未来先端, 4 群馬大・食健康セ)
Kanako Shimamoto¹, Rui Kawahara¹, Naoyuki Tsuchida¹, Toshiyuki Takagi², Hiroshi Takahashi¹, Hideki Amii^{1,3}, Masashi Sonoyama^{1,3,4} (*1 Grad. Sch. Sci. Tech., Gunma Univ., 2 AIST, 3 GIAR, Gunma Univ., 4 GUCFW, Gunma Univ.*)

- [2-06-1403*](#) 全反射赤外分光法による kappa-オピオイド受容体のリガンド認識機構研究
ATR-FTIR study of ligand recognition on kappa opioid receptor
○岩田 聖矢¹, 鮎 洗平¹, 片山 耕大¹, 寿野 良二², 寿野 千代², 小林 拓也², 辻本 浩一³, 岩田 想³, 神取 秀樹¹ (1 名工大・院工, 2 関医大・院医, 3 京大・院医)
Seiya Iwata¹, Kohei Suzuki¹, Kota Katayama¹, Ryoji Suno², Chiyo Suno², Takuya Kobayashi², Koichi Tsujimoto³, So Iwata³, Hideki Kandori¹ (¹*Grad. Sch. Eng., Tech. Inst. Nagoya*, ²*Grad. Sch. Med., Univ. Med. Kansai*, ³*Grad. Sch. Med., Univ. Kyoto*)
- [2-06-1415*](#) アクチノバクテリア門の細菌がもつ新規ロドプシン群
A novel cluster of microbial rhodopsin present in terrestrial *Actinobacteria*
○上野 真琴¹, 林 史夫², 菊川 峰志³, 園山 正史^{1,4,5} (1 群馬大・院理工, 2 群馬大・機器分析セ, 3 北大・院先端生命科学, 4 群馬大・未来先端, 5 群馬大・食健康セ)
Mako Ueno¹, Fumio Hayashi², Takashi Kikukawa³, 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.*)
- [2-06-1427*](#) Heterotrimer formation of MdtB and MdtC, transporter components of the bacterial xenobiotic efflux complex
Kenichiro Kashihara¹, Hirotaka Tajima^{2,3}, Masatoshi Nishikawa³, Yoshiyuki Sowa^{1,2,3}, Ikuro Kawagishi^{1,2,3} (¹*Grad. Sch. Eng., Hosei Univ.*, ²*Res. Cent. Micro-Nano Tech.*, ³*Dept. Front. Biosci.*)
- [2-06-1439*](#) 非天然基質の触媒を実現するシトクロム P450BM3 の酸化型中間体の構造解析
Structure of a heme-oxy intermediate of cytochrome P450BM3 catalyzing a non-natural substrate
○桑野 わ子¹, 長尾 聡¹, 當倉 武彦², Joshua Stanfield³, 笠井 千枝³, 有安 真也³, 荘司 長三³, 杉本 宏², 久保 稔¹ (1 兵県大・院理学, 2 理研・SPring-8, 3 名大・院理学)
Wako Kuwano¹, Satoshi Nagao¹, Takechiko Tosha², Stanfield Joshua³, Chie Kasai³, Shinya Ariyasu³, Osami Shoji³, Hiroshi Sugimoto², Minoru Kubo¹ (¹*Grad. Sch. Sci., Univ. Hyogo*, ²*Spring-8, RIKEN*, ³*Grad. Sch. Sci., Nagoya Univ.*)
- [2-06-1451*](#) Conformational dynamics of *E. coli* Cytidine Repressor DNA Binding domain studied by Single-molecule Fluorescence Spectroscopy
Shrutarshi Mitra^{1,2}, Hiroyuki Oikawa^{1,2}, Divya Rajendran³, Athi N. Naganathan³, Satoshi Takahashi^{1,2} (¹*Institute for Multidisciplinary Research for Advanced Materials., Tohoku University*, ²*Department of Chemistry., Graduate School of Science., Tohoku University*, ³*Department of Biotechnology., Bhupat & Jyoti Mehta School of Biosciences., Indian Institute of Technology, Madras*)
- [2-06-1503*](#) 全原子分子動力学シミュレーションによるヒト L 型アミノ酸トランスポーター LAT1-CD98hc 複合体の構造変化と輸送機序の解明
Transport mechanism of human LAT1-CD98hc complex studied by all-atom MD
○吉田 夏海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 R-CCS)
Natsumi Yoshida¹, Toru Ekimoto¹, Tsutomu Yamane², Mitsunori Ikeguchi^{1,2} (¹*Dept. of Med. Life Sci., Yokohama City Univ.*, ²*RIKEN R-CCS*)
- [2-06-1515*](#) (1S6-4) 分子シミュレーションによるオレキシン 2 受容体-G タンパク質複合体の動的性質の研究
(1S6-4) Dynamics of Orexin2 Receptor and G-protein Complex with Molecular Dynamics Simulations
○横井 駿, 光武 亜代理 (明治大学 理工学研究科 物理学専攻)
Shun Yokoi, Ayori Mitsutake (*Department of Physics, School of Science and Technology, Meiji University*)

座長：光武 亜代理 (明治大学), 柴田 幹大 (金沢大学)

Session Chairs: Ayori Mitsutake (Meiji Univ.), Mikihiko Shibata (Kanazawa Univ.)

- [2-06-1600](#) 大腸菌 UvrD C 末端アミノ酸欠損変異体の DNA 巻き戻しダイナミクス
DNA-unwinding dynamics of *Escherichia coli* UvrD lacking C-terminal amino acids
○横田 浩章 (光産創大)
Hiroaki Yokota (*Grad. Sch. Creation New Photon. Indust.*)
- [2-06-1612](#) 悪性高熱症を引き起こす RyR1 チャネル中間領域変異による細胞の高熱感受性
Cellular heat hypersensitivities caused by mutation in the middle region of the RyR1 channel implicated in malignant hyperthermia
○劉 楚傑¹, 山澤 徳志子², 大山 廣太郎^{3,4}, 原田 慶恵^{5,6}, 鈴木 団⁵ (¹ 阪大院・理・生物, ² 慈恵医大・医, ³ 量研・高崎研, ⁴ JST・さきがけ, ⁵ 阪大・蛋白研, ⁶ 阪大・QIQB)
Chujie Liu¹, Toshiko Yamazawa², Kotaro Oyama^{3,4}, Yoshie Harada^{5,6}, Madoka Suzuki⁵ (¹Dept Biol Sci, Grad Sch Sci, Osaka Univ, ²Jikei Univ Sch Med, ³QST, ⁴PRESTO, ⁵JST, ⁶IPR, Osaka Univ, ⁶QIQB, Osaka Univ)
- [2-06-1624](#) 一分子蛍光測定を用いた SARS-CoV-2 N タンパク質と RNA の結合様式
Structural characterization of RNA upon the binding with SARS-CoV-2 N protein by single molecule fluorescence measurements
○鈴木 怜和^{1,2}, 小井川 浩之^{1,2}, 高橋 聡^{1,2} (¹ 東北大・多元研, ² 東北大院・生命科学)
Leo Suzuki^{1,2}, Hiroyuki Oikawa^{1,2}, Satoshi Takahashi^{1,2} (¹IMRAM, Tohoku Univ., ²Grad. Sch. Life Sci., Tohoku Univ.)
- [2-06-1636](#) Molecular mechanism of MutS sliding on DNA explored by coarse-grained molecular dynamics simulations
Keisuke Inoue, Shoji Takada, Tsuyoshi Terakawa (*Department of Biophysics, Graduate School of Science, Kyoto University*)
- [2-06-1648](#) Processive Motion of Lambda Exonuclease revealed by Reactive Coarse-Grained Molecular Dynamics Simulation
Toru Niina, Shoji Takada (*Grad. Sch. Sci., Univ. Kyoto*)
- [2-06-1700](#) DNA 結合に伴うヘテロクロマチンタンパク質 HP1 の天然変性領域の ESR 動的構造解析
Structural Dynamics of Intrinsically Disordered Region of HP1 upon DNA Binding Studied by Spin Labeling ESR Spectroscopy
末武 勲^{2,3,4}, 佐藤 和信⁵, 武藤 梨沙⁶, 三島 優一², 工位 武治⁵, 川上 徹², 北條 裕信², 藤原 敏道², 宮田 真人¹, ○荒田 敏昭^{1,2} (¹ 阪市大・院理・生物, ² 阪大・蛋白研, ³ 中村学園大・院栄養, ⁴ 阪大・ツインリサーチセンター, ⁵ 阪市大・院理・化学, ⁶ 福岡大・理・物理)
Isao Suetake^{2,3,4}, Kazunobu Sato³, Risa Mutoh⁶, Yuichi Mishima², Takeji Takui⁵, Tohru Kawakami², Hironobu Hojo², Toshimichi Fujiwara², Makoto Miyata¹, **Toshiaki Arata**^{1,2} (¹Dept. Biol., Grad. Sch. Sci., Osaka City Univ., ²IPR, Osaka Univ., ³Grad. Sch. Nutrition, Nakamura Gakuen Univ., ⁴Twin Res. Ctr., Osaka Univ., ⁵Dept. Chem., Grad. Sch. Sci., Osaka City Univ., ⁶Dept. Phys., Fac. Sci., Fukuoka Univ.)
- [2-06-1712](#) 高速原子間力顕微鏡による膜中 TRPV1 チャネルの動態観察
Dynamics of transient receptor potential vanilloid1 (TRPV1) in lipid bilayer observed by high speed atomic force microscopy (HS-AFM)
○向 大地¹, Yimeng Zhao⁴, 柴田 幹大^{2,3}, 服部 素之⁴, 角野 歩^{2,3} (¹ 金沢大・院新学術創生研究科ナノ生命科学専攻, ² 金沢大 WPI-NanoLSI, ³ 金沢大新学術創成研究機構, ⁴ 復旦大生命科学学院)
Daichi Mukai¹, Zhao Yimeng⁴, Mikihiko Shibata^{2,3}, Motoyuki Hattori⁴, Ayumi Sumino^{2,3} (¹Dept. of Nano Life Sci., Grad. Sch. of Frontier Sci. Initiative, Univ. Kanazawa, ²WPI-NanoLSI, Univ. Kanazawa, ³Institute for Frontier Sci. Initiative, Univ. Kanazawa, ⁴Sch. of Life Sci., Univ. Fudan)

- [2-06-1724](#) カリウムチャンネル KcsA の開閉にともなう構造変化
Conformational Changes of KcsA K⁺ Channel upon Gating
○高崎 寛子¹, 清水 啓史², 安永 卓生³ (¹ 阪大・蛋白質研, ² 福井大・医, ³ 九工大・情報工)
Hiroko Takazaki¹, Hirofumi Shimizu², Takuo Yasunaga³ (¹*IPR, Univ. Osaka*, ²*Fac. Med. Sci., Univ. Fukui*, ³*Grad. Sch. Comp. Sci. Syst. Eng., KIT*)
- [2-06-1736](#) チトクロム酸化酵素を活性化する Higd1a の作用機序に関する分光学的研究
Spectroscopic study on the action mechanism of Higd1a for activating cytochrome c oxidase
○松村 和香¹, 柳澤 幸子¹, 伊藤 (新澤) 恭子¹, 西田 優也², 長尾 壮将², 新谷 泰範², 久保 稔¹ (¹ 兵庫県大・院生命理学, ² 国循・分子薬理)
Waka Matsumura¹, Sachiko Yanagisawa¹, Kyoko Shinzawa-Itoh¹, Yuya Nishida², Takemasa Nagao², Yasunori Shintani², Minoru Kubo¹ (¹*Grad. Sch. Life Sci., Univ. Hyogo, Japan*, ²*Molecular Pharmacology, NCVC, Japan*)
- [2-06-1748](#) ストップフローラマン・吸収分光計を用いたインドールアミン 2,3 ジオキシゲナーゼの反応中間体の研究
Investigation of reaction intermediates of indoleamine 2,3-dioxygenase by using a stopped-flow Raman/absorption spectrometer
○河村 味奈, 名定 加峰, 柳澤 幸子, 久保 稔 (兵庫県大・院生命理)
Mina Kawamura, Kaho Nasada, Sachiko Yanagisawa, Minoru Kubo (*Grad. Sch. Life Sci., Univ. Hyogo, Japan*)

13:15~15:39 Ch07

2G07A 筋肉・分子モーター II

Muscle & Molecular motor II

座長：西坂 崇之 (学習院大学), 飯野 亮太 (分子科学研究所)

Session Chairs: Takayuki Nishizaka (Gakushuin Univ.), Ryota Iino (IMS)

- [2-07-1315*](#) キネシン・ダイニンによる軸索輸送速度の極値統計解析
Extreme value analysis of the velocity of axonal transport by kinesin and dynein
○直井 拓磨¹, 加川 裕貴¹, 名木野 貴美子¹, 丹羽 伸介², 林 久美子^{1,3} (¹ 東北大・院工・応物, ² 東北大・学際研, ³ JST さきがけ)
Takuma Naoi¹, Yuki Kagawa¹, Kimiko Nagino¹, Shinsuke Niwa², Kumiko Hayashi^{1,3} (¹*Dep. Appl. Phys., Grad. Sch. Eng., Tohoku Univ.*, ²*FRIS, Tohoku Univ.*, ³*JST, PRESTO*)
- [2-07-1327*](#) 野生型と疾患変異型から構成されるヘテロダイマー KIF1A の 1 分子解析
Single molecule analysis of heterodimers composed of wild-type KIF1A and disease-associated KIF1A
○北 智輝¹, 穴澤 ゆず², 林 久美子^{1,3}, 丹羽 伸介^{2,4} (¹ 東北大・院工, ² 東北大・院生命科学, ³ JST・さきがけ, ⁴ 東北大・学際研)
Tomoki Kita¹, Yuzu Anazawa², Kumiko Hayashi^{1,3}, Shinsuke Niwa^{2,4} (¹*Grad. Eng., Tohoku Univ.*, ²*Grad. Life. Sci., Tohoku Univ.*, ³*PRESTO., JST*, ⁴*FRIS., Tohoku Univ.*)
- [2-07-1339*](#) キネシンとチューブリン C 末端との間の長距離引力
Long-range attraction between kinesin and C-terminal tail of tubulin
○田口 裕大, 庄司 響平, 大貫 隼, 高野 光則 (早大・物理応物)
Yuta Taguchi, Kyohei Shoji, Jun Ohnuki, Mitsunori Takano (*Dept. of Pure & Appl. Phys., Grad. Sch. Adv. Sci. & Eng., Waseda Univ.*)
- [2-07-1351*](#) A novel photochromic compound inhibits mitotic kinesin Eg5 in three isomerization states
Md Alrazi Islam, Shinsaku Maruta (*Grad.Sch.Eng., Soka University*)

- [2-07-1403*](#) **ネガティブ染色電子顕微鏡法により明らかにされた繊毛ダイニンの新規構造**
Novel isolated ciliary dynein structure revealed by negative stain EM
 ○雷 宜慈¹, 今井 洋¹, 山本 遼介¹, 下 理恵子¹, 上村 慎治², 八木 俊樹³, 梶村 直子⁵, 廣瀬 未果⁴, 加藤 貴之⁴, 光岡 薫⁵, 昆 隆英¹ (¹ 阪大・院理, ² 中大・理工・生命, ³ 県立広島大・生命環境, ⁴ 阪大・蛋白研, ⁵ 阪大・超高压電顕センター)
Yici Lei¹, Hiroshi Imai¹, Ryosuke Yamamoto¹, Rieko Shimo¹, Shinji Kamimura², Toshiki Yagi³, Naoko Kajimura⁵, Mika Hirose⁴, Takayuki Kato⁴, Kaoru Mitsuoka⁵, Takahide Kon¹ (¹*Dept. Biol. Sci., Grad. Sch. Of Sci., Osaka Univ.*, ²*Dept. Biol. Sci., Chuo Univ.*, ³*Dept. Life Sci., Prefect. Univ. Hiroshima*, ⁴*Inst. Of Protein Res., Osaka Univ.*, ⁵*Res. Ctr. UHVEM, Osaka Univ.*)
- [2-07-1415*](#) **細菌アクチン MreB の ATP 加水分解機構**
ATP hydrolysis mechanism of bacterial actin MreB
 ○高橋 大地¹, 藤原 郁子^{1,2,3}, 今田 勝巳⁴, 宮田 真人^{1,2} (¹ 大市大・院理, ² 大市大・複合先端, ³ 長岡技術大・生物工学, ⁴ 阪大・院理)
Daichi Takahashi¹, Ikuko Fujiwara^{1,2,3}, Katsumi Imada⁴, Makoto Miyata^{1,2} (¹*Grad. Sch. Sci., Osaka City Univ.*, ²*OCARINA, Osaka City Univ.*, ³*Dept. Bioeng., Nagaoka Univ. Tech.*, ⁴*Grad. Sch. Sci., Osaka Univ.*)
- [2-07-1427*](#) **ミオシン 1c が駆動する F-アクチン回転運動の 3 次元観察**
Corkscrew motion of F-actin driven by myosin-1c observed via three-dimensional optical tracking microscope
 ○佐藤 優成¹, 吉村 孝平², 松田 恭平¹, 原口 武士³, 山岸 雅彦¹, 須河 光弘¹, 伊藤 光二^{2,3}, 矢島 潤一郎¹ (¹ 東京大学大学院 総合文化研究科 広域科学専攻, ² 千葉大・院・融合理工・生物, ³ 千葉大・院・理学・生物)
Yusei Sato¹, Kohei Yoshimura², Kyohei Matsuda¹, Takeshi Haraguchi³, Msahiko Yamagishi¹, Mitsuhiro Sugawa¹, Kohji Ito^{2,3}, Junichiro Yajima¹ (¹*Dep. of Life Sciences, Graduate School of Arts and Sciences, The University of Tokyo*, ²*Dep. of Biology, Chiba Uni.*, ³*Dep. of Biology, Chiba Uni.*)
- [2-07-1439*](#) **滑らかに回転するバクテリアべん毛モーターの軸-軸受け相互作用を立体構造から紐解く**
Structural and functional analysis of the molecular bushing of the bacterial flagellar motor and the interactions with the rod
 ○山口 智子^{1,2}, 牧野 文信^{1,3}, 宮田 知子¹, 南野 徹¹, 加藤 貴之^{1,4}, 難波 啓一^{1,2,5,6} (¹ 阪大・生命機能, ² 理研・生命機能科学, ³ 日本電子(株), ⁴ 阪大・蛋白研, ⁵ 理研・放射光科学, ⁶ 阪大・日本電子 YOKOGUSHI 協働研)
Tomoko Yamaguchi^{1,2}, Fumiaki Makino^{1,3}, Tomoko Miyata¹, Tohru Minamino¹, Takayuki Kato^{1,4}, Keiichi Namba^{1,2,5,6} (¹*Grad. Sch. Frontier Biosci, Osaka Univ.*, ²*RIKEN BDR*, ³*JEOL Ltd.*, ⁴*IPR, Osaka Univ.*, ⁵*RIKEN Spring-8*, ⁶*JEOL YOKOGUSHI Res. Alliance Lab., Osaka Univ.*)
- [2-07-1451*](#) **IV型線毛収縮マシナリーは回転運動を生み出すか？**
Does the machinery of type IV pili retraction work as a rotary motor?
 ○佐久間 大輔¹, 中根 大介², 鹿毛 あずさ¹, 西坂 崇之¹ (¹ 学習院・物理, ² 電通大・基盤理工学専攻)
Daisuke Sakuma¹, Daisuke Nakane², Azusa Kage¹, Takayuki Nishizaka¹ (¹*Dept. Phys., Gakushuin Univ.*, ²*Dept. Eng. Sci., Univ. of Electro-Communications*)
- [2-07-1503*](#) **Cell-free スクリーニングに向けた F₁-ATPase の in vitro 合成及び 1 分子回転観察系の構築**
In vitro synthesis of F₁-ATPase and construction of single molecule rotation assay system for cell-free screening
 ○田口 真衣, 上野 博史, 野地 博行 (東大・院工・応化)
Mai Taguchi, Hiroshi Ueno, Hiroyuki Noji (*Appl. Chem., Grad. Sch. Eng., Univ. Tokyo*)
- [2-07-1515*](#) **人工回転分子モーターの設計とその自律的運動のシミュレーション**
Novel design of artificial molecular rotary motor and simulation of its autonomous motion
 ○伊藤 健太¹, 佐藤 佑介², 鳥谷部 祥一¹ (¹ 東北大・院工, ² 東北大・学際研)
Kenta Ito¹, Yusuke Sato², Sho Toyabe¹ (¹*Grad. Sch. Eng., Tohoku Univ.*, ²*FRIS, Tohoku Univ.*)

[2-07-1527](#) Insight into cooperative structural remodeling of the flagellar rotor ring complex responsible for directional switching

Tohru Minamino¹, Miki Kinoshita¹, Keiichi Namba^{1,2,3} (¹*Grad. Sch. Frontier Biosci, Osaka Univ.*,
²*RIKEN Spring-8*, ³*RIKEN BDR*)

16:00~18:36 Ch07

2G07B 筋肉・分子モーターⅢ

Muscle & Molecular motor Ⅲ

座長：岩城 光宏（理化学研究所），鳥澤 嵩征（国立遺伝学研究所）

Session Chairs: Mitsuhiro Iwaki (RIKEN), Takayuki Torisawa (NIG)

[2-07-1600](#) 筋節長ナノ計測と電子顕微鏡ライブイメージングで捉えた心筋細胞の筋節振動の力学特性
Mechanical properties of cardiomyocyte sarcomeric oscillations captured by sarcomere length nanometry and electron microscope live imaging

○新谷 正嶺（中部大・生命医科学）

Seine Shintani (*Dept. of Biomedical Sciences., Chubu Univ.*)

[2-07-1612](#) 高圧力により誘発される心筋細胞の非典型的収縮

High hydrostatic pressure induces unconventional cardiomyocyte contraction

○山口 陽平¹, 西山 雅祥², 金子 智之¹, 入部 玄太郎¹, 成瀬 恵治³, 森松 賢順³ (¹旭医大・生理学,
²近大・理工学・物理学,³岡大・院医歯薬学・システム生理学)

Yohei Yamaguchi¹, Masayoshi Nishiyama², Toshiyuki Kaneko¹, Gentaro Iribe¹, Keiji Naruse³,
Masatoshi Morimatsu³ (¹*Dept. Physio., Asahikawa Med Univ.*, ²*Dept. Physics., Kindai Univ.*, ³*Dept. Cardio. Physio., Grad. Sch. Med. Dent. Pharma., Univ. Okayama*)

[2-07-1624](#) 演題取り消し

[2-07-1636](#) Dynamics and coordination of the lever-arm swing of muscle myosin in the artificial myosin filament

Hiroki Fukunaga^{1,2}, Masashi Ohmachi², Takumi Washio^{4,5}, Keisuke Fujita^{1,2}, Hiroaki Takagi⁶,
Keigo Ikezaki⁷, Toshio Yanagida^{1,2,8}, Mitsuhiro Iwaki^{2,3} (¹*FBS, Univ. Osaka*, ²*Riken, BDR, IFRc, Univ. Osaka*,
⁴*UT-Heart Inc.*, ⁵*FC, Univ. Tokyo*, ⁶*Nara Med. Univ.*, ⁷*Univ. Tokyo*, ⁸*NICT*)

[2-07-1648](#) Trimethylamine-N-oxide (TMAO)がミオシンの熱安定性に与える効果

Effects of trimethylamine-N-oxide (TMAO) on the thermal stability of myosin

○茶園 茂（日本大学文理学部生命科学科）

Shigeru Chaen (*Department of Biosciences, College of Humanities and Sciences, Nihon University*)

[2-07-1700](#) 再構築したダイニン-微小管複合体の屈曲運動

Active beating of a reconstituted dynein-microtubule complexes

グイード イザベラ¹, 石橋 健太², ボーデンシャッツ エーベンハルド¹, ビルファン アンドレ³,
ゴールスタニアン ラミン¹, 榊原 斉², 大岩 和弘^{2,4} (¹マックスプランク研究所, ²NICT 未来
ICT 研究所, ³ヨーゼフ・ステファン研究所, ⁴兵庫県大・院理学)

Isabella Guido¹, Kenta Ishibashi², Eberhard Bodenschatz¹, Andrej Vilfan³, Ramin Golestanian¹,
Hitoshi Sakakibara², **Kazuhiro Oiwa**^{2,4} (*MPI. Dynamics Self-Organization*, ²*Nat. Inst. Info. Commun. Technol., Adv. ICT Res. Inst.*, ³*Jozef Stefan Inst.*, ⁴*Grad. Sch. Sci., Univ. Hyogo*)

[2-07-1712](#) 細胞質ダイニンとその制御タンパク質が紡錘体形成時に示す集積動態の時空間的定量

Spatiotemporal quantification of mitotic accumulation of cytoplasmic dynein I and its regulators at the spindle region

○鳥澤 嵩征^{1,2}, 木村 暁^{1,2} (¹遺伝研・細胞建築, ²総研大・遺伝学)

Takayuki Torisawa^{1,2}, Akatsuki Kimura^{1,2} (¹*Cell Arch. Lab., Natl. Inst. Genet.*, ²*Dept. Genet., SOKENDAI*)

- [2-07-1724](#) クライオ電顕で明らかになった外腕ダイニンの構造変化と活性化機構
Cryo-EM reveals remodeling and activation mechanisms of the outer arm dynein complex
久保 進太郎¹, Yang Shun Kai¹, Black Corbin S¹, Dai Daniel¹, Valente-Paterno Melissa¹, Gaetrig Jacek²,
○市川 宗巖³, Bui Khanh Huy¹ (¹マギル大学, ²ジョージア大学, ³奈良先端科学技術大学院大学)
Shintaroh Kubo¹, Shun Kai Yang¹, Corbin S Black¹, Daniel Dai¹, Melissa Valente-Paterno¹,
Jacek Gaetrig², **Muneyoshi Ichikawa**³, Khanh Huy Bui¹ (¹McGill University, ²University of Georgia,
³Nara Institute of Science and Technology)
- [2-07-1736](#) クラミドモナスにおける軸糸ダイニンの活性調節
Regulation of axonemal dynein motor activity in Chlamydomonas
○近藤 裕祐, 八木 俊樹 (県広大・院生命)
Yusuke Kondo, Toshiki Yagi (*Grad. bio. sci., Prefect. Univ. Hiroshima*)
- [2-07-1748](#) 翻訳後修飾によるダイニンの運動制御に関する粗視化 MD 計算
Regulating dynein motility controlled by post-translational modification revealed by coarse-grained MD simulation
○久保 進太郎^{1,2}, カーン フィ ブイ¹ (¹マギル大・医, ²東大・医)
Shintaroh Kubo^{1,2}, Bui Khanh Huy¹ (¹Dept. of Anatomy and Cell Biol., McGill Univ., ²Grad. Sch. of Med., The Univ. of Tokyo)
- [2-07-1800](#) Noise-induced acceleration of a molecular motor, kinesin-1
Takayuki Ariga¹, Keito Tateishi¹, Michio Tomishige², Daisuke Mizuno³ (¹Grad. Sch. Med., Yamaguchi Univ., ²Dept. Phys. Sci., Aoyama Gakuin Univ., ³Dept. Phys., Kyushu Univ.)
- [2-07-1812](#) Cytoskeletal component microtubules function as mechano-sensor to regulate intracellular transport
Syeda Rubaiya Nasrin¹, Christian Ganser², Arif Md. Rashedul Kabir¹, Kazuki Sada^{1,3},
Takefumi Yamashita⁴, Mitsunori Ikeguchi⁵, Takayuki Uchihashi^{3,6}, Akira Kakugo^{1,3} (¹Fac. Sci, Hokkaido Univ., Hokkaido., ²Dept. Creative Res., Nat. Inst. Nat. Sci., Okazaki, Aichi., ³Grad. Sch. Chem. Sci. Engg, Hokkaido Univ. Hokkaido., ⁴Res. Cent. Adv. Sci. Tech., Univ. Tokyo, Tokyo., ⁵Grad. Sch. Med. Life Sci, Yokohama City Univ., Yokohama., ⁶Dept. Phys. Struc. Biol. Res. Cent., Nagoya Univ., Nagoya.)
- [2-07-1824](#) 神経疾患を引き起こす KIF1A/UNC-104 変異体の軸索輸送とシナプス分布異常の関係
Axonal transport by pathogenic KIF1A/UNC-104 mutants cause abnormal synapse distributions
○加川 裕貴¹, 佐々木 瞭¹, 穴澤 ゆず², 丹羽 伸介³, 林 久美子^{1,4} (¹東北大・院工学, ²東北大・院生命科学, ³東北大・学際研, ⁴JST さきがけ)
Yuki Kagawa¹, Ryo Sasaki¹, Yuzu Anazawa², Shinsuke Niwa³, Kumiko Hayashi^{1,4} (¹Grad. Sch. Eng., Tohoku Univ., ²Grad. Life Sci., Tohoku Univ., ³FRIS, Tohoku Univ., ⁴JST, PRESTO)

13:15~15:39 Ch08

2G08A 細胞生物 II、骨格 II

Cell biology II, Cytoskeleton II

座長：鈴木 健一 (岐阜大学), 小松 英幸 (九州工業大学)

Session Chairs: Kenichi Suzuki (Gifu Univ.), Hideyuki Komatsu (Kyutech)

[2-08-1315*](#) 損傷した細胞を用いて計測する細胞内粒子動態と細胞死の関係

Relations between Motions of Intracellular Particles and Cell Death in Damaged Cells

○太田 英暁, 樋口 秀男 (東大・院理)

Hideaki Ota, Hideo Higuchi (*Grad. Sch. Sci., The Univ. of Tokyo*)

- [2-08-1327*](#) 興奮系 Ras の制御に関わる GEF の網羅的解析
Comprehensive analysis of GEFs involved in the regulation of a Ras excitable system
○岩本 浩司¹, 松岡 里実^{1,2,3}, 上田 昌宏^{1,2,3} (¹ 阪大・院理・生物科学, ² 阪大・院生命機能, ³ 理研生命機能科学研究センター)
Koji Iwamoto¹, Satomi Matsuoka^{1,2,3}, Masahiro Ueda^{1,2,3} (¹*Dept. of Biol. Sci., Grad. Sch. of Sci., Univ. of Osaka*, ²*Grad. Sch. of Front. Biosci., Univ. of Osaka*, ³*BDR, RIKEN*)
- [2-08-1339*](#) フォロワー細胞の先端端への割り込みによる上皮細胞集団の拡大
Leading Edge Expansion in Migrating Cell Sheet by Follower Cell's Interruption
○岩永 美咲¹, 沖村 千夏¹, 櫻井 建成², 岩橋 好昭¹ (¹ 山口大・院創成科学, ² 武蔵野大・工)
Misaki Iwanaga¹, Chika Okimura¹, Tatsunari Sakurai², Yoshiaki Iwadate¹ (¹*Grad. Sch. Sci. Tech., Yamaguchi Univ.*, ²*Dept. Math. Eng., Musashino Univ.*)
- [2-08-1351*](#) Oligomerization of neuronal receptors is essential for assembly and function of the synapse
Saahil Acharya¹, Taka A. Tsunoyama¹, Irina Meshcheryakova¹, Aya Nakamura¹, Hiroko Hijikata¹, Yuri Nemoto¹, Takahiro K. Fujiwara², Akihiro Kusumi¹ (¹*Membrane Cooperativity Unit, Okinawa Institute of Science and Technology Graduate University (OIST), Okinawa, Japan*, ²*Institute for Integrated Cell-Material Sciences (WPI-iCeMS), Kyoto University, Kyoto, Japan*)
- [2-08-1403*](#) Investigating the contribution of nuclear size on chromatin dynamics in interphase during *C. elegans* embryogenesis
Aiya K. Yesbolatova¹, Takahiro Sakaue², Akatsuki Kimura¹ (¹*Cell Architecture Laboratory, National Inst. of Genetics, Grad. Univ. for Advanced Studies*, ²*Department of Physics and Mathematics, Aoyama Gakuin University*)
- [2-08-1415](#) アクティブな界面摩擦と流体抵抗の幾何学的バランスが決めるアクトミオシン液滴の自発運動
Geometric trade-off between interfacial active friction and passive fluid drag determines the motility of actomyosin droplets
○坂本 遼太¹, イズリ ジャン², 島本 勇太³, 宮崎 牧人^{4,5,6,7}, 前多 裕介¹ (¹ 九大・院理, ² ミネソタ大・物理, ³ 遺伝研, ⁴ 京大白眉, ⁵ 京大・物理, ⁶ キュリー研, ⁷ JST PRESTO)
Ryota Sakamoto¹, Ziane Izri², Yuta Shimamoto³, Makito Miyazaki^{4,5,6,7}, Yusuke Maeda¹ (¹*Grad. Sch. Sci., Kyushu Univ.*, ²*Sch. Phys. Astro., Univ. Minnesota*, ³*Nat. Inst. Genetics*, ⁴*Hakubi Ctr., Kyoto Univ.*, ⁵*Dept. Phys., Kyoto Univ.*, ⁶*Inst. Curie*, ⁷*PRESTO, JST*)
- [2-08-1427*](#) アクトミオシン収縮力の光操作による細胞質分裂中の表層張力の機能解析
Optogenetic relaxation of actomyosin contractility uncovers mechanistic roles of cortical tension during cytokinesis
○山本 啓^{1,2,3}, 三浦 晴子^{2,3}, 近藤 洋平^{1,2,3}, 青木 一洋^{1,2,3} (¹ 総合研究大学院大学, ² 基礎生物学研究所, ³ 生命創成探究センター)
Kei Yamamoto^{1,2,3}, Haruko Miura^{2,3}, Yohei Kondo^{1,2,3}, Kazuhiro Aoki^{1,2,3} (¹*ISOKENDAI*, ²*NIBB*, ³*ExCELLS*)
- [2-08-1439*](#) 原子間力顕微鏡によるホヤ神経胚の力学マッピング
Mapping mechanical properties of ascidian embryo during neurulation by atomic force microscopy
○坪山 洋介, 松尾 智大, 岡嶋 孝治 (北大・院情報科学)
Yosuke Tsuboyama, Tomohiro Matsuo, Takaharu Okajima (*Grad. Info. Sci. & Tech. Univ. Hokkaido*)
- [2-08-1451*](#) 高速イメージングで明らかにする *Volvox carteri* の鞭毛メタクロナル波による力発生機構
Mechanism of Force Generation by Flagellar Metachronal Waves in *Volvox carteri* Revealed by High-speed Imaging
○上村 直輝, 島袋 勝弥 (宇部高専・物質)
Naoki Uemura, Katsuya Shimabukuro (*Chem. Bio. Eng., NIT Ube College*)

- [2-08-1503*](#) 細胞外小胞の標的細胞への選択的結合機構：1粒子追跡法による解明
Mechanisms of selective binding of small extracellular vesicles to recipient cells as revealed by single-particle tracking
○磯貝 樹¹, 廣澤 幸一朗², 正 彩乃³, 木塚 康彦^{2,4}, 横田 康成⁵, 鈴木 健一^{2,4} (¹岐阜大・院・自科技, ²岐阜大・iGCORE, ³岐阜大・応生, ⁴科技振・CREST, ⁵岐阜大・工)
Tatsuki Isogai¹, Koichiro M. Hirosawa², Ayano Sho³, Yasuhiko Kizuka^{2,4}, Yasunari Yokota⁵, Kenichi G. N. Suzuki^{2,4} (¹Grad. Sch. Nat Sci Tech., Gifu Univ., ²iGCORE, Gifu Univ., ³Dept. App Bio Sci., Gifu Univ., ⁴CREST, JST, ⁵Dept. Eng., Gifu Univ.)
- [2-08-1515](#) Effect of a sudden change of confined environments in collective cell migration of epithelial cells
Masaharu Endo¹, Mitsuru Sentoku², Kenji Yasuda^{1,2,3} (¹Dept. Phys., Sch. Adv. Sci. & Eng., Waseda Univ., ²Dept. Pure & Appl. Phys., Grad. Sch. Adv. Sci. & Eng., Waseda Univ., ³Org. Univ. Res. Initiatives, Waseda Univ.)
- [2-08-1527](#) A suppressor mutation of a *Chlamydomonas* cilia-less mutant suggests a novel role of Bld10p, an essential protein for centriole assembly
Yuki Nakazawa¹, Masafumi Hirono² (¹STG, OIST, ²Dept. Frontier Biosci., Hosei Univ.)

16:00~18:12 Ch08

2G08B 細胞生物：分子モーター

Molecular motor

座長：岩楯 好昭（山口大学），今田 勝巳（大阪大学）

Session Chairs: Yoshiaki Iwadate (Yamaguchi Univ.), Katsumi Imada (Osaka Univ.)

- [2-08-1600](#) ストレスファイバの直動回転変換モデル
Conversion of linear contraction of stress fibers into rotation in migrating cells
○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 Okimura¹, Shu Akiyama¹, Tatsunari Sakurai², Yoshiaki Iwadate¹ (¹Dept. Biol., Yamaguchi Univ., ²Dept. Math. Eng., Musashino Univ.)
- [2-08-1612](#) 海洋性ビブリオ菌において細胞極の目印タンパク質 HubP がべん毛本数制御因子 FlhG の ATPase 活性に与える影響
Effect of the polar landmark protein HubP on ATPase activity of FlhG, a flagellar number regulator of *Vibrio alginolyticus*
○郝 雨希¹, 竹川 宜宏², 本間 道夫¹, 小嶋 誠司¹ (¹名大・院理・生命理学, ²阪大・院理・高分子科学)
Yuxi Hao¹, Norihiro Takekawa², Michio Homma¹, Seiji Kojima¹ (¹Div. Biol. Sci., Grad. Sch. Sci., Nagoya Univ., ²Dept. Macromol. Sci., Grad. Sch. Sci., Osaka Univ.)
- [2-08-1624](#) 細菌べん毛のフック-フィラメント連結部にフィラメントキャップが結合した複合体の構造
Structure of the hook-filament junction with the filament cap in the bacterial flagellum
○竹川 宜宏¹, 池田 篤志¹, 宮田 知子², 牧野 文信^{2,3}, 難波 啓一^{4,5,6}, 今田 勝巳¹ (¹阪大・院理・高分子科学, ²阪大・院生命機能, ³日本電子(株), ⁴理研・生命機能, ⁵理研・SPRING-8, ⁶阪大・日本電子 YOKOGUSHI 協働研)
Norihiro Takekawa¹, Atsushi Ikeda¹, Tomoko Miyata², Fumiaki Makino^{2,3}, Keiichi Namba^{4,5,6}, Katsumi Imada¹ (¹Dept. Macromol. Sci., Grad. Sch. Sci., Osaka Univ., ²Grad. Sch. Frontier Biosci., Osaka Univ., ³JEOL Ltd., ⁴BDR, RIKEN, ⁵SPRING-8, RIKEN, ⁶JEOL YOKOGUSHI Res. Alliance. Lab., Osaka Univ.)
- [2-08-1636](#) 蛍光染色法による大腸菌べん毛の挙動の観察
Observation of behavior of flagella in *Escherichia coli* by using fluorescence staining
○中植 達也, 蔡 榮淑, 石島 秋彦, 福岡 創 (大阪大・生命機能研究科)
Tatsuya Nakae, Yong-Suk Che, Akihiko Ishijima, Hajime Fukuoka (Grad. Sch. Frontier Biosci. Osaka Univ.)

- [2-08-1648](#) 織毛基部と軸糸の位相板を用いたクライオ電顕法による構造解析
3D structure of the basal body and the axoneme from motile cilia reconstructed by cryo-electron tomography with the phase plate
○石川 尚, 苗加 彰, ツイマーマン ノエミ (パウル・シェラー研究所)
Takashi Ishikawa, Akira Noga, Noemi Zimmermann (*Paul Scherrer Institute*)
- [2-08-1700](#) フックキャップ蛋白質の輸送はフック蛋白質の輸送を促進する
Secretion of the hook cap protein enhances secretion of the hook protein
○五十嵐 玲香, 竹川 宜宏, 今田 勝巳 (阪大・院理・高分子科学)
Reika Igarashi, Norihiro Takekawa, Katsumi Imada (*Dept. Macromol. Sci., Grad. Sch. Sci., Osaka Univ.*)
- [2-08-1712](#) Search for domain in chemoreceptor to cause coordination of rotational switching between flagellar motors
Hiroto Kozono, Yong-Suk Che, Hajime Fukuoka, Akihiko Ishizima (*Grad. Sch. Frontier Bio Sci., Osaka Univ.*)
- [2-08-1724](#) 鞭毛内構造のラセン配置は鞭毛上の場所に依存する
The Helical Arrangement of Axonemal Structures Depends on the Region of the Flagellum
○榎原 斉¹, 石橋 健太², 岩本 裕之³, 小嶋 寛明¹, 大岩 和弘^{1,4} (¹情報通信研究機構 バイオ ICT 研究室, ²大阪大 CiNet, ³高輝度光科学研究センター, ⁴兵庫県立大 生命理学)
Hitoshi Sakakibara¹, Kenta Ishibashi², Hiroyuki Iwamoto³, Hiroaki Kojima¹, Kazuhiro Oiwa^{1,4} (¹*Bio-ICT Lab., Nat. Inst. Inf. Com. Tech.*, ²*CiNet, Osaka Univ.*, ³*Spring-8, JASRI*, ⁴*Life Sci. Univ. Hyogo*)
- [2-08-1736](#) 受容体アレイのメチル化レベルの変化は大腸菌べん毛モーター間の回転方向転換の同調を引き起こす
Change in methylation level in receptor array causes coordinated reversal of flagellar motors on a single Escherichia coli cell
内田 裕美子¹, 濱元 樹², 蔡 榮淑¹, 石島 秋彦¹, 福岡 創¹ (¹阪大・院生命機能, ²沖縄科学技術大学院大学)
Yumiko Uchida¹, Tatsuki Hamamoto², Yong-Suk Che¹, Akihiko Ishijima¹, **Hajime Fukuoka**¹ (¹*Grad. Sch. Frontier Biosci. Osaka Univ.*, ²*OIST Grad. Univ.*)
- [2-08-1748](#) 受容体の協調性を崩す変異型/野生型受容体の比率の定量化とべん毛モーターの協調性
Quantification for mutant/WT receptors ratio that collapses receptor cooperativity and switching coordination between flagellar motors
○粟 沙里, 内田 裕美子, 福岡 創, 石島 秋彦, 蔡 榮淑 (大阪大・院生命機能)
Shiori Awa, Yumiko Uchida, Hajime Fukuoka, Akihiko Ishijima, Yong-Suk Che (*Grad. Sch. Frontier Biosci. Osaka Univ.*)
- [2-08-1800](#) *Bacillus subtilis* 由来べん毛固定子蛋白質 MotS のナトリウム依存的構造変化
Sodium-dependent conformational change of flagellar stator protein MotS from *Bacillus subtilis*
○上堀 まりあ¹, 山口 綾香¹, 竹川 宜宏¹, 南野 徹², 今田 勝巳¹ (¹阪大・院理・高分子科学, ²阪大・院生命機能)
Maria Uehori¹, Ayaka Yamaguchi¹, Norihiro Takekawa¹, Tohru Minamino², Katsumi Imada¹ (¹*Dept. Macromol. Sci., Grad. Sch. Sci., Osaka Univ.*, ²*Grad. Sch. Frontier Biosci., Osaka Univ.*)

座長：細川 千絵 (大阪市立大学), 工藤 卓 (関西学院大学)

Session Chairs: Chie Hosokawa (Osaka City Univ.), Suguru Kudoh (Kwansei Gakuin Univ.)

[2-09-1315](#) 線虫 *C. elegans* の低温馴化多様性を制御する神経回路の解析

Neural circuit regulating the diversity of cold acclimation in *C. elegans*

○岡畑 美咲¹, 吉名 佐和子², 水口 洋平³, Wei Aguan D.⁴, 豊田 敦³, 三谷 昌平², 三浦 徹¹, 太田 茜¹, 久原 篤^{1,5} (¹甲南大学統合ニューロバイオロジー研究所,²東京女子医大,³国立遺伝学研究所,⁴Seattle Children's Research Inst.,⁵日本医療研究開発機構)

Misaki Okahata¹, Sawako Yoshina², Yohei Minakuchi³, Aguan D. Wei⁴, Atsushi Toyoda³, Shohei Mitani², Toru Miura¹, Akane Ohta¹, Atsushi Kuhara^{1,5} (¹*Inst. for Integrative Neurobio.*, *Konan Univ.*, ²*Tokyo Women's Med. Univ.*, ³*National Inst. of Genetics*, ⁴*Seattle Children's Research Inst.*, ⁵*PRIME, AMED*)

[2-09-1327](#) 海馬で合成される男性・女性ホルモンやストレスホルモンによる記憶シナプスの早い non-genomic な制御

Rapid non-genomic modulation of synapses by hippocampus-synthesized androgen, estrogen and stress steroid

○川戸 佳^{1,2}, 相馬 ミカ^{1,2}, 池田 真理^{1,2}, 斎藤 稔² (¹順天堂大・医,²日大文理・生命)

Suguru Kawato^{1,2}, Mika Soma^{1,2}, Mari Ikeda^{1,2}, Minoru Saito² (¹*Grad. Sch. Med, Juntendo Univ.*, ²*Dept. Bio, Nihon Univ.*)

[2-09-1339](#) *C. elegans* homologue of HADH involved in human mitochondrial fatty acid metabolism regulates neural function in temperature acclimation

Akihisa Fukumoto¹, Misaki Okahata¹, Yohei Minakuchi², Atsushi Toyoda², Akane Ohta¹, Atsushi Kuhara^{1,3} (¹*Grad. Sch. Sci., Konan Univ.*, ²*Natl. Inst. of Genetics, Japan.*, ³*PRIME, AMED*)

[2-09-1351](#) 神経回路をステップワイズに構築するためのアガロース微細加工技術の開発

Stepwise neuronal network pattern formation in agarose during cultivation using non-destructive microneedle photothermal microfabrication

○渡部 治樹, 下田 賢司, 田中 悠平, 安田 賢二 (早大・院先進・物理応物)

Haruki Watanabe, Kenji Simoda, Yuhei Tanaka, Kenji Yasuda (*Dept. Pure & Appl. Phys., Grad. Sch. Adv. Sci. & Eng., Waseda Univ.*)

[2-09-1403](#) 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

○中西 大斗, 藤井 雅史, 粟津 暁紀 (広島大・院統合生命科学)

Taito Nakanishi, Masashi Fujii, Akinori Awazu (*Graduate School of Integrated Sciences for Life, Univ. Hiroshima*)

[2-09-1415](#) Development of agarose microfabrication technology using Joule heat of micrometer-sized ionic current

Kenji Shimoda, Haruki Watanabe, Kenji Yasuda (*Dept. Pure & Appl. Phys., Grad. Sch. Adv. Sci. & Eng., Waseda Univ.*)

- [2-09-1427](#) 自己学習型ニューロロボットののための、培養神経回路網における連想学習再現の試み
An attempt to reproduce associative learning on a cultured neuronal network for development of a self-learning neurobots
趙 恩明², ○工藤 卓^{1,2} (¹関西学院大学 工学部 知能・機械工学課程 神経知能工学研究室,² 関西学院大学大学院 理工学研究科 人間システム工学専攻 神経知能工学研究室)
Enming Zhao², **Suguru N. Kudoh**^{1,2} (¹Laboratory for Neuronal Intelligence Engineering (NI LAB), Artificial Intelligence and Mechanical Engineering Course, Department of Engineering, Kwansei Gakuin University, ²Laboratory for Neuronal Intelligence Engineering (NI LAB), Department of Human System Interaction, School of Science and Technology, Kwansei Gakuin University.)
- [2-09-1439](#) ミミズ非連合学習におけるセロトニンの関与
Serotonin-dependent mechanism of non-associative learning in earthworm *Eisenia fetida*
○北村 美一郎, 中原 敏彰, 高橋 輝 (関東学院大・理工・数物)
Yoshihiro Kitamura, Toshiaki Nakahara, Hikaru Takahashi (*Dept Math Sci Phys, Col Sci Eng, Kanto Gakuin Univ*)
- [2-09-1451](#) マウススライス標本で電位感受性色素を用いてイメージングされた嗅周囲皮質 (PC)と嗅内野 (EC)との皮質神経振動
Cortical oscillations in entorhinal and perirhinal cortices imaged with voltage-sensitive dye in slice preparations of mice
○富永 貴志¹, 富永 洋子¹, 梶原 利一² (¹徳島文理大・神経研,² 明治大・理工学部・電気電子生命)
Takashi Tominaga¹, Yoko Tominaga¹, Riichi Kajiwara² (*Inst. Neurosci., Tokushima Bunri Univ.,²Dept.Electro. Bioinfo., Sch. Sci. Tech., Meiji Univ.*)

16:00~18:12 Ch09

2G09B 神経回路、化学受容・行動

Neural circuit, Chemoreception & Behavior

座長：村山 能宏 (東京農工大学), 権田 幸祐 (東北大学)

Session Chairs: Yoshihiro Murayama (Tokyo Univ. of Agric. and Tech.), Kohsuke Gonda (Tohoku Univ.)

- [2-09-1600*](#) Bull's eye 型プラズモニックチップによる神経細胞表面グルタミン酸受容体分子の光捕捉
Optical trapping of glutamate receptors on neuronal cells with a bull's eye-type plasmonic chip
○小泉 喬史¹, 永末 智也², 田和 圭子², 細川 千絵¹ (¹大阪市大・院理学,² 関学大・院理工)
Takashi Koizumi¹, Tomoya Nagasue², Keiko Tawa², Chie Hosokawa¹ (*Grad. Sch. Sci., Osaka City Univ.,²Grad. Sch. Sci. Tech., Kwansei Gakuin Univ.*)
- [2-09-1612*](#) モノアラガイの味覚嫌悪学習に対する緑茶由来カテキン混合物の影響
The combined effect of green tea-derived catechins on taste aversive conditioning in *Lymnaea*
○松岡 英樹¹, 伊藤 綾香², 斎藤 稔², 小松崎 良将¹ (¹日大・院・理工学・物理学,² 日大・院・総合基礎科学・相関理化学)
Hideki Matsuoka¹, Ayaka Itoh², Minoru Saito², Yoshimasa Komatsuzaki¹ (*Dept. Phys., Grad. Sch. Sci. and Tech., Nihon Univ.,²Dept. Corr. Study in Phys. and Chem., Grad. Sch. Integ. Basic Sci., Nihon Univ.*)
- [2-09-1624*](#) 開放系空間における脂質膜上のアミロイドβ凝集挙動の単分子観察
Single Molecule Observation of Amyloid β on Lipid Membrane under Open Space
○飯田 茜¹, 並河 英紀² (¹山形大院理工,² 山形大理工)
Akane Iida¹, Hideki Nabika² (*Grad. Sch. Sci. Eng., Yamagata Univ.,²Fac. Sci., Yamagata Univ.*)
- [2-09-1636*](#) クロストリジウム属細菌走化性システムの大腸菌再構成系の確立
Reconstitution of a *Clostridium* chemosensory system in *Escherichia coli*
○小池 祥平, 眞鍋 昇大, 大越 奨, 西山 宗一郎, 浦上 弘 (新潟薬科大・応用生命科学・食品安全学)
Shohei Koike, Shota Manabe, Susumu Ogoshi, So-ichiro Nishiyama, Hiroshi Urakami (*Fac. App. Life Sci., Niigata Univ. Pharm. App. Life Sci.*)

- [2-09-1648*](#) 大腸菌細胞側面膜領域における走化性受容体クラスター形成
Chemotaxis receptor clusters in the lateral membrane region of *Escherichia coli* cells
○井上 綾乃¹, 伊藤 那奈¹, 田島 寛隆³, 西川 正俊², 曾和 義幸^{1,2,3}, 川岸 郁朗^{1,2,3} (¹法政大・院理工・生命機能, ²法政大・生命・生命機能, ³ナノテクセンター)
Ayano Inoue¹, Nana Ito¹, Hiroataka Tajjima³, Nishikawa Masatoshi², Yoshiyuki Sowa^{1,2,3}, Ikuro Kawagishi^{1,2,3} (¹Grad. Sch. Sci. & Eng., Hosei Univ., ²Dept. Frontier Biosci., Hosei Univ., ³Res. Cen. Micro-Nano Tech., Hosei Univ.)
- [2-09-1700*](#) 神経細胞における早期遺伝子制御の定量的解析
Quantitative analysis of immediate early genes regulation in neuron
○伊藤 夏穂, 岡田 眞里子 (大阪大学蛋白質研究所)
Kaho Itoh, Mariko Okada (Institute for Protein Research, Osaka University)
- [2-09-1712](#) 蟻の蟻道合流時における意思決定とその意義について
A movement strategy of a single ant when entering a pheromone trail
○崎山 朋子, 坂本 悠太 (創価大・理工)
Tomoko Sakiyama, Yuta Sakamoto (Soka University)
- [2-09-1724](#) ボルボックスの鞭毛停止確率の照度依存性
Light intensity dependence of flagellar stop probability of *Volvox*
○原田 啓吾, 村山 能宏 (農工大・院工・物理システム工学)
Keigo Harada, Yoshihiro Murayama (Applied Physics, Tokyo Univ. of Agri. and Tech.)
- [2-09-1736](#) 緑藻 *Volvox* 目における細胞数と走光性の関係
Relationship between cell number and phototaxis in green algae *Volvox*
○坪内 聖樹, 村山 能宏 (農工大・院工・物理システム工学)
Masaki Tsubouchi, Yoshihiro Murayama (Applied Physics, Tokyo Univ. of Agri. and Tech.)
- [2-09-1748](#) 単細胞緑藻クラミドモナスの負の重力走性メカニズム
Mechanisms of negative gravitaxis in the unicellular green alga *Chlamydomonas reinhardtii*
○鹿毛 あずさ¹, 大森 俊宏², 菊地 謙次², 石川 拓司², 西坂 崇之¹ (¹学習院大・物理, ²東北大・ファインメカニクス)
Azusa Kage¹, Toshihiro Omori², Kenji Kikuchi², Takuji Ishikawa², Takayuki Nishizaka¹ (¹Dept. Physics, Gakushuin Univ., ²Dept. Finemechanics, Tohoku Univ.)
- [2-09-1800](#) 線虫 *C. elegans* の低温順化を司る神経回路における温度受容情報伝達
Thermosensory signaling in neural circuit underlying cold acclimation of *C. elegans*
○太田 茜¹, 本村 晴佳¹, 久原 篤^{1,2} (¹甲南大・理工生物・統合ニューロバイオロジー研, ²国立研究開発法人日本医療研究開発機構 AMED)
Akane Ohta¹, Haruka Motomura¹, Atsushi Kuhara^{1,2} (¹Dept. of Biology, Inst. of Integral Neurobio, Konan Univ., ²PRIME, AMED)

13:15~15:15 Ch10

2G10A 生体膜・人工膜 II

Biological & Artificial membrane II

座長：森垣 憲一 (神戸大学), 中野 実 (富山大学)

Session Chairs: Kenichi Morigaki (Kobe Univ.), Minoru Nakano (Univ. of Toyama)

- [2-10-1315*](#) 両親媒性タンパク質とリン脂質から構成された非対称小胞の形成
Formation of asymmetric vesicles composed of amphiphilic protein and phospholipid
○鈴木 允人, 神谷 厚輝 (群大・院理工)
Masato Suzuki, Koki Kamiya (Facut. Sci. Tech., Univ. Gunma)

- [2-10-1327*](#) ホスファチジルコリン二重膜特性におよぼす疎水鎖結合様式の影響
Effect of hydrophobic chain-linkage type of phosphatidylcholines on their bilayer membranes
○中尾 俊樹¹, 後藤 優樹², 倉科 昌², 玉井 伸岳², 安澤 幹人², 松木 均² (¹徳島大院先端技術科学教育, ²徳島大院社会産業理工学)
Toshiki Nakao¹, Masaki Goto², Masashi Kurashina², Nobutake Tamai², Mikito Yasuzawa², Hitoshi Matsuki² (¹*Grad. Sch. Advan. Tech. & Sci, Tokushima Univ.*, ²*Grad. Sch. Tech. Indus. & Soc. Sci, Tokushima Univ.*)
- [2-10-1339*](#) 浸透圧下における粘弾性ベシクルの構造変化解析
Morphological deformation of viscoelastic vesicle under osmotic stress
○丸山 朋輝¹, 森 健^{2,3}, 片山 佳樹^{2,3,4}, 岸村 顕広^{2,4} (¹九大シス生, ²九大院工, ³九大未来セ, ⁴九大分子システムセ)
Tomoki Maruyama¹, Takeshi Mori^{2,3}, Yoshiki Katayama^{2,3,4}, Akihiro Kishimura^{2,4} (¹*Fac. of System Life Science, Kyushu Univ.*, ²*Dept. of Applied Chem., Fac. of Eng., Kyushu Univ.*, ³*Ctr. for Future Chem., Kyushu Univ.*, ⁴*Ctr. for Molecular Systems, Kyushu Univ.*)
- [2-10-1351*](#) (3S5-4) 放射光円二色性・直線二色性・蛍光異方性により明確化された生体膜に誘起されたマガイニン 2β 凝集体の特徴
(3S5-4) Membrane-Induced β-Aggregates of Magainin 2 Characterized by Circular Dichroism, Linear Dichroism, and Fluorescence Anisotropy
○熊代 宗弘¹, 末永 翔磨¹, 松尾 光一² (¹広大・院理学, ²広大・放射光)
Munehiro Kumashiro¹, Shoma Suenaga¹, Koishi Matsuo² (¹*Grad. Sch. Sci., Hiroshima Univ.*, ²*HiSOR, Hiroshima Univ.*)
- [2-10-1403*](#) クラミドモナス封入巨大リポソームの光応答性運動
Motion response of *Chlamydomonas*-containing giant liposomes to optical signal
○汐見 駿佑, 林 真人, 金子 智行 (法政大学 大学院 理工学研究科 生命機能学専攻 再構成細胞学研究室 (LaRC))
Shunsuke Shiomi, Masahito Hayashi, Tomoyuki Kaneko (*LaRC, FB, Grad. Sch. Sci. & Eng., Hosei Univ.*)
- [2-10-1415](#) Membrane viscosity of heterogeneous multi component liposome
Yuka Sakuma (*Grad. Sch. Sci., Tohoku Univ.*)
- [2-10-1427](#) 膜相転移への影響からクロロゲン酸のリン脂質ホスファチジルコリン膜表面結合様式を探る
Binding mode of chlorogenic acid to phosphatidylcholine bilayer revealed by its effect on the lipid bilayer phase transition
熊川 恵理, 矢島 芳起, ○高橋 浩 (群馬大・理工)
Eri Kumagawa, Yoshiki Yajima, **Hiroshi Takahashi** (*Grad. Sch. Sci. & Tech., Gunma Univ.*)
- [2-10-1439](#) コレステロールが支持脂質二重膜の単層膜特異的な脂質拡散に与える影響
Leaflet-specific lipid diffusion of a supported lipid bilayer in the presence of cholesterol
○佐藤 昌樹, 坂口 美幸, 山口 祥一, 乙須 拓洋 (埼玉大・院理工)
Masaki Sato, Miyuki Sakaguchi, Shoichi Yamaguchi, Takuhiro Otosu (*Grad. Sch. Sci. Eng., Saitama Univ.*)
- [2-10-1451](#) 部分フッ素化ジエーテル型リン脂質の膜物性の解析
Analysis of membrane properties of partially fluorinated diether phospholipid membrane
○蟻坂 知佳¹, 宮崎 真也¹, 高木 俊之², 高橋 浩¹, 網井 秀樹^{1,3}, 園山 正史^{1,2,4} (¹群馬大・院理工学, ²産業技術総合研究所, ³群馬大・未来先端, ⁴群馬大・食健康セ)
Chika Arisaka¹, Masaya Miyazaki¹, Toshiyuki Takagi², Hiroshi Takahashi¹, Hideki Amii^{1,3}, Masashi Sonoyama^{1,2,4} (¹*Grad. Sch. Sci. Tech., Gunma Univ.*, ²*AIST*, ³*GIAR, Gunma Univ.*, ⁴*GUCFW, Gunma Univ.*)
- [2-10-1503](#) Theoretical Study of GM1 gangliosides assembly caused by Cholesterol: Structural Analysis by Coarse-grained Model
Daiki Shibata, Hidemi Nagao, Kazutomo Kawaguchi (*Graduate School of Natural Science and Technology, Kanazawa University*)

座長：山崎 昌一（静岡大学），松尾 光一（広島大学）

Session Chairs: Masahito Yamazaki (Shizuoka Univ.), Koichi Matsuo (Hiroshima Univ.)

- 2-10-1600** 抗菌ペプチド・マガニン2の巨大リポソーム中のポア形成に対する浸透圧の効果
Effect of osmotic pressure (Π) on antimicrobial peptide magainin 2 (Mag)-induced pore formation in giant unilamellar vesicles (GUVs)
○ピラエムディマスム¹, サハサミロンクマール¹, オアラシッドエムディマムン¹, 山崎 昌一^{1,2,3} (1 静大・創造院, 2 静大・電研, 3 静大・院理)
Md. Masum Billah¹, Samiron Kumar Saha¹, Md. Mamun Or Rashid¹, Masahito Yamazaki^{1,2,3} (1 *Grad. Sch. Sci. Tech., Shizuoka Univ.*, 2 *Res. Inst. Ele., Shizuoka Univ.*, 3 *Grad. Sch. Sci., Shizuoka Univ.*)
- 2-10-1612** 蛍光ラベルされていない抗菌ペプチド PGLa の巨大リポソーム内へのポア形成なしの侵入
Entry of nonlabeled Antimicrobial Peptide PGLa into giant unilamellar vesicle (GUV) lumens without Pore Formation
○アリエムディハズラット¹, シューママドビラタ¹, 道羅 英夫², 山崎 昌一^{1,3,4} (1 静大・創造院, 2 静大・グリーン研, 3 静大・電研, 4 静大・院理)
Md. Hazrat Ali¹, Madhab Lata Shuma¹, Hideo Dohra², Masahito Yamazaki^{1,3,4} (1 *Grad. Sch. Sci. Tech., Shizuoka Univ.*, 2 *Res. Inst. Green Sci. Tech., Shizuoka Univ.*, 3 *Res. Inst. Ele., Shizuoka Univ.*, 4 *Grad. Sch. Sci., Shizuoka Univ.*)
- 2-10-1624** 抗菌ペプチドの殺菌活性のための最小相互作用時間
Minimum Interaction Time for Bactericidal Activity of Antimicrobial Peptides (AMPs)
○ホセイ NFアーザナ¹, 山崎 昌一^{1,2,3} (1 静大・創造院, 2 静大・電研, 3 静大・院理)
Farzana Hossain¹, Masahito Yamazaki^{1,2,3} (1 *Grad. Sch. Sci. Tech., Shizuoka Univ.*, 2 *Res. Inst. Ele., Shizuoka Univ.*, 3 *Grad. Sch. Sci., Shizuoka Univ.*)
- 2-10-1636** 抗菌ペプチドを模倣した膜活性抗菌剤の設計と作用機構
Design of membrane-active antimicrobial agent by mimicking natural antimicrobial peptides and its action mechanism
○安原 主馬, 楫 瑞基, 木畑 秀仁, 中野 卓斗, ラッペンゲナエル (奈良先端大院・物質)
Kazuma Yasuhara, Mizuki Kaji, Hideto Kibata, Takuto Nakano, Gwenael Rapenne (*Div. Mat. Sci., Nara Inst. Sci. Tech.*)
- 2-10-1648** 脂質分子の特性に依存するマガニン2の膜結合構造
Membrane-Bound Conformations of Magainin 2 depending on the Inherent Characteristics of Lipid Molecules
○辻 怜河¹, 熊代 宗弘², 松尾 光一³ (1 広大院先進理工科学, 2 広大院理学, 3 広大院放射光)
Ryoga Tsuji¹, Munehiro Kumashiro², Koichi Matsuo³ (1 *Grad. Sch. Adv. Sci. Eng., Hiroshima Univ.*, 2 *Grad. Sch. Sci., Hiroshima Univ.*, 3 *HiSOR., Hiroshima Univ.*)
- 2-10-1700** 抗菌ペプチドのダブル・コオペラティブ効果
Antimicrobial peptide double cooperativity
○杉原 加織¹, ドラブ エバ² (1 東大生研, 2 ジュネーブ大学)
Kaori Sugihara¹, Ewa Drab² (1 *IIS, Univ. Tokyo*, 2 *Univ. Geneva*)
- 2-10-1712** Crowding conditions induce clustering of diffusive molecules inside artificial cells
Yuki Kanakubo¹, Chiho Watanabe², Miho Yanagisawa¹ (1 *Univ. Tokyo*, 2 *Hiroshima Univ.*)
- 2-10-1724** 細胞サイズのミクロな膜閉じ込めによる相分離と分子拡散の制御
Phase separation and molecular diffusion modulated by cell-size micrometric membrane confinement
○渡邊 千穂^{1,2}, 柳澤 実穂² (1 広大院・統合生命科学, 2 東大院・総合文化・先進)
Chiho Watanabe^{1,2}, Miho Yanagisawa² (1 *Hiroshima Univ.*, 2 *Univ. Tokyo*)

- [2-10-1736](#) 流れ環境下で生じる非対称脂質膜が引き起こす細胞サイズのリポソームへの分子濃縮
Abiotic molecular transport against a concentration gradient caused by flow-induced membrane asymmetry of cell-sized liposomes
○杉山 博紀¹, 大崎 寿久^{2,3}, 竹内 昌治^{2,4}, 豊田 太郎^{5,6} (¹自然科学研究機構・ExCELLS, ²東大・生産研, ³神奈川産技研, ⁴東大院・情理, ⁵東大院・総合, ⁶生物普遍性連携研究機構)
Hironori Sugiyama¹, Toshihisa Osaki^{2,3}, Shoji Takeuchi^{2,4}, Taro Toyota^{5,6} (¹ExCELLS, NIBB, ²IIS, UTokyo, ³KISTEC, ⁴Grad. Sch. Info Sci. Tech., UTokyo, ⁵Grad. Sch. Arts and Sci., UTokyo, ⁶UBI, UTokyo)
- [2-10-1748](#) 環境酸素濃度による大腸菌封入巨大リポソームの形態制御
Motion control of *E. coli*-containing giant liposome using environmental oxygen concentration
○林 真人, 早川 舞, 金子 智行 (法政大・生命科学)
Masahito Hayashi, Mai Hayakawa, Tomoyuki Kaneko (Dept. Frontier Biosci., Hosei Univ.)

13:15~15:39 Ch11
2G11A 光合成 I、光応答タンパク質：DNA I
Photosynthesis I, Light sensitive proteins: DNA I

座長：藤井 律子 (大阪市立大学), 栗栖 源嗣 (大阪大学)
Session Chairs: Ritsuko Fujii (Osaka City Univ.), Genji Kurisu (Osaka Univ.)

- [2-11-1315](#) *Arthrospira platensis* の red Chl について
The red chlorophyll of *Arthrospira platensis*
○松永 恭子¹, 本多 未来¹, 長尾 遼², 沈 建仁², 秋本 誠志³, 鞆 達也⁴ (¹東京理科大学理学部, ²岡山大学異分野基礎研究所, ³神戸大学大学院理学研究科, ⁴東京理科大学大学院理学研究科)
Kyoko Matsunaga¹, Miku Honda¹, Ryo Nagao², Jian-Ren Shen², Seiji Akimoto³, Tatsuya Tomo⁴
(¹Faculty of Science, Tokyo University of Science, Tokyo, Japan, ²Research Institute for Interdisciplinary Science and Graduate School of Natural Science and Technology, Okayama University, Okayama, Japan, ³Graduate School of Science, Kobe University, Hyogo, Japan, ⁴Graduate School of Science, Tokyo University of Science, Tokyo, Japan)
- [2-11-1327](#) In-vitro reconstruction of light-harvesting complexes of siphonous green alga, *Codium fragile*
Chiari Akiyama¹, Naoko Norioka², Naohiro Oka³, Yumiko Yamano⁴, Tetsuko Nakaniwa², Hideaki Tanaka^{2,5}, Genji Kurisu^{2,5}, Ritsuko Fujii^{1,6} (¹Grad. Sch. Sci., Osaka City Univ., ²Inst. Protein Res., Osaka Univ., ³BIRC, Tokushima Univ., ⁴Lab. Org. Chem. Life Sci., Kobe Pharm. Univ., ⁵Grad. Sch. Sci., Osaka Univ., ⁶ReCAP, Osaka City Univ.)
- [2-11-1339](#) フィコビリソームのフィコシアニン 6 量体内のエネルギーマ移動におけるリンカータンパク質の役割
The role of the linker protein in energy transfer within the phycocyanin hexamer of phycobilisome
○菊地 浩人 (日本医大・物理)
Hiroto Kikuchi (Dept. of Phys. Nippon Med. Sch.)
- [2-11-1351*](#) 励起スペクトル顕微鏡と超解像イメージングで明らかになったステート遷移におけるチラコイド膜の不規則な構造変化
Irregular Transformation of Thylakoid upon State Transition as Revealed by Excitation Spectral and Super-Resolution Microcopy
○張 先駿¹, 藤田 祐輝¹, 金田 直也¹, 得津 隆太郎², 皆川 純², 叶 深², 柴田 穰² (¹東北大学・院理学, ²基礎生物研究所)
XianJun Zhang¹, Yuki Fujita¹, Naoya Kaneda¹, Ryutarou Tokutsu², Jun Minagawa², Shen Ye², Yutaka Shibata² (¹Grad. Sci. Uni. Tohoku, ²National Institute for Basic Biology)
- [2-11-1403*](#) 光合成電子伝達経路の鉄硫黄錯体における電子アクセプター／ドナー鉄サイト
Electron Acceptor-Donor Iron Sites in the Iron-Sulfur Cluster of Photosynthetic Electron-Transfer Pathways
○神田 知樹¹, 斉藤 圭亮^{1,2}, 石北 央^{1,2} (¹東京大・院工, ²東京大・先端研)
Tomoki Kanda¹, Keisuke Saito^{1,2}, Hiroshi Ishikita^{1,2} (¹Grad. Eng., Univ. Tokyo, ²RCAST, Univ. Tokyo)

- [2-11-1415*](#) 光合成反応中心における複数のプロトン移動経路の同定と各経路の機能解明
Mechanism of the formation of proton transfer pathways in photosynthetic
○菅生 優¹, 斉藤 圭亮^{1,2}, 石北 央^{1,2} (¹東大院・応化,²東大・先端研)
Yu Sugo¹, Keisuke Saito^{1,2}, Hiroshi Ishikita^{1,2} (¹*Department of Applied Chemistry, Univ. Tokyo,*
²*Research Center for Advanced Science and Technology, Univ. Tokyo.*)
- [2-11-1427*](#) 低温ラマン分光法による Photoactive Yellow Protein の初期中間体の構造決定
Structural determination of initial intermediate of Photoactive Yellow Protein by low-temperature Raman spectroscopy
○志賀 大将¹, 藤澤 知績², Hoff Wouter D³, 海野 雅司² (¹佐賀大・院・先進健康科学,²佐賀大・理工,³オクラハマ州立大)
Daisuke Shiga¹, Tomotsumi Fujisawa², Wouter D Hoff³, Masasi Unno² (¹*Grad. Sch. Adv. Health Sci., Saga Univ,* ²*Fac. Sci. Eng., Saga. Univ,* ³*Oklahoma State Univ*)
- [2-11-1439*](#) bZIP 型転写因子 Photozipper における光誘起二量体形成過程の高速 AFM 観察
High-speed AFM observation on the light-induced dimerization of a bZIP transcription factor, Photozipper
○辻 明宏¹, 山下 隼人¹, 久富 修², 阿部 真之¹ (¹阪大・院基礎工,²阪大・院理)
Akihiro Tsuji¹, Hayato Yamashita¹, Osamu Hisatomi², Masayuki Abe¹ (¹*Grad. Sch. of Eng. Sci., Osaka Univ.,* ²*Grad. Sch. of Sci., Osaka Univ.*)
- [2-11-1451*](#) AUREO1 の二量体における水素結合の役割
The role of hydrogen bonds in stabilization of AUREO1 dimer
○足立 裕美子, 中島 碩士, 永野 優大, 久富 修 (大阪大学・院理)
Yumiko Adachi, Hiroto Nakajima, Yuta Nagano, Osamu Hisatomi (*Grad. Sch. Sci., Univ. Osaka*)
- [2-11-1503](#) AUREO1 における発色団 FMN のリビトールリン酸の役割
The role of ribitol-phosphate of the chromophore (FMN) in AUREO1
○久富 修, 永野 優大 (阪大・院理)
Osamu Hisatomi, Yuta Nagano (*Grad. Sch. Sci., Osaka Univ.*)
- [2-11-1515](#) 褐藻類シオミドロ Aureochrome - 3 の光反応
Photoreaction of Aureochrome-3 in a brown alga, *E. siliculosus*
○永野 優大, 足立 裕美子, 久富 修 (阪大・院理)
Yuta Nagano, Yumiko Adachi, Osamu Hisatomi (*Grad. Sch. of Sci., Osaka Univ.*)
- [2-11-1527](#) 光誘起電子移動反応を引き起こす LOV ドメイン変異体
Photoreaction of mutated LOV domain that causes light-induced electron transfer
○岩田 達也¹, 高野 史明¹, 濱田 守彦², 神取 秀樹³, 伊関 峰生¹, 小堀 康博² (¹東邦大・薬,²神戸大・分子フォト,³名工大・生命・応化)
Tatsuya Iwata¹, Fumiaki Takano¹, Morihiko Hamada², Hideki Kandori³, Mineo Iseki¹, Yasuhiro Kobori² (¹*Dept. Phar. Sci., Toho Univ.,* ²*Mol. Photo. Res. Cent. Kobe U.,* ³*Dept. Life Sci. Appl. Chem., NITech*)

座長：三野 広幸 (名古屋大学), 久富 修 (大阪大学)

Session Chairs: Hiroyuki Mino (Nagoya Univ.), Osamu Hisatomi (Osaka Univ.)

- [2-11-1600](#) 光合成水分解系における翻訳後アミノ酸変換のメカニズム
Mechanism of post-translational amino-acid conversion in the photosynthetic water-oxidizing complex
○松原 巧¹, 鈴木 健裕², 嶋田 友一郎¹, 北島(井原) 智美¹, 長尾 遼^{1,3}, 堂前 直², 野口 巧¹ (¹ 名大・院理, ² 理研 CSRS, ³ 岡大・異分野研)
Takumi Matsubara¹, Takchiro Suzuki², Yuichiro Shimada¹, Tomomi Kitajima-Ihara¹, Ryo Nagao^{1,3}, Naoshi Dohmae², Takumi Noguchi¹ (¹*Grad. Sch. Sci., Nagoya Univ.*, ²*RIKEN CSRS*, ³*RIIS, Okayama Univ.*)
- [2-11-1612](#) 光化学系 II における第二キノン電子受容体 Q_B への 2 段階プロトン移動の時間分解赤外分光検出
Time-resolved infrared detection of two-step proton transfer to the secondary quinone electron acceptor Q_B in photosystem II
○伊藤 帆奈美, 加藤 佑樹, 野口 巧 (名古屋大・院理)
Honami Ito, Yuki Kato, Takumi Noguchi (*Grad. Sch. Sci, Univ. Nagoya*)
- [2-11-1624](#) 光合成光化学系 II 酸素発生系中間状態 g = 5 S₂ 状態の熱的安定性
Thermodynamically stability of the g = 5 S₂ states in the Oxygen Evolving Complex of Photosystem II
○三野 広幸 (名古屋大・院理)
Hiroyuki Mino (*Grad. School Sci., Nagoya Univ.*)
- [2-11-1636](#) 嫌気性緑色硫黄光合成細菌における Rieske/cytb 複合体と c 型シトクロム間の構造機能相関の解析
Structure-function relationships between the Rieske/cytb complex and c-type cytochromes in anaerobic photosynthetic green sulfur bacteria
○岸本 拓¹, 浅井 智広², 武藤 梨沙³, 田中 秀明⁴, 宮ノ入 洋平⁴, 栗栖 源嗣⁴, 大岡 宏造¹ (¹ 阪大・院理, ² 立命大・生命, ³ 福岡大・理, ⁴ 阪大・蛋白質研)
Hiraku Kishimoto¹, Chihiro Azai², Risa Mutoh³, Hideaki Tanaka⁴, Yohei Miyanoiri⁴, Genji Kurisu⁴, Hirozo Oh-oka¹ (¹*Grad. Sch. Sci., Osaka Univ.*, ²*Col. Life Sci., Ritsumeikan Univ.*, ³*Fac. Sci., Fukuoka Univ.*, ⁴*Inst. Protein Res., Osaka Univ.*)
- [2-11-1648](#) プラストシアニンとシトクロム f の複合体形成に関する理論的研究
Theoretical study of complex formation of Plastocyanin and Cytochrome f
○川口 一朋, 長尾 秀実 (金沢大学理工研究域)
Kazutomo Kawaguchi, Hidemi Nagao (*Institute of Science and Engineering, Kanazawa University*)
- [2-11-1700](#) A. marina の光化学系 I の光捕集機構：T. elongatus の光化学系 I との比較
The light harvesting mechanism of A. marina Photosystem I reaction center: comparison with T. elongatus Photosystem I
○木村 明洋¹, 鬼頭 宏任², 浜口 祐³, 米倉 功治³, 川上 恵典³, 菓子野 康浩⁴, 伊藤 繁¹ (¹ 名大院理, ² 神戸大, ³ 理研, ⁴ 兵庫県大)
Akihiro Kimura¹, Hirotaka Kitoh², Tasuku Hamaguchi³, Koji Yonekura³, Keisuke Kawakami³, Yasuhiro Kashino⁴, Shigeru Itoh¹ (¹*Grad. Sch. Sci., Naoya Univ.*, ²*Kove Univ.*, ³*RIKEN*, ⁴*Univ. Hyogo*)
- [2-11-1712](#) Quantitative measurements of the redox chemistry of a flavin cofactor in photolyases and cryptochromes
Yuhei Hosokawa, Hiroyoshi Morita, Mai Nakamura, Shigenori Iwai, Junpei Yamamoto (*Grad. Sch. Eng. Sci., Osaka Univ.*)

- [2-11-1724](#) Light-induced movements of amino acid residues in *Chlamydomonas reinhardtii* animal-like cryptochrome and their roles in photoreduction
Mai Nakamura, Yuhei Hosokawa, Shigenori Iwai, Junpei Yamamoto (*Grad. Sch. Eng. Sci., Univ. Osaka*)
- [2-11-1736](#) 時間分解赤外分光法による(6-4)光修復酵素の光修復中間体の計測
 Time-resolved IR spectroscopic detection of a photorepair intermediate in (6-4) photolyase
 ○棚野 亜衣¹, 山田 大智¹, 山元 淳平², 久保 稔¹ (¹ 兵庫県大・院理, ² 阪大・院基礎工)
Ai Kadono¹, Daichi Yamada¹, Junpei Yamamoto², Minoru Kubo¹ (¹*Grad. Sch. Sci., Univ. Hyogo, Japan*, ²*Grad. Sch. Eng. Sci., Osaka Univ., Japan*)
- [2-11-1748](#) クリプトクロムが触媒する DNA 光修復反応のマイクロフロー・フラッシュ紫外可視分光解析
 Microflow-flash UV-vis spectroscopic analysis of DNA photorepair reaction catalyzed by cryptochrome
 ○前野 達海¹, 山田 大智¹, 山元 淳平², 久保 稔¹ (¹ 兵庫県大・院生命理学, ² 阪大・院基礎工)
Tatsumi Maeno¹, Daichi Yamada¹, Junpei Yamamoto², Minoru Kubo¹ (¹*Grad. Sch. Sci., Univ. Hyogo*, ²*Grad. Sch. Eng. Sci., Osaka Univ.*)
- [2-11-1800](#) Molecular insight into photoactivation of BLUF photoreceptor from QM/MM free energy calculation
Masahiko Taguchi, Shun Sakuraba, Chan Justin, Hidetoshi Kono (*Inst. Quant. Life Sci., QST*)
- [2-11-1812](#) 可視光照射下での DNA 二重鎖切断に対する水素分子の保護効果
 Effect of molecular hydrogen on DNA double-strand breaks under irradiation of visible light
 ○浅野 達哉¹, 波多野 雄治², 下谷内 宏統¹ (¹ 富山大・院理工学教育, ² 富山大・水素同位体)
Tatsuya Asano¹, Yuji Hatano², Hiroto Shimoyachi¹ (¹*Grad. Sch. Sci., Univ. Toyama*, ²*Hydrogen Isotope Research., Univ. Toyama*)

13:15~15:27 Ch12

2G12A ロドプシン：性質・機能II、構造I

Rhodopsins: Characteristics and function II, Structure I

座長：片山 耕大 (名古屋工業大学), 永田 崇 (東京大学)

Session Chairs: Kota Katayama (Nagoya Inst. of Tech.), Takashi Nagata (The Univ. of Tokyo)

- [2-12-1315](#) レチナール光異性化酵素として働く動物ロドプシンの分光学的解析
 UV-Vis spectroscopic analysis of animal rhodopsins acting as a retinal photoisomerase
 ○森本 直也¹, 永田 崇^{1,2}, 井上 圭一¹ (¹ 東大・物性研究所, ² JST・さきがけ)
Naoya Morimoto¹, Takashi Nagata^{1,2}, Keiichi Inoue¹ (¹*Inst. Solid State Phys., Univ. Tokyo*, ²*JST, PRESTO*)
- [2-12-1327](#) 高温環境由来のアーキアから発見されたシゾロドプシンの熱安定性研究
 Thermal stability of schizorhodopsin discovered from archaea derived from high-temperature environment
 ○川崎 佑真¹, 今野 雅恵^{1,2}, 井上 圭一¹ (¹ 東大・物性研, ² JST・さきがけ)
Yuma Kawasaki¹, Masae Konno^{1,2}, Keiichi Inoue¹ (¹*ISSP, Univ. Tokyo*, ²*PRESTO, JST*)

- [2-12-1339](#) シグナルペプチドを持つ Marine group II 古細菌由来 Clade-C ロドプシンの分子特性
Molecular properties of Clade-C rhodopsins with signal peptides derived from Marine Group II archaea (Ca. Poseidoniales)
○今野 雅恵^{1,2}, Bu Xu³, Apoorva Prabhu⁴, Yang Liu⁵, Meng Li⁵, Oded Bèjà⁶, Chuanlun Zhang³, Christian Rinke⁴, Lu Fan³, 井上 圭一¹ (¹東大・物性研, ²JST・さきがけ, ³Dept. Ocean Sci. Eng., SUSTech, ⁴Australian Centre for Ecogenomics, Sch. Chem. Mol. Biosci., Univ. Queensland, ⁵Inst. Adv. Study, Shenzhen Univ, ⁶Technion - Israel Inst. Tech)
- Masae Konno**^{1,2}, Bu Xu³, Apoorva Prabhu⁴, Yang Liu⁵, Meng Li⁵, Oded Bèjà⁶, Chuanlun Zhang³, Christian Rinke⁴, Lu Fan³, Keiichi Inoue¹ (¹ISSP, Univ. Tokyo, ²PRESTO, JST, ³Dept. Ocean Sci. Eng., SUSTech, ⁴Australian Centre for Ecogenomics, Sch. Chem. Mol. Biosci., Univ. Queensland, ⁵Inst. Adv. Study, Shenzhen Univ, ⁶Technion - Israel Inst. Tech)
- [2-12-1351](#) バクテリオロドプシンの光反応サイクルにおける 2 種類の O 中間体の存在
Existence of two substates in the O intermediate of the bacteriorhodopsin photocycle
○神山 勉¹, 井原 邦夫² (¹名古屋大学理学研究科, ²名古屋大学遺伝子実験施設)
Tsutomu Kouyama¹, Kunio Ihara² (¹Graduate School of Science, Nagoya University, ²Center for Gene Research, Nagoya University)
- [2-12-1403](#) 固体 NMR による暗順応状態ミドルロドプシンのレチナル発色団の構造解析
Structure of a retinal chromophore of dark-adapted middle rhodopsin as studied by solid-state NMR spectroscopy
○川村 出^{1,2}, 関 隼斗², 但馬 聖也¹, 横野 義輝², 重田 安里寿², 沖津 貴志³, 和田 昭盛³, 内藤 晶², 須藤 雄気⁴ (¹横国大・院理工, ²横国大・院工, ³神戸薬大・生命有機化学, ⁴岡山大・院医歯薬)
Izuru Kawamura^{1,2}, Hayto Seki², Seiya Tajima¹, Yoshiteru Makino², Arisu Shigeta², Takashi Okitsu³, Akimori Wada³, Akira Naito², Yuki Sudo⁴ (¹Grad. Sch. Eng. Sci., Yokohama Natl. Univ., ²Grad. Sch. Eng., Yokohama Natl. Univ., ³Kobe Pharm. Univ., ⁴Grad. Sch. Med. Dent. Pharm. Sci., Okayama Univ.)
- [2-12-1415](#) 天然アニオンチャネルロドプシン GtACR1 のイオン輸送過程に関する理論的研究
Theoretical study on ion conduction of natural anion channel rhodopsin GtACR1
○鹿倉 啓史, 成 誠, 林 重彦 (京大・院・理)
Takafumi Shikakura, Cheng Cheng, Shigehiko Hayashi (*Grad. Sch. Sci., Kyoto Univ.*)
- [2-12-1427](#) チャネルロドプシンのカチオン伝導の分子動力学研究
Molecular dynamics study of cation conduction in channelrhodopsin
○大貫 隼, 林田 拓登, 広本 拓麻, 高野 光則 (早大・先進理工・物理応物)
Jun Ohnuki, Takuto Hayashida, Takuma Hiromoto, Mitsunori Takano (*Dept. of Pure & Appl. Phys., Grad. Sch. Adv. Sci. & Eng., Waseda Univ.*)
- [2-12-1439](#) Sodium-ion transportation mechanism of a light-driven sodium pump rhodopsin investigated by step-scan time-resolved FTIR spectroscopy
Sahoko Tomida¹, Akimori Wada², Hideki Kandori^{1,3}, Yuji Furutani^{1,3} (¹Nagoya Institute of Technology, ²Kobe Pharmaceutical University, ³OptoBio Technology Research Center, Nagoya Institute of Technology)
- [2-12-1451](#) Color Tuning of Microbial Rhodopsin Proteins: Combined Spectroscopic and QM/MM Modeling Studies
Maria del Carmen Marin Perez¹, Konno Masae^{1,2}, Laura Pedraza-Gonzalez³, Luca De Vico³, Massimo Olivucci^{3,4}, Keiichi Inoue¹ (¹Univ. Tokyo / ISSP, ²Japan Sci. Tech. Agency / PRESTO, ³Univ. Siena / Biotech., Chem. and Phar. Depart., ⁴BGSU / Chem. Depart.)
- [2-12-1503](#) Swing motion of Arg108 residue as a gating mechanism of *Indibacter alkaliphilus* Na⁺ pump rhodopsin
Yukino Sato¹, Tsubasa Hashimoto¹, Koji Kato², Yoshikazu Tanaka³, Yoshiki Tanaka⁴, Tomoya Tsukazaki⁴, Takashi Tsukamoto^{1,5}, Makoto Demura^{1,5}, Min Yao^{1,5}, Takashi Kikukawa^{1,5} (¹Grad. Sch. Life Sci., Hokkaido Univ., ²RIIS, Okayama Univ., ³Grad. Sch. Life Sci., Tohoku Univ., ⁴Grad. Sch. Biol. Sci., NAIST, ⁵Fac. Adv. Life Sci., Hokkaido Univ.)

- [2-12-1515](#) DTG ロドプシンの X 線結晶構造解析
X-ray crystallographic analysis on DTG rhodopsin
○井上 圭一¹, 鈴木 花野², 今野 雅恵^{1,3}, Reza Bagherzadeh¹, Andrey Rozenberg⁴,
María del Carmen Marin¹, Oded Bèjà⁴, 村田 武士^{2,5} (1 東大・物性研,² 千葉大・院理学,³ JST・さきがけ,⁴ イスラエル工科大,⁵ 千葉大・分子キラリテイ研究センター)
Keiichi Inoue¹, Kano Suzuki², Masae Konno^{1,3}, Reza Bagherzadeh¹, Andrey Rozenberg⁴,
María del Carmen Marin¹, Oded Bèjà⁴, Takeshi Murata^{2,5} (1 *Inst. Solid State Phys., Univ. Tokyo*, 2 *Grad. Sch. Sci., Chiba Univ.*, 3 *PRESTO, JST*, 4 *Techion*, 5 *Mol. Chirality Res. Cntr; Chiba Univ.*)

16:00~18:36 Ch12

2G12B ロドプシン：光制御 II、性質・機能 III、構造 II

Rhodopsins: Optical control II, Characteristics and function III, Structure II

座長：菊川 峰志 (北海道大学), 古谷 祐詞 (名古屋工業大学)

Session Chairs: Takashi Kikukawa (Hokkaido Univ.), Yuji Furutani (Nagoya Inst. of Tech.)

- [2-12-1600*](#) 表面増強赤外吸収分光解析によるセンサリーロドプシン II—トランスデューサータンパク質融合タンパク質の光誘起構造変化

Light-induced conformational change of pSRII-pHtrII fusion protein analyzed by surface-enhanced infrared spectroscopy

○唐 静一¹, Insyeerah Binti Muhammad Jauhari², 古谷 祐詞^{1,3} (1 名工大・院工,² 名工大・工学,³ 名工大・オプトバイオ)

Jingyi Tang¹, Insyeerah Binti Muhammad Jauhari², Yuji Furutani^{1,3} (1 *Grad. Eng. Nagoya Inst. Tech.*, 2 *Dept. Eng. Nagoya Inst. Tech.*, 3 *Opt. Tech. Nagoya Inst. Tech.*)

- [2-12-1612*](#) LED システムを用いたロドプシン蛍光の観察と膜電位の長時間イメージングへの適用

Detection of membrane potential-dependent rhodopsin fluorescence with LED system for long-term imaging

○川西 志歩¹, 小島 慧一^{1,2}, 洪川 敦史¹, 坂本 雅行³, 須藤 雄気^{1,2} (1 岡山大・院医歯薬 (薬),² 岡山大・医歯薬学域,³ 京都大・院生命科学)

Shiho Kawanishi¹, Keiichi Kojima^{1,2}, Atsushi Shibukawa¹, Masayuki Sakamoto³, Yuki Sudo^{1,2} (1 *Grad. Sch., Med. Dent. & Pharm. Sci., Okayama Univ.*, 2 *Grad. Sch., Med. Dent. & Pharm. Sci., Okayama Univ.*, 3 *Grad. Sch., Biostudies, Kyoto Univ.*)

- [2-12-1624*](#) 内向きプロトンポンプ型ロドプシン RmXeR を用いた光誘起崩壊リポソーム (LiDL) の開発
Development of light-induced disruptive liposome (LiDL) with an inward proton pump rhodopsin RmXeR

○恒石 泰地¹, 小島 慧一^{1,2}, 窪田 文佳³, 山田 勇磨³, 須藤 雄気^{1,2} (1 岡山大・院医歯薬 (薬),² 岡山大・医歯薬学域,³ 北海道大・院薬学研究院)

Taichi Tsuneishi¹, Keiichi Kojima^{1,2}, Fumika Kubota³, Yuma Yamada³, Yuki Sudo^{1,2} (1 *Grad. Sch. of Med., Dent. & Pharm. Sci., Okayama Univ.*, 2 *Grad. Sch. of Med., Dent. & Pharm. Sci., Okayama Univ.*, 3 *Grad. Sch. of Pharm. Sci., Hokkaido Univ.*)

- [2-12-1636*](#) 青色吸収型プロテオロドプシンにおける異常な pH 依存的長波長シフトの解明

Mechanism of anomalous pH-dependent color change in blue-proteorhodopsin from *Vibrio caribbeanicus*

○澄川 瑞季¹, 吉住 玲¹, 内橋 貴之², 神取 秀樹¹ (1 名工大・院工,² 名大・院理)

Mizuki Sumikawa¹, Rei Abe-Yoshizumi¹, Takayuki Uchihashi², Hideki Kandori¹ (1 *Nagoya Inst. Tech.*, 2 *Dept of phys, Nagoya univ*)

- [2-12-1648*](#) 様々な内向きおよび外向きプロトンポンプロドプシンの電気生理学的解析
Electrophysiological analysis of inward and outward proton pump rhodopsins
○奥山 あかり, 細島 頌子, 角田 聡, 神取 秀樹 (名工大・院工)
Akari Okuyama, Shoko Hososhima, Satoshi Tsunoda, Hideki Kandori (*Grad. Sch. Eng., Nagoya Inst. Tech.*)
- [2-12-1700*](#) TAT ロドプシンの Ca²⁺センサー機能
Ca²⁺ sensing function of TAT rhodopsin
○杉本 哲平, 片山 耕大, 神取 秀樹 (名工大・院工)
Tepei Sugimoto, Kota Katayama, Hideki Kandori (*Grad. Sch. Univ. Nagoya Institute of Technology*)
- [2-12-1712*](#) 光と苦味のセンサーとしてはたらくキイロシヨウジヨウバエ Rh7 の赤外分光研究
FTIR study of Drosophila Rh7, a light and bitter taste sensor
○渡辺 航平, 片山 耕大, 神取 秀樹 (名工大・院工)
Kohei Watanabe, Kota Katayama, Hideki Kandori (*Grad. Sch. Eng., Nagoya Inst. Tech.*)
- [2-12-1724*](#) 全長型アニオンチャンネルロドプシンの機能解析
Functional Characterization of *Guillardia theta* Anion Channelrhodopsin 1 with its Full-Length Sequence
○大木 優也¹, 大竹 峻平², 佐藤 千乃², 渡邊 拓真¹, 渡辺 稷¹, 出村 誠³, 菊川 峰志³, 塚本 卓³
(¹北海道大学理学部, ²北海道大学生命科学院, ³北海道大学先端生命科学研究院)
Yuya Ohki¹, Ryouhei Ohtake², Yukino Sato², Takuma Watanabe¹, Jo Watanabe¹, Makoto Demura³, Takashi Kikukawa³, Takashi Tsukamoto³ (*¹School of Science, Hokkaido University, ²Graduate School of Life Science, Hokkaido University, ³Faculty of Advanced Life Science, Hokkaido University*)
- [2-12-1736*](#) ラマン光学活性による微生物型ロドプシン単量体と多量体におけるレチナールシッフ塩基の構造解析
Conformational analysis of retinal Schiff base of a microbial rhodopsin in monomeric and oligomeric forms using Raman optical activity
○西川 航平¹, 藤澤 知績², 海野 雅司², 須藤 雄気³, 小島 慧一³, 仲間 政樹³ (¹佐賀大・院・先進健康, ²佐賀大・理工, ³岡大・院・医歯薬(薬))
Kohei Nishikawa¹, Tomotsumi Fujisawa², Masashi Unno², Yuki Sudo³, Keiichi Kojima³, Masaki Nakama³ (*¹Grad. Sch. Adv. Health. Sci., Saga Univ., ²Fac. Sci. Eng., Saga Univ., ³Grad. Sch. of Med. Dent. & Pharm. Sci. Okayama Univ.*)
- [2-12-1748*](#) 近赤外光を吸収する新規酵素ロドプシン(RhGC)の反応特性
Reaction characteristics of near-infrared light absorbing enzyme rhodopsin (RhGC)
○石川 和季¹, 細島 頌子¹, 杉浦 雅大¹, ブラウン レオニード S², 角田 聡², 神取 秀樹¹ (¹名古屋工業大学 大学院工学研究科, ²グエルフ大学 物理学部)
Kazuki Ishikawa¹, Shoko Hososhima¹, Masahiro Sugiura¹, Leonid S Brown², Satoshi Tsunoda², Hideki Kandori¹ (*¹Graduate School of Engineering, Nagoya Institute of Technology, ²the Department of Physics, University of Guelph.*)
- [2-12-1800*](#) ロドプシングアニル酸シクラーゼ (Rh-GC) の光反応ダイナミクス
Photoreaction Dynamics of Rhodopsin Guanylate Cyclase (Rh-GC)
○杉浦 雅大¹, 角田 聡¹, 二又 葉音², 志甫谷 渉², 濡木 理², 神取 秀樹¹, 古谷 祐詞¹ (¹名工大・院工, ²東大・院理)
Masahiro Sugiura¹, Satoshi Tsunoda¹, Haon Futamata², Wataru Shihoya², Osamu Nureki², Hideki Kandori¹, Yuji Furutani¹ (*¹Nagoya Inst. Tech., ²Grad. Sch. Sci., Tokyo Univ.*)
- [2-12-1812*](#) ヘリオロドプシン特有の波長制御メカニズムの構造基盤
Structural basis for unique color tuning mechanism in heliorhodopsin
○田中 達基¹, Singh Manish², 志甫谷 渉¹, 山下 恵太郎¹, 神取 秀樹², 濡木 理¹ (¹東大・院理, ²名工大・院工)
Tatsuki Tanaka¹, Manish Singh², Wataru Shihoya¹, Keitaro Yamashita¹, Hideki Kandori², Osamu Nureki¹ (*¹Grad. Sch. of Sci., Univ. of Tokyo, ²Grad. Sch. of Eng., Nagoya Inst. of Tech.*)

- [2-12-1824*](#) アニオンチャネルロドプシンのプロトンを介したアニオン透過機構の解明
Proton-mediated gating mechanism of anion channelrhodopsin-1
○辻村 真樹¹, 小島 慧², 川西 志歩², 須藤 雄気², 石北 央^{1,3} (¹東大・理工,²岡山大・院医歯薬,³東大・先端研)
Masaki Tsujimura¹, Keichi Kojima², Shiho Kawanishi², Yuki Sudo², Hiroshi Ishikita^{1,3} (¹Grad. Sch. Eng., Univ. Tokyo, ²Grad. Sch. Med. Dent. Pharm., Okayama Univ., ³RCAST, Univ. Tokyo)

13:15~15:39 Ch13

2G13A 生命の起源、生態

Origin of life, Ecology

座長：今井 正幸（東北大学），市橋 伯一（東京大学）

Session Chairs: Masayuki Imai (Tohoku Univ.), Norikazu Ichihashi (The Univ. of Tokyo)

- [2-13-1315](#) ペプチド核酸の Taq ポリメラーゼに対する鑄型活性を利用したタンパク質から DNA への転写活性の検出

Detection of transcription activity of amino acids into DNA using Peptide Nucleic Acid (PNA) as a template for *Taq* DNA polymerase

○桑山 秀一（筑波大学生命環境系）

Hidekazu Kuwayama (*University of Tsukuba, Faculty of Life and Environmental Sciences*)

- [2-13-1327](#) 飢餓状態における解糖系の振動現象

Role of Glycolytic Oscillation in Starvation

○波多野 誠司¹, 永田 昇¹, 車 兪澈², 川勝 年洋¹, 今井 正幸¹ (¹東北大院理,²海洋研究開発機構)

Seiji Hatano¹, Noboru Nagata¹, Yutetsu Kuruma², Toshihiro Kawakatsu¹, Masayuki Imai¹ (¹Grad. Sch. Sci., Tohoku Univ., ²Japan Agency for Marine-Earth Science and Technology)

- [2-13-1339](#) 人工 RNA 複製システムのダーウィン進化による複雑化

Evolutionary complexification of an artificial RNA replication system

○水内 良^{1,2}, 古林 太郎³, 市橋 伯一^{1,4,5} (¹東大・先進科学,²JST・さきがけ,³東大・応用科学,⁴東大・生命,⁵東大・普遍性)

Ryo Mizuuchi^{1,2}, Taro Furubayashi³, Norikazu Ichihashi^{1,4,5} (¹Komaba Inst. Sci., Univ. Tokyo, ²JST, PRESTO, ³Appl. Chem., Univ. Tokyo, ⁴Life Sci., Univ. Tokyo, ⁵Univ. Biol. Inst., Univ. Tokyo)

- [2-13-1351](#) Mechanism of chiral-selective aminoacylation of an RNA minihelix studied by quantum mechanics/molecular mechanics free energy simulations

Tadashi Ando^{1,2}, Takato Masui¹ (¹Adv. Eng., Tokyo Univ. Sci., ²Res. Ins. Sci. Tech., Tokyo Univ. Sci.)

- [2-13-1403](#) 単純なペプチドから RNA ポリメラーゼコアドメインへの進化過程の実験的再現

Reconstructing the evolutionary pathway of the core domain in RNA polymerases from simple peptide

○八木 創太, 田上 俊輔（理研・生命機能科学研究センター）

Sota Yagi, Shunsuke Tagami (*Center for Biosystems Dynamics Research, RIKEN*)

- [2-13-1415](#) 細菌の群集がしめす適応的な表現型構造

Adaptive phenotypic structures of bacterial communities

○鈴木 誉保¹, 松井 求¹, 岩崎 渉² (¹東大・理,²東大・新領域)

Takao Suzuki¹, Motomu Matsui¹, Wataru Iwasaki² (¹Grad. Sch. Sci., UTokyo, ²Grad. Sch. Front. Sci., UTokyo)

- [2-13-1427*](#) (1S10-3) アミノ酸配列と連携した原始生体膜の成長

(1S10-3) Growth of Primitive Cell Membrane Coupled with Amino Acid Sequence

○馬場 晶子¹, オルソン ウルフ², 今井 正幸¹ (¹東北大・院理学,² Lund 大・院理学)

Akiko Baba¹, Ulf Olsson², Masayuki Imai¹ (¹Grad. Sch. Sci., Univ. Tohoku, ²Grad. Sch. Sci., Univ. Lund)

- [2-13-1439*](#) 鋳型重合と連携したベシクルの自己生産サイクル：自律的なプロトセルの構築を目指して
 Reproduction cycles of vesicle coupled with template polymerization: toward autonomous synthetic protocell
 ○栗栖 実¹, 片山 涼介¹, 佐久間 由香¹, ワルデ ピーター², 今井 正幸¹ (¹ 東北大・院理学, ² Dept. Materials Sci., ETH Zurich)
Minoru Kurisu¹, Ryosuke Katayama¹, Yuka Sakuma¹, Peter Walde², Masayuki Imai¹ (¹ Grad. Sch. Sci., Tohoku Univ., ² Dept. Materials Sci., ETH Zurich)
- [2-13-1451*](#) (1S10-7) 多相液滴のコアを用いた人工細胞内転写反応場の構築
 (1S10-7) Development of a transcription field in the artificial cell by the core of multiphase droplets
 ○友原 貴志, 皆川 慶嘉, 野地 博行 (東大院・工 応用化学)
Kanji Tomohara, Yoshihiro Minagawa, Hiroyuki Noji (Dept. Appl. Chem., Grad. Sch. Eng., Univ. Tokyo)
- [2-13-1503*](#) 多段階酵素反応による DNA 液滴ベース人工細胞の分裂制御
 Controlled division of DNA-droplet-based artificial cells coupled with enzymatic reaction cascade
 ○丸山 智也¹, 山本 陽大², 瀧ノ上 正浩^{1,2} (¹ 東京工業大学 生命理工学院 生命理工学系, ² 東京工業大学 情報理工学院 情報工学系)
Tomoya Maruyama¹, Akihiro Yamamoto², 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)
- [2-13-1515*](#) 無細胞翻訳系を用いた DNA の自己複製による相分離液滴の形成
 Formation of phase-separated droplets by DNA self-replication using cell-free protein synthesis system
 ○藪田 萌, 皆川 慶嘉, 野地 博行 (東京大・院応用化学)
Moe Yabuta, Yoshihiro Minagawa, Hiroyuki Noji (Dept. App. Chem., Grad. Sch. Eng., Univ. Tokyo)
- [2-13-1527*](#) 共通要素は解糖系とタンパク質合成系の共役再構成系の動態を制御する
 Common elements regulate the dynamics of the conjugated system of glycolysis and protein-synthesis reconstituted *in vitro*
 ○佐藤 岳, 木下 紗季, 山田 貴大, 舟橋 啓, 土居 信英, 藤原 慶 (慶大・院理工)
Gaku Sato, Saki Kinoshita, Takahiro Yamada, Akira Funahashi, Nobuhide Doi, Kei Fujiwara (Grad. Sch. Sci. Technol. Univ. Keio)

16:00~18:00 Ch13

2G13B 分子遺伝、ゲノム生物学 III

Molecular genetics, Genome biology III

座長：田端 和仁 (東京大学), 土方 敦司 (長浜バイオ大学)

Session Chairs: Kazuhito Tabata (The Univ. of Tokyo), Atsushi Hijikata (Nagahama Inst. of Bio-Sci. and Tech.)

- [2-13-1600*](#) 胚発生期に海馬の細胞運命を決定する動的な分子制御ネットワークの構築
 A Dynamic Molecular Regulatory Network to Determine Hippocampal Cell Fate during Embryogenesis
 ○王 梓, 岡田 真里子 (阪大・蛋白研・細胞システム研)
Zi Wang, Mariko Okada (Lab. of Cell Sys., IPR, Osaka Univ.)
- [2-13-1612*](#) DNA1 分子からの無細胞遺伝子発現ノイズ解析
 Noise analysis of cell-free gene expression from single-molecule DNA
 ○野呂 聖弥, 皆川 慶嘉, 野地 博行 (東京大・院応用化学)
Seiya Noro, Yoshihiro Minagawa, Hiroyuki Noji (Dept. App. Chem., Grad. Sch. Eng., Univ. Tokyo)

- [2-13-1624*](#) 発現量ノイズの伝搬を利用した隠れた相互作用の検出
Capturing hidden regulation by utilizing expression noise propagation
○伊藤 冬馬^{1,2}, 牧野 能士³ (¹総研大・生命基礎生物, ²東北大・理学部生物, ³東北大・院生命)
Thoma Itoh^{1,2}, Takashi Makino³ (¹*Department of Basic Biology, School of Life Science, The Graduate University for Advanced Studies, SOKENDAI*, ²*Department of Biology, Faculty of Science, Tohoku University*, ³*Graduate School of Life Sciences, Tohoku University*)
- [2-13-1636](#) 左右軸決定における、マウスノード不動繊毛への機械刺激依存的な *Cer12* mRNA 分解の活性化
Mechanical stimuli to a mouse nodal immotile cilium activate *Cer12* mRNA decay for left-right symmetry breaking
○加藤 孝信¹, 大森 俊宏², 水野 克俊³, 石川 拓司², 濱田 博司¹ (¹理化学研究所 生命機能科学研究センター, ²東北大学大学院工学研究科 ファインメカニクス専攻, ³福井大学 医学部)
Takanobu A Katoh¹, Toshihiro Omori², Katsutoshi Mizuno³, Takuji Ishikawa², Hiroshi Hamada¹ (¹*BDR, Riken*, ²*Dept. Finemechanics, Grad. Sch. Eng., Tohoku University*, ³*School of Medical Sciences, University of Fukui*)
- [2-13-1648](#) G146V 変異アクチンのサプレッサー変異はクレフト周辺に位置する
Intragenic suppressor mutations of G146V mutant actin are located around the nucleotide binding cleft
○湯本 天嗣¹, 横尾 岳彦², 上田 太郎¹ (¹早稲田大学 理工学術院 先進理工学研究科 物理専攻, ²産業技術総合研究所 生物プロセス研究部門)
Tenji Yumoto¹, Takehiko Yoko-o², Taro Q.P. Uyeda¹ (¹*Dept. physics, School of Advanced Science and Engineering, Waseda Univ.*, ²*Inst. AIST, Bioprod. Res.*)
- [2-13-1700](#) 転写因子の動的な集合体形成はエンハンサーの長距離間相互作用を媒介する
Dynamic clustering of transcription factors mediates long-range regulatory communication in *Drosophila* embryos
○川崎 洗司, 深谷 雄志 (東京大・定量生命科学研究所・遺伝子発現ダイナミクス研究分野)
Koji Kawasaki, Takashi Fukaya (*Inst. for Quantitative Biosciences, Research Center for Biological Visualization, Univ. of Tokyo*,)
- [2-13-1712](#) 中立的な競争とニッチを伴う幹細胞のクローン増殖に関する生物物理学的モデル
Biophysical model for clonal expansion of stem cells with neutral competition and niches
○中牟田 旭^{1,2}, 吉戸 香奈^{2,4}, 本田 直樹^{2,3,4} (¹理学部, 京都大学, 日本, ²生命科学研究所, 京都大学, 日本, ³自然科学研究機構生命創成研究センター, 日本, ⁴統合生命科学研究科, 広島大学, 日本)
Asahi Nakamuta^{1,2}, Kana Yoshido^{2,4}, Naoki Honda^{2,3,4} (¹*Graduate School of Biostudies, Kyoto University, Japan*, ²*Graduate School of Biostudies, Kyoto University, Japan*, ³*Exploratory Research Center on Life and Living Systems (ExCELLS), National Institutes of Natural Sciences, Japan*, ⁴*Graduate School of Integrated Science for Life, Hiroshima University, Japan*)
- [2-13-1724](#) 自己組織化過程における細胞の挙動解析
A dynamic self-organization of single cells
○渡辺 隆太, 堀川 凜一, 城所 龍, 野崎 庄太, 守山 裕大, 三井 敏之 (青学大・院理工学)
Ryuta Watanabe, Riichi Horikawa, Ryu Kidokoro, Shota Nozaki, Yuuta Moriyama, Toshiyuki Mitsui (*Dept. Phys., Aoyama Gakuin Univ.*)
- [2-13-1736](#) ヒト胚発生を模倣するための単純化された反応拡散 in vitro モデル実験系
Simplified reaction-diffusion in vitro model to mimic human embryonic development
○大沼 清 (長岡技術科大・生物機能工学)
Kiyoshi Ohnuma (*Bioeng., Nagaoka Univ Tech*)

- [2-13-1748](#) 分子動力学法による MED26 の天然変性蛋白質認識メカニズムの検討
Molecular dynamics study on multiple binding modes of MED26 to recognize intrinsically disordered proteins
○後藤 聡志¹, 笠原 浩太², 高橋 秀尚³, 肥後 順一⁴, 高橋 卓也² (¹立命館大・院・生命,²立命館大・生命,³横浜市大・院・医,⁴立命館大・総研機構)
Satoshi Goto¹, Kota Kasahara², Hidechisa Takahashi³, Junichi Higo⁴, Takuya Takahashi² (¹*Grad. Sci. Life Sci., Ritsumeikan Univ.*, ²*Coll. Life. Sci., Ritsumeikan Univ.*, ³*Grad. Sch. Med., Yokohama City Univ.*, ⁴*Res. Org. Sci. Tech., Ritsumeikan Univ.*)

13:15~15:15 Ch14

2G14A 数理生物学・非平衡・生体リズムII

Mathematical biology, Nonequilibrium state & Biological rhythm II

座長：安田 賢二 (早稲田大学), 野口 博司 (東京大学)

Session Chairs: Kenji Yasuda (Waseda Univ.), Hiroshi Noguchi (The Univ. of Tokyo)

- [2-14-1315*](#) ヒト iPSC 細胞由来ニューロンの神経突起伸長過程における駆動力のゆらぎ解析
Fluctuation analysis of driving forces for development processes of neurites of human iPSC-derived neurons
○前田 成海¹, 柴崎 雄介¹, 白川 由佳², 斎藤 稔^{1,2} (¹日大院・総合基礎科学,²日大・文理・自然研)
Narumi Maeda¹, Yusuke Shibasaki¹, Yuka Shirakawa², Minoru Saito^{1,2} (¹*Grad. Sch. of Integ. Bas. Sci., Nihon Univ.*, ²*Nat. Inst., Nihon Univ.*)
- [2-14-1327*](#) 画像データから上皮細胞の力学パラメータを推定する手法の開発
Image-based parameter estimation for epithelial mechanics
○荻田 豪士^{1,2}, 近藤 武史¹, 井川 敬介^{2,3}, 上村 匡¹, 石原 秀至^{4,5}, 杉村 薫^{2,3,5} (¹京大・生命,²東大・理・生物,³京大・物質-細胞統合システム拠点,⁴東大・総合文化,⁵東大・生物普遍性研究機構)
Goshi Ogita^{1,2}, Takefumi Kondo¹, Keisuke Ikawa^{2,3}, Tadashi Uemura¹, Shuji Ishihara^{4,5}, Kaoru Sugimura^{2,3,5} (¹*Grad. Sch. Bio., Kyoto Univ.*, ²*Grad. Sch. Sci., Univ. Tokyo.*, ³*CeMS, Kyoto Univ.*, ⁴*Grad. Sch. Arts and Sci., Univ. Tokyo.*, ⁵*UBI, Univ. Tokyo.*)
- [2-14-1339*](#) 細胞区画内のセルフリー遺伝子発現における液液相分離現象とぬれ効果
Liquid-liquid phase separation and wetting in compartmentalized cell-free expression reactions
○加藤 修三¹, Garenne David², Noireaux Vincent², 前多 裕介¹ (¹九大・理,²ミネソタ大・物理)
Shuzo Kato¹, David Garenne², Vincent Noireaux², Yusuke Maeda¹ (¹*Dept. Phys., Kyushu Univ.*, ²*Sch. Phys. Astro., Univ. of Minnesota*)
- [2-14-1351*](#) プロトセル空間における反応拡散波の示す時空間パターンの頑健性と可塑性
Robustness and plasticity of spatiotemporal patterning by a reaction-diffusion wave entrapped in protocells
○高田 咲良¹, 義永 那津人^{2,3}, 土居 信英¹, 藤原 慶¹ (¹慶應大・理工,²東北大・AIMR,³産総研・MathAM-OIL)
Sakura Takada¹, Natsuhiko Yoshinaga^{2,3}, Nobuhide Doi¹, Kei Fujiwara¹ (¹*Dept. Biosci. Info., Keio Univ.*, ²*AIMR, Tohoku Univ.*, ³*MathAM-OIL, AIST*)

- [2-14-1403*](#) ミトコンドリア呼吸鎖の活性と熱発生メカニズム解析
Mechanistic analysis of mitochondrial respiratory activity and heat generation
○鯨岡 郁雄¹, 向柴 巧¹, Namari Nuning¹, 武安 光太郎^{2,3}, 中村 潤児^{2,3} (¹筑波大学理工情報生命学術院数理物質科学研究群国際マテリアルズイノベーション学位プログラム, ²筑波大学数理物質系, ³筑波大学エネルギー物質科学研究センター)
Ikuo Kujiraoka¹, Taku Mukoshiba¹, Nuning Namari¹, Kotaro Takeyasu^{2,3}, Junji Nakamura^{2,3}
(¹Graduate school of science and technology, Univ. Tsukuba, ²Faculty of pure and applied sciences, Univ. Tsukuba, ³Tsukuba research center for energy materials science, Univ. Tsukuba)
- [2-14-1415](#) インシュリンシグナルは線虫のスケールフリー行動を制御する
Scale-free behaviors of *C. elegans* is shaped by insulin signaling
○Arata Yukinobu¹, 志賀 樹², 池田 優作³, 木村 啓志³, ユリツァ ペテル¹, 清野 健², 佐甲 靖志¹
(¹理研・開拓・佐甲細胞, ²阪大・院基礎工, ³東海大・工)
Yukinobu Arata¹, Itsuki Shiga², Yusaku Ikeda³, Hiroshi Kimura³, Peter Jurica¹, Ken Kiyono², Yasushi Sako¹ (¹CPR, Cell. Info., RIKEN, ²Grad. Sch. Eng. Sci., Osaka Univ., ³Sch. Eng., Tokai Univ.)
- [2-14-1427](#) 2種細胞群間の境界パターン形成の動態モデル構築と定量解析
Physical model construction and quantitative analysis of boundary pattern formation between binary cell groups
○森 功佑, 安井 優平, 粟津 暁紀, 藤井 雅史 (広島大・統合生命科学研究科)
Kosuke Mori, Yuhei Yasui, Akinori Awazu, Masashi Fuji (Department of Mathematical and Life Sciences, Graduate School of Integrated Sciences for Life, Hiroshima University)
- [2-14-1439](#) 特異点をもつ2次元領域における細胞配向とトポロジカル欠陥
Cell Alignment and Topological Defects in Two-Dimensional Geometries with Corner Singularities
○宮廻 裕樹¹, 佐藤 弘之², 奈良 高明^{1,2} (¹東大・院情報理工, ²東大・工学部)
Hiroki Miyazaki¹, Hiroyuki Sato², Takaaki Nara^{1,2} (¹Grad. Sch. IST, Univ. Tokyo, ²Sch. Eng., Univ. Tokyo)
- [2-14-1451](#) Representation and inference of cell growth and division by neural-network-aided point processes
Atsushi Kamimura, Tetsuya J. Kobayashi (Institute of Industrial Science, The University of Tokyo)
- [2-14-1503](#) 波打つ場が誘起する上皮細胞の集団運動と秩序形成
Collective motion of active epithelial cells induced by wave-like hydrogel folds
○前多 裕介¹, 繁田 和幸¹, 福山 達也¹, 高橋 陸², 田中 あや² (¹九大・物理, ²NTT 物性基礎研, 分子生体機能)
Yusuke Maeda¹, Kazuyuki Shigeta¹, Tatsuya Fukuyama¹, Riku Takahashi², Aya Tanaka² (¹Kyushu Univ., Dept. Phys., ²NTT, BRL/BMC)

16:00~17:48 Ch14

2G14B 数理生物学・非平衡・生体リズム III

Mathematical biology, Nonequilibrium state & Biological rhythm III

座長：笹井 理生 (名古屋大学), 望月 敦史 (京都大学)

Session Chairs: Masaki Sasai (Nagoya Univ.), Atsushi Mochizuki (Kyoto Univ.)

- [2-14-1600](#) 遺伝子発現制御ネットワークモデルのダイナミクス定量解析
Quantitative analysis of gene regulatory network dynamics
○井上 雅世¹, 金子 邦彦² (¹明治大・総合数理, ²東大・総合文化)
Masayo Inoue¹, Kunihiko Kaneko² (¹IMS, Meiji Univ., ²Univ. of Tokyo)
- [2-14-1612](#) Boolean modeling and state analysis of gene regulatory networks
Yoshiaki Horiike, Shin Fujishiro, Masaki Sasai (Dept. Appl. Phys., Nagoya Univ.)

- [2-14-1624](#) Effects of epigenetic modifications on the intermediate states of epithelial-mesenchymal transitions
Kenichi Hagiwara, Masaki Sasai (*Dept of Appl. Phys., Nagoya Univ*)
- [2-14-1636](#) 出芽酵母のDNA二本鎖切断時における染色体動態の数値モデル
 Mathematical model of chromosomal dynamics in budding yeast during DNA double strand break
 ○中畑 伸児郎, 藤井 雅史, 粟津 暁紀 (広島大学大学院 統合生命科学研究科)
Shinjiro Nakahata, Masashi Fujii, Akinori Awazu (*Graduate School of Integrated Sciences for Life, Hiroshima University*)
- [2-14-1648](#) ES細胞のクロマチンドメイン変化による染色体動態制御のモデル
 A model for regulation of chromosome dynamics in mouse ES cells by chromatin domain changes
 ○小本 哲史, 藤井 雅史, 粟津 暁紀 (広島大・院統合生命科学)
Tetsushi Komoto, Masashi Fujii, Akinori Awazu (*Grad. Sch. Integrated Sciences for Life, Univ. Hiroshima*)
- [2-14-1700](#) Lifetime analysis of nucleotides bound to KaiC
Damien Stephane Simon^{1,2}, Atsushi Mukaiyama^{1,2}, Yoshihiko Furuike^{1,2}, Shuuji Akiyama^{1,2} (*Institute for Molecular Science, ²SOKENDAI*)
- [2-14-1712](#) 代謝漏出による微生物の共存共栄戦略
 The advantage of leakage of essential metabolites and resultant symbiosis of diverse microbes
 ○山岸 純平¹, 斉藤 稔^{2,3}, 金子 邦彦^{1,3} (¹東京大・院総合文化, ²自然研・生命創成探究, ³東京大・生物普遍性)
Jumpei Yamagishi¹, Nen Saito^{2,3}, Kunihiro Kaneko^{1,3} (*Grad. Sch. of Arts and Sci., Univ. Tokyo, ²ExCELLS, NINS, ³UBI, Univ. Tokyo*)
- [2-14-1724](#) がん進行にともなう代謝変化のネットワーク構造に基づく解析
 Network structure-based analysis of metabolic changes associated with cancer progression
 ○菱田 温規^{1,2}, 服部 鮎奈¹, 伊藤 貴浩¹, 望月 敦史¹ (¹京都大学ウイルス・再生医科学研究所, ²京都大学大学院理学研究科)
Atsuki Hishida^{1,2}, Ayuna Hattori¹, Takahiro Ito¹, Atsushi Mochizuki¹ (*Institute for Frontier Life and Medical Sciences, Kyoto University, ²Graduate School of Science, Kyoto University*)
- [2-14-1736](#) ステージ特異的な細胞周期調節機構の、ネットワーク構造に基づく解明
 Independent regulation of the G₁-S and G₂-M transition realized by topology of the cell cycle network
 ○山内 悠平, 望月 敦史 (京都大学ウイルス再生医科学研究所 数理生物学分野)
Yuhei Yamauchi, Atsushi Mochizuki (*Department of Mathematical Biology, Kyoto University*)

13:15~15:39 Ch15
 2G15A 計測II
 Measurements II

座長：小松崎 民樹 (北海道大学), 酒井 誠 (岡山理科大学)
 Session Chairs: Tamiki Komatsuzaki (Hokkaido Univ.), Makoto Sakai (Okayama Univ. of Sci.)

- [2-15-1315*](#) 全神経活動リアルタイム計測のための全自動全神経細胞捕捉システムの開発
 Development of a whole neural network tracking system for real-time high-resolution light-field imaging in freely behaving *C. elegans*
 ○前岡 遥花, 執行 航希, 杉 拓磨 (広島大学)
Haruka Maoka, Kazuki Shigyou, Takuma Sugi (*Univ. Hiroshima*)

- [2-15-1327*](#) 繊毛虫 *Tetrahymena* における螺旋遊泳行動の三次元観察
Direct three-dimensional observation of helical swimming behavior of the ciliate *Tetrahymena*.
○丸茂 哲聖, 山岸 雅彦, 矢島 潤一郎 (東大・総合文化)
Akisato Marumo, Masahiko Yamagishi, Junichiro Yajima (*Grad. Arts & Sci., Univ. Tokyo*)
- [2-15-1339*](#) Structure-based analysis and evolution of a monomerized red-color chromoprotein from jellyfish *Olindias formosa* for bioimaging
Le Zhai (*Graduate School of Frontier Bioscience, Osaka University*)
- [2-15-1351*](#) 酸化ストレス下の単一生細胞における液-液相分離のラマンイメージング測定
Raman imaging of liquid-liquid phase separation in a living single cell under oxidative stress
○澁谷 蓮¹, 梶本 真司^{1,2}, 中林 孝和¹ (¹ 東北大・薬, ²JST さきがけ)
Ren Shibuya¹, Shinji Kajimoto^{1,2}, Takakazu Nakabayashi¹ (¹*Fac. Pharm. Sci., Univ. Tohoku*, ²*JST PRESTO*.)
- [2-15-1403*](#) ラマンおよび自家蛍光顕微鏡による生細胞内の薬剤ナノ粒子の代謝過程の観測
Observation of metabolism of drug nanoparticles in living cells using Raman and autofluorescence microscopy
○町田 雅斗¹, 杉村 俊紀², Farsai Taemaitree³, 小関 良卓³, 笠井 均³, 梶本 真司^{1,2,4}, 中林 孝和^{1,2} (¹ 東北大学大学院薬学部, ² 東北大学院薬学研究科, ³ 東北大多元物質科学研究所, ⁴JST さきがけ)
Masato Machida¹, Toshiki Sugimura², Taemaitree Farsai³, Yoshitaka Koseki³, Hitoshi Kasai³, Shinji Kajimoto^{1,2,4}, Takakazu Nakabayashi^{1,2} (¹*Faculty of Pharmaceutical Sciences, Tohoku University*, ²*Graduate School of Pharmaceutical Sciences, Tohoku University*, ³*Institute of Multidisciplinary Research for Advanced Materials, Tohoku University*, ⁴*JST PRESTO*)
- [2-15-1415*](#) ラマンイメージングと Deep Learning の融合によるラベルフリー細胞内解析手法の開発
Development of label-free intracellular analysis methods by integrating Raman imaging and deep learning
○高橋 大智¹, 梶本 真司^{1,2}, 中林 孝和¹ (¹ 東北大・院薬, ²JST さきがけ)
Hiroaki Takahashi¹, Shinji Kajimoto^{1,2}, Takakazu Nakabayashi¹ (¹*Grad. Sch. Pharm. Sci., Tohoku Univ.*, ²*JST PRESTO*)
- [2-15-1427*](#) 構造化照明超解像ラマン顕微鏡の構築と生細胞への応用
Construction of a structured illumination super-resolution Raman microscope and application to a living cell
○阿部 陽¹, 梶本 真司^{1,2}, 中林 孝和¹ (¹ 東北大・院薬, ²JST さきがけ)
Akira Abe¹, Shinji Kajimoto^{1,2}, Takakazu Nakabayashi¹ (¹*Grad. Sch. Pharm. Sci., Univ. Tohoku*, ²*JST PRESTO*)
- [2-15-1439*](#) 情報理論を取り入れた手法によるラマン分光イメージ中での化学的空間不均一性の解析
Analysis of chemical heterogeneity in Raman spectral image with information theory
○近藤 僚哉¹, N.Taylor James², Clement Jean-Emmanuel², 水野 雄太^{1,2,3}, 藤田 克昌⁴, 原田 義規⁵, 小松崎 民樹^{1,2,3} (¹ 北大・院総合化学, ² 北大・電子科学研, ³ 北大・WPI-ICReDD, ⁴ 大阪大・院工学研究科, ⁵ 京都府立医大)
Ryoya Kondo¹, James N.Taylor², Jean-Emmanuel Clement², Yuta Mizuno^{1,2,3}, Katsumasa Fujita⁴, Yoshinori Harada⁵, Tamiki Komatsuzaki^{1,2,3} (¹*Grad. Sch. Sci. & Tec., Hokkaido Univ.*, ²*Res. Inst. electron Sci., Hokkaido Univ.*, ³*WPI-ICReDD, Hokkaido Univ.*, ⁴*Grad. Sch. Tec., Osaka Univ.*, ⁵*Kyoto Pre. Univ. Med.*)
- [2-15-1451](#) A sample preparation method using the resin-embedding for digital holographic microscopy
Yuki Ide¹, Yuji Matsukawa¹, Shigeki Mayama², Kazuo Umemura¹ (¹*Tokyo Univ. Sci.*, ²*Tokyo Gakugei Univ.*)

[2-15-1503](#) 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内ケラチタンパク質の選択的観察

Selective IR super-resolution imaging of keratin proteins in biological samples by micro-spectroscopy based on non-linear optical process

○高橋 広奈, 伊田 哲也, 片山 康平, 酒井 誠 (岡山理大・理)

Hirona Takahashi, Tetsuya Ida, Kohei Katayama, Makoto Sakai (*Grad. Sch. Sci., Okayama Univ. of Sci.*)

[2-15-1515](#) 相関顕微鏡法 (CLEM) による同一試料観察に向けた相関・位置合わせ精度の改善

Improvement of correlation and alignment accuracy toward the same sample observation by CLEM

○五味 潤 由貴¹, 江副 里紗², 高崎 寛子^{1,3}, 本多 康久¹, 山本 八生起¹, 森本 雄祐¹, 安永 卓生¹ (¹ 九工大・情報工学・物理情報, ² 九工大・情報工学・生命情報, ³ 大阪大学・蛋白質)

Yuki Gomibuchi¹, Risa Ezoe², Hiroko Takazaki^{1,3}, Yasuhisa Honda¹, Yaoki Yamamoto¹, Yusuke V. Morimoto¹, Takuo Yasunaga¹ (¹*Dept. of Phys. Info. Tech., Kyushu Inst. Tech.*, ²*Dept. of Biosci. Bioinfo., Kyushu Inst. Tech.*, ³*IPR. Osaka Univ.*)

[2-15-1527](#) 診療録からの症状半自動抽出システムの開発

Development of semi-automatic phenotype extraction system from medical records

○地引 芳乃¹, 土肥 栄祐², 仁宮 洸太^{3,4}, 藤原 豊史⁵, 佐々木 貴規¹ (¹ 明治大・院・先端数理, ² 新潟大・脳研究所・生命科学リソース研究センター・脳病態解析分野, ³ 国立保健医療科学院, ⁴ 東京大・院・薬, ⁵ ライフサイエンス統合データベースセンター)

Yoshino Jibiki¹, Eisuke Dohi², Kota Ninomiya^{3,4}, Toyofumi Fujiwara⁵, Takanori Sasaki¹ (¹*Fac. Adv. Math. Sci., Meiji Univ.*, ²*Dept. Neuroscience Disease, Brain Research Inst., Niigata Univ.*, ³*Natl. Inst. Public Health.*, ⁴*Grad. Sch. Pharm. Sci., The Univ. of Tokyo.*, ⁵*DBCLS*)

16:00~18:36 Ch15

2G15B 計測 IV

Measurements IV

座長：前島 一博 (国立遺伝学研究所), 徳永 万喜洋 (東京農工大学)

Session Chairs: Kazuhiro Maeshima (NIG), Makio Tokunaga (Tokyo Univ. of Agric. and Tech.)

[2-15-1600](#) グラフェン電界効果トランジスタ表面におけるノイラミニダーゼ反応の電氣的バイオセンシング
Electrical Biosensing for Neuraminidase Reaction at the Surface of Graphene Field-Effect Transistors

○小野 亮生^{1,2}, 鎌田 果歩¹, 林 亮太¹, Piacenti Alba Rosa³, Gabbutt Calum³, 宮川 成人⁴, 山本 佳織¹, Sriwilajaroen Nongluk⁵, 平松 宏明⁶, 金井 康¹, 小山 知弘^{1,7}, 井上 恒一¹, 牛場 翔太⁴, 品川 歩⁴, 木村 雅彦⁴, 中北 愼一⁸, 河原 敏男⁶, 家 裕隆¹, 渡邊 洋平⁹, 鈴木 康夫⁶, 千葉 大地^{1,7}, Contera Sonia³, 松本 和彦¹ (¹ 阪大・産研, ² JST・さきがけ, ³ オックスフォード大・物理学, ⁴ (株) 村田製作所, ⁵ タマサート大・医学, ⁶ 中部大・生命健康科学, ⁷ 阪大・CSR, ⁸ 香川大・総合生命セ, ⁹ 京府医大・院医学)

Takao Ono^{1,2}, Kaho Kamada¹, Ryota Hayashi¹, Alba Rosa Piacenti³, Calum Gabbutt³, Naruto Miyakawa⁴, Kaori Yamamoto¹, Nongluk Sriwilajaroen⁵, Hiroaki Hiramatsu⁶, Yasushi Kanai¹, Tomohiro Koyama^{1,7}, Koichi Inoue¹, Shota Ushiba⁴, Ayumi Shinagawa⁴, Masahiko Kimura⁴, Shin-ich Nakakita⁸, Toshio Kawahara⁶, Yutaka Ie¹, Yohei Watanabe⁹, Yasuo Suzuki⁶, Daichi Chiba^{1,7}, Sonia Contera³, Kazuhiko Matsumoto¹ (¹*SANKEN, Osaka Univ.*, ²*JST-PRESTO*, ³*Dept. Phys., Univ. Oxford*, ⁴*Murata Mfg.*, ⁵*Fac. Med., Thammasat Univ.*, ⁶*Col. LHS, Chubu Univ.*, ⁷*CSR, Osaka Univ.*, ⁸*LSRC, Kagawa Univ.*, ⁹*Grad. Sch. Med. Sci., KPUM*)

- [2-15-1612](#) Diffusion of LLPS Droplets Consisting of Poly(PR) Dipeptide Repeats and RNA on Chemically Modified Glass Surface
Chen Chen¹, Kohsuke Kanekura², Yuhei Hayamizu³ (¹*Tokyo Tech., Earth-Life Science Institute*, ²*Tokyo Medical University, Department of Molecular Pathology*, ³*Tokyo Tech., School of Materials and Chemical Technology*)
- [2-15-1624](#) 多次元 *in vitro* 酵素スクリーニング法の開発
 Development of multidimensional *in vitro* enzyme screening system
 ○本田 信吾¹, 皆川 慶嘉², 野地 博行^{1,2}, 田端 和仁² (¹東大・院工バイオ,²東大・院工応化)
Shingo Honda¹, Yoshihiro Minagawa², Hiroyuki Noji^{1,2}, Kazuhito Tabata² (¹*Dept. Bioeng., Grad. Sch. Eng., Univ. Tokyo*, ²*Dept. Appl. Chem., Grad. Sch. Eng., Univ. Tokyo*)
- [2-15-1636](#) リコンビナント LOX-1 受容体に結合する LDL の特性
 Physical properties of low-density lipoproteins recognized by recombinant LOX-1 receptor
 ○武田 晴治¹, 後潟 夏菜子², 濱向 青緒¹, スバキョ アグス³, 高須賀 太一² (¹北科大・薬,²北大・食資源,³北大・情報科学)
Seiji Takeda¹, Kanajo Ushirogata², Ao Hamamuki¹, Agus Subagyo³, Taichi Takasuka² (¹*Dept. Pharm., Hokkaido Univ. of Sci.*, ²*Grad. Sch. GFR., Hokkaido University*, ³*Grad. Sch. Info. Sci. Tech., Hokkaido University*)
- [2-15-1648](#) インターカレーターは生きた細胞内のクロマチンの動きを抑制する
 Intercalator suppresses chromatin motion in living human cells
 ○伊藤 優志, 大塚 碧, 前島 一博 (遺伝研)
Yuji Itoh, Aoi Otsuka, Kazuhiro Maeshima (*NIG*)
- [2-15-1700](#) Localized in vivo Mechanical Characterisation of Normal and Abnormal Cell Nuclei by Atomic Force Microscopy
Sivashanmugan Kundan¹, Takehiko Ichikawa¹, Eishu Hirata^{1,2}, Mohammad Shahidul Alam¹, Mohammad Mubarak Hosain¹, Tetsuya Shirokawa¹, Keisuke Miyazawa^{1,3}, Kazuki Miyata^{1,3}, Takeshi Fukuma^{1,3} (¹*WPI Nano Life Science Institute (WPI-NanoLSI), Kanazawa University, Kakuma-Machi, Kanazawa, 920-1192, Japan*, ²*Division of Tumor Cell Biology and Bioimaging, Cancer Research Institute of Kanazawa University, Kakuma-Machi, Kanazawa, 920-1192, Japan*, ³*Division of Electrical Engineering and Computer Science, Kanazawa University, Kakuma-Machi, Kanazawa, 920-1192, Japan*)
- [2-15-1712](#) Development of a method for quantitative profiling of microRNAs in single exosomes
Cinya Chung¹, Ryo Iizuka², Takashi Funatsu¹ (¹*Grad. Sch. Pharm. Sci., Univ. Tokyo*, ²*Dept. Biol. Sci., Grad. Sch. Sci., Univ. Tokyo*)
- [2-15-1724](#) 1 分子超解像イメージングを用いた RNA ポリメラーゼ II とクロマチンのナノスケール相互作用解析
 Single-molecule super-resolution analysis for nano-scale interaction between RNA polymerase II and chromatin
 ○伊藤 由馬, 徳永 万喜洋 (東工大・生命理工学院)
Yuma Ito, Makio Tokunaga (*Sch. Life Sci. Tech., Tokyo Tech.*)
- [2-15-1736](#) (3S6-2) 微小電気穿孔法を用いた細胞膜の機械特性と遺伝子発現の統合解析
 (3S6-2) A combined analysis of membrane-mechanical phenotyping and transcriptomics using nanoelectroporation
 ○塩見 晃史, 金子 泰洗ボール, 西川 香里, 新宅 博文 (理研・開拓・白眉)
Akifumi Shiomi, Taikopaul Kaneko, Kaori Nishikawa, Hirofumi Shintaku (*Hakubi, CPR, RIKEN*)
- [2-15-1748](#) 1 分子超解像イメージングによる細胞周期がもたらすヘテロクロマチンの構造変化
 Structural changes in heterochromatin involved in cell cycle using single-molecule and super-resolution imaging
 ○中野 真徳, 伊藤 由馬, 徳永 万喜洋 (東工大・生命理工学院)
Masanori Nakano, Yuma Ito, Makio Tokunaga (*Sch. Life Sci. Tech., Tokyo Inst. Tech.*)
- [2-15-1800](#) Genetically encodable tool for live-imaging and manipulation of endogenous RNAs in living cells
Akira Takai¹, Yasushi Okada^{1,2} (¹*BDR, RIKEN*, ²*Dept. Phys., Grad. Sch. Sci., Univ. Tokyo*)

- [2-15-1812](#) 異なる翻訳後修飾を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 with different epigenetic modifications
○廣瀬 仁教, 伊藤 由馬, 徳永 万喜洋 (東工大・生命理工学院)
Masanori Hirose, Yuma Ito, Makio Tokunaga (*Sch. Life Sci. Tech., Tokyo Tech*)
- [2-15-1824](#) 核小体タンパク質の生細胞1分子イメージングを用いたRNAに依存した相分離動態の定量解析
Single-molecule imaging analysis of RNA-dependent dynamics of phase-separated nucleolar proteins in living cells
伊藤 由馬, Sirisukhodom Supanut, ○徳永 万喜洋 (東工大・生命理工学院)
Yuma Ito, Supanut Sirisukhodom, Makio Tokunaga (*Sch. Life Sci. Tech., Tokyo Tech*)

13:15~15:39 Ch16
2G16A 計測 III
Measurements III

座長：古寺 哲幸 (金沢大学), 内橋 貴之 (名古屋大学)

Session Chairs: Noriyuki Kodera (Kanazawa Univ.), Takayuki Uchihashi (Nagoya Univ.)

- [2-16-1315*](#) Development of a genetically encoded fluorescent indicator for molecular crowding with large dynamic range and high sensitivity
Shinya Sakai (*Graduate School of Frontier Bioscience, Osaka University*)
- [2-16-1327*](#) ヨーロッパモノアラガイの咀嚼調節ニューロンのカルシウムイメージングー味覚嫌悪学習前後のカルシウムシグナルの比較ー
Fluorescence calcium imaging for the feeding modulatory neuron of the pond snail
○伊藤 綾香¹, 小松崎 良将², 斎藤 稔¹ (¹ 日本大学・院・総合基, ² 日大・理工)
Ayaka Itoh¹, Yoshimasa Komatsuzaki², Monoru Saito¹ (¹ *Grad. Sch. of Integ. Bas. Sci., Nihon Univ.*, ² *Coll. Sci. Tech., Nihon Univ.*)
- [2-16-1339*](#) 細胞内温度イメージングを用いた神経分化機構の解明
Elucidation of Neural Differentiation Using Intracellular Temperature Imaging
○中馬 俊祐^{1,2}, 岡部 弘基^{3,4}, 原田 慶恵^{2,5} (¹ 阪大院・理・生物, ² 阪大・蛋白研, ³ 東大院・薬, ⁴ JST さきがけ, ⁵ 阪大・IQB)
Shunsuke Chuma^{1,2}, 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 *IQB Osaka Univ.*)
- [2-16-1351*](#) 高速 AFM によるヒストン H2A-DNA 相互作用およびその凝集性のリアルタイムダイナミクスの解明
Investigation of real-time dynamic histone H2A-DNA interaction and H2A-DNA condensation/de-condensation using high-speed AFM
○西出 梧朗¹, Lim Keesiang², 小林 亜紀子^{2,3}, 羽澤 勝治^{2,3}, 中山 隆宏², 古寺 哲幸², 安藤 敏夫², Wong Richard^{2,3} (¹ 金沢大学大学院新学術創成研究科ナノ生命科学専攻博士前期課程, ナノ精密医学・理工学卓越大学院プログラム, ² 金沢大学ナノ生命科学研究所, ³ 金沢大学新学術創成研究機構)
Goro Nishide¹, Keesiang Lim², Akiko Kobayashi^{2,3}, Masaharu Hazawa^{2,3}, Takahiro Nakayama², Noriyuki Kodera², Toshio Ando², Richard Wong^{2,3} (¹ *Division of Nano Life Science in the Graduate School of Frontier Science Initiative, WISE Program for Nano-Precision Medicine, Science, and Technology Kanazawa University*, ² *WPI-Nano Life Science Institute, Kanazawa University*, ³ *Cell-Bionomics Research Unit, Institute for Frontier Science Initiative, Kanazawa University*)

- [2-16-1403*](#) Development of the nanoendoscopy AFM technique for visualizing inter-cellular structures in living cells
Mohammad Shahidul Alam¹, Marcos Penedo^{2,5}, Tetsuya Shirokawa³, Mohammad Mubarak Hosain¹, Takahiko Ichikawa², Keisuke Miyazawa^{2,3}, Kazuki Miyata^{1,2,3}, Chikashi Nakamura⁴, Takeshi Fukuma^{1,2,3}
¹Graduate school of frontier science initiative, Division of Nano Life Science, Kanazawa University, ²Nano Life Science Institute (WPI-NanoLSI), Kanazawa University., ³Graduate school of natural Science and technology, Division of Electrical Engineering and Computer Science, Kanazawa University., ⁴National Institute of Advanced Industrial Science and Technology (AIST), ⁵Laboratory for Bio- and Nano-Instrumentation, Swiss Federal Institute of Technology Lausanne (EPFL), Lausanne, Switzerland.)
- [2-16-1415*](#) レーザー照射による固液界面でのリポソームの捕捉と破壊
 Capture and rupture of liposomes at the solid-liquid interface by laser irradiation
 ○内田 匠 (東大院・理学系研究科)
Takumi Uchida (*Grad. Sch. Sci., The Univ. of Tokyo*)
- [2-16-1427*](#) パッチクランプ機能付き高速 AFM の開発
 Development of Patch-Clamp High-speed Atomic Force Microscopy
 ○松原 猛¹, 渡辺 信嗣², 梅田 健一², 角野 歩², 安藤 敏夫², 古寺 哲幸² (¹金沢大・院ナノ生命, ²金沢大・WPI-NanoLSI)
- Takeru Matsubara**¹, Shinji Watanabe², Kenichi Umeda², Ayumi Sumino², Toshio Ando², Noriyuki Kodera² (¹Grad. Sch. NanoLS., Kanazawa Univ., ²WPI-NanoLSI, Kanazawa Univ.)
- [2-16-1439*](#) CALHM2 をナノポアとして用いた多様なサイズの分子検出法の開発
 Development of a variety size of molecule detection method using CALHM2 as a nanopore
 ○中村 宗太郎, 山崎 洋人, 志甫 谷 涉, 濡木 理, 上村 想太郎 (東京大学・大学院理学系研究科生物学専攻)
Sotaro Nakamura, Hirohito Yamazaki, Wataru Shihoya, Osamu Nureki, Sotaro Uemura (*Department of Biological Sciences, The University of Tokyo*)
- [2-16-1451](#) 曲率の大きいエッジを持つナノポアと DNA の相互作用
 Pathways for DNA into sharp-edged nanopores
 ○高野 辰, 吉川 匠, 松木 翔, 市野 新葉, 守山 裕大, 三井 敏之 (青学大・理工)
Shin Takano, Takumi Yoshikawa, Sho Matsuki, Shimba Ichino, Yuuta Moriyama, Toshiyuki Mitsui (*Dept. of Phys. Aoyama Gakuin Univ.*)
- [2-16-1503](#) 力学ストレス印加下におけるタンパク質の動態イメージングのための高速 AFM 用基板伸縮システムの開発
 Development of Substrate Stretching System for High-Speed AFM for Dynamic Imaging of Proteins under Mechanical Stress
 ○詹 豊嶽, 黒崎 涼, 内橋 貴之 (名古屋大・院理学)
Fengyueh Chan, Ryo Kurosaki, Takayuki Uchihashi (*Grad. Sch. Sci., Nagoya Univ.*)
- [2-16-1515](#) Photothermally enhanced single molecule nanopore sensing
Hirohito Yamazaki, Sotaro Uemura (*Department of Biological Sciences*)
- [2-16-1527](#) Hidden Markov Modeling of Biomolecular Conformational Dynamics from Atomic Force Microscopy Time-Series Images
Tomonori Ogane, Yasuhiro Matsunaga (*Grad. Sch. of Eng. Sci., Saitama Univ.*)

座長：岡 浩太郎（慶應義塾大学），小嶋 寛明（情報通信研究機構）
Session Chairs: Kotaro Oka (Keio Univ.), Hiroaki Kojima (NICT)

- [2-16-1600](#) 自動化1分子イメージングシステムによる受容体動態の大規模解析
Large-scale analysis of receptor behaviors with automated single-molecule imaging system
○廣島 通夫^{1,2}, 渡邊 大介³, 上田 昌宏³ (¹ 理研 BDR, ² 理研 CPR, ³ 阪大・生命機能)
Michio Hiroshima^{1,2}, Daisuke Watanabe³, Masahiro Ueda³ (¹RIKEN BDR, ²RIKEN CPR, ³FBS Osaka Univ.)
- [2-16-1612](#) 超解像顕微鏡の分解能を向上する事後処理の計算補償光学顕微鏡法
Post-processing, computational adaptive optics for 3D super-resolution microscopy
○松田 厚志（情報通信研究機構未来 ICT 研究所）
Atsushi Matsuda (*Advanced ICT Research Institute, National Institute of Information and Communications Technology*)
- [2-16-1624](#) 細菌が形成する動くバイオフィルムの ASEM と cryo-TEM による観察
Mobile biofilm formed by bacteria was observed using ASEM and cryo-TEM
○佐藤 主税¹, 納谷 昌実¹, 笠畑 尚喜¹, 佐藤 真理¹, 佐藤 啓子² (¹産総研・健康医工学, ²長崎大・医歯薬学)
Chikara Sato¹, Masami Naya¹, Naoki Kasahata¹, Mari Sato¹, Keiko Sato² (¹Health Medical Res. Inst., AIST, ²Graduate School Biomedical Sciences, Univ. Nagasaki)
- [2-16-1636](#) 蛍光イメージング法によるケラチノサイト細胞内 Mg²⁺ 動態の可視化
Visualization of intracellular Mg²⁺ dynamics in keratinocytes by fluorescent imaging
○藤田 圭吾¹, 新藤 豊¹, 勝田 雄治², 後藤 真紀子², 堀田 耕司¹, 岡 浩太郎¹ (¹慶應義塾大学大学院理工学研究科, ²資生堂グローバルイノベーションセンター)
Keigo Fujita¹, Yutaka Shindo¹, Yuji Katsuta², Makiko Goto², Kohji Hotta¹, Kotaro Oka¹ (¹Grad. Sch. Sci. and Tech. Keio Univ., ²Shiseido Global Innovation Center)
- [2-16-1648](#) 細胞内温度分布の追跡が単一細胞内の遅いエネルギー散逸を明らかにする
Tracking Intracellular Temperature Mapping Reveals Slow Energy Dissipation in Single Cells
○寶田 雅治¹, 岡部 弘基^{1,2}, 船津 高志¹ (¹東大・院薬, ²JST さきがけ)
Masaharu Takarada¹, Kohki Okabe^{1,2}, Takashi Funatsu¹ (¹Grad. Sch. of Pharm. Sci., The Univ of Tokyo, ²JST, PRESTO)
- [2-16-1700](#) High temporal observation of CheY-binding and dissociation during rotational switching of a single flagellar motor
Taro Yuri, Yumiko Uchida, Yong-Suk Che, Akihiko Ishijima, Hajime Fukuoka (*Grad. Sch. Frontier Bio Sci. Osaka Univ*)
- [2-16-1712](#) 細胞内の温度変動に対する微小管の寄与
The contribution of microtubules on intracellular temperature variations
○上田 健史¹, 柳 昂志¹, 岡部 弘基^{1,2}, 船津 高志¹ (¹東京大学大学院・薬学系研究科, ²JST さきがけ)
Takeshi Ueda¹, Takashi Yanagi¹, Koki Okabe^{1,2}, Takashi Funatsu¹ (¹Grad. Sch. Pharm., Univ. Tokyo, ²JST PRESTO)
- [2-16-1724](#) 大腸菌走化性応答適応過程 (CW バイアス) を簡単かつリアルタイムに数値化するポータブル顕微鏡システムの構築
Construction of a portable microscope system that easily and in real time digitizes E. coli chemotaxis adaptation process (CW bias)
○田中 裕人, 数田 恭章, 矢野 亜美奈, 小嶋 寛明（情報通信研究機構 未来 ICT 研究所 神戸フロンティア研究センター）
Hiroto Tanaka, Yasuaki Kazuta, Amina Yano, Hiroaki Kojima (*Adv ICT Res Inst, NICT*)

- [2-16-1736](#) 細胞内の温度変化に対する高分子の影響の解明
Elucidation of the effect of macromolecules on temperature changes in cells
○永井 駿作¹, 岡部 弘基^{1,2}, 船津 高志¹ (¹東大・院薬, ²JST さきがけ)
Shunsaku Nagai¹, Koki Okabe^{1,2}, Takashi Funatsu¹ (¹*Grad. Sch. of Pharm. Sci., The Univ of Tokyo*, ²*JST, PRESTO*)
- [2-16-1748](#) Influence of Intra-Cellular Nanoendoscopy-AFM Measurements on Cell Viability and Functions
Mohammad Mubarak Hosain¹, Mohammad Shahidul Alam¹, Ichikawa Takehiko¹, Marcos Penedo^{1,2}, Tetsuya Shirokawa³, Sivashanmugan Kundan¹, Keisuke Miyazawa^{1,3}, Kazuki Miyata^{1,3}, Fukuma Takeshi^{1,3} (¹*Division of Nano Life Science Institute (WPI-NanoLSI) and Nano Life Science Institute, Kanazawa University*, ²*Laboratory for Bio- and Nano-Instrumentation, Swiss Federal Institute of Technology Lausanne (EPFL), Lausanne, Switzerland*, ³*Division of Electrical Engineering and Computer Science, Kanazawa University*)
- [2-16-1800](#) Fluorometric digital ATPase assay with single-enzyme detection sensitivity
Hiroshi Ueno, Mio Sano, Mayu Hara, Hiroyuki Noji (*Grad. Sch. Eng., Univ. Tokyo*)
- [2-16-1812](#) 補償光学系を用いた1分子輝点3次元位置精度の改善のシミュレーション研究
A simulation study to evaluate improvement of three-dimensional localization precision of single molecule images using adaptive optics
○周 翔, 伊藤 由馬, 徳永 万喜洋 (東工大・生命理工学院)
Xiang Zhou, Yuma Ito, Makio Tokunaga (*Sch. Life Sci. Tech., Tokyo Tech*)
- [2-16-1824](#) Plunus Lanessiana から抽出した色素のpH依存蛍光特性と水素化アモルファスシリコン上での薄膜
A pH depend fluorescent properties of pigment extracted from Plunus Lanessiana and the thin film on hydrogenated amorphous silicon film
○辻内 裕¹, 秋山 洗佑¹, 和泉 真生¹, 木村 聡見¹, 高田 一範¹, 増本 博² (¹秋田大・物質科学, ²東北大・学際研)
Yutaka Tsujiuchi¹, Koyu Akiyama¹, Mao Izumi¹, Satomi Kimura¹, Kazunori Takada¹, Hiroshi Masumoto² (¹*Grad. Mat. Sci. Univ. Akita*, ²*Fris. Univ. Tohoku*)

3日目 (11月27日(土)) / Day 3 (Nov. 27 Sat.)

13:30~15:30 Ch01
3G01 タンパク質：一般 VI
Protein: General VI

座長：後藤 祐児 (大阪大学), 出村 誠 (北海道大学)
Session Chairs: Yuji Goto (Osaka Univ.), Makoto Demura (Hokkaido Univ.)

- [3-01-1330](#) Towards understanding eukaryotic and prokaryotic protein interactions in loop regions
Lin Zhang¹, Hafumi Nishi^{1,2,3} (¹*Graduate School of Information Sciences, Tohoku University*, ²*Faculty of Core Research, Ochanomizu University*, ³*Tohoku Medical Megabank Organization, Tohoku University*)
- [3-01-1342](#) 超音波照射を利用した夾雑物存在下におけるβ2ミクログロブリンのアミロイド線維形成反応の研究
Study on amyloid fibril formation of β2-microglobulin in presence of concomitants by ultrasonication assay
○中島 吉太郎¹, 山口 圭一¹, 山本 卓², 荻 博次³, 後藤 祐児³ (¹阪大・国際医工情報センター, ²新潟大・医, ³阪大・院工)
Kichitaro Nakajima¹, Keiichi Yamaguchi¹, Suguru Yamamoto², Hirotosugu Ogi³, Yuji Goto³ (¹*Global Center for Med. Eng. Info., Osaka Univ.*, ²*Med. Sch., Niigata Univ.*, ³*Grad. Sch. Eng., Osaka Univ.*)

- [3-01-1354](#) CRAF は 14-3-3 結合サイトへの変異で N-/C-端ドメインを含む分子内複合体の状態が変わる
Mutations in 14-3-3 binding sites affect the intramolecular complex formation of CRAF involving its N- and C-terminus domains
○岡本 憲二, 佐甲 靖志 (理研・CPR)
Kenji Okamoto, Yasushi Sako (CPR, RIKEN)
- [3-01-1406](#) Dynamic Residue Interaction Network Analysis of Primary Mutations in Protease that Confer Drug Resistance in HIV-1
Ryouga Miyawaki, Mohini Yadav, Norihumi Yamamoto (Chiba Tech)
- [3-01-1418](#) β シート内における隣接ストランド間の $C\alpha$ 間距離の解析
Analysis of $C\alpha$ distances between adjacent strands in β -sheets
○鈴木 博実 (明治大・農)
Hiroimi Suzuki (Sch. Agri., Meiji Univ.)
- [3-01-1430](#) 生物分子モーターベースの群れは、貨物をロード・デリバリー・アンロードする分子トランスポーターとしての役割を果たす
Construction of biomolecular motor-based swarm as a molecular transporter to load-deliver-unload cargo
○Aker Mousumi¹, Keya Jakia Jannat¹, Kabir Arif Md. Rashedul¹, Inoue Daisuke², Hess Henry³, Sada Kazuki¹, Kuzuya Akinori⁴, Asanuma Hiroyuki⁵ (¹北海道大学理学部, ²九州大学デザイン学部, ³コロンビア大学医用生体工学科, ⁴関西大学大学院化学物質工学研究科, ⁵名古屋大学大学院工学研究科)
Mousumi Akter¹, Jakia Jannat Keya¹, Arif Md. Rashedul Kabir¹, Daisuke Inoue², Henry Hess³, Kazuki Sada¹, Akinori Kuzuya⁴, Hiroyuki Asanuma⁵ (¹Fac. Sci., Univ. Hokkaido, ²Fac. Des., Univ. Kyushu, ³Dep. Biomed. Eng., Univ. Columbia, ⁴Grad. Sch. Chem. Mat. Eng., Univ. Kansai, ⁵Grad. Sch. Eng., Univ. Nagoya)
- [3-01-1442](#) Relationship between the acceptor specificity and the loop structure of catalytic domain in bacterial glucansucrases
Takafumi Inoue, Ko-hei Yano, Hideyuki Komatsu (Dept. of Bioscience and Bioinformatics, Kyushu Inst. Tech.)
- [3-01-1454](#) ヒト S100A3 の変異体を用いた四量体構造解析に向けた研究
Research for tetramer structure analysis using mutants of human S100A3
○飯田 泰由¹, 井手 賢司^{1,2}, 海野 昌喜^{1,2} (¹茨大・院理工, ²茨大・フロンティア)
Hiroyuki Iida¹, Kenji Ite^{1,2}, Masaki Unno^{1,2} (¹Grad. Sci. Eng., Ibaraki Univ., ²iFRC, Ibaraki Univ.)
- [3-01-1506](#) アミロイド β (16-22)ペプチドのアミロイド線維形成メカニズムの解明
Elucidation of the mechanism of amyloid fibril formation of amyloid- β (16-22) peptide
○山崎 萌 (富山大・院薬)
Moe Yamazaki (Faculty of Pharmaceutical Sciences, University of Toyama)
- [3-01-1518](#) 抗体製剤の凝集体形成に及ぼす物理化学的製剤特性の影響
Effect of Physicochemical Formulation Properties on the Formation of aggregate in Antibody Preparations
○三谷 麻綺, 末友 裕行, 和湯 千紘, 細川 俊仁 (協和キリン株式会社 パイオ生産技術研究所)
Maki Mitani, Hiroyuki Suetomo, Chihiro Wayu, Toshihito Hosokawa (Bio Process Research and Development Laboratories, Kyowa Kirin Co., Ltd.)

座長：田中 元雅 (理化学研究所), 新井 宗仁 (東京大学)

Session Chairs: Motomasa Tanaka (RIKEN), Munechito Arai (Univ. of Tokyo)

[3-02-1330](#) Structural intermediates in rotary V/A-ATPase from initial to steady state visualized by time-resolved cryo-electron microscopy

Atsuko Nakanishi^{1,2}, Jun-ichi Kishikawa^{1,3}, Tomohiro Nishizawa^{4,5}, Kaoru Mitsuoka², Ken Yokoyama¹ (¹*Dept. of Life Sci., Kyoto Sangyo Univ.*, ²*Res. Ctr. for UHVEM, Osaka Univ.*, ³*Inst. for Protein Res., Osaka Univ.*, ⁴*Dept. of Bio. Sci., Grad. Sch. of Sci., Univ. of Tokyo.*, ⁵*Grad. Sch. of Med. Life Sci., Yokohama City Univ.*)

[3-02-1342](#) ポンプ型チャネルロドプシン ChRmine のイオン透過機構の構造基盤

Structural basis for channel conduction in the pump-like channelrhodopsin ChRmine

○岸 孝一郎¹, Kim Yoon², 福田 昌弘¹, 草木 迫 司³, Thadhani Elina^{2,4}, Byrne Eamon², Paggi Joseph⁴, Ramakrishnan Charu⁵, 松井 俊貴¹, 山下 恵太郎⁶, 永田 崇^{7,8}, 今野 雅恵^{7,8}, Wang Peter², 井上 昌俊², Benster Tyler², 植村 智子⁹, Liu Kehong⁹, 柴田 幹大¹⁰, 野村 紀通⁹, 岩田 想^{9,11}, 瀧木 理³, Dror Ron^{4,12}, 井上 圭一⁷, Deisseroth Karl^{2,5,13,14}, 加藤 英明^{1,3,15} (¹東大院・総合文化研究科, ²Department of Bioengineering, Stanford University., ³東大院・理学系研究科, ⁴Department of Computer Science, Stanford University., ⁵CNC Program, Stanford University., ⁶MRC Laboratory of Molecular Biology, Cambridge Biomedical Campus., ⁷東京大学物性研究所, ⁸さきがけ-科学技術振興機構, ⁹京都大学大学院医学系研究科, ¹⁰金沢大学新学術創成研究機構, ¹¹理化学研究所放射光科学研究センター, ¹²Institute for Computational and Mathematical Engineering, Stanford University., ¹³Howard Hughes Medical Institute, Stanford University., ¹⁴Department of Psychiatry and Behavioral Sciences, Stanford University., ¹⁵創発的研究支援事業-科学技術振興機構)

Koichiro Kishi¹, Yoon Kim², Masahiro Fukuda¹, Tsukasa Kusakizako³, Elina Thadhani^{2,4}, Eamon Byrne², Joseph Paggi⁴, Charu Ramakrishnan⁵, Toshiki Matsui¹, Keitaro Yamashita⁶, Takashi Nagata^{7,8}, Masae Konno^{7,8}, Peter Wang², Masatoshi Inoue², Tyler Benster², Tomoko Uemura⁹, Kehong Liu⁹, Mikihiro Shibata¹⁰, Norimichi Nomura⁹, So Iwata^{9,11}, Osamu Nureki³, Ron Dror^{4,12}, Keiichi Inoue⁷, Karl Deisseroth^{2,5,13,14}, Hideaki Kato^{1,3,15} (¹*Komaba Institute for Science, The University of Tokyo.*, ²*Department of Bioengineering, Stanford University.*, ³*Department of Biological Sciences, Graduate School of Science, The University of Tokyo.*, ⁴*Department of Computer Science, Stanford University.*, ⁵*CNC Program, Stanford University.*, ⁶*MRC Laboratory of Molecular Biology, Cambridge Biomedical Campus.*, ⁷*The Institute for Solid State Physics, The University of Tokyo.*, ⁸*PRESTO, Japan Science and Technology Agency.*, ⁹*Department of Cell Biology, Graduate School of Medicine, Kyoto University.*, ¹⁰*High-speed AFM for Biological Application Unit, Institute for Frontier Science Initiative, Kanazawa University.*, ¹¹*RIKEN SPring-8 Center.*, ¹²*Institute for Computational and Mathematical Engineering, Stanford University.*, ¹³*Howard Hughes Medical Institute, Stanford University.*, ¹⁴*Department of Psychiatry and Behavioral Sciences, Stanford University.*, ¹⁵*FOREST, Japan Science and Technology Agency.*)

[3-02-1354](#) Structural analysis of amyloid disaggregation reaction by the novel FT-IR technique

Takashi Nomura¹, Yoshiko Nakagawa^{1,2}, Yusuke Komi¹, Shingo Tamai^{1,3}, Motomasa Tanaka¹ (¹*CBS, Riken*, ²*Dept. of Life Sci. & Tech., Tokyo Tech.*, ³*Biomed. Sci. & Eng., Grad. Sch. of Med. & Dent. Sci., TMDU*)

- [3-02-1406](#) X線結晶構造解析による2機能的ミモシン合成酵素の反応機構解明に向けて
Structural Insights into Catalytic Reaction Mechanism for bifunctional enzyme, Mimosine Synthase, from *Leucaena leucocephala*
○堀谷 正樹^{1,2}, 前田 理沙¹, 大貝 茂希², 福田 雅一^{2,3}, 屋 宏典^{2,4}, 杉本 宏⁵ (¹佐大・農,² 鹿大・院連合農,³ 琉大・院農,⁴ 琉大・熱帯生物圏研究セ,⁵ 理研・播磨)
Masaki Horitani^{1,2}, Risa Maeda¹, Shigeki Oogai², Masakazu Fukuta^{2,3}, Hirotsugu Oku^{2,4}, Hiroshi Sugimoto⁵ (¹Fac. of Agri., Saga Univ., ²United Grad. Agri. Sci., Kagoshima Univ., ³Grad. Sch. Agri., Univ. Ryukyuu, ⁴Trop. Bios. Res. Cent., Univ. Ryukyuu, ⁵Harima Inst., Riken)
- [3-02-1418](#) 酸化型及び還元型の cryptdin 4 の抗菌活性発現に關与する構造の解析
Structural analysis to clarify antimicrobial mechanisms of oxidized and reduced cryptdin-4
○耿 偉銘, 王 一, 宋 雨迟, 闫 少男, 杨 文典, 相沢 智康 (北大生命科学院蛋白質科学研究所)
Weiming Geng, Yi Wang, Yuchi Song, Shaonan Yan, Wendian Yang, Tomoyasu Aizawa (Grad. Sch. of Life Sci, Hokkaido Univ)
- [3-02-1430](#) Crystal Structure of Soluble Family II Inorganic Pyrophosphatase Revealed the Mechanism of Catalysis and Structure Dynamics
Kantaro Sakamoto¹, Hiroshi Sugimoto², Masaki Horitsni¹ (¹Grad. Sch. Agric., Univ. Saga, ²Harima Inst., Riken)
- [3-02-1442](#) 単粒子解析における投影パラメーター分布推定と初期モデル生成
Estimation of projection parameter distribution and initial model generation in single particle analysis
○馬水 信弥^{1,2}, 安永 卓生¹ (¹九工大・院情工,² (株) システムインフロンティア)
Nobuya Mamizu^{1,2}, Takuo Yasunaga¹ (¹Grad. Sch. Comp. Sci., Kyushu Inst. Tech., ²System in frontier Inc.)
- [3-02-1454](#) クモ糸フィブロインからなるナノファイバー構造の解明
Nanofiber Structure Composed of Spider Silk Fibroin
○梶本 遥也¹, 岡本 悠介¹, 米澤 健人², 佐藤 健大³, 山崎 洋一¹, 藤間 祥子¹, 上久保 裕生^{1,2,4} (¹奈良先端大・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,³ スパイバー (株), ⁴ 高エネ機構・物構研)
Haruya Kajimoto¹, Yusuke Okamoto¹, Kento Yonezawa², Takehiro Sato³, Yoichi Yamazaki¹, Sachiko Toma¹, Hironari Kamikubo^{1,2,4} (¹NAIST, MS, ²NAIST, CDG, ³Spiber Inc., ⁴KEK, IMSS)

13:30~15:30 Ch03

3G03 タンパク質：計算 IV

Protein: Simulation IV

座長：清水 伸隆 (高エネルギー加速器研究機構), 奥村 久士 (分子科学研究所)

Session Chairs: Nobutaka Shimizu (KEK), Hisashi Okumura (IMS)

- [3-03-1330](#) The conformational stability analysis of dengue virus envelope domain III(ED3) wild type and its mutants by molecular dynamics simulation
Jingwen Xian¹, Hiromichi Tsurui², Atsushi Kurotani³, Yutaka Kuroda¹ (¹Tokyo University of Agriculture and Technology, ²Department of Immunological Diagnosis, Juntendo University School of Medicine, ³Center for Sustainable Resource Science, RIKEN Institute)
- [3-03-1342](#) Analysis of amino acid sequence variation in the RBD of SARS-CoV-2
Cheng ZhiRui¹, Yutaka Kuroda¹, Atsushi Kurotani² (¹Tokyo University of Agriculture and Technology, ²Center for Sustainable Resource Science, RIKEN Institute)

- [3-03-1354](#) SEC-SAXS/紫外可視分光で測定した行列データの自動解析ソフトウェア開発
Development of software for automatic processing of matrix data measured with SEC-SAXS/UV-Vis. spectroscopy
米澤 健人^{1,2}, 高橋 正剛¹, 小山 恵史¹, 谷田部 景子¹, 永谷 康子¹, 清水 伸隆¹ (¹高エネ機構・物構研・放射光, ²奈良先端大・CDG)
Kento Yonezawa^{1,2}, Masatsuyo Takahashi¹, Keishi Oyama¹, Keiko Yatabe¹, Yasuko Nagatani¹,
Nobutaka Shimizu¹ (¹PF, IMSS, KEK, ²CDG, NAIST)
- [3-03-1406](#) 質問学習を活用した HLA class II 結合性ペプチドの予測
Prediction of HLA class II-binding peptides by training with query learning
○宇高 恵子¹, 茶畑 守富¹, 尾上 広祐², 山下 慶子², 田中 雄希² (¹高知大・医・免疫, ²AI Drug Development Division, NEC)
Keiko Udaka¹, Morito Chabata¹, Kousuke Onoue², Yoshiko Yamashita², Yuki Tanaka² (¹Department of Immunology, School of Medicine, Kochi University, ²AI Drug Development Division, NEC)
- [3-03-1418](#) 抗原-抗体界面の塩橋の安定性と その役割に関する理論的研究
A theoretical study on the salt bridge stability in the antigen-antibody interface and its effect
○山下 雄史 (東大・先端研)
Takefumi Yamashita (RCAST, Univ. Tokyo)
- [3-03-1430](#) シアニディオシゾン由来 Branching Enzyme の MD シミュレーションによる構造解析
Molecular Dynamics Simulation of Starch Branching Enzyme Derived from *Cyanidioschyzon merolae*
○成山 幸助¹, 野口 瑤^{1,3}, 中島 基邦¹, 山田 寛尚^{2,3}, 森河 良太¹, 高須 昌子¹, 藤原 祥子¹ (¹東葉大生命, ²東葉大薬, ³統数研)
Kosuke Nariyama¹, Yoh Noguchi^{1,3}, Motokuni Nakajima¹, Hironao Yamada^{2,3}, Ryota Morikawa¹, Masako Takasu¹, Shoko Fujiwara¹ (¹Sch. of Life Sci., Tokyo Univ. of Pharm. and Life Sci., ²Sch. of Pharm., Tokyo Univ. of Pharm. and Life Sci., ³The Institute of Statistical Mathematics)
- [3-03-1442](#) サポシン B と脂質分子の分子動力学シミュレーション
Molecular dynamics simulations of Saposin B with a bound lipid
○城田 松之 (東北大・院医)
Matsuyuki Shiota (Grad. Sch. Med., Tohoku Univ.)
- [3-03-1454](#) Capturing drastic state transitions of biological macromolecules by molecular dynamics simulation and nonlinear dimensionality reduction
Mao Oide¹, Yuji Sugita^{1,2,3} (¹CPR, RIKEN, ²BDR, RIKEN, ³R-CCS, RIKEN)
- [3-03-1506](#) 分子動力学シミュレーションによって明らかになった SLC26A9 塩化物イオントランスポーターのゲート運動機構
Mechanism of the gating motion of SLC26A9 chloride ion transporter revealed by the molecular dynamics simulations
○大森 聡¹, 花園 裕矢², 西 羽美^{1,3}, 木下 賢吾^{1,4,5} (¹東北大・院・情報・応用・生命, ²医科歯科大・難治疾患研, ³お茶の水大・基幹研究院, ⁴東北大・メディカルメガバンク, ⁵東北大・加齢研)
Satoshi Omori¹, Yuya Hanazono², Hafumi Nishi^{1,3}, Kengo Kinoshita^{1,4,5} (¹GSIS, Tohoku Univ., ²Med. Res. Inst., Tokyo Medical and Dental Univ., ³Faculty of Core Res., Ochanomizu Univ., ⁴ToMMo, Tohoku Univ., ⁵Inst. of Dev. Aging and Cancer, Tohoku Univ.)
- [3-03-1518](#) 微小管つぎ目領域におけるチューブリン構造集団の全原子分子動力学シミュレーションによる解析
Tubulin conformational ensemble in seam region of microtubule investigated by all-atom molecular dynamics simulation
○梅澤 公二^{1,2}, 古田 尚之¹, 轟 拓磨¹ (¹信大・総合理工, ²信大・バイオメディカル研)
Koji Umezawa^{1,2}, Naoyuki Furuta¹, Takuma Todoroki¹ (¹Grad. Sch. of Sci. & Tech., Shinshu Univ., ²IBS, Shinshu Univ.)

座長：堀谷 正樹 (佐賀大学), 黒田 裕 (東京農工大学)

Session Chairs: Masaki Horitani (Saga Univ.), Yutaka Kuroda (Tokyo Univ. of Agric. and Tech.)

- [3-04-1330](#) Recombinant production and antibacterial activity assay of reduced and oxidized cryptdin-6
Shaonan Yan, Yuchi Song, Yi Wang, Weiming Geng, Wendian Yang, Tomoyasu Aizawa (*Graduate School of Life Sciences, Hokkaido University*)
- [3-04-1342](#) gREST 法による Nanobody CDR H3 ループ構造のサンプリング
 Enhanced Conformational Sampling of Nanobody CDR H3 Loops by Generalized Replica-Exchange with Solute Tempering
 ○東田 連, 松永 康佑 (埼玉大・院理工学)
- [3-04-1354](#) Ren Higashida, Yasuhiro Matsunaga (*Grad. Sch. Sci. Eng., Saitama Univ.*)
 一分子蛍光法による RNA 結合と液滴形成に伴う LAF-1 RGG 構造変化の解明
 Single molecule fluorescence investigations on the structure transitions of LAF-1 RGG upon the RNA binding and the droplet formation
 ○藤田 かなな^{1,2}, 木村 美智子^{1,2}, 高橋 泰人^{1,2}, 高橋 聡^{1,2}, 小井川 浩之^{1,2} (¹ 東北大・多元研, ² 東北大・院生命科学)
- [3-04-1406](#) Kanna Fujita^{1,2}, Michiko Kimura^{1,2}, Hiroto Takahashi^{1,2}, Satoshi Takahashi^{1,2}, Hiroyuki Oikawa^{1,2} (*¹IMRAM, Tohoku Univ., ²Grand. Sch. Life Sci., Tohoku Univ.*)
 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 mechanisms of cold-adapted glucokinase
 ○矢持 紅音¹, 浅香 里緒², 杉本 宏³, 渡邊 啓一², 堀谷 正樹² (¹ 佐賀大・院先進健康, ² 佐賀大・農, ³ 理研・SPring-8)
- [3-04-1418](#) Akane Yato¹, Rio Asaka², Hiroshi Sugimoto³, Keiichi Watanabe², Masaki Horitani² (*¹Grad. Sch. Adv. Hea. Sci., Saga Univ., ²Agr., Saga Univ., ³RIKEN, SPring-8 center*)
 Studies on Cry j 7, a Novel Allergen from Japanese cedar
- [3-04-1430](#) Jignkang Zheng, Tomona Iizuka, Tomoyasu Aizawa (*Grad. Sch. Life Sci., Hokkaido Univ.*)
 Amyloid accumulation dynamics in physiological condition
- [3-04-1442](#) Masahiro Kuragano, Shinya Yamanaka, Kiyotaka Tokuraku (*Grad. Sch. Eng., Muroran Inst. of Tech.*)
 ラッサウイルスの表面タンパク質を覆う糖鎖の構造ダイナミクス
 Structure and dynamics of glycans on Lassa virus envelop protein
 ○李 秀榮¹, 水口 賢司^{1,2} (¹ 医薬健康研, ² 阪大蛋白研)
- [3-04-1454](#) Suyong Re¹, Kenji Mizuguchi^{1,2} (*¹ArCHER, NIBIOHN, ²IPR, Osaka Univ.*)
 PSD95-PDZ3 の一残基置換による高温での可逆的なオリゴマー (RO) 形成の阻害およびアミロイド線維の抑制
 Blocking PSD95-PDZ3's amyloidogenesis through point mutations that inhibit high-temperature reversible oligomerization (RO)
 ○早乙女 友規^{1,2,3}, Onchaiya Sawaros¹, 目崎 太一³, Martinez Jose⁴, 城所 俊一³, 黒田 裕^{1,2} (¹ 東農工大・生命工, ² 東農工大・GIR, ³ 長岡技大・生物機能, ⁴ グラナダ大学・物化)
- Tomonori Saotome**^{1,2,3}, Sawaros Onchaiya¹, Taichi Mezaki³, Jose Martinez⁴, Shun-ichi Kidokoro³, Yutaka Kuroda^{1,2} (*¹Dept. of Biotech. and Life Sci., Tokyo Univ. of Agric. and Tech., ²Insti. of Glob. Innov. Res., Tokyo Univ. of Agric. and Tech., ³Dept. of Bio., Nagaoka Univ. of Tech., ⁴Dept. of Phys. Chem. and Insti. of Biotech., Univ. of Granada.*)

座長：富樫 祐一（立命館大学），片平 正人（京都大学）

Session Chairs: Yuichi Togashi (Ritsumeikan Univ.), Masato Katahira (Kyoto Univ.)

[3-05-1330](#) Free Energy Landscape of RNA Binding Dynamics in Start Codon Recognition by Eukaryotic Ribosomal Pre-Initiation Complex

Takeru Kameda¹, Katsura Asano^{2,3,4}, Yuichi Togashi^{1,5} (¹*College of Life Sciences, Ritsumeikan University*, ²*Molecular Cellular and Developmental Biology Program, Division of Biology, Kansas State University*, ³*Hiroshima Research Center for Healthy Aging (HiHA)*, ⁴*Graduate School of Integrated Sciences for Life, Hiroshima University*, ⁵*RIKEN Center for Biosystems Dynamics Research (BDR)*.)

[3-05-1342](#) 構造レベルでの RRF と tRNA によるリボソームリサイクリングの解明

Structural basis for ribosome recycling by RRF and tRNA

○丹澤 豪人^{1,2}, Zhou Dejian³, Lin Jinzhong³, Matthieu G. Gagnon^{2,4} (¹阪大・蛋白研,²テキサス州立大・医・微生物学/免疫学,³復旦大・中山医院・生命科学,⁴テキサス州立大・医・シーリー構造生物学/生物物理学センター)

Takehito Tanzawa^{1,2}, Dejian Zhou³, Jinzhong Lin³, Gagnon Matthieu G.^{2,4} (¹*Inst., for Protein Res., Osaka Univ.*, ²*Dept. of Microbiol. & Immunol., Univ. of Texas Med. Branch*, ³*Schl. of Life Sci., Zhongshan Hospital, Fudan Univ.*, ⁴*Sealy Center for Struct. & Biophys., Univ. of Texas Med. Branch*)

[3-05-1354](#) DNA 複製一分子観察にむけた酵母レプリソームの DNA 結合の評価

Evaluation of DNA binding of yeast replisome toward single-molecule observation of DNA replication

○寺川 まゆ, 寺川 剛（京大・院理学）

S. Mayu Terakawa, Tsuyoshi Terakawa (*Grad. Sci. Kyoto Univ.*)

[3-05-1406](#) 薬剤耐性機構の解明に向けた、クライオ電子顕微鏡解析による NTM リボソームへのマクロライド結合様式の解明

Elucidation of the binding mode of a macrolide antibiotic to NTM ribosome for understanding drug resistance mechanism by using cryo-EM

○橋本 翼¹, 高田 希美¹, 千足 啄馬¹, 深野 華子², 山本 健太郎², 鈴木 仁人³, 星野 仁彦², 横山 武司¹, 田中 良和¹ (¹東北大・院生命,²感染研・ハンセン病研究センター,³感染研・薬剤耐性研究センター)

Tsubasa Hashimoto¹, Nozomi Takada¹, Takuma Chiashi¹, Hanako Fukano², Kentaro Yamamoto², Masato Suzuki³, Yoshihiko Hoshino², Takeshi Yokoyama¹, Yoshikazu Tanaka¹ (¹*Grad. Sch. Life Sci., Tohoku Univ.*, ²*Leprosy Res. Center, Nat. Ins. of Infectious Diseases*, ³*AMR Center, Nat. Ins. of Infectious Diseases*)

[3-05-1418](#) In-cell NMR 法によるヒト生細胞内環境下の核酸の塩基対ダイナミクスの解析

In-cell NMR study on the base pair dynamics of nucleic acid in the living human cells

○山置 佑大^{1,2}, 永田 崇^{1,2}, 近藤 敬子¹, 阪本 知樹², 高見 昇平², 片平 正人^{1,2} (¹京大・エネルギー理工研,²京大・院エネルギー科学)

Yudai Yamaoki^{1,2}, Takashi Nagata^{1,2}, Keiko Kondo¹, Tomoki Sakamoto², Shohei Takami²,

Masato Katahira^{1,2} (¹*Inst. Adv. Energy, Kyoto Univ.*, ²*Grad. Sch. Energy Sci., Kyoto Univ.*)

[3-05-1430](#) c-MYC 遺伝子のグアニン四重鎖の圧力変性に関する FTIR 研究

FTIR study of pressure-induced denaturation of the guanine quadruplex of the c-MYC gene

○宮内 滉平¹, 山置 佑大², 今村 比呂志¹, 加藤 稔¹ (¹立命館大・院生命科学,²京都大・エネルギー理工)

Kohei Miyauchi¹, Yudai Yamaoki², Hiroshi Imamura¹, Minoru Kato¹ (¹*Grad. Sch. Life Sci., Univ. Ritsumei*, ²*Advanced Energy Inst., Univ. Kyoto*)

[3-05-1442](#) Simultaneous monitoring of DNA, RNA, and DNA:RNA hybrid G-quadruplexes, and their interaction with arginine-glycine-rich peptide by NMR
Chihiro Nakayama^{1,2}, Yudai Yamaoki^{1,2}, Keiko Kondo¹, Takashi Nagata^{1,2}, Masato Katahira^{1,2} (¹*Inst. Adv. Energy, Kyoto Univ.*, ²*Grad. Sch. Energy Sci., Kyoto Univ.*)

13:30~14:42 Ch06

3G06 筋肉・分子モーターⅣ

Muscle & Molecular motor Ⅳ

座長：野地 博行（東京大学），福岡 創（大阪大学）

Session Chairs: Hiroyuki Noji (The Univ. of Tokyo), Hajime Fukuoka (Osaka Univ.)

[3-06-1330](#) 生体運動メカニズムの統一的理解
Unified Understanding of Active Motions Driven by Proteins
○福元 孝晋¹, 佐々木 一夫², 樋口 秀男³ (¹東大・理・物理, ²東北大・工・応物, ³東大・理・物理)

Takakuni Fukumoto¹, Kazuo Sasaki², Hideo Higuchi³ (¹*Grad. Sch. Sci., Univ. Tokyo*, ²*Grad. Sch. Eng., Univ. Tohoku*, ³*Grad. Sch. Sci., Univ. Tokyo*)

[3-06-1342](#) Molecular dynamics simulations of the yeast condensin holo complex towards elucidation of the mechanism of DNA loop extrusion

Hiroki Koide, Shoji Takada, Tsuyoshi Terakawa (*Kyoto Univ. Dep. of Science Takada Lab.*)

[3-06-1354](#) ショウジョウバエの左右非対称性を制御する Myosin1C と Myosin1D の解析
Molecular analysis of Myosin1C and Myosin1D, determinants of left-right asymmetry in *Drosophila*

○吉村 考平¹, 原口 武士¹, 伊美 拓真¹, 山口 明日香², 前田 知那美², 松野 健治², 伊藤 光二¹ (¹千葉大・院融合理工, ²大阪大学・院理学研究科)

Kohei Yoshimura¹, Takeshi Haraguchi¹, Takuma Imi¹, Asuka Yamaguchi², Chinami Maeda², Kenji Matsuno², Kohji Ito¹ (¹*Grad. Sch. Sci., Univ. Chiba*, ²*Grad. Sch. Sci., Univ. Osaka*)

[3-06-1406](#) 病原性大腸菌 EPEC 有する III 型分泌装置の ATPase 複合体の機能解析
Functional analysis of ATPase complex in Type Three Secretion System of Enteropathogenic *Escherichia coli*

○鈴木 綾¹, 多治見 祐希², 黒崎 涼², 上野 博史¹, 内橋 貴之², 野地 博行¹ (¹東大・院工学系・応用化学専攻, ²名大・院理学・物質理学専攻)

Aya Suzuki¹, Yuki Tajimi², Ryo Kurosaki², Hiroshi Ueno¹, Takayuki Uchihashi², Hiroyuki Noji¹ (¹*Dept. Appl. Chem., Grad. Sch. Eng., Univ. Tokyo*, ²*Dept. Matl. Sci., Grad. Sch. Sci., Nagoya Univ.*)

[3-06-1418](#) 高速原子間力顕微鏡と電子顕微鏡によるダイナクチンサイドアームのダイナミクスの可視化
Visualization of conformational dynamics of dynactin sidearm by high-speed AFM and negative stain EM

○斎藤 慧^{1,2}, Ganser Christian³, 小林 琢也⁴, 村山 尚⁴, 内橋 貴之^{3,5}, 豊島 陽子⁶ (1 遺伝研・物理細胞生物学, 2 総研大・遺伝学, 3 自然科学研究機構・生命創成探究センター, 4 順天堂大・医・薬理, 5 名大・院理, 6 東大・総合文化)

Kei Saito^{1,2}, Christian Ganser³, Takuya Kobayashi⁴, Takashi Murayama⁴, Takayuki Uchihashi^{3,5}, Yoko Y. Toyoshima⁶ (¹*Phys. Cell Lab., Natl. Inst. Genet.*, ²*Dept. Genet., SOKENDAI*, ³*ExCELLS, NINS*, ⁴*Dept. Pharmacology, Juntendo Univ. Sch. Med.*, ⁵*Grad. Sch. Sci., Nagoya Univ.*, ⁶*Grad. Sch. Arts Sci., Univ. Tokyo*)

[3-06-1430](#) 高度好塩菌アーキアの回転モーターにおける化学走性
Chemotaxis of the archaeal motor in *Haloferax volcanii*

○木下 佳昭, 渡邊 力也 (理化学研究所 開拓研究本部)

Yoshiaki Kinoshita, Rikiya Watanabe (*CPR, RIKEN*)

座長：上田 太郎（早稲田大学），宮田 真人（大阪市立大学）

Session Chairs: Taro Ueda (Waseda Univ), Makoto Miyata ()

[3-07-1330](#) 無細胞タンパク質発現系による生体分子モーターの試験管内合成とデザイン

In vitro synthesis and design of biomolecular motors by cell-free protein expression system

○井上 大介¹, 大橋 慧介^{2,3}, 高須賀 太一^{2,3}, 角五 彰⁴ (¹九州大学大学院芸術工学研究院, ²北海道大学大学院国際食資源学院, ³北海道大学大学院農学研究院, ⁴北海道大学大学院理学研究院)

Daisuke Inoue¹, Keisuke Ohashi^{2,3}, Taichi Takasuka^{2,3}, Akira Kakugo⁴ (¹Faculty of Design, Kyushu University, ²Graduate School of Global Food Resources, Hokkaido University, ³Research Faculty of Agriculture, Hokkaido University, ⁴Faculty of Science)

[3-07-1342](#) (1S1-3) Engineering of hybrid kinesin-1 dimer with synthetic linker by tuning the neck linker length

Jakia Jannat Keya¹, Akasit Visootsat¹, Akihiro Otomo¹, Sanghun Han², Kazushi Kinbara², Ryota Iino¹ (¹Institute for Molecular Science, National Institutes of Natural Sciences, ²School of Life Science and Technology, Tokyo Institute of Technology)

[3-07-1354](#) 微小管群ロボット操作のための人工 DNA フェロモンの開発

Designed DNA pheromone for automatic controlling of microtubules swarming

○松本 大輝¹, 西山 晃平², 川又 生吹^{1,4}, 村田 智¹, 角五 彰^{2,3}, 野村 M. 慎一郎¹ (¹東北大学大学院・工学研究科・ロボティクス専攻, ²北海道大学大学院・総合化学院, ³北海道大学大学院・理学研究院・化学部門, ⁴お茶の水女子大学・基幹研究院・自然科学系)

Daiki Matsumoto¹, Kohei Nishiyama², Ibuki Kawamata^{1,4}, Satoshi Murata¹, Akira Kakugo^{2,3}, Shin-ichiro M. Nomura¹ (¹Department of Robotics, Graduate School of Engineering, Tohoku University, ²Graduate School of Chemical Sciences and Engineering, Hokkaido University, ³Department of Chemistry, Faculty of Science, Hokkaido University, ⁴Natural Science Division, Faculty of Core Reserch, Ochanomizu University)

[3-07-1406](#) ポリエチレングリコールを用いたアクトミオシン運動の輸送能力試験

Test on in vitro transport capacity of actomyosin using polyethylene glycols

○砂田 悠真, 羽鳥 晋由 (山形大・院・理工)

Yuma Sunada, Kuniyuki Hatori (*Grad. Sch. Sci. Eng., Yamagata Univ.*)

[3-07-1418](#) In vitro でのアクチンフィラメントへの lifeact-GFP の不均一かつ安定的な結合の観察

Uneven and stable binding of lifeact-GFP to actin filaments observed in vitro

○青木 優也, 山崎 陽祐, 上田 太郎 (早稲田大学 先進理工学研究所 物理専攻)

Yuuya Aoki, Yousuke Yamazaki, Taro Q.P. Uyeda (*Dept. Physics, Waseda Univ*)

[3-07-1430](#) Photocontrol of small GTPase Ras using its regulatory factor GEF modified with photochromic azobenzene derivative

Yuichi Imamura, Nobuyuki Nishibe, Yuichi Imamura (*Grad.Sch.Eng., Univ. Soka*)

座長：岡嶋 孝治 (北海道大学), 山下 隼人 (大阪大学)

Session Chairs: Takaharu Okajima (Hokkaido Univ.), Hayato Yamashita (Osaka Univ.)

- [3-08-1330](#) 細胞内物質輸送を理解する新しい接近方：機械学習とイメージング技術の応用について
Understanding of vesicle transport using machine learning and image processing technology
○Lee Seohyun¹, Kim Hyuno¹, 石川 正俊¹, 樋口 秀男² (¹東京大学 情報基盤センター データ科学研究部門, ²東京大学 理学系研究科 物理学科)
Seohyun Lee¹, Hyuno Kim¹, Masatoshi Ishikawa¹, Hideo Higuchi² (¹*Data Science Reserach Division, Information Technology Center, The University of Tokyo*, ²*Department of Physics, Graduate School of Science, The University of Tokyo*)
- [3-08-1342](#) 原子間力顕微鏡による上皮ドームの力学解析
Mechanical analysis of epithelial dome using atomic force microscopy
○茂村 研太, 繁富 (栗林) 香織, スバギョ アグス, 末岡 和久, 岡嶋 孝治 (北海道大学・情報科学研究院)
Kenta Shigemura, Kaori Kuribayashi-Shigetomi, Agus Subagy, Kazuhisa Sueoka, Takaharu Okajima (*Grad. Sch. Inform. Sci., Univ. Hokkaido*)
- [3-08-1354](#) Observations of structural change in epithelial dome under constant electric field
Mataka Nagano, Miyu Ogawa, Yuki Fujii, Takaharu Okajima (*Grad. Sch. Inform. Sci. and Tech., Univ. Hokkaido*)
- [3-08-1406](#) 極性形成に関わる膜タンパク質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
○笠井 倫志¹, 根本 悠宇里² (¹岐阜大・糖鎖生命コア研, ²沖縄科技大院)
Rinshi Kasai¹, Yuri Nemoto² (¹*iGCORE, Gifu Univ.*, ²*OIST*)
- [3-08-1418](#) 酵母 G1 期核内での染色体分布とそのフラクタル次元に関する X 線回折イメージング
X-ray diffraction imaging study on the distribution and fractal dimensions of chromosomes in yeast nuclei in G1 phase
○上江洲 奏^{1,2} (¹慶應・理工, ²理研・RSC)
So Uezu^{1,2} (¹*Dept. Phys., Keio Univ.*, ²*RSC, RIKEN*)
- [3-08-1430](#) 蛍光顕微鏡複合型高速 AFM による細胞のナノ粒子取り込み過程の計測
The cellular uptake observation of nanoparticles by high-speed AFM combined with fluorescent microscopy
○松井 爽斗¹, 山下 隼人¹, 辻 明宏¹, 山口 明日香², 鈴木 団³, 阿部 真之¹ (¹阪大・院基礎工学, ²阪大・院理学, ³阪大・蛋白質研)
Akito Matsui¹, Hayato Yamashita¹, Akihiro Tsuji¹, Asuka Yamaguchi², Madoka Suzuki³, Masayuki Abe¹ (¹*Grad. Sch. Eng. Sci., Osaka Univ.*, ²*Grad. Sch. Sci., Osaka Univ.*, ³*IPR Osaka Univ.*)
- [3-08-1442](#) 細胞外小胞のサブタイプと取り込み経路の解明：超解像顕微鏡法と 1 粒子追跡法による研究
Subtypes of small extracellular vesicles and their uptake routes as revealed by super-resolution microscopy and single-particle tracking
○廣澤 幸一朗¹, 横田 康成², 鈴木 健一^{1,3} (¹岐阜大学 糖鎖生命コア研究所, ²岐阜大学 工学部 電気電子・情報工学科, ³CREST, JST)
Koichiro M. Hirose¹, Yasunari Yokota², Kenichi G.N. Suzuki^{1,3} (¹*iGCORE, Gifu Univ.*, ²*Dept. Eng., Gifu Univ.*, ³*CREST, JST*)
- [3-08-1454](#) Measuring the conformational changes in clathrin light chain at single sites of endocytosis with FLIM-FRET-CLEM
Kazuki Obashi, Kem Sochacki, Marie-Paule Strub, Justin Taraska (*National Heart, Lung, and Blood Institute, National Institutes of Health*)

- [3-08-1506](#) Application of photothermal agarose microfabrication technology for spatiotemporal analysis of collective cell migration
Mitsuru Sentoku, Hiromichi Hashimoto, Kenji Yasuda (*Dept. Pure & Appl. Phys., Grad. Sch. Adv. Sci. & Eng., Waseda Univ.*)
- [3-08-1518](#) 原子間力顕微鏡の往復フォースカーブを用いた初期発生胚のレオロジーマッピング
 Mapping rheological parameters of embryonic cells during early developmental stages using atomic force microscopy force curves
 ○松尾 智大, 坪山 洋介, 横堀 恵美, 藤井 裕紀, 岡嶋 孝治 (北海道大・院情報科学)
Tomohiro Matsuo, Yosuke Tsuboyama, Megumi Yokobori, Yuki Fujii, Takaharu Okajima (*Grad. Info. Sci. & Tech., Univ. Hokkaido*)

13:30~15:06 Ch09
 3G09 細胞生物 III
 Cell biology III

座長：澤井 哲 (東京大学), 三井 敏之 (青山学院大学)

Session Chairs: Satoshi Sawai (The Univ. of Tokyo), Toshiyuki Mitsui (Aoyama Gakuin Univ.)

- [3-09-1330](#) tau-RNA 液滴形成の熱量解析
 Calorimetric study of RNA-induced formation of tau droplet
 ○松田 貫, 鹿嶋 純太, 小松 英幸 (九州工大・情報工・生命化学情報)
Kan Matsuda, Junta Kashima, Hideyuki Komatsu (*Dept. of Bioscience and Bioinformatics, Kyushu Inst. Tech.*)
- [3-09-1342](#) 心毒性検査法の効率化を目指したハイスループット薬剤応答解析
 High-throughput cardiotoxicity detection system for simultaneously analysis of 64 samples
 ○鬼頭 健太郎, 田所 直樹, 林 真人, 金子 智行 (法政大学 生命科学部 生命機能学科 再構成細胞学研究室)
Kentaro Kito, Naoki Tadokoro, Masahito Hayashi, Tomoyuki Kaneko (*LaRC, FB, Hosei Univ*)
- [3-09-1354](#) リアルタイムフィードバック機構を内蔵した心臓細胞への機械的刺激システム
 Development of a mechanical device for stimulus on cardiac cells with feedback control system
 ○佐々木 亜優, 万本 和輝, 城所 龍, 野崎 庄太, 守山 裕大, 三井 敏之 (青学大・理工学)
Ayu Sasaki, Kazuki Mammoto, Ryu Kidokoro, Shota Nozaki, Yuuta Moriyama, Toshiyuki Mitsui (*Dept. Phys., Aoyama Gakuin Univ.*)
- [3-09-1406](#) リアルタイムフィードバック制御による力学的刺激に影響を受けた心筋細胞の拍動変化
 Change in phase stability of cardiac cell clusters affected by to mechanical stimulus with feedback control
 ○野崎 庄太, 城所 龍, 小島 快斗, 佐々木 亜優, 守山 裕大, 三井 敏之 (青学大・院理工学)
Shota Nozaki, Ryu Kidokoro, Kaito Kojima, Ayu Sasaki, Yuuta Moriyama, Toshiyuki Mitsui (*Dept. Phys., Aoyama Gakuin Univ.*)
- [3-09-1418](#) 機械学習を用いた細胞の集団運動ダイナミクスの次元圧縮とメカノバイオロジー的な効果
 Dimension compression and mechanobiological effects of collective cell movement dynamics using machine learning
 ○藤崎 弘士^{1,4}, 小田切 健太^{2,4}, 末谷 大道³, 高田 弘弥^{1,4}, 小川 令^{1,4} (¹日医大, ²専修大, ³大分大, ⁴AMED-CREST)
Hiroshi Fujisaki^{1,4}, Kenta Odagiri^{2,4}, Hiromichi Suetani³, Hiroya Takada^{1,4}, Rei Ogawa^{1,4} (¹Nippon Med. Sch., ²Senshu Univ., ³Oita Univ., ⁴AMED-CREST)
- [3-09-1430](#) 初期二ワトリ胚における中胚葉細胞の動的網目構造の自己組織化
 Dynamical network structure formation of mesoderm cells in early chick embryo
 ○多羅間 充輔, 仲矢 由紀子, 柴田 達夫 (理研 BDR)
Mitsusuke Tarama, Yukiko Nakaya, Tatsuo Shibata (*RIKEN BDR*)

- [3-09-1442](#) 細胞性粘菌の細胞型特異的な運動形状ダイナミクスの定量的解析
Quantitative analysis of cell-type specific morphology dynamics in *Dictyostelium discoideum*
○村山 菜月¹, 桑名 悟史², 上道 雅仁², 橋村 秀典², 澤井 哲² (¹東京大・院理,²東京大・院総文)
Natsuki Murayama¹, Satoshi Kuwana², Masahito Uwamichi², Hidenori Hashimura², Satoshi Sawai²
(¹Grad. Sch. Sci., Univ. Tokyo, ²Grad. Sch. Arts & Sci., Univ. Tokyo)
- [3-09-1454](#) 納豆菌が生産する水溶性メナキノン-7の構造研究
Structural study of water-soluble complex of menaquinone-7 produced by *Bacillus subtilis natto*
○茶竹 俊行¹, 柳澤 泰任², 村上 理沙², 大杉 忠則³, 須見 洋行³, 奥田 綾¹, 守島 健¹,
井上 倫太郎¹, 杉山 正明¹ (¹京大・複合研,²千葉科大・薬学,³倉敷芸科学大・生命科学)
Toshiyuki Chatake¹, Yasuhide Yanagisawa², Risa Murakami², Tadanori Ohsugi³, Hiroyuki Sumi³,
Aya Okuda¹, Ken Morishima¹, Rintaro Inoue¹, Masaaki Sugiyama¹ (¹KURNS, Kyoto Univ., ²Fac. Pharm.,
Chiba Inst. Sci., ³Dep. Life Sci., Kurashiki Univ. Sci. Arts)

13:30~15:06 Ch10

3G10 生体膜・人工膜Ⅳ

Biological & Artificial membrane IV

座長：井出 徹（岡山大学），岩本 真幸（福井大学）

Session Chairs: Toru Ide (Okayama Univ.), Masayuki Iwamoto (Univ. of Fukui)

- [3-10-1330](#) 脂質二分子膜への有毒物質の吸着
Adsorption of toxic molecules into lipid bilayer membranes
○吉田 一也, 藤原 尚史 (山形大・院理工学)
Kazunari Yoshida, Naofumi Fujiwara (Grad. Sch. Sci Eng., Yamagata University)
- [3-10-1342](#) 膜曲率依存的な KcsA チャネル構造変化を蛍光ラベルで検出する
Fluorescence detection of membrane curvature-induced structural changes in the KcsA potassium channel
植木 美鈴, ○岩本 真幸 (福井大・医・分子神経科学)
Misuzu Ueki, **Masayuki Iwamoto** (Dept. Mol. Neurosci., Facul. Med. Sci., Univ. Fukui)
- [3-10-1354](#) 金プローブを用いた自動チャネル電流測定装置の開発
Development of an automated system for measuring channel currents using a gold probe
○平野 美奈子¹, 富田 正久², 高橋 雅佳子¹, 川島 信幸³, 井出 徹⁴ (¹光産創大・光産業創成,²トムズ工房,³(株) システック,⁴岡大・院ヘルシステム)
Minako Hirano¹, Masahisa Tomita², Chikako Takahashi¹, Nobuyuki Kawashima³, Toru Ide⁴ (¹GPI,
²Tom's factory, ³SYSTEC Corporation, ⁴Grad Sch Interdiscip Sci Engr Health Syst, Okayama Univ.)
- [3-10-1406](#) アガロースゲルビーズを用いた新規チャネル電流測定法の開発
Development of a novel channel current measurement method using agarose gel beads
○朝倉 真実¹, 山本 大樹¹, 平野 美奈子², 井出 徹¹ (¹岡山大・院ヘルシステム統合科学研究科,²光産業創成大学院大・光バイオ分野)
Mami Asakura¹, Daiki Yamamoto¹, Minako Hirano², Toru Ide¹ (¹Grad. Sch. Health Sys., Okayama Univ., ²Photo-Bio. GPI)
- [3-10-1418](#) チャネル電流測定のためのゲルビーズ上の人工膜の形成
Artificial bilayers on a hydrogel bead for channel current recordings
○山本 大樹¹, 朝倉 真実¹, 平野 美奈子², 井出 徹¹ (¹岡山大・院ヘルシステム統合科学研究科,²光産業創成大学院大・光バイオ分野)
Daiki Yamamoto¹, Mami Asakura¹, Minako Hirano², Toru Ide¹ (¹Grad. Sch. Health Sys., Okayama Univ., ²Photo-Bio. GPI)
- [3-10-1430](#) Analysis of water permeability of human Aquaporin6 using moving membrane method
Takahisa Maki¹, Shigetoshi Oiki², Masayuki Iwamoto¹ (¹Dept. Mol. Neurosci., Facul. Med. Sci., Univ. Fukui, ²Biomed. Imaging. Res. Ctr., Univ. Fukui)

[3-10-1442](#) Thermo-responsive deformable liposomes, towards micron scale bio-hybrid robotics
Richard James Archer, Shinichiro Nomura, Satoshi Murata (*Tohoku University Graduate School of Engineering Department of Robotics*)

[3-10-1454](#) Adhesion of giant liposomes with cells using lipid-conjugated DNA towards DNA-mediated fusion
Sho Takamori, Hisatoshi Mimura, Toshihisa Osaki, Shoji Takeuchi (*Kanagawa Institute of Industrial Science and Technology*)

13:30~15:30 Ch11

3G11 光応答タンパク質：細胞
Light sensitive proteins: Cell

座長：上久保 裕生 (奈良先端科学技術大学院大学), 寺嶋 正秀 (京都大学)

Session Chairs: Hironari Kamikubo (NIST), Masahide Terazima (Kyoto Univ.)

[3-11-1330](#) Intermolecular interaction dynamics between PYPs and downstream PYP-binding proteins
Suhyang Kim¹, Yusuke Nakasone¹, Akira Takakado², Yoichi Yamazaki³, Hironari Kamikubo³, Masahide Terazima¹ (¹*Grad. Sch. Sci., Univ. Kyoto*, ²*Grad. Sch. Sci., Univ. Gakushuin*, ³*Div. Mat. Sci., NAIST*)

[3-11-1342](#) RcPYP の複合体形成反応に対する塩濃度効果

Effect of salt concentration on the complex formation reaction of RcPYP

○ 橋原 陽子¹, 山崎 洋一¹, 米澤 健人², 藤間 祥子¹, 上久保 裕生^{1,2,3} (¹奈良先端大・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,³高エネ機構・物構研)

Yoko Narahara¹, Yoichi Yamazaki¹, Kento Yonezawa², Sachiko Toma¹, Hironari Kamikubo^{1,2,3} (¹*NAIST, MS*, ²*NAIST, CDG*, ³*KEK, IMSS*)

[3-11-1354](#) 発色団水素結合を欠損した桂皮酸導入 RcPYP の光反応・相互作用

Photoreaction and interaction of cinnamic acid-incorporated RcPYP lacking chromophore hydrogen bond

○ 大久保 海¹, 山崎 洋一¹, 米澤 健人², 藤間 祥子¹, 上久保 裕生^{1,2,3} (¹奈良先端大・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,³高エネ機構・物構研)

Kai Okubo¹, Yoichi Yamazaki¹, Kento Yonezawa², Sachiko Toma¹, Hironari Kamikubo^{1,2,3} (¹*NAIST, MS*, ²*NAIST, CDG*, ³*KEK, IMSS*)

[3-11-1406](#) 赤色光照射による植物光受容蛋白質フィトクロム A の構造変化

Red-light induced structural changes in plant photoreceptor protein phytochrome A

大出 真央^{1,2}, 中迫 雅由^{1,2} (¹慶應大・物理,²理研・播磨)

Mao Oide^{1,2}, Masayoshi Nakasako^{1,2} (¹*Dept. Phys., Keio Univ.*, ²*RSC, RIKEN*)

[3-11-1418](#) 部位特異的変異導入によるビリル結合光センサー RcaE の光変換機構の解析

Analysis of the proton transfer mechanism of the bilin-based photosensor RcaE by site-directed mutagenesis

○ 広瀬 侑, 加茂 尊也, 浴 俊彦 (豊橋技術科学大学 応用化学・生命工学系)

Yuu Hirose, Takanari Kamo, Toshihiko Eki (*Toyohashi Univ. of Tech. Appl. Chem. & Life Sci.*)

[3-11-1430](#) 高速 AFM によるグラナ膜に内在する PSII 側方運動の可視化

Visualizing the lateral mobility of photosystem II in grana membrane by HS-AFM

○ 井手 美里¹, 山本 大輔² (¹福岡大・院理,²福岡大・理)

Misato Ide¹, Daisuke Yamamoto² (¹*Grad. Sch. Sci., Fukuoka Univ.*, ²*Fac. Sci., Fukuoka Univ.*)

- [3-11-1442](#) パターン化人工膜におけるチラコイド膜再構築技術の開発
 Reconstitution of thylakoid membrane in a patterned model membrane
 ○楠 祐佳¹, 高木 大輔², 秋本 誠志³, 前川 昌平³, 森垣 憲一^{1,4} (¹ 神大・院農学, ² 摂南大・農学, ³ 神大・院理学, ⁴ 神大・バイオシグナル総合研究センター)
Yuka Kusunoki¹, Daisuke Takagi², Seiji Akimoto³, Syouhei Maekawa³, Kenichi Morigaki^{1,4} (¹ *Grad. Sch. Agr., Univ. Kobe*, ² *Agr., Univ. Setsunan*, ³ *Grad. Sch. Sci., Univ. Kobe*, ⁴ *Bio signal Research Center, Univ. Kobe*)
- [3-11-1454](#) ストリークカメラを検出器とした細胞内局所での時間分解顕微蛍光分光
 Microscopic Time-Resolved Fluorescence Spectroscopy within a Single Chloroplast based on the Streak Camera
 ○藤田 祐輝, 張 先駿, 金田 直也, 柴田 穰 (東北大・理学研究科)
Yuki Fujita, XianJun Zhang, Naoya Kaneda, Yutaka Shibata (*Grad. Sch. Sci., Univ. Tohoku*)
- [3-11-1506](#) 二光子顕微鏡法での AMPK イメージングと ATP イメージングで見たマウス桿体視細胞の代謝回復
 Two-Photon AMPK and ATP Imaging Reveals Metabolic Recovery in Mouse Rod Photoreceptor Cells
 ○佐藤 慎哉^{1,2}, 何 家洲¹, 山本 正道², 隅山 健太³, 小長谷 有美⁴, 寺井 健太⁵, 松田 道行^{1,5,6} (¹ 京都大・院生命, ² 国立循環器病研究センター研究所, ³ 理研・大阪, ⁴ コーネル大・医, ⁵ 京都大・院医, ⁶ 京都大・iCeMS)
Shinya Sato^{1,2}, Jiazhou He¹, Masamichi Yamamoto², Kenta Sumiyama³, Yumi Konagaya⁴, Kenta Terai⁵, Michiyuki Matsuda^{1,5,6} (¹ *Grad. Sch. Biostudies, Kyoto Univ.*, ² *National Cerebral and Cardiovascular Center Research Institute*, ³ *Osaka Inst., Riken*, ⁴ *Weill Cornell Med.*, ⁵ *Grad. Sch. Med., Kyoto Univ.*, ⁶ *iCeMS, Kyoto Univ.*)
- [3-11-1518](#) マイクロビーム用いた細胞質損傷を起因とした防御的な細胞応答の解析
 Microbeam irradiation and analysis on cytoplasm damage induced defensive cellular response
 ○小西 輝昭¹, 小林 亜利紗^{1,2}, 大澤 大輔¹, 及川 将一^{1,2}, 王 军³ (¹ 量子科学技術研究開発機構 シングルセル応答解析グループ, ² 量子科学技術研究開発機構 静電加速器運転室, ³ 高磁場イオンビーム物理生物学拠点研究所 中国科学院)
Teruaki Konishi¹, Alisa Kobayashi^{1,2}, Daisuke Ohsawa¹, Masakazu Oikawa^{1,2}, Jun Wang³ (¹ *Single Cell Radiation Biology Group, National Institutes for Quantum and Radiological Science and Technology*, ² *Electrostatic Accelerator Operation Section, National Institutes for Quantum and Radiological Science and Technology*, ³ *Key Laboratory of High Magnetic Field and Ion Beam Physical Biology, Chinese Academy of Sciences*)

13:30~14:54 Ch12
 3G12 ゲノム生物学 IV
 Genome biology IV

座長：白井 剛 (長浜バイオ大学), 藤原 慶 (慶應義塾大学)
 Session Chairs: Tsuyoshi Shirai (Nagahama Inst. of Bio-Sci. and Tech.), Kei Fujiwara (Keio Univ.)

- [3-12-1330](#) 細胞内シグナリング経路を表したタンパク質間相互作用の有向グラフ
 Directed Protein-Protein Interaction Network Representing Intracellular Signaling Pathways
 ○曹 文若, 小池 亮太郎, 太田 元規 (名古屋大学・情報学研究科)
Wenruo Cao, Ryotaro Koike, Motonori Ota (*Grad. Sch. Info., Univ. Nagoya*)
- [3-12-1342](#) ジペプチドのエネルギー準位統計と分子進化
 Energy level statistics of dipeptides and molecular evolution
 ○山中 雅則 (日大・理工)
Masanori Yamanaka (*CST, Nihon Univ.*)

- [3-12-1354](#) グラフニューラルネットワークを使ったタンパク質-補酵素結合予測
Protein-cofactor binding prediction with graph neural networks
○塩生 真史, 土方 敦司 (長浜バイオ・バイオサイエンス)
Masafumi Shionyu, Atsushi Hijikata (*Fac. Biosci., Nagahama Inst. Bio-Sci. Tech.*)
- [3-12-1406](#) 単一インフルエンザウイルス集団中のヘマグルチニンゲノム配列の分布測定
Heterogeneity of Hemagglutinin Gene within Single-Plaque Population of Influenza Virus Revealed by Single-Molecule Sequencing Method
○玉尾 研二¹, 末次 正幸², 野地 博行¹, 田端 和仁¹ (¹東大・院工・応化,²立教大・院理・生命理学)
Kenji Tamao¹, Masayuki Suetsugu², Hiroyuki Noji¹, Kazuhito Tabata¹ (¹*Appl. Chem., Grad. Sch. Eng., Univ. Tokyo*, ²*Dept. Life. Sci., Col. Sci., Univ. Rikkyo*)
- [3-12-1418](#) 疾患-タンパク質-ドラッグのネットワークグラフを用いた新しい創薬ターゲット予測法
A new method to predict potential drug targets using a disease-protein-drug network graph
○土方 敦司, 塩生 真史, 白井 剛 (長浜バイオ大)
Atsushi Hijikata, Masafumi Shionyu, Tsuyoshi Shirai (*Nagahama Inst. Bio-Sci. Tech.*)
- [3-12-1430](#) Revisiting structural and functional features of phosphorylation sites
Hafumi Nishi^{1,2,3} (¹*Grad. Sch. Info. Sci., Tohoku Univ.*, ²*Fac. Core Res., Ochanomizu Univ.*, ³*ToMMO, Tohoku Univ.*)
- [3-12-1442](#) 回転並進同変なニューラルネットワークを用いた蛋白質間相互作用部位予測の検討
Towards protein interface prediction using roto-translation equivariant neural network
○中村 司 (学振 PD/東北大・院情報科学)
Tsukasa Nakamura (*JSPS-PD/Grad. Sch. Info. Sci., Tohoku Univ.*)

13:30~14:42 Ch13

3G13 計測 VI

Measurements VI

座長：相沢 智康 (北海道大学), 真壁 幸樹 (山形大学)

Session Chairs: Tomoyasu Aizawa (Hokkaido Univ.), Koki Makabe (Yamagata Univ.)

- [3-13-1330](#) Whole-mount cryo-TEM 観察による *Mycobacterium avium* 株間の菌体基礎形態情報の比較検討
Comparison of fundamental cell morphology between strains of *Mycobacterium avium* examined with whole-mount cryo-TEM
○山田 博之¹, 近松 絹代¹, 青野 昭男¹, 村田 和義², 宮崎 直幸^{2,3}, 香山 容子⁴, 御手洗 聡^{1,5} (¹ (公財) 結核予防会結核抗酸菌,² 生理学研究所,³ 大塚製薬,⁴ (株) テラベース,⁵ 長崎大)
Hiroyuki Yamada¹, Kinuyo Chikamatsu¹, Akio Aono¹, Kazuyoshi Murata², Naoyuki Miyazaki^{2,3}, Youko Kayama⁴, Satoshi Mitarai^{1,5} (¹*Dept. Mycobacterium Ref. Res., RIT, JATA*, ²*NIPS*, ³*Ohtsuka Pharm.*, ⁴*Terabase Inc.*, ⁵*Nagasaki Univ.*)
- [3-13-1342](#) 液中 AFM による肺がん細胞の薬剤耐性獲得に伴うナノスケール表面構造変化の解明
Changes in Nanoscale Surface Structures of Lung Cancer Cells Associated with Acquisition of Drug Resistance Investigated by In-Liquid AFM
○北村 太樹¹, 福田 康二², 宮澤 佳甫¹, 日笠山 拓¹, 原田 昌征¹, 矢野 聖二², 福岡 剛士¹ (¹ 金沢大学ナノ生命科学研究所,² 金沢大学がん進展制御研究所)
Taiki Kitamura¹, Koji Fukuda², Keisuke Miyazawa¹, Taku Higayama¹, Masayuki Harada¹, Seiji Yano², Takeshi Fukuma¹ (¹*Nano Life Science Institute (WPI-NanoLSI), Kanazawa University*, ²*Cancer Research Institute, Kanazawa University*)

[3-13-1354](#)

生体高分子の3D-AFM像の走査速度依存性の理論予測

A theoretical prediction of dependency of three-dimensional atomic force microscopy images of biopolymers on scanning velocity

○炭竈 享司^{1,2}, フェデリーチ フィリポ^{3,4}, ガオ デイヴィッド^{3,5}, フォスター アダム^{2,4}, 福岡 剛士^{2,6} (¹JST さきがけ, ²金沢大・ナノ生命科学研究所, ³ナノレイヤー・リサーチ・コンピューティング, ⁴アールト大・応用物理, ⁵ノルウェー科学技術大・物理, ⁶金沢大・電子情報科学)

Takashi Sumikama^{1,2}, Filippo Federici Canova^{3,4}, David Z. Gao^{3,5}, Adam S. Foster^{2,4}, Takeshi Fukuma^{2,6} (¹PRESTO, JST, ²Nano Life Sci. Inst., Kanazawa Univ., ³Nanolayers Research Computing Ltd., ⁴Dept. of Appl. Phys., Aalto Univ., ⁵Dept. of Phys., Norwegian Univ. of Sci. and Tech., ⁶Div. of Elect. Eng. and Comput. Sci., Kanazawa Univ.)

[3-13-1406](#)

NMRメタボロームを用いた昆虫食に関する研究

Research of Entomophagy by NMR-based Metabolomics

○甘 莉, 宋子豪, 大西 裕季, 久米田 博之, 熊木 康裕, 相沢 智康 (北大・院生命科学)

Li Gan, Zihao Song, Yuki Ohnishi, Hiroyuki Kumeta, Yasuhiro Kumaki, Tomoyasu Aizawa (*Grad. Sch. Life Sci., Univ. Hokkaido*)

[3-13-1418](#)

Application of low field, benchtop NMR for discriminating metabolic signature of DSS-induced colitis model mice from the healthy

Zihao Song¹, Yuki Ohnishi¹, Seiji Osada², Li Gan¹, Hiroyuki Kumeta¹, Yasuhiro Kumaki¹, Kiminori Nakamura¹, Tokiyoshi Ayabe¹, Kazuo Yamauchi³, Tomoyasu Aizawa¹ (¹Grad. Sch. Life Sci., Univ. Hokkaido, ²Nakayama Co., Ltd., ³Instrumental Analysis Section, OIST)

[3-13-1430](#)

Manganese-enhanced MRI enables early detection of neuroinflammation in the rat brain

Sosuke Yoshinaga¹, Satoshi Fujiwara¹, Shigeto Iwamoto¹, Sayaka Shibata², Aiko Sekita², Nobuhiro Nitta², Tsuneo Saga², Ichio Aoki², Hiroaki Terasawa¹ (¹Fac. Life Sci., Kumamoto Univ., ²NIRS, QST)

13:30~14:30 Ch14

3G14 計測 VII

Measurements VII

座長：永山 國昭 (N-EM ラボラトリーズ), 昆 隆英 (大阪大学)

Session Chairs: Kuniaki Nagayama (N-EM Labs LLC), Takahide Kon (Osaka Univ.)

[3-14-1330](#)

透過型電子顕微鏡の最大感度をもたらす φ ヒルベルト位相板

φ-Hilbert Phase Plates That Assure the Highest Sensitivity of Transmission Electron Microscopy

○永山 國昭 (N-EM ラボラトリーズ株式会社)

Kuniaki Nagayama (*N-EM Laboratories*)

[3-14-1342](#)

ナノスケール量子計測を用いたラベルフリー脂質二重層相転移計測

Label-free phase change detection of lipid bilayers using nanoscale diamond magnetometry

○石綿 整^{1,2}, 渡邊 宙志^{1,3}, 花島 慎弥⁴, 岩崎 孝之², 波多野 睦子² (¹ さきがけ JST, ² 東工大 工学部, ³ 慶應大学 量子コンピューティングセンター, ⁴ 大阪大学 理学部 化学科)

Hitoshi Ishiwata^{1,2}, Hiroshi C. Watanabe^{1,3}, Shinya Hanashima⁴, Takayuki Iwasaki², Mutsuko Hatano² (¹PRESTO JST, ²School of Engineering, Tokyo Institute of Technology, ³Quantum Computing Center, Keio University, ⁴Department of Chemistry, Graduate School of Science, Osaka University)

[3-14-1354](#) 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を用いたガスセンサシステム

Gas sensor system using composite molecular film of fatty acid and coumarin enhanced by hydrogenated amorphous silicon

○畠山 晃¹, 島崎 海理¹, 麦田 修¹, 佐藤 匠朗¹, 白須 健大¹, 増本 博², 込内 裕¹ (¹ 秋田大・物質科学, ² 東北大・学際研)

Hikaru Hatakeyama¹, Kairi Shimazaki¹, Shu Mugita¹, Takuro Sato¹, Kenta Shirasu¹, Hiroshi Masumoto², Yutaka Tsujiuchi¹ (¹*Grad. Mat. Sci. Univ. Akita*, ²*Fris. Univ. Tohoku*)

[3-14-1406](#) 電子顕微鏡を利用した繊維状蛋白質の解離定数の新規測定法の開発

Development of a new method to measure dissociation constant of filamentous protein complexes by electron microscopy

○渡邊 真人¹, 今井 洋¹, 宮田 知子³, 牧野 文信^{3,4}, 武藤 悦子⁵, Gerle Christoph², 光岡 薫⁶, 栗栖 源嗣², 難波 啓一³, 昆 隆英¹ (¹ 阪大・院理・生物科学, ² 阪大・蛋白研, ³ 阪大・生命機能, ⁴ 日本電子, ⁵ 中大・理工, ⁶ 阪大・超高压電顕センター)

Masato Watanabe¹, Hiroshi Imai¹, Tomoko Miyata³, Fumiaki Makino^{3,4}, Etsuko Muto⁵, Christoph Gerle², Kaoru Mitsuoka⁶, Genji Kurisu², Keiichi Namba³, Takahide Kon¹ (¹*Grad. Sch. Sci., Osaka Univ.*, ²*IPR, Osaka Univ.*, ³*Grad. Sch. Frontier Biosci., Osaka Univ.*, ⁴*JEOL*, ⁵*Chuo Univ.*, ⁶*Res. Ctr. UHVEM, Osaka Univ.*)

[3-14-1418](#) Visualizing individual dengue virus maturation states using high-speed atomic force microscopy

Steven John McArthur, Noriyuki Kodera (*WPI-Nano Life Sciences Inst., Kanazawa Univ.*)

[1S1-1](#) (1-07-1418) Dissociation mechanism of IF_1 from mitochondrial ATP synthase revealed by single-molecule analysis and manipulation

Ryohei Kobayashi, Hiroshi Ueno, Hiroyuki Noji (*Appl. Chem., Grad. Sch. Eng., Univ. Tokyo*)

IF_1 is a regulatory protein for mitochondrial ATP synthase, which inhibits ATP hydrolysis by inserting its N-terminus into the $\alpha_3\beta_3$ interface of the F_1 motor. Although biochemical assay and structural analysis have contributed to elucidate how IF_1 blocks catalysis of F_1 , the reverse reaction, IF_1 release, has not been well studied. To elucidate how IF_1 is released from F_1 , we have performed the single-molecule rotation assay of F_1 with magnetic tweezers, enabling to manipulate rotation of F_1 by applying external force. Our results indicated that ATP synthesis reaction by F_1 promotes IF_1 release. We have also revealed that the probability of IF_1 release strongly correlated with the stall angle, suggesting that it is tightly coupled with the elementary reactions of F_1 .

[1S1-2](#) Engineering biomolecular motors

Zev Bryant (*Department of Bioengineering, Stanford University*)

Molecular motors lie at the heart of biological processes ranging from DNA replication to cell migration. We use single-molecule tracking and manipulation to characterize the structural dynamics of these nanoscale assemblies, and further challenge our understanding by designing and testing structural variants with novel properties that expand the functional range of known biomolecular machines. In the process, we are developing an engineering capacity for molecular motors with tunable and dynamically controllable physical properties, providing a toolkit for precise perturbations of mechanical functions in vitro and in living cells.

[1S1-3](#) (3-07-1342) Engineering of hybrid kinesin-1 dimer with synthetic linker by tuning the neck linker length

Jakia Jannat Keya¹, Akasit Visootsat¹, Akihiro Otomo¹, Sanghun Han², Kazushi Kinbara², Ryota Iino¹ (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 dimer by conjugating with a synthetic linker through the neck-linker regions. Single-molecule fluorescence imaging of a hybrid revealed unidirectional processive motion with the velocity of 202 nm/s and run length of 1084 nm at 1 mM ATP, although lower than those of the wild-type (690 nm/s and 2740 nm). By removing 9 additional glycine linkers and 1 amino acid residue of the neck linker from the original hybrid, velocity and run length increased to 362 nm/s and 1930 nm respectively, indicating the critical role of neck linker length for fast and long processive motion. By tuning the neck linker and synthetic linker lengths, we are trying to further improve the velocity and run length of the hybrid kinesin-1 to outperform the wild-type.

[1S1-4](#) Deciphering the function of activating adaptors in the motor-driven transport of mitochondria and autophagosomes

Erika Holzbaur (*University of Pennsylvania Perelman School of Medicine*)

The axons of neurons are maintained by the active transport of organelles along the microtubule cytoskeleton, driven by the molecular motors cytoplasmic dynein and kinesin. Organelles such as mitochondria and autophagosomes co-purify with both dynein and kinesin motors, which independently drive movement to either the microtubule minus- or plus-end. We are interested in how the activities of opposing dynein and kinesin motors are coordinately regulated on an organelle by adaptor and scaffolding proteins. Here, I will focus on the role of TRAK2 in regulating dynein and kinesin motors on mitochondria, and the role of HAP1 in regulating motors on autophagosomes, using single molecule assays and live cell imaging to better understand organelle transport in neurons.

1S1-5 A rogue kinesin that destroys microtubules in cells

Kristen Verhey^{1,2}, Yang Yue¹, Lynne Blasius¹, Breane Budaitis¹ (¹*Department of Cell & Developmental Biology, University of Michigan Medical School*, ²*Department of Biophysics, University of Michigan*)

Recent work on kinesins has raised the possibility that the physical act of motors walking on microtubules creates stress in the microtubule lattice. Whether processive motility of kinesin and/or dynein motors creates stress and/or defects in the microtubule lattice in cells has not been determined. Here, we describe a kinesin-1 mutant that causes microtubule destruction when expressed in cells. Using in vitro assays, we show that the mutant motor is unable to promote rescues in microtubule dynamics assays and generates large defects in the microtubule lattice in microtubule repair assays. These findings suggest that the mutant is an unnatural or rogue motor whose activity would have been selected against during evolution.

1S1-6 Analyses of KIF1A-associated neuronal disorder by genetics and single molecule assays

Shinsuke Niwa (*FRIS, Tohoku Univ.*)

KIF1A is a motor protein that transports synaptic vesicle precursors. Mutations in KIF1A lead to broad range of neuronal diseases such as spastic paraplegia and intellectual disability. These diseases caused by KIF1A mutations are called KIF1A-associated neuronal disorder (KAND). We have analyzed KAND mutations to reveal the molecular mechanism of axonal transport and search for therapeutic approaches for neuronal diseases. Disease model worms generated by CRISPR/cas9 as well as single molecule analyses of mutant KIF1A revealed that KAND is caused by both gain-of-function and loss-of-function mechanisms, suggesting that the amount of transport is strictly regulated. The combinatorial approach revealed important physical parameters of KIF1A in the axonal transport.

1S1-7 In Vitro Reconstitution of Kinesin-1 Activation

Kyoko Chiba (*FRIS, Tohoku Univ.*)

Kinesin-1 is a microtubule motor complex composed of two kinesin heavy chains (KHC) and two kinesin light chains (KLC). Autoinhibition is an important mechanism for Kinesin-1 regulation, but the molecular details remain unclear. Using in vitro reconstitution, we show that KLC strongly inhibits the kinesin-microtubule interaction via an independent mechanism from the previously reported tail-motor interaction within KHC. The motility of Kinesin-1 was recovered by addition of cargo-adaptor proteins that binds to KLC and further enhanced by a non-motor MAP protein. Our results suggest that Kinesin-1 is regulated by a two-factor mechanism comprised of intramolecular allosteric regulation, as well as intermolecular kinesin-adaptor and kinesin-MAP interactions.

1S2-1 Molecular pattern recognition in DNA-based artificial neural networks

Lulu Qian (*Caltech*)

Recognizing specific patterns of molecular signals is an essential type of function required for information-processing circuits in biological organisms. DNA-based neural networks have been developed to perform molecular pattern recognition within biochemical environments. Here we show a systematic implementation of winner-take-all neural networks using DNA strand-displacement reactions. We demonstrate the classification of 100-bit patterns shown as handwritten digits. Patterns with up to 30 flipped bits compared to the “remembered” digits can still be successfully recognized. Our results suggest the possibility of embedding molecular circuits within biochemical environments to classify highly complex and noisy information based on similarity to a memory.

1S2-2 Computer designed organisms

Josh Bongard (*Dept. Computer Sci., Univ. of Vermont*)

Creating an artificial cell may require design help from artificial intelligence methods. So, I will present our work on creating AI that can design biological robots: mm-sized collections of frog skin and heart muscle tissue. The AI method receives as input a mathematical description of what the “xenobot” should do, and the AI then searches the space of all possible frog tissue rearrangements that will result in a simulated xenobot that performs that task. The most promising xenobot designs are then sent to a human microsurgeon, who builds those xenobots using a cellular construction kit. We have found that this AI / microsurgeon team can create xenobots that walk, swim, perform collective behaviors, and can remember and report back on what they have seen.

1S2-3 化学反応ネットワークと連携したベシクルの再生産 Reproduction of vesicle coupled with chemical reaction network

Masayuki Imai¹, Minoru Kurisu¹, Peter Walde² (¹*Dep. Phys., Tohoku Univ.*, ²*Dep. Materials, ETH Zurich*)

The life is a network of chemical reactions to reproduce itself, which is composed of three essential domains. (1) energy production domain, which synthesizes energy currencies from glucose, (2) processing of genetic information domain, which replicates the information molecule DNA and synthesizes proteins via RNA, and (3) membrane reproduction domain, which synthesizes membrane molecules and realizes growth and division. We have constructed an artificial minimal cell system equipped three equivalent domains using non-biological molecules. A key of this system is “template” polymerization on membrane, where polymer encodes the membrane molecules and encourage selective membrane growth. We will discuss physical background of this minimal cell system.

1S2-4 Mesoscale DNA-based machines powered by artificial metabolism

Shogo Hamada (*Dept. of Robotics, Tohoku Univ.*)

Metabolism plays a key role in life by dynamically generating materials from a continuous flux of matter and energy. Mimicking such a system could lead to molecular robots with life-like characteristics. As a first step towards the goal, we have developed dynamic DNA materials with artificial metabolism. Coupling synthesis and assembly of DNA achieved autonomous generation and degeneration of patterns. A new class of machines was realized by programming behaviors of the material. Two types of behaviors, emergent locomotion and racing, were implemented. Other applications, such as pathogen detection, were also demonstrated. A discussion includes potential future perspectives on artificial metabolism and ongoing attempts related to the vision of chemical AI.

1S2-5 ケミカル AI 構築に向けた修飾アデニンの光環化付加反応による人工核酸の光制御 Photoregulation of Artificial Nucleic Acid via Photo-Cycloaddition of Modified Adenine Residues for Chemical AI

Keiji Murayama¹, Yuuhei Yamano², Hiroyuki Asanuma¹ (¹*Grad. Sch. Eng., Nagoya Univ.*, ²*IMRAM, Tohoku Univ.*)

For achievement of chemical AI, effective photoregulation system that can control signal information by light-stimulus is highly important. We developed photocontrol of duplex formation between the artificial serinol nucleic acid (SNA) and RNA, using a photo-responsive nucleobase 8-pyrenylvinyl adenine (P^VA). When the P^VA-SNA/RNA duplex was irradiated with 455 nm light, almost complete dissociation of the duplex was attained via intrastrand [2+2] photocycloaddition, and 340 nm light restored duplex formation by cycloreversion. This is first example of use of photocycloaddition and cycloreversion to photo-regulate canonical duplex formation and dissociation reversibly at constant temperature.

IS3-1 銅・亜鉛スーパーオキシドディスムターゼの成熟化におけるシステイン残基の役割
A dual role of cysteine residues in the maturation of prokaryotic Cu/Zn-superoxide dismutase

Yoshiaki Furukawa (*Dept. Chem., Keio Univ.*)

Bacterial Cu/Zn-superoxide dismutase (SodC) is an enzyme catalyzing the disproportionation of superoxide radicals, to which the binding of copper and zinc ions and the formation of an intramolecular disulfide bond are essential. Here, we show that the disulfide-reduced SodC can secure a copper ion as well as a zinc ion through the thiolate groups. Furthermore, the disulfide-reduced SodC was found to bind cuprous and cupric ions more tightly than SodC with the disulfide bond. Based upon the experiments *in vitro*, therefore, we propose a mechanism for the activation of SodC, in which the conserved Cys residues play a dual role: the acquisition of a copper ion for the enzymatic activity and the formation of the disulfide bond for the structural stabilization.

IS3-2 時間分解分光法を用いたヘム ABC トランスポーター BhuUV-T における輸送過程の速度論的解析
Kinetic analysis of the transport in heme ABC transporter; BhuUV-T, by time-resolved spectroscopy

Tetsunari Kimura (*Grad. Sch. Sci., Kobe Univ.*)

Structural analyses of ABC transporters have clarified their stable conformations bound with nucleotides, suggesting the alternating access mechanism, in which the conformational change of transmembrane domain induced by the ATP binding/hydrolysis reaction is the key step of the transport. Complementary observations in structural and functional dynamics along the reaction axis is necessary to substantiate the mechanism, allocrites are chemically silent during the transport, indicating that the observation of allocrite transport is difficult. In this study, dynamics of the heme ABC transporter; BhuUV-T complex, was kinetically investigated due to the changes in spectrum of its allocrite; heme, along the binding manner, and the detailed mechanism will be discussed.

IS3-3 Computational study of the structural–function relationship of heme proteins

Yu Takano¹, Hiroko X. Kondo², Yusuke Kanematsu³ (¹*Grad. Sch. Info. Sci., Hiroshima City Univ.*, ²*Fac. Eng., Kitami Inst. Tech.*, ³*Grad. Sch. Adv. Sci. Eng., Hiroshima Univ.*)

Heme proteins are involved in various biochemical functions. More than 5000 heme protein structures have been reported and deposited in Protein Data Bank (PDB). Given the recent accelerating increase of the available data, the combination of statistical analysis and molecular simulation on heme proteins will pave the way to seek how they make excellent use of their hemes to control their functions. We report a study of the structural–function relationship of heme proteins, in particular heme porphyrin distortion, with the combination of statistics, machine learning, and quantum chemical calculation.

IS3-4 SR-Ca²⁺-ATPase における E1/E2 転移の反応座標の解析
Analysis of reaction pathway in E1/E2 transition of SR-Ca²⁺-ATPase

Chigusa Kobayashi¹, Yasuhiro Matsunaga², Jaewoon Jung^{1,3}, Yuji Sugita^{1,3,4} (¹*RIKEN, R-CCS*, ²*Grad. Sch. Sci. Eng., Saitama Univ.*, ³*RIKEN, CPR*, ⁴*RIKEN, BDR*)

Sarcoplasmic reticulum (SR) Ca²⁺-ATPase (SERCA) transports two Ca²⁺ across the membrane against a 10⁴ times concentration gradient by utilizing ATP hydrolysis. Although X-ray structures of the E1P and E2P states have been revealed, the atomic-level details of the intermediates and pathways have not been elucidated. In this study, we perform simulation with a mean-force string to calculate the minimum free energy pathway between two states. We also analyze the reaction pathway and the relationship between their domains. The simulations show a series of structural changes starting from the cytoplasmic domains, gradually occurring in loops between the cytoplasmic domains and the TM helices, and then in the Ca²⁺ binding site.

1S3-5 Design of staphylococcal two-component pore forming toxin to change pore formation property

Nouran Ghanem^{1,2}, Takashi Matsui^{1,3}, Jun Kaneko⁴, Tomomi Uchikubo-Kamo², Mikako Shirouzu², Tsubasa Hashimoto¹, Tomohisa Ogawa^{1,4}, Tomoaki Matsuura⁵, Po-Ssu Huang⁶, Takeshi Yokoyama^{1,2}, **Yoshikazu Tanaka**¹ (¹Graduate School of Life Sciences, Tohoku University, ²Laboratory for Protein Functional and Structural Biology, RIKEN Center for Biosystems Dynamics Research, ³School of Science, Kitasato University, ⁴Graduate School of Agricultural Science, Tohoku University, ⁵Earth-Life Science Institute, Tokyo Institute of Technology, ⁶Department of Bioengineering, Stanford University)

Staphylococcus aureus expresses several hemolytic pore-forming toxins (PFTs). PFTs are expressed as soluble monomers and assemble to form a transmembrane β -barrel pore in the erythrocyte cell membrane. It remains challenging to design PFTs with a β -barrel pore because their formation requires large conformational changes. In this study, to investigate the design principles of the β -barrel pore, chimeric mutants composed of the outer membrane domains of one-component PFT and a stem of two-component PFTs were prepared. Biochemical characterization showed that one of them assembles as a one-component PFT, while another can participate as both one- and two-component PFT. Based on these observations, the role of the domains of these PFTs is discussed.

1S3-6 放射光顕微システムによる細胞内小分子イメージングと医学応用の試み
Visualization of intracellular small molecules using synchrotron radiation and its trials for medical application

Mari Shimura (*Nat. Cent. for Global Health and Med.*)

Omics for disease analyses have been conducted even at single cell level; however, studies of the intracellular distribution of small molecules are not well understood. We have developed a scanning X-ray fluorescence microscope system (SXF) at SPring-8 (Harima, Riken) that can reliably determine the cellular distribution of multiple elements at organelle-level. We successfully developed methods for imaging intracellular fatty acids by labeling with a single element and SXFM. We demonstrate SXFM, and discuss the possibility for medical application, e.g., a drug screening, diagnosis or prognosis of diseases. 1. Matsuyama S, *et al*, *JAAS*, 35, 2020. 2. Shimura M, *et al*, *FASEB J.* 30, 2016. 3. Imai R, *et al*, *Scientific Report*, 2016. 4. Shimura M, *et al*, *Cancer Res.* 65, 2005.

1S4-1 高速 AFM による一分子動態イメージングデータと分子シミュレーション
High-speed-AFM imaging of single-molecule dynamics and molecular simulation

Takayuki Uchihashi^{1,2} (¹Graduate School of Science, Nagoya University, ²ExCELLS, NINS)

Advances in high-speed atomic force microscopy have enabled us to directly visualize dynamic various dynamic actions of individual molecules under physiological conditions. While HS-AFM provides information on global structural dynamics of a protein, it is often difficult to understand the molecular mechanisms behind the observed dynamics due to the limited spatial and temporal resolution and the inability to visualize the internal molecular structure. Therefore, in order to truly understand the phenomena observed by HS-AFM at the molecular level, collaboration with computational science is essential. In this talk, I will introduce recent studies on the integration of high-speed AFM images and computational simulation.

1S4-2 高速原子間力顕微鏡データと分子シミュレーションのデータ同化による動的構造解析
Dynamic structure analysis by data assimilation combining high-speed atomic force microscopy data and molecular simulations

Sotaro Fuchigami¹, Yasuhiro Matsunaga², Shoji Takada¹ (¹Grad. Sch. of Science, Kyoto Univ., ²Fac. of Engin., Saitama Univ.)

High-speed atomic force microscopy (HS-AFM) is an outstanding technique to observe structural dynamics of a single biomolecular system at work in real time and with nanometer resolution. However, its spatiotemporal resolution is not enough to reveal atomic details. In the present study, we focused on walking myosin V along actin filament and aim to provide detailed information on its structural dynamics using single-molecule measurement data by HS-AFM. First, we performed coarse-grained molecular dynamics simulation of modeled myosin V in three different states many times. Then, we constructed Markov state model (MSM) describing its walking dynamics using obtained trajectories. Finally, we performed a hidden Markov model analysis using experimental data and MSM.

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- [1S4-3](#) 分子モーターの化学力学共役モデルのベイズ推定
Bayesian inference of the chemomechanical coupling model of molecular motors

Kei-ichi Okazaki (*Inst. for Mol. Sci.*)

The mechanism of biomolecular motors has been elucidated using single-molecule experiments for visualizing motor motion. However, it remains elusive that how changes in the chemical state during the catalytic cycle of motors lead to unidirectional motions. In this study, we use single-molecule trajectories to estimate an underlying diffusion model with chemical-state-dependent free energy profile in the Bayesian inference framework. We develop a novel framework based on a hidden Markov model, wherein switching among multiple energy profiles occurs reflecting the chemical state changes in motors. The method is tested using simulation trajectories and applied to single-molecule trajectories of molecular motors such as chitinase and kinesin.

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- [1S4-4](#) DNA上や相分離複合体内でのタンパク質ダイナミクスの単分子計測と分子動力学解析
Single molecule and molecular dynamics characterization of protein action along DNA and in liquid droplets

Kiyoto Kamagata (*IMRAM, Tohoku Univ.*)

DNA-binding proteins are involved in the cell fate regulation. How do DNA-binding proteins search for and recognize the target sequence on genomic DNA? To solve this question, we visualized the movements of several proteins along DNA using single-molecule fluorescence microscopy coupled with DNA garden. I will focus on complex dynamics of Nhp6A and its bypass over obstacles bound to DNA, which is supported by molecular dynamics simulations. In addition, p53 undergoes liquid-liquid phase separation. How are guest proteins recruited into p53 droplets? How do they move within the droplets? We investigated the uptake and dynamics property of guest proteins using single-molecule fluorescence microscopy coupled with molecular dynamics simulations. I will present our findings.

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- [1S4-5](#) 光子相関計測で解き明かす生体分子のマイクロ秒構造・機能ダイナミクス
Microsecond Structural and Functional Dynamics of Biomolecules Revealed by Photon Correlation Measurements

Kunihiko Ishii (*Mol. Spectrosc. Lab., RIKEN*)

Single-molecule FRET (smFRET) is a powerful technique to elucidate structural and functional dynamics of biomolecules. However, the time resolution of smFRET measurement has been typically limited to the millisecond time scale. Two-dimensional fluorescence lifetime correlation spectroscopy (2D FLCS), recently developed by us, is able to detect a fast structural dynamics taking place in a few microsecond time scale, by analyzing temporal correlation of photon emission events from different conformers. In this talk, I will present a few applications of 2D FLCS, in which (1) the mechanisms of protein folding were studied and (2) biologically relevant dynamics of a functional RNA molecule was elucidated.

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- [1S4-6](#) 生物分子モーターの再デザインと計測
Re-designing and measuring biomolecular motors

Ken'ya Furuta (*Advanced ICT, NICT*)

Living organisms use fast intracellular logistics that are powered by biological molecular motors, which can be potential microscale actuators. A limitation is that neither motors nor cytoskeletal filaments can be re-designed. To overcome this limitation, we constructed a new variety of "possible" motor systems. The tracks can be cytoskeletal tracks that are not compatible with original motors or even artificial DNA nanotubes. Our strategy will open the way to systematic research on the mechanisms of biomolecular motors and to nanotechnological applications, including microscopic robots that undergo sequential procedure, computation, and synthesis of chemical compounds according to the programmed code incorporated into DNA tracks.

[1S4-7](#) 一分子計測からたんぱく質のエネルギー地形の階層性を抽出する
Capturing hierarchical features in protein energy landscape from single molecule time series

Tamiki Komatsuzaki^{1,2} (¹*RIES, Hokkaido Univ.*, ²*WPI-ICReDD, Hokkaido Univ.*)

Hierarchical features of the energy landscape of the folding/unfolding behavior of adenylate kinase are elucidated in terms of single-molecule fluorescence resonance energy transfer measurements. The core in constructing the energy landscape from single-molecule time-series is the application of rate-distortion theory, which naturally considers the effects of measurement noise and sampling error etc. Energy landscapes are constructed as a function of observation time scale, revealing multiple partially folded conformations at small time scales that are situated in a superbasin. As the time scale increases, these denatured states merge into a single basin, demonstrating the coarse-graining of the energy landscape as observation time increases.

[1S5-1](#) Large-scale transcriptome analysis at single cell level

Piero Carninci (*RIKEN Center for Integrative Medical Sciences*)

Long non-coding RNAs (lncRNAs) play key roles in genomic regulation. To understand it, we developed the CAGE technology, which identifies transcription start sites generally overlapping promoters, enhancers and lncRNAs, quantitatively measuring their activity genome-wide. Using CAGE, we broadly explored such regulatory elements activity in a large panel of human and mouse primary cells in FANTOM5 and created a large knockdown data set of lncRNAs to explore lncRNA functions in FANTOM6. We are also working with Human Cell Atlas (HCA) to create a comprehensive transcriptional regulatory map of all human cells at single cell level. We developed single cell CAGE and bioinformatics pipeline for the 10X Genomics platform, which promises an acute power of analysis.

[1S5-2](#) 機械学習によるシングルセル・ダイナミクスからの生物学的原理の解読
Deciphering Biological Principles from Single-cell Dynamics by Machine Learning

J. Tetsuya Kobayashi (*IIS, UTokyo*)

Discovering patterns and rules from single-cell dynamics is an important but non-trivial task. In this talk, we show two examples of how we can use machine learning for this purpose. We mainly focus on how growth and replication are controlled at the single-cell level. In the first part, we show an application of latent state inference to characterize growth mode and its transition over cellular lineages. In the second part, we will show another approach by using a deep neural network, with which the size control law of microbes can be extracted only from data. These examples demonstrate how machine and deep learning can assist us in searching for and characterizing cellular states, their dynamical rules, and relations among multiple observables and their combinations.

[1S5-3](#) ネットワーク化計測によるプール型細胞解析
Networked measurement for pooled cell analysis

Sadao Ota^{1,2} (¹*RCAT, Univ. Tokyo*, ²*Thinkcyte Inc*)

Pooled formats in biological assays are holds high potential in scalability, throughput, reduction of the reagent usages and cost, resolutions down to single cells levels, and the small batch effect. Considering these, future pooled formats may enable powerful automated platforms. In today's talk, I introduce a ghost cytometry-based cell phenotyping and a pooled screening platform enabled by the ghost cytometry-based high throughput cell sorter. Ghost cytometry is a flow cytometric technology which employs machine learning methods to analyze cells based on their image information without image reconstruction, either in fluorescence or label-free modes. If I have time, I may be introducing a novel platform enabling multiplexed networked measurement.

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- 1S5-4** 情報理論解析による細胞間のばらつきを活かした正確な応答制御機構の解明
Information analysis reveals that cell-to-cell variability can improve the accuracy of the control of biological responses

Takumi Wada¹, Ken-ichi Hironaka², Shinya Kuroda^{2,3} (¹Center for iPS Research and Application, Kyoto Univ., ²Grad. Sch. Sci., Univ. Tokyo, ³Grad. Sch. Front. Sci., Univ. Tokyo)

The heterogeneity in cellular responses has been regarded as noise that reduces accurate information transmission. The heterogeneity consists of intracellular variation caused by stochasticity of biochemical reactions, and intercellular variation caused by differences in gene expression (i.e., cell-to-cell variability). However, the intercellular variation has the potential to enable accurate control of the cellular response by increasing the gradualness of the response. This means that a tissue with cells that exhibit different responses has a wider dynamic range for interpreting stimulation intensity. This response diversity effect is a previously unappreciated mechanism enabling multicellular organisms to use cell-to-cell variability as information, not noise.

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- 1S5-5** 一細胞プロテオーム解析を目指した三次元一分子イメージングによるバイオ分析法の開発
3D single-molecule imaging-based bioanalyses towards single-cell proteomics

Sooyeon Kim^{1,2}, Latiefa Kamarulzaman^{1,3}, Yuichi Taniguchi^{1,2,3} (¹RIKEN, BDR, ²iCeMS, Kyoto Univ., ³Grad. Sch. Front. Biosci., Osaka Univ.)

Cells even with the same genome are known to exhibit varied protein expression profiles depending on their surroundings and phase. To obtain phenotype information at cellular level, analyzing single-cell proteins is the most direct choice. Nonetheless, its infinitesimal amount (~300 picogram), vast kinds (> 30,000), and difficulty in amplification make single-cell proteomics technically challenging. Herein, we developed single-molecule fluorescence gel electrophoresis with a light-sheet microscope that can image each protein molecule embedded in a gel. As a result, tens of protein bands from a single-cell sample were successfully distinguished. We believe this method is beneficial for studying cell differentiation, tracing stage transition, and cancer diagnostics.

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- 1S6-1** ヒトプロスタグランジン受容体 EP3-G タンパク質複合体の構造解析
Structural insights into the human Prostaglandin E2 receptor EP3- Gi signaling complex

Ryoji Suno (*Dept. Med., Kansai Med. Univ.*)

Prostaglandin receptors are involved in a wide range of functions such as inflammation, immune response, reproduction, and cancer. Here, we report the cryo-EM structure of the human EP3-Gi signaling complex at a resolution of 3.4 Å and revealed the structural changes due to G protein binding and the binding mode of G proteins. We compared the EP3-Gi complex with previously reported EP2 / EP4-Gs complex structures and investigated the differences in amino acid residues at each receptor site with which the G protein interacts. Mutant analysis of these amino acid residues revealed that the specific amino acid residues of the second intracellular loop and TM5 contribute to the selectivity of G proteins.

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- 1S6-2** Back and forth between purified and cellular systems for GPCR biology

Asuka Inoue (*Grad. Sch. Pharm., Tohoku Univ.*)

In cells, GPCRs are regulated by a series of factors and their behaviors may differ from those in purified systems. Over years, our lab has spent efforts to establish and standardize GPCR tools that enable reliable measurement of individual GPCR signaling in cells. These include TGF α shedding assay, NanoBiT-G-protein dissociation assay, a panel of GPCR effector-KO cells (G-protein, β -arrestin, GRK), etc. For example, these tools are useful for mutant experiments of not only validation studies of structural analyses, but also screening/construct optimization studies. In this presentation, I will present these GPCR analysis tools that have illuminated structural GPCRs. In addition, I will show recent advance of understanding a novel mode of signal bias regulation.

1S6-3 Spatiotemporal Determinants and Allosteric Communication Modulate the Ligand Bias in GPCRs

Nagarajan Vaidehi (*Chair, Department of Computational & Quantitative Medicine, Beckman Research Institute of the City of Hope, Duarte, CA*)

The G-protein coupled receptor (GPCR) interactions with the G protein or b-arrestin are inherently transient, dynamic and exhibit exquisite selectivity or promiscuity. These selectivity or promiscuity determinants emerge from the dynamics of the GPCR:G protein complexes. Using molecular dynamics simulations with FRET experiments we show that the spatio-temporal components play a critical role in explaining the selective coupling of GPCRs towards G proteins and b-arrestins. We have delineated the residue networks involved in allosteric communication from the ligand binding site to the G protein or b-arrestin coupling site. Knowledge of these residue networks would allow us to design ligands that are specific or “biased” to a given signaling pathway. Such “biased ligands” are therapeutically desirable and would enable design of drugs with minimal side effects.

1S6-4* (2-06-1515) 分子シミュレーションによるオレキシン 2 受容体-G タンパク質複合体の動的性質の研究
(2-06-1515) Dynamics of Orexin2 Receptor and G-protein Complex with Molecular Dynamics Simulations

Shun Yokoi, Ayori Mitsutake (*Department of Physics, School of Science and Technology, Meiji University*)

Orexin2 receptor (OX2R) is classified as a class A G-protein-coupled receptor (GPCR) and belongs to the group of orexinergic systems. The OX2R is involved in the regulation of feeding behavior and sleep-wake rhythm to give some examples. Such kinds of neurological processes are caused by GPCR activation. Although the structure of the OX2R has been clarified, the atomic-level mechanisms of GPCR and G-protein activation remain unknown. Here, we performed and analyzed several microsecond-scale molecular dynamics (MD) simulations. In this poster, we first show the results of the MD simulations and investigate the dynamics of OX2R and G-protein complex. Then, we discuss implications for the activation mechanism of OX2R and for the binding mechanism of G-protein.

1S6-5 配位ケモジェネティクスによる GPCR 型グルタミン酸受容体の活性制御
Coordination chemogenetics for direct activation of GPCR-type glutamate receptors in brain tissue

Shigeki Kiyonaka (*Grad. Sch. Eng., Nagoya Univ.*)

Direct activation methods of cell-surface receptors are highly desired for clarifying physiological roles of the receptors. However, subtype-selective ligands are very limited because of the high-homology among the receptor subtypes. Here, we develop a novel chemogenetic method for direct activation of metabotropic glutamate receptor 1 (mGlu1) having essential roles in cerebellar function in brain. Our screening identified a mGlu1 mutant, which was directly activated by palladium complexes. Notably, a palladium complex showing low cytotoxicity successfully induced mGlu1-dependent synaptic plasticity in the mice.

1S6-6* (2-01-1451) アデノシン A_{2A} 受容体の不活性型構造を安定化するための all- α 融合パートナータンパク質のゼロからの合理デザイン
(2-01-1451) De novo design of an alpha-helical fusion partner protein to stabilize adenosine A_{2A} receptor in the inactive state

Masaya Mitsumoto^{1,2}, Kanna Sugaya³, Kazuki Kazama³, Ryosuke Nakano³, Takahiro Kosugi^{1,2,4}, Takeshi Murata³, Nobuyasu Koga^{1,2,4} (¹SOKENDAI, ²IMS, NINS, ³Grad. Sch. of Sci. and Eng., Chiba Univ., ⁴ExCELLS, NINS)

GPCRs are known for low stability and large conformational changes upon transitions between multiple states. Here, we aim to rationally stabilize one of the class A GPCRs, adenosine A_{2A} receptor (A_{2A}R), in a targeted state. For class A GPCRs, the transmembrane helices 5 and 6 (TM5 and TM6) connected by the intracellular loop 3 (ICL3) exhibit large conformational changes. Therefore, we computationally de novo designed an all- α fusion partner protein FiX1, designed to be fused to the TM5 and TM6 of the inactive-state A_{2A}R without kinks or intervening loops. Experimentally, FiX1 was found to be folded into unique shape and form helical structures even around 100°C, and the fusion of A_{2A}R with FiX1 was found to be stabilized in the inactive state as designed.

1S6-7 Conformational dynamics upon ligand binding in muscarinic acetylcholine receptor revealed by FTIR spectroscopy

Kota Katayama^{1,2} (¹*Grad. Sch. Eng., Nagoya Inst. Tech.*, ²*PRESTO, JST*)

The intrinsic efficacy of ligand binding to GPCRs reflects the ability of the ligand to differentially activate its receptor to cause a physiological effect. Here we use attenuated total reflection-Fourier transform infrared (ATR-FTIR) spectroscopy to examine the ligand-dependent conformational changes in the human M₂ muscarinic acetylcholine receptor (M₂R). We show that different ligands affect conformational alteration appearing at the C=O stretch of amide-I band in M₂R. Notably, ATR-FTIR signals strongly correlated with G-protein activation levels in cells. Together, we propose that amide-I band serves as an infrared probe to distinguish the ligand efficacy in M₂R and paves the path to rationally design ligands with varied efficacy towards the target GPCR.

1S7-1 Secondary-probe based DNA-PAINT super-resolution imaging for unlimited multiplexing

Mahipal Ganji (*Department of Biochemistry, Indian Institute of Science, Bangalore, India*)

Biological systems emerge from the coordinated activities of a multitude of macromolecular interactions. To understand those emerging properties, we need to visualize the comprehensive distribution, stoichiometry, and interacting partners in their native environment. However, current imaging modalities do not allow to image a large number of targets with high-resolution. DNA-PAINT is a versatile technique that not only provides close to molecular resolution but also allows for multiplexed imaging beyond the number of spectrally well-separated fluorophores. Based on the DNA nanotechnology approach, we will present novel implantation of DNA-PAINT for “unlimited” multiplexed imaging of a large number of targets in a single sample.

1S7-2 1分子イメージングで迫るヒト染色体の動的組織化
Single molecule imaging unveils the dynamic organization of the human chromosomes

Kayo Hibino¹, Yuji Sakai², Masato Kanemaki¹, Kazuhiro Maeshima¹ (¹*Natl. Inst. Genet. & SOKENDAI*, ²*Univ. Tokyo*)

The mitotic chromosome condensation during cell division is a dramatic reorganization of the long thin genome chromatin polymers (several centimeters) into compact short chromosomes (several micrometers). The processes of chromosome condensation were thought to be mediated by the chromatin looping, which requires condensin and topoisomerase II α (TopoII α), however, the underlying mechanism remains unclear. Here, by using single nucleosome imaging in living human cells, we measured local nucleosome dynamics during the condensation. Combining with simulation studies, we discuss how condensin and TopoII α involve the chromosome condensation in an intracellular environment from the biophysical aspect.

1S7-3 BAR domain protein function in plasma membrane remodeling during embryogenesis

Richa Rikhy (*Biology, IISER, Pune, India*)

BAR domain containing proteins play a role in various plasma membrane remodeling events seen in endocytosis, cell migration and cell division. We have found a role for BAR domain containing protein GRAF in restricting actomyosin ring contractility in cellularization in *Drosophila* embryogenesis. GRAF contains the BAR, PH, RhoGAP and SH3 domains and recruits to the contractile ring at early stages of cellularization. GRAF loss of function mutants show an increase in actomyosin based contractility in a RhoGAP domain dependent manner. This phenotype is suppressed in RhoGEF2 and Rho kinase mutants. Our data together show that GRAF regulates the rate of actomyosin contractility thereby promoting adhesion during cellularization.

1S7-4**上皮集団遊走におけるメカノケミカルフィードバック**
Mechanochemical feedbacks in collective cell migration of epithelial cells

Tsuyoshi Hirashima^{1,2}, Naoya Hino^{2,4}, Daniel Boocock⁴, Michiyuki Matsuda^{2,3}, Edouard Hannezo⁴ (¹*The Hakubi Center, Kyoto Univ*, ²*Grad Sch Biostudies, Kyoto Univ*, ³*Grad Sch Med, Kyoto Univ*, ⁴*IST Austria*)

Collective cell migration offers a rich field of research for cellular biology and non-equilibrium physics, but it remains unclear how mechanical and chemical signaling are integrated at the cellular level to give rise to such collective behaviors. We address this by focusing on the spatiotemporal patterns of cell density and intracellular signaling activity ERK, which appear both in vitro and in vivo during collective cell migration. We propose a simple mathematical model, supported by mechanical and optogenetic perturbation experiments, showing that patterns can be quantitatively explained by a mechanochemical coupling between active cellular tensions and the mechanosensitive ERK signaling.

1S7-5**Dynamics of active-polar gels on curved surfaces**

Vijay Kumar Krishnamurthy¹, Siddharth Jha², Swapnil Kole², Sriram Ramaswamy² (¹*International Centre for Theoretical Sciences, Bengaluru*, ²*Indian Institute of Science, Bengaluru*)

Active deformable surfaces are widely found in living matter -- the prime examples being the cortex-membrane composite structure at the cellular level and sheets of epithelial tissues in developing organisms. Mechanical stresses generated by nonequilibrium activity drive the shape changes of these surfaces. We study the dynamics of an active polar gel confined to a curved manifold. We find a variety of interesting phases, even on stationary surfaces, that result from the coupling of the density and orientational fields to the underlying geometry. We show that surface curvature can control the localization of topological defects. Our flexible computational approach can easily be extended to active surfaces with non-trivial shapes.

1S7-6**Compositional identity and robustness of autocatalytic RNA reaction networks in coacervate protocells**

Shashi Thutupalli^{1,2} (¹*National Centre for Biological Sciences, Tata Institute for Fundamental Research*, ²*International Centre for Theoretical Sciences, Tata Institute for Fundamental Research*)

We encapsulate a self-reproducing RNA system within coacervate compartments where catalytic RNAs result from the autocatalytic assembly of the constituent smaller RNA fragments. The compartments locally enhance the concentrations of the RNA fragments, resulting in a concomitant rate enhancement of the self-assembly process. This self-assembly occurs both by self- and cross-catalysis, allowing us to construct complex networks of RNA self-reproducers. The coacervate compartments transiently protect the chemical networks from perturbations due to external, parasitic catalysts. Our results establish a compartmentalised chemical system possessing a compositional identity that exists at a balance between robustness and the variability required for the chemical evolution.

1S7-7***C. elegans* の集団運動**
Collective motion of *C. elegans*

Ken H. Nagai¹, Hiroshi Ito², Takuma Sugi³ (¹*JAIST*, ²*Kyushu University*, ³*Hiroshima University*)

Unclear is what kinds of collective motion of animals can be described by simple descriptions like the Vicsek model, since animals generically have little experimentally easily-controllable parameters. To study collective motion of one of the model animals, *Caenorhabditis elegans*, we developed a new cultivation method with which highly concentrated worms formed dynamical networks. We proposed a minimal model with two characteristics found in isolated worm's motion: long-time memory of rotation rate, and nematic alignment of two worms after collision. The simple model reproduced the formation of the dynamical network and the responses to various external perturbations well, which indicates that the two characteristics mainly govern the collective motion of *C. elegans*.

1S8-1 Nonthermal Excitation Effects Mediated by Sub-Terahertz Radiation on Biomolecular Hydration Dynamics and Reactions

Masahiko Imashimizu¹, Yuji Tokunaga¹, Masahito Tanaka², Jun-ichi Sugiyama³ (¹*CMB, AIST*, ²*NMRI, AIST*, ³*NMRI, AIST*)

At physiological temperatures in aqueous solution, fast fluctuating dynamics of biomolecules and coupled water molecules occur in the terahertz (THz) and sub-THz frequency range. Recent our studies have suggested that the externally applied alternating electromagnetic field with (sub)-THz frequency nonthermally influences biomolecular functions. If such a phenomenon indeed occurs, one needs to assume a very slow relaxation pathway in which (sub)-THz excitation energy must be retained and localized in the biomolecule-water interface (i.e. hydration water) until the timedomains relevant to the expression of biomolecular functions. However, this notion appears to be inconsistent with the conventional physicochemical view of water dynamics.

1S8-2 荷電フィラメント周りの協同的水分子運動 -マイクロ波誘電緩和とラマン OH 伸縮/ベンディング分光-
Collective water behavior around charged filaments by microwave dielectric relaxation and Raman OH-stretching/bending bands spectroscopy

Makoto Suzuki (*IMRAM, Tohoku Univ.*)

The hydrating water dynamics is affected by the electric field and structural barrier (vdw) of the solute and cosolvents. The properties of hydration water were observed by high-resolution microwave dielectric relaxation spectroscopy (DRS) as showing dual hydration layers of restrained water and hyper-mobile water around alkali-halide ions, F-actin, charged polymers and dsDNA. The properties of the hydration water have been also measured by high-precision Raman OH-stretching/HOH-bending bands spectroscopy which could observe the Fermi resonance of OH-stretching mode and HOH-bending overtone, indicating collective dynamics among water molecules around the charged filaments. It suggests the importance of various collective modes of water clusters around solute molecules.

1S8-3* (2-02-1624) 水和水の OH 伸縮振動バンドに基づく生体保護作用を持つ小分子の水素結合強化作用の評価
(2-02-1624) Hydrogen bond strengthening effect of stabilizing osmolytes investigated by OH stretching band of hydration water

Fumiki Matsumura¹, Toshiyuki Shikata², Yuichi Ogawa¹, Tetsuhito Suzuki¹, Naoshi Kondo¹, Keiichiro Shiraga¹ (¹*Grad. Sch. Agri., Kyoto Univ.*, ²*Grad. Sch. Agri., Tokyo Univ. of Agriculture and Technology*)

Although number of studies have addressed its importance, general understanding of the protein-stabilizing effects of osmolytes on water hydrogen bond strength is yet to be reached. In this study, with the aid of dielectric relaxation spectroscopy in the microwave region, we determined the OH stretching band of water molecules around stabilizing osmolytes: trehalose and Trimethylamine-N-oxide (TMAO). We found that these stabilizing osmolytes let surrounding water molecules enhance the red-side of the OH stretching intensity, which clearly shows that both trehalose and TMAO strengthen hydrogen bonds of water surrounding them. This result indicates that water molecules with strong hydrogen bond can be an essential characteristic of stabilizing osmolytes.

1S8-4 高圧力下誘電分光測定による全濃度範囲におけるグリセロール水溶液の過冷却水のダイナミクスに関する研究
High-pressure dielectric study of dynamics of supercooled water in whole concentration range glycerol-water mixtures

Kaito Sasaki (*Dept. Phys. Sch. Sci., Tokai Univ.*)

The so-called two-state model is sometimes adopted to understand the properties of liquid water. Using the idea of polyamorphism, in which the presence of high- and low-density amorphous (HDA and LDA) states of water, it can be considered that the two states correspond to the two amorphous states. Therefore, clarifying the properties of HDA and LDA water is essential to understand liquid water and water around solute molecules such as biomolecules and possibly to understand the function of the water-surrounded biomolecules. In this talk, I would like to introduce the physical properties of water in the amorphous states with our dielectric spectroscopy results of the entire concentration range of aqueous glycerol solutions at low temperatures and high pressures.

[1S8-5](#) The role of water for biomolecular dynamics; slaving versus plasticization

Jan Swenson¹, Silvina Cerveny^{1,2} (¹*Chalmers University of Technology*, ²*Donostia International Physics Center*)

It is well-known that biomolecules, such as proteins, need water to function. In fact, the life we know about needs water. However, the exact role of water for the motions and functions of biomolecules is still debated. Experiments have shown that protein and water dynamics are strongly coupled, but with water motions occurring on a considerably faster time scale (the so-called slaving behavior). This is in contrast to most aqueous solutions where water acts as a plasticizer of the solute molecules. Here, we discuss differences between the slaving and plasticization phenomena and whether slaving is unique for protein hydration water or not, with the aim to understand the key factors for observing the biologically important slaving behavior.

[1S8-6](#) Hydration shells of biomolecules: dynamics and biochemical function

Damien Laage^{1,2,3,4} (¹*Ecole Normale Supérieure*, ²*CNRS*, ³*PSL Univ.*, ⁴*Sorbonne Univ.*)

Water is considered to be indispensable to life, but a molecular understanding of its role in protein function has remained elusive. We will show that theory and simulations provide a molecular description of protein hydration dynamics in agreement with experimental observations. The hydration shell is slower than bulk water and the molecular origin of this slowdown can be precisely determined. In a complementary study, we focus on the influence of water on protein function, to understand why water enhances enzyme catalytic activity. Water is usually depicted as a lubricant which facilitates conformational transitions. Through the study of a paradigm enzyme in a non-aqueous solvent, we will assess the molecular validity of this picture.

[1S8-7](#) 低含水率媒質中の水和水の室温ガラス状態
Glass-like state of hydration water in aqueous mediums with low water contents at room temperature

Hiroshi Murakami (*Inst. Quantum life Sci., QST*)

Various aqueous mediums, such as cytoplasm and solution of biomolecules, exhibit glass transitions at around room temperature with low water contents. The glassy states are believed to play an important role in biological functions, for example, quiescence of organisms due to suppression of metabolic reactions. Despite hydration water working synergistically with solute molecules in their reactions, it remains unclear how the hydration water behaves in those aqueous mediums. Moreover, it is still challenging to distinguish hydration water from bulk-like one in aqueous solutions. Here we show that hydration water becomes glass-like in a nanometer-sized aqueous medium with low water contents at room temperature, and the biological relevance of the result is discussed.

[1S9-1](#) 蛍光性タンパク質温度センサーを用いた生体内温度分布の可視化とその意義の解明
Visualization and understanding of subcellular thermodynamics using fluorescent protein-based thermosensors

Reiko Sakaguchi^{1,2} (¹*Univ of Occupational and Environmental Health*, ²*Grad Sch Engineering, Kyoto Univ.*)

Thermoregulation to maintain body temperature is essential for life. Multiple mechanisms of thermogenesis have been proposed in different subcellular organelles. However, visualizing thermogenesis directly in organelles has been challenging. In this presentation, we introduce genetically encoded, GFP-based thermosensors (tsGFPs) that can visualize thermogenesis in specific organelles in live cells. In tsGFPs, the coiled-coil structure of thermosensing protein transmits conformational changes to GFP to convert temperature changes into quantifiable fluorescence changes. The protein-based tsGFPs can be specifically expressed in distinct organelles by the attachment of targeting signals. Thus, tsGFPs are powerful tools to noninvasively assess thermogenesis in live cells.

IS9-2 Single-molecule dynamics of TRPV1 channel upon activation with different stimuli

Hirofumi Shimizu (*Div. Int. Physiol. Univ. Fukui. Fac. Med. Sci.*)

Transient receptor potential vanilloid 1 (TRPV1) channel is a well-known sensor protein for various stimuli such as heat, pH, and vanilloids. To investigate its motion during function, we utilized a diffracted X-ray tracking method that can track conformational changes of a protein with high temporal (sub-millisecond) and spatial (~0.1°) resolutions. In the presence of capsaicin, enhanced molecular fluctuations and large twisting motions of TRPV1 were observed, which were inhibited by an antagonist. The twisting motions were also observed under low pH or high-temperature conditions. In this presentation, we describe the experimental setup and discuss the motions related to the activation.

IS9-3 電位依存性 H⁺チャネルの温度感受性ゲーティングの構造基盤
Structural Basis for Temperature-Sensitive Gating of Voltage-Gated H⁺ Channels

Yuichiro Fujiwara (*Grad. Sch. Med., Kagawa Univ.*)

The voltage-gated H⁺ channel (Hv) is mainly expressed in immune cells, the physiological functions of which are temperature sensitive. Earlier studies showed that the properties of Hv, including H⁺ conductance and gating, are highly temperature dependent. We have reported that Hv assembles as a homo-dimeric channel, which is mediated by the coiled-coil assembly domain in the cytoplasmic C terminus. The interaction between the two protomers was important for the temperature sensitivity. Electrophysiological analysis of the mutant Hv showed that the temperature dependence was closely related to the structural change during gating. In this symposium, I will discuss structural bases of the cooperative gating and thermosensitive properties of Hv.

IS9-4 温度感受性チャネル TRPM5 の温度依存的活性化及び不活性化
Temperature-dependent activation and inactivation of TRPM5 channel

Kunitoshi Uchida (*Dept. Environ. Life Sci., Sch. Food Nutr. Sci., Univ. Shizuoka.*)

TRPM5 is a monovalent cation-permeable channel activated by intracellular Ca²⁺, and its activity is enhanced by temperature increases. In this study, we analyzed the temperature dependency of TRPM5 by using whole-cell patch-clamp recording. We found that TRPM5 is activated and irreversibly inactivated upon heat stimulation. The mechanism of temperature-dependent inactivation could be different from that of voltage-dependent inactivation. Next, we analyzed TRPM5 protein electrophysiologically by using planar lipid bilayer (PLB) method. Temperature-dependent activation and inactivation of TRPM5 were also observed in PLB method, suggesting that other molecules contained in cells could not be required for temperature-dependent activation and inactivation of TRPM5.

IS9-5 両生類の生態的な棲み分けに起因した温度感覚の進化的変化とその分子機構
The evolutionary tuning of thermal perception related to habitat selection in frogs

Shigeru Saito^{1,2,3}, Claire Saito^{1,2}, Takeshi Igawa⁴, Shohei Komaki⁵, Makoto Tominaga^{1,2,3} (*¹Dep. Cell Signaling, Natl. Inst. Physiol. Sci., ²Thermal Biol., ExCELLS, ³Dept. Physiol. Sci., SOKENDAI, ⁴Amphibian Res. Center, Hiroshima Univ., ⁵Iwate Tohoku Med. Megabank Org.*)

In order to examine the role of thermal perception in environmental adaptation, tadpoles of five frog species that are spatially and temporally inhabit different thermal niches were compared. The upper thermal limits as well as avoidance temperatures of tadpoles were determined by behavioral assay. These two parameters were positively correlated with each other, and the species differences were consistent with thermal niches of each species. In addition, functional characterizations of heat sensor TRPA1 revealed that its activity and sensitivity shifted with the avoidance temperature of the species. Combined, our findings suggest that functional shift in the heat sensor played a crucial role in thermal adaptation processes.

[1S9-6](#) てんかん原性域の局所発熱は TRPV4 活性化を介して病態悪化を引き起こす
Temperature elevation in epileptogenic foci exacerbates the disease through TRPV4 activation

Koji Shibasaki (*Lab. Neurochem., Univ. Nagasaki*)

We generated a model of partial epilepsy in wild type (WT) or TRPV4KO mice, and measured electroencephalogram (EEG). The frequencies of epileptic EEG in WT mice were significantly larger than those in TRPV4KO mice. These results strongly indicate that TRPV4 activation is involved in disease progression. We expected that the disease progression enhanced hyperexcitability, and lead to local hyperthermia. To confirm it, we developed a new device to measure exact brain temperature only in restricted local area. From the recording results by the new device, we revealed that the brain temperatures in epileptogenic zones were dramatically elevated compared with normal regions. Furthermore, we demonstrated that the temperature elevation was critical for disease progression.

[1S10-1](#) Assembly of Primitive Liquid Crystal Peptide/DNA Coacervates

Tommy Z Jia^{1,2}, Tommaso P Fraccia³ (¹*Earth-Life Science Institute, Tokyo Institute of Technology*, ²*Blue Marble Space Institute of Science*, ³*Institut Pierre-Gilles de Gennes, Chimie Biologie et Innovation, ESPCI Paris*)

Compartmentalization supported the assembly and evolution of protocells on early Earth. Recent trends have investigated membraneless droplets as primitive compartments. Here, we introduce a membraneless peptide/DNA coacervate where the structural complexity can be increased through incorporation of DNA liquid crystals (LC). LC-coacervates form through peptide-DNA binding (coacervation) and DNA stacking (LC formation), and can transition through all known LC mesophases through variations in salinity, heat, and hydration. We predict that the increased structural complexity of LC phases applied to coacervates could help to increase the functional complexity of primitive compartment systems, perhaps even extending applications to modern engineering fields.

[1S10-2](#) 相分離を介して原始細胞モデル液滴を形成する核酸スキヤフォールド
Nucleic acid scaffolds that undergo phase separation into liquid droplets serving as primitive cell models

Shunsuke Tomita¹, Masahiro Mimura^{1,2}, Yoichi Shinkai³, Ryoji Kurita^{1,2} (¹*Health Med. Inst., AIST*, ²*Grad. Sch. of Pure and Appl. Sci., Univ. Tsukuba*, ³*Biomed. Res. Inst., AIST*)

Liquid droplets formed via liquid-liquid phase separation of oppositely charged polyions, also referred to as 'complex coacervates', exhibit fluidic properties that enable their reversible and rapid formation in response to changes in the surrounding environments, as well as the selective concentration or exclusion of particular molecules within the droplet phase. Therefore, such liquid droplets may possibly be key to the emergence of the earliest lifeforms through prebiotic organization. In this talk, we present our recent studies on the role of structure of nucleic acids, e.g., constituent moieties, primary sequences, and higher-order structures, as scaffolds of droplets formed with cationic polypeptide chains, and discuss their relevance to the origin of life.

[1S10-3*](#) (2-13-1427) アミノ酸配列と連携した原始生体膜の成長
(2-13-1427) Growth of Primitive Cell Membrane Coupled with Amino Acid Sequence

Akiko Baba¹, Ulf Olsson², Masayuki Imai¹ (¹*Grad. Sch. Sci., Univ. Tohoku*, ²*Grad. Sch. Sci., Univ. Lund*)

Evolution is change shifted toward greater fitness over time. The fitness is a measure of replication rate and is determined by genetic information: sequence of nucleotide or amino acid in nucleic acid or protein. Therefore, to elucidate relationship between the fitness and the genetic information is essential to understand the evolution. We believe that the simplest relationship has emerged in the prebiotic era, when fatty acid vesicles coexist with numerous primitive molecules such as nucleotides, amino acids, and peptides. Here, we demonstrate amino acids and peptides encourage the growth of fatty acid vesicles. Especially, the growth rate strongly depends on the type of amino acids and amino acid sequence in peptides, which might be the origin of evolution.

[1S10-4](#) 高分子混雑した細胞モデル中の分子挙動決定因子としての細胞サイズ
Cell size as a key determinant of molecular behaviors in macromolecular crowding artificial cells

Chiho Watanabe^{1,2}, Miho Yanagisawa² (¹*Hiroshima Univ.*, ²*Univ. Tokyo*)

Artificial cells are essential tools for understanding life from a bottom-up approach. We aim to understand the role of the “cell size”, which is in principle, micrometers to tens of micrometers. To this aim, we employ polymer droplets covered with a lipid membrane that can examine together the cell-size effect and the macromolecular crowding. Recently, we discovered that the cell size confinement can control the degree of molecular diffusion coupled with high polymer concentration which models macromolecular crowding in real cells. In addition, we found that membrane physicochemical properties, i.e., lipid composition, also affect the cell-size dependent diffusion. Further, we shall discuss the cell-size effect on liquid-liquid phase separation (LLPS).

[1S10-5](#) Multiple fusion barriers for fatty acid protocells

Anna Wang¹, Tetsuya Yomo², Lauren Lowe¹, Daniel WK Loo¹, Yaam Deckel¹ (¹*School of Chemistry and the Australian Centre for Astrobiology, UNSW Sydney, Australia*, ²*Institute of Biology and Information Science, Biomedical Synthetic Biology Research Center, School of Life Sciences, East China Normal University, Shanghai, China*)

Lipid bilayers are central to living organisms. Prior to the existence of phospholipids, it is likely that primitive cells on Earth were made of simpler molecules such as fatty acids. These vesicles are highly dynamic, including enhanced fluidity and flip-flop. Membrane fusion is critical for sharing contents, as well as remodelling processes such as division, endocytosis, and exocytosis. Here we discuss attempts to attain full fusion between fatty acid vesicles. We use a recently reported method to generate solutions of giant fatty acid vesicles and find that in addition to being extremely colloidally stable, the dynamic nature of the membranes can counterintuitively also limit full fusion. We will then discuss strategies for further studies.

[1S10-6](#) 人工細胞における細胞内構造形成の不安定性
Understanding the instability of intracellular organization in synthetic cells

Yusuke Maeda (*Kyushu Univ., Dept. Phys.*)

A living cell is a highly organized molecular system in nature, which stores genetic information in the genome and many proteins for its self-reproduction. An intracellular organization is vital for the emergence of such a complex system in protocells or synthetic cells; however, the lack of quantitative experimental tools has hindered the understanding of those structures from interactions of a relatively small number of molecules. To address this aim, we build synthetic cells as physical modeling of the instability of intracellular organization. Our synthetic cells show symmetry-breaking and instability from the uniformly dissolved state. Two types of molecular interactions relevant to instabilities, active force generation and phase separation, are discussed.

[1S10-7*](#) (2-13-1451) 多相液滴のコアを用いた人工細胞内転写反応場の構築
(2-13-1451) Development of a transcription field in the artificial cell by the core of multiphase droplets

Kanji Tomohara, Yoshihiro Minagawa, Hiroyuki Noji (*Dept. Appl. Chem., Grad. Sch. Eng., Univ. Tokyo*)

In this work, we developed core-shell structured droplets as compartments for artificial cells and found out if the core of the droplets could serve as a field of enzymatic reactions and rectify the reaction pathway. First, we demonstrate that the mixture of three polymers, intrinsically disordered protein, dextran, and PEG, generates core-shell structured droplets by liquid-liquid phase separation. Next, we have engineered this system so that the core of the droplet, the IDP-rich phase, can incorporate proteins, including enzymes. Finally, NTP and DNA, both substrates for transcription, were observed to be naturally recruited into the IDP-rich phase. Based on these results, we are now trying to conduct transcription inside the core of this artificial cell compartment.

1S11-1 X-ray free electron lasers reveal the molecular mechanism for water oxidation in photosystem II

Michi Suga, Yoshiki Nakajima, Hongjie Li, Jian-Ren Shen (*Okayama Univ.*)

Photosynthetic water oxidation is catalyzed by the Mn_4CaO_5 -cluster/ Mn_4CaO_6 -cluster of Photosystem II (PSII) through a linear four oxidation intermediates of *Si*-state cycle (S_i , $i = 0-4$). To reveal the molecular details in the water oxidation reaction, we analyzed the X-ray-free laser (XFEL) structures of PSII in different S states using fixed-target serial femtosecond crystallography (SFX) time-resolved SFX with an XFEL provided by the SACLA. The structural changes in PSII between the different S-states or during the progression of the S-state reveal the detail of the mechanism of photosynthetic water oxidation by the cooperative action of substrate water access, proton release, and O=O bond formation. I would show our results in recent years.

1S11-2 Involvement of conserved amino acids in ion transport pathways of multidrug and toxic compound extrusion (MATE) transporter

Keiko Shinoda¹, Hisashi Kawasaki¹, Satoshi Murakami², Sagar Raturi³, Asha V. Nair³, Himansha Singh³, Boyan Bai³, Hendrik W. van Veen³ (¹*AgTECH, GSALS, UTokyo*, ²*Sch. of Life Sci. and Tech., Tokyo Inst. of Tech.*, ³*Dept. of Pharmacology, Univ. of Cambridge*)

MATE is a multidrug extrusion transporter that export a large class of antibiotic and toxic compounds using a concentration gradient of Na ions or protons. In the NorM subfamily of MATE, three acidic amino acids (Asp36, Glu255, and Asp371) are conserved and are expected to play important functions. To investigate how these conserved acidic amino acids relates to the dynamics of NorM proteins and ion transport, we performed molecular dynamics (MD) simulations for NorM-VC and NorM-PS. It has been experimentally shown that NorM-VC transports either Na ions or protons, whereas NorM-PS transports only protons. MD simulations suggest that the protonation of conserved amino acids is involved in the transport of Na ions.

1S11-3 ギャップ結合タンパク質のナノディスクにおける構造
Structures of gap junction proteins in nanodiscs

Atsunori Oshima^{1,2} (¹*CeSPI, Nagoya Univ.*, ²*Grad. Sch. Pharm. Sci.*)

Gap junction channels form intercellular conduits with a large pore size whose closed and open states regulate communication between adjacent cells. We show the cryo-electron microscopy structures of *Caenorhabditis elegans* innexin-6 gap junction proteins in detergent or nanodisc. In a nanodisc-reconstituted structure of the wild-type innexin-6 (INX-6) hemichannel, flat double-layer densities obstruct the channel pore. The structure in detergent reveals the N-terminal funnels, suggesting an open form. Together with molecular dynamics simulations and electrophysiology functional assays, our results provide insight into the closure of the INX-6 hemichannel in a lipid bilayer before docking of two hemichannels.

1S11-4 Molecular mechanisms involved in the regulation of the Circadian Clock

Florence Tama^{1,2,3} (¹*RIKEN Center for Computational Science*, ²*Department of Physics, Nagoya University*, ³*Institute of Transformative Bio-Molecules*)

A circadian rhythm is a natural, internal process “clock” that regulates cellular responses to the environment and disruption of this cycle has been linked to a variety of diseases. However, the molecular mechanism of regulation of this internal biological clock which involves complex interactions between transcription factors, period genes, cryptochromes and several other associated factors remains poorly understood. We have been studying clock proteins involved in the maintenance of the circadian rhythm. In particular, we have studied mammalian cryptochrome proteins and demonstrated that differences in dynamics around their secondary pocket could be responsible for functional divergence in terms of transcriptional repression and period length observed *in vivo*.

1S11-5 XFEL analyses of molecular mechanism and structure in DNA photolyase photoreduction**Yoshitaka Bessho**^{1,2} (¹*Academia Sinica, IBC*, ²*RIKEN Spring-8 Center*)

DNA photolyases are flavoenzymes that repair UV-induced DNA pyrimidine dimer damage. Blue light activates the enzyme by the photoreduction of its FAD cofactor. To clarify the photoreduction mechanism of photolyase, we used the femtosecond pulses of the SACLA X-ray Free-Electron Laser (XFEL) as a probe. The damage-free crystal structure revealed the exact arrangement of the water molecule clusters adjacent to the U-shaped FAD cofactor. We also observed time-dependent buckling and twisting in the isoalloxazine ring of the FAD cofactor in different redox states. Our molecular movies showed how the protein environment of redox cofactors organizes multiple electron and proton transfer events in an ordered fashion. At this symposium, we will report our latest results.

1S11-6 蛋白質結合解離ダイナミクスの分子動画
Molecular movie of protein association/dissociation dynamics**Akio Kitao** (*Sch. Life Sci. Tech., Tokyo Tech.*)

Association and dissociation of proteins with other molecules are important molecular processes in biomolecular systems. We constructed molecular simulation procedures to investigate protein association/dissociation dynamics by using the combination of parallel cascade selection molecular dynamics (PaCS-MD) and the Markov state model (MSM), namely PaCS-MD/MSM. These procedures enable us to calculate free energy profile of dissociation/association, binding affinity and flux of dissociation/association pathways. Recently, we are applying this method to investigate dissociation and association dynamics of large molecular systems, e.g., protein-protein and protein-DNA complexes, as well as protein-ligand complexes. I will report recent results obtained by PaCS-MD/MSM.

1S12-1 Biophysics of Infectious Diseases: How are the carriers of abnormal hemoglobin protected from severe malaria?**Motomu Tanaka**^{1,2} (¹*Heidelberg University, Institute of Physical Chemistry*, ²*Kyoto University, Center for Integrative Medicine and Physics*)

Over 0.5 million people in the world die through malaria every year. Malaria-infected erythrocytes adhere to the surface of microvasculature and escape from splenic clearance, which enables them to spread the infection. It is widely known that people carrying the sickle cell hemoglobin (HbAS) or hemoglobin C (HbAC) are protected from severe malaria. As the progression of malaria alters both biochemical and biophysical properties of human red blood cells, we combined several experimental and analytical tools to unravel the underlying mechanism how the nature provides HbAS and HbAC carriers with the survival benefit from the view point of physics.

1S12-2 形成外科学 とメカノバイオロジー —物理的的刺激が創傷治癒や組織再生に与える役割—
Plastic Surgery and Mechanobiology —The Role of Mechanical Forces on Wound Healing,
Tissue Repair and Regeneration—**Rei Ogawa** (*Department of Plastic, Reconstructive and Aesthetic Surgery, Nippon Medical School*)

Mechanobiology is an emerging field of science which focuses on the way that physical forces and changes in cell or tissue mechanics contribute to development, physiology, and disease. Cells convert intrinsic and extrinsic mechanical stimuli into electrical signals through mechanosensors such as mechanosensitive ion channels, cell adhesion molecules, and actin filaments. This signal conversion results in accelerated cell proliferation and matrix maturation during the course of tissue growth. Skin and soft tissues are organs those are always affected by mechanical forces, thus physicians need to know the mechanobiology for surgery, wound healing and tissue repair and regeneration.

[1S12-3](#) 計算流体力学を用いた心血管系疾患に対する患者固有解析
Patient-specific analyses by computational fluid dynamics for cardiovascular diseases

Hiroshi Suito (*AIMR, Tohoku Univ.*)

In blood vessels with congenital heart diseases, characteristic flow structures are formed, in which pulsating flows affect strongly on wall shear stresses and energy dissipation patterns. In this talk, we present computational analyses for blood flows in patient-specific cases, through which we aim at understanding the relationships between differences in geometries and in energy dissipations. Our present targets include an aortic coarctation case and a Norwood surgery for hypoplastic left heart syndrome. These analyses yield deeper understandings in clinical medicine.

[1S12-4](#) 質量分析イメージングの病理学応用
Pathology application of mass spectrometry imaging

Tatsuaki Tsuruyama^{1,2} (¹*Kyoto University, graduate school of medicine*, ²*Radiation effect Reseach Foundation*)

Imaging mass spectrometry (IMS) has been rarely used to examine human pathology specimens. However, we developed a new pretreatment method for preparing tissue sections for IMS. We identified histone H2A as a colon cancer marker. Further, the correlation analysis of IMS signal patterns and intensities of the regions of interest (ROI) identified new biomarkers such as triphosphate synthase alpha subunit, myosin-6/7, aortic actin, and the myosin light chain 3 in the heart infarcted region. Besides, hierarchical cluster analysis (IMS-HCA) suggested the new protein markers of brain tumorigenesis. IMS application may be a promising technique for the identification of biomarkers for pathological studies.

[1S12-5](#) 光トモグラフィーと生物物理
Optical tomography and biophysics

Manabu Machida (*Hamamatsu University School of Medicine*)

Optical tomography is an imaging modality with near-infrared light. Light propagation in biological tissue is governed by the radiative transport equation or diffusion equation. We can obtain reconstructed images of absorption and scattering coefficients by solving inverse problems for these equations. The inverse problem of optical tomography is known to be severely ill-posed. In this talk, I will present an algorithm of simulated annealing for optical tomography. Moreover, I will discuss the interaction between light and biological tissue. For example, functional neuroimaging by light becomes possible through the neurovascular coupling. The study of the light-tissue interaction in biophysics will accelerate the technology of optical tomography in medicine.

[1S13-1](#) はじめに：「シンギュラリティ生物学」とは？
Introduction: What is "Singularity Biology"?

Hiroko Bannai (*Waseda Univ., Fac. Sci. Eng.*)

"Singularity biology" is the biology that deals with biological events that can alter the entire system by very rare elements. We define these biological phenomena as "singularity phenomena". In this symposium, the speakers will introduce various biological phenomena that are candidates for "Singularity Phenomena" including algal behavior, stem cell differentiation, organogenesis, and neurological disorder. The speakers will share novel viewpoints and methodologies that enable us to elucidate the mechanism of "singularity phenomena".

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- [1S13-2](#) あまのじゃく細胞から紐解く緑藻クラミドモナス走光性の生理的意義
Significance of phototaxis in the unicellular green alga *Chlamydomonas reinhardtii* revealed by “perverse” cells

Ken-ichi Wakabayashi^{1,2} (¹*CLS, Tokyo Tech*, ²*LST, Tokyo Tech*)

Chlamydomonas reinhardtii is the unicellular green alga that exhibits phototaxis by controlling ciliary movements after photoreception at the eyespot. We found that its sign of phototaxis is positive when the amount of cellular reactive oxygen species (ROS) increases and is negative when it decreases. However, this regulation seems to be suicidal, because more ROS would be produced by perceiving higher light. We are trying to solve this mystery by two approaches: (1) phenotyping mutants that show the opposite sign of phototaxis to the wild type, and (2) observing fluctuation in the sign of phototaxis in wild-type cells after prolonged light exposure. No clear answer has yet been obtained, but I will discuss the results we have obtained.

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- [1S13-3](#) シンギュラリティ細胞の脱分化による幹細胞集団維持機構の解明
Homeostasis of stem cell populations maintained by rare de-differentiating subsets

Mio Nakanishi (*Grad. Sch. Med.*)

Stem and progenitor cells change their individual roles in tissue homeostasis dramatically according to the tissue status. In hematopoietic system for example, the multipotent progenitors and the stem cells are majorly contributing to the homeostasis at steady state and regenerative phases, respectively. Nonetheless, mechanisms underlying the balancing between stem cells and progenitors are largely unknown. Recently I found a progenitor-like subset in human pluripotent stem cell cultures, that regulates the stem vs progenitor balance in the culture through its de-differentiation to the stem cell subset. In this talk, I will describe this newly-revealed mechanism that potentially underlying homeostasis of pluripotent- and adult stem cell populations.

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- [1S13-4](#) Self-patterning of brain organoids

Kent Imaizumi (*Department of Physiology, Keio University School of Medicine*)

Organoids can establish *in vivo*-like tissue structures in a dish. The brain is patterned into distinct regions, and we found that this patterning was spontaneously self-organized within brain organoids. In this study, we examine how this self-patterning takes place during the development of organoids from a homogeneous population of stem cells. We found that there were a small number of morphogen-secreting cells within brain organoids, and these *singularity* cells were initially randomly distributed, but were eventually localized to a single place, giving rise to stable organoid-wide morphogen gradients. We will discuss the underlying mechanisms of spontaneous assembly of morphogen-secreting cells.

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- [1S13-5](#) 免疫応答を介したアルツハイマー病発症への寄与の解明
Involvement in the development of Alzheimer's disease through activation of systemic immune response

Minako Ito, Ryusei Kaneko (*Med. Inst. Bioreg., Kyusyu Univ.*)

In neurodegenerative diseases such as Alzheimer's disease (AD), the appearance and accumulation of aggregates of Amyloid beta (A β) and phosphorylated Tau is triggered by some stimulus such as an immune response. Inflammatory bowel disease was also reported to be a risk factor for dementia in humans, but the mechanism remains unclear. The aim of this study is to develop novel therapeutic strategies by clarifying the immune responses that regulate the expansion of cells expressing A β and phosphorylated Tau. We found that colitis enhanced the pathogenesis of AD, and immune cells were infiltrated in the brains and dura maters of mice models of AD by using scRNAseq, suggesting the involvement of immune responses in the development of neurological diseases.

[1S13-6](#) 社会性アメーバの時空間自己組織化過程におけるシンギュラリティ ~AMATERAS1.0 で実現した定量トランススケール解析~
Quantitative trans-scale analysis of a singularity in spatiotemporal self-organization of social amoeba by using AMATERAS1.0

Taishi Kakizuka¹, Yusuke Hara², Taro Ichimura¹, Takeharu Nagai^{1,3}, Kazuki Horikawa² (¹OTLI, Osaka Univ., ²Adv. Res. Prom. Cen., Tokushima Univ., ³SANKEN, Osaka Univ.)

Rotating spirals are spatiotemporal self-organization patterns at population level resulting from signal propagation among excitable constituents, but the mechanism of their spontaneous formation remains elusive. Here, we observed cAMP signaling among about 130,000 living cells of social amoeba by our trans-scale-scope, AMATETAS1.0. We found that the mesoscale structure of excitability, which formed spontaneously during development, played an essential role in causing spirals. Furthermore, quantitative trans-scale analysis revealed a cellular level mechanism for generating the structured excitability; not only less than 1% of the cells acted as leaders, but less than 10 % acted as followers, working together to make a singularity that triggers critical transition.

[1S14-1](#) ケモフォレシス・エンジン：ATPase 駆動型カーゴ輸送の理論
Chemophoresis Engine: Theory of ATPase-driven Cargo Transport

Takeshi Sugawara¹, Kunihiko Kaneko^{1,2} (¹UBI, Univ. Tokyo, ²Grad. Sch. Arts Sci., Univ. Tokyo)

The formation of macromolecule patterns has recently been observed in bacterial cells, and its relevance as intracellular morphogen has been demonstrated in the case of bacterial cell division. These studies have discussed how cargos maintain positional information provided by chemical gradients. However, how cargo transports are directly mediated by such gradients remains unknown. Based on the previously proposed mechanism of chemotaxis-like behavior of cargos (referred to as chemophoresis), we introduce the *chemophoresis engine* as a physicochemical mechanism of cargo motion, which transforms chemical free energy to directed motion through the catalytic ATP hydrolysis. We propose its possible role as a universal principle of hydrolysis-driven intracellular transports.

[1S14-2](#) サルモネラのべん毛運動と走化性
Flagellar motility and chemotaxis in *Salmonella*

Yusuke V. Morimoto^{1,2} (¹Fac. Comp. Sci. and Sys. Eng., Kyushu Inst. Tech., ²PRESTO, JST)

E. coli and *Salmonella* are propelled by rotating flagella to swim in liquid environments. The basal body is located at the base of the flagellar filament and works as a rotary motor. The flagellar motor rotates in both counterclockwise (CCW) and clockwise (CW) directions. When one or more motors switch the rotational direction from CCW to CW, the cells change the swimming direction. Then bacterial cells carry out chemotaxis by a biased random walk toward various chemicals, pH, and temperature. These systems are commonly conserved in *E. coli* and *Salmonella*, but with some differences. This presentation will focus on these differences and discuss them from the perspective of *Salmonella* research.

[1S14-3](#) Near-critical tuning of conformational spread revealed by single-cell FRET in bacterial chemoreceptor arrays

Johannes M. Keegstra¹, Fotios Avgidis¹, Yuval Mullah¹, John S. Parkinson², Thomas Shimizu¹ (¹AMOLF Institute, Amsterdam, The Netherlands, ²Department of Biology, University of Utah, Salt Lake City, USA)

Dynamics of allosteric complexes are crucial for signal processing by protein networks, but direct observation of switches between distinct conformational states has been limited to relatively small assemblies such as ion channels. Using in vivo FRET, we discovered spontaneous switches in the activity of *E. coli* chemosensory arrays, huge membrane-associated protein complexes comprising thousands of proteins. Analysis of the temporal statistics using a conformational spread model revealed coupling energies within 3% of the Ising phase transition, indicating that these bacterial sensory arrays are poised at criticality. These results demonstrate how even the simplest biological systems can enhance performance by tuning their nonlinear dynamics close to a critical point.

1S14-4 Subpopulation of chemotactic cells with extremely high sensitivity

Satomi Matsuoka^{1,2,3}, Masahiro Ueda^{1,2} (¹*Grad. Sch. Frontier Biosciences, Osaka Univ.*, ²*RIKEN, BDR*, ³*PRESTO, JST*)

Chemotaxis is a fundamental function seen universally in vast kinds of eukaryotic cells in complicated natural environments. To understand the highly responsive yet flexible mechanism for the gradient sensing and motility biasing, it is required to quantify the movement under the chemoattractant gradient generated in a reproducible manner. Using a microfluidic device that enables a large-scale observation of individual cells' movement under the same gradients, we revealed a subpopulation of *Dictyostelium discoideum* cells showed higher sensitivity to chemoattractant, cAMP, than the rest of the cells. It became clear that at least 6 cAMP molecules are sufficient for biasing the motility, suggesting an underlying mechanism resilient to molecular noises.

1S14-5 初期胚組織はモルフォゲン勾配のノイズを感知し修復する能力を備えている
Embryonic cell community senses and eliminates the noise of morphogen gradient

Yuki Akieda (*Hom. Reg., RIMD, Osaka Univ.*)

Morphogen signaling forms an activity gradient and instructs cell identities to pattern developing tissues. However, developing tissues stochastically may produce cells with unfit morphogen signaling and consequent noisy morphogen gradients. Here we show that embryonic cell community actively corrects such noisy morphogen gradients. Zebrafish imaging analyses of the Wnt morphogen signaling gradient, which acts as a morphogen to establish embryonic anterior-posterior patterning, identify that unfit cells with abnormal Wnt activity spontaneously appear. Unfit cells are eliminated by apoptosis via cell-cell communication. This elimination is required for proper gradient formation and patterning. I'd like to introduce our recent progress of this study.

1S14-6 ゼブラフィッシュ胚におけるモルフォゲン分布の制御
Spatiotemporal regulation of morphogen distribution in zebrafish embryo

Hidehiko Inomata, Hiroki Hamada, Setsuko Kanamura (*BDR., Riken*)

During the developmental processes, complex tissues of the embryo are formed by secreted proteins such as morphogen. Morphogens are secreted by the producing cells and diffuse through the extracellular space, forming a concentration gradient. It is known that cells differentiate into various tissues depending on local morphogen concentration. We have developed a novel method for spatiotemporal regulation of morphogen distribution in the embryo. Furthermore, we found that perturbation of morphogen distribution disrupts pattern formation in zebrafish embryos. We think that this method will be an effective tool for understanding the interactive mechanisms of morphogen dynamics and tissue patterning.

2S1-1 クライオ電子顕微鏡によるクロススケール構造解析
Cross-scale structural studies by cryo-electron microscopy

Masahide Kikkawa (*The University of Tokyo*)

Since 2017, the University of Tokyo has offered cryo-electron microscopy for structural analysis to researchers and companies throughout Japan as part of the AMED/BINDS. At present, nearly 50 projects are being supported, and six companies are also using the facility. In our facility, we use three cryo-EM methods to perform cross-scale observation ranging from atoms to cellular structures. Single particle analysis is used to observe biological molecules, microED is for atomic resolution structures of tiny crystals, and cryo-electron tomography is used for cellular structures. In this symposium, I would like to show the recent results using the three methods and discuss what is necessary for further utilization of the cryo-EM shared facility.

[2S1-2](#) 高速データ収集と原子分解能を両立したクライオ電子顕微鏡撮影法と酸化修飾グラフェングリッド
High throughput atomic resolution cryoEM analysis by multi-hole imaging and epoxidized graphene grid

Keiichi Namba (*Grad. Sch. Frontier Biosci., Osaka Univ., RIKEN BDR & SPring-8*)

CryoEM image analysis has become a powerful tool for life/medical sciences. Single particle image analysis can easily determine macromolecular structures beyond 2Å. We developed a cryoTEM “CRYO ARM” with JEOL over the last decade and solved the structure of apoferritin at 1.53Å from about 900 images collected in one day. Now we developed a new TEM control software, multi-hole imaging with a GATAN K3 camera allows 22,000 images to be collected in one day and allowed us to determine the apoferritin structure at 1.29Å from images collected over 15 hours. We also developed an epoxidized graphene grid to solve denaturation and preferred orientation problems at the air-water interface and solved the structure of GroEL at 1.99Å from just 500 images collected in 1 hour.

[2S1-3](#) Cryo-EM ネットワークと産学連携
Industry-academia collaboration with the cryo-EM network

Toshiya Senda¹, Takeshi Murata², Kenji Iwasaki³ (¹*SBRC, IMSS, KEK*, ²*Grad. Sch. Sci, Chiba Univ.*, ³*TARA, Univ. Tsukuba*)

Cryo-EM has become an essential tool for structural biology in the last decade, and the importance of cryo-EM is rapidly increasing in the pharmaceutical industry. However, the number of high-end cryo-EM machines has been limited due to their installation cost. To accelerate the shared use of cryo-EM in Japan, we have associated the cryo-EM network with the support of AMED. In addition, we have organized an academia-industry collaboration in the non-competitive area of pharmaceutical research. In FY2021, cryo-EM machines that pharmaceutical companies can use are being installed at the TARA center of Tsukuba University. We will present the current status and future direction of the collaboration.

[2S1-4](#) COVID-19等の感染症に対する治療薬・ワクチン開発を目指したBSL3クライオ電子顕微鏡を軸とする北大創薬拠点
BSL3 Cryo-EM facility of Hokkaido Univ. Drug Discovery Base for the Development of Therapeutics and Vaccines against COVID-19

Katsumi Maenaka (*Facult. Pharm.Sci., Hokkaido Univ.*)

Center for Research and Education on Drug Discovery (CRED) of Hokkaido University has established an integrated drug discovery system. With regard to structural analyses, we started cryo-electron microscopy (cryo EM) collaboration with Univ. of Oxford in 2013. In 2017-19, we introduced the 200 keV cryo EM, Glacios and FIB/SEM Aquilos. In 2020-21, we have introduced two 300 keV cryo EM, Krios G4, at BSL2 and BSL3 facilities with support for AMED BINDS. We are conducting single particle analysis, cryo electron tomography for viruses, cells, and tissues, and MicroED for organic compounds to develop therapeutics and vaccines against COVID-19. In this talk, I would like to outline current state and future plan of cryo-electron microscopes at Hokkaido University.

[2S1-5](#) 東北大学の最新クライオ電子顕微鏡の活用と共同利用について
New 300kV Cryo EM of Tohoku University: application and public utilization

Seizo Koshiba^{1,2,3}, Kengo Kinoshita^{1,2,4}, Masayuki Yamamoto^{1,2,3} (¹*INGEM, Tohoku Univ.*, ²*ToMMo, Tohoku Univ.*, ³*Grad. Sch. Med., Tohoku Univ.*, ⁴*Grad. Sch. Info., Tohoku Univ.*)

Cryo electron microscopy (Cryo EM) is an indispensable tool in modern structural biology. Tohoku University recently installed a new 300kV Cryo EM system (CRYO ARM 300 II, JEOL) in Advanced Research Center for Innovations in Next-Generation Medicine (INGEM) and many high-quality data have been already obtained. Moreover, our Cryo EM system cooperates with the supercomputer system of Tohoku Medical Megabank Organization. Cryo EM data are directly transferred to the storage system of the supercomputer and users can use the powerful computer resources (including GPU units) for the analysis of the obtained data. We will open our Cryo EM system to the public this autumn and expect that our system will be widely used by many institutes and companies.

[2S1-6](#) 九州・西日本エリアにおける創薬支援を目指したクライオ電顕ネットワーク
Cryo-EM network aiming to support drug discovery in the Kyushu / West Japan area

Kouta Mayanagi (*Medical Institute of Bioregulation, Kyushu Univ.*)

Two high-end cryoEMs (200 kV & 300 kV) will be installed this year at the Pharmaceutical Research Institute, Kyushu University, which is the Library Screening Section (leader: Shigehiro Ohdo) of the AMED BINDS. Using these two new EMs together with the cryo-EM Polara (MIB, Kyushu Univ.), we will promote research support for researchers in academia and pharmaceutical companies in the Kyushu / West Japan areas. Taking advantage of the characteristics of the Library Screening Section of BINDS, we aim to focus on research support for drug discovery research, such as structural analysis using libraries. In addition, we are also planning to utilize the supercomputer ITO to build a standard single particle analysis environment, easy and convenient for beginners.

[2S2-1](#) 質量分析法によるミトコンドリアタンパク質複合体の解析
Mass spectrometry-based methods for analysing the mitochondrial interactome in mammalian cells

Takumi Koshiba (*Dep. Sci., Chem., Fukuoka Univ.*)

Protein-protein interactions are essential biologic processes that occur at inter- and intracellular levels. To gain insight into the various complex cellular functions of these interactions, it is necessary to assess them under physiologic conditions. Recent advances in various proteomic technologies allow to investigate protein-protein interaction networks in living cells. The combination of proximity-dependent labelling and chemical cross-linking will greatly enhance our understanding of multi-protein complexes that are difficult to prepare, such as organelle-bound membrane proteins. In the symposium, we describe our current understanding of mass spectrometry-based proteomics mapping methods for elucidating mitochondrial protein complexes in living cells.

[2S2-2](#) ミトコンドリア膜融合反応の試験管内再構成
In vitro reconstitution of mitochondrial membrane fusion

Tadato Ban¹, Naotada Ishihara² (¹*Inst. of Life Sci., Kurume Univ.*, ²*Dept. of Biol. Sci., Grad. Sch. of Sci., Osaka Univ.*)

Mitochondria are highly dynamic organelles that move and fuse to regulate their shape, size, and fundamental functions. In mammalian cells, the large mitochondrial GTPases Mitofusin (Mfn) and OPA1 play a critical role in mitochondrial membrane fusion. However, how these GTPases mediate membrane fusion remains unclear because of the difficulty in preparing active recombinant proteins. To address these issues, we have established a method to prepare sufficient amounts of recombinant Mfn and OPA1 using the BmNPV bacmid-silkworm expression system and developed in vitro reconstitution of membrane fusion. In this symposium, we will discuss the role of GTP hydrolysis, the contribution of lipid membranes, and the molecular mechanism of mitochondrial membrane fusion.

[2S2-3](#) 熱力学的解離速度分析法を用いた光化学系I三量体間の結合エネルギーの解析
Investigation on the thermodynamic dissociation kinetics of Photosystem I trimer to determine the binding strengths of each protomer

Hisako Kawai¹, Eunchul Kim² (¹*Fac. Sci., Univ. Yamagata*, ²*NIBB*)

Photosystem I (PSI) mediates the light-driven charge separation and generating a highly negative redox potential, which is utilized to produce organic matter. In cyanobacteria, PSI forms both trimer and monomer (Kubota et al. BBA, 2010) and the PSI monomer/trimer ratio, which is determined by environmental conditions, is regarded to modulate the photosynthetic activity. However, the mechanisms to regulate the dissociation and reorganization of PSI protomer remains unclear because the methods for evaluate the binding energy of the membrane protein complexes have been limited. In this study, we will describe the activation energy for the dissociation of PSI protomers which estimated by the thermodynamic dissociation kinetics analysis (Kim et al. JPCB 2018, JPCL2019).

[2S2-4](#) (1-15-1330) 細胞膜中の TRPV1・TRPV4 チャンネルの 1 分子動態の比較解析
(1-15-1330) Comparative analysis of single-molecule dynamics of TRPV1 and TRPV4 channels in living cells

Masataka Yanagawa^{1,2}, Yutaro Kuwashima^{1,3}, Mitsuhiro Abe¹, Michio Hiroshima^{1,4}, Masahiro Ueda^{4,5}, Makoto Arita^{3,6,7}, Yasushi Sako¹ (¹Riken CPR, ²JST, PRESTO, ³Faculty Pharm., Keio Univ., ⁴Riken BDR, ⁵Grad. Sch. Front. Biosci., Osaka University, ⁶Riken IMS, ⁷Grad. Sch. Med. Life Sci., Yokohama City Univ.)

TRPV channels are multimodal sensor of various stimuli, including temperature and chemicals. Here we undertook single-molecule time-lapse imaging of TRPV1 and TRPV4 in HEK293 cells. In the resting state, TRPV4 was more likely to form higher-order oligomers within immobile membrane domains than TRPV1. TRPV1 became immobile upon activation, followed by its gradual endocytosis. In contrast, TRPV4 was rapidly internalized after agonist stimulation. The selective loss of immobile higher-order oligomers from the cell surface through endocytosis increased the proportion of the fast-diffusing state for both subtypes. Our results provide a possible mechanism for the different rates of endocytosis of TRPV1 and TRPV4 based on the membrane domain localization.

[2S2-5](#) マルチ機能性光受容膜タンパク質・ロドプシンによる生命機能の光制御
Optical control of biological activities with multi-functional photoreactive membrane protein rhodopsin

Yuki Sudo (Grad. Sch. Med. Dent. Pharm. Sci., Okayama Univ.)

In life science, methods to control biological activities with stimuli have been widely utilized to understand their molecular mechanisms. Light has the advantage of a high spatiotemporal resolution that allows for the precise control of biological activities. Photoactive membrane protein rhodopsin absorbs visible light and that light absorption triggers photoisomerization of the chromophore retinal, leading to protein functions such as ion pumps, ion channels, transcriptional regulators and enzymes. In addition, rhodopsins are widely utilized as fundamental molecular tools for optogenetics. I introduce here the molecular basis of representative rhodopsin molecules and their applications for optogenetics. Refs. (2020) JPCL, Biophys. J., Sci. Rep., JPCB, (2021) Sci. Rep.

[2S2-6](#) (1-02-1506) Cryo-EM analysis provides new mechanistic insight into ATP binding to Ca²⁺-ATPase SERCA2b

Yuxia Zhang¹, Satoshi Watanabe¹, Akihisa Tsutsumi², Hiroshi Kadokura¹, Masahide Kikkawa², Kenji Inaba¹ (¹Institute of Multidisciplinary Research for Advanced Materials, Tohoku University, ²Graduate School of Medicine, The University of Tokyo)

SERCA2b is a ubiquitous SERCA family member that conducts Ca²⁺ uptake from the cytosol to the ER. Herein, we present a 3.3 Å resolution cryo-EM structure of human SERCA2b in the E1·2Ca²⁺ state, revealing a new conformation for Ca²⁺-bound SERCA2b with a more compact cytosolic domain arrangement than the crystal structure of SERCA1a. Notably, ATP binding residues of SERCA2b in this state are located at similar positions to those in the E1·2Ca²⁺-ATP state, hence the cryo-EM structure likely represents a preformed state prior to ATP binding. With several lines of biochemical evidence, we propose and discuss a novel mechanism of ATP binding to SERCA2b.

[2S2-7](#) Rhythmic ATP release from the cyanobacterial circadian clock protein KaiC revealed by real-time monitoring of bioluminescence

Risa Mutoh¹, Takahiro Iida¹, Kiyoshi Onai² (¹Fac. Sci., Fukuoka Univ., ²Grad. Sch. Agr., Kyoto Univ.)

The cyanobacterial circadian clock oscillator is composed of three clock proteins called KaiA, KaiB, and KaiC. KaiC subunit has a duplicated structure, which is composed of N-terminal and C-terminal domains. Each domain has a series of ATPase motifs, that is ATP binds to twelve sites in KaiC hexamer. Here, we monitored the release of ATP from wild-type and mutant KaiCs as a bioluminescence in real time using a firefly luciferase assay *in vitro*. We observed the oscillation of ATP release from KaiC even without KaiA and KaiB. This oscillation was enhanced and suppressed by KaiB and KaiA, respectively. These results suggest that ATP release from KaiC acts on generating a fundamental oscillation in the clock system.

2S3-1 海馬台からの経路選択的な情報送出：投射先を光同定した大規模活動計測による解析
Projection-identified large-scale recording reveals pathway-specific information outflow from the subiculum

Takuma Kitanishi^{1,2} (¹*Grad. Sch. Med., Osaka City Univ.*, ²*PRESTO, JST*)

The hippocampus conveys a variety of spatial information. However, how the information is distributed to multiple downstream areas remains unknown. We investigated this by identifying axonal projections using optogenetics during large-scale extracellular recordings from the rat subiculum, the major hippocampal output structure. Subicular neurons demonstrated a noise-resistant representation of place, speed, and trajectory. Speed and trajectory information was selectively sent to the retrosplenial cortex and nucleus accumbens, respectively. Place information was distributed uniformly to the retrosplenial cortex, nucleus accumbens, anteroventral thalamus, and medial mammillary body. Thus, the subiculum robustly routes diverse spatial information to downstream areas.

2S3-2 概日光受容の新規メカニズムと光遺伝学への応用
Mechanism of circadian photoreception and its application for optogenetics.

Arisa Hirano, Tohru Takahashi, Takeshi Sakurai (*Faculty of Medicine, University of Tsukuba*)

CRYPTOCHROME (CRY) is a principal clock component in the molecular feedback loop of the mammalian clock system, while CRY of other species such as fly and plants acts as a photoreceptor. We have shown a missense mutation in the *hCRY2* FAD binding loop causes Familial Advanced Sleep Phase (Hirano et al., *eLife*, 2017). The mutation in *Cry2* gene altered the phase resetting by light, and we currently try to clarify the function of mammalian CRY in photoreception. By using conditional knockout mice, we have assessed the physiological role of CRY1 proteins in mouse retina for the circadian entrainments. At the molecular level, we also found that CRY1 interacts with G protein signaling molecule and enhances the signaling mediated by OPN4 in cell culture.

2S3-3 視覚再生に向けた暗活性・光不活性化 GPCR 型光遺伝学ツールの開発
Development of a dark-active, light-inactivated GPCR-based optogenetic tool for vision restoration

Takashi Nagata^{1,2} (¹*Inst. Solid State Phys., Univ. Tokyo*, ²*JST, PRESTO*)

Most animal rhodopsins function as light-activated G protein-coupled receptors (GPCRs), which have been used as optogenetic tools for controlling intracellular signaling cascades. We previously demonstrated that peropsin, an all-*trans*-retinal-binding rhodopsin, acts as a dark-active, light-inactivated GPCR upon replacement of its intracellular domain. This unique property of peropsin may enable a new approach for vision restoration. In the presentation, we will present the strategy for developing a peropsin-based optogenetic tool for vision restoration. Based on the strategy, we obtained peropsin-based tools that activate the Go-type G protein, which could be useful for restoring the light-sensitiveness of retinal interneurons after photoreceptor degeneration.

2S3-4 Development of photoinactivatable protein kinases to manipulate plant cell growth

Hiromasa Shikata^{1,2} (¹*Dev. Plant Environmental Responses, NIBB*, ²*PRESTO, JST*)

Protein kinases regulate various cellular processes by phosphorylating their downstream targets. We have studied roles of AGC kinases on the plant development and cell growth. Some of the AGC kinases are involved in the growth of root hairs and pollen tubes, which undergo typical polarized cell growth. We found that polar localization of the kinases on the plasma membrane correlates closely with re-orientation of root hair growth, suggesting that the kinases could regulate the growth direction. To demonstrate it, we have developed optogenetic tools to directly control the kinase activity at the subcellular level. One of the tools utilizes a LOV2 domain and its interacting motif which we identified to negatively regulate AGC kinase activity by blue light.

[2S3-5](#) 培養細胞、分裂酵母、線虫における細胞内シグナル伝達系の光操作
Optical control of cell signaling in cultured cells, fission yeast, and worms

Kazuhiro Aoki^{1,2} (¹NIBB, NINS, ²ExCELLS, NINS)

The light-induced dimerization (LID) system, in which photoresponsive proteins are rapidly and reversibly dimerized in response to light, allows controlling protein-protein interactions and cell signaling. One of the red/far-red responsive LID systems, phytochrome B (PhyB)-phytochrome interacting factor (PIF), has a unique property of controlling both association and dissociation by light on the second time scale, but PhyB requires a linear tetrapyrrole chromophore such as phycocyanobilin (PCB), and such chromophores are present only in higher plants and cyanobacteria. Here, we demonstrate an efficient biosynthesis of PCB and its application to the control of cell signaling in mammalian cells, fission yeast, and *C. elegans*.

[2S3-6](#) 多様なシアノバクテリオクロム光受容体の発見と改変
Discovery and engineering of diverse cyanobacteriochrome photoreceptors

Rei Narikawa (*Grad. Scho. Biol. Sci., Tokyo Metro. Univ.*)

Cyanobacteriochrome photoreceptors are a distant relative of plant canonical photoreceptors, phytochromes, and are highly diversified in their spectral properties. Only the GAF domain is needed for chromophore incorporation and proper photoconversion. Here, especially focusing on the binding chromophore species, I will provide three topics on the discovery and engineering of the cyanobacteriochromes. The first one is the rational conversion of the cyanobacteriochrome GAF domains to accept the mammalian intrinsic biliverdin chromophore. The second one is the evolution-inspired design of multicolored photoswitches from a single cyanobacteriochrome GAF domain. Finally, I introduce atypical cyanobacteriochrome GAF domains incorporating novel chromophore, isophycocyanobilin.

[2S4-1](#) コヒーシンのリング構造とゲノム機能
Opening cohesin's ring structure is essential for genome functions

Tomoko Nishiyama (*Grad. Sch. Sci., Nagoya Univ.*)

Sister chromatid cohesion is a fundamental event to ensure the genome stability. Cohesion is mediated by a ring-shaped cohesin complex, which topologically holds two DNAs together. This topological association creates a structural obstacle to genome-wide chromosomal events such as replication or transcription. However, how cohesin circumvents being an obstacle is unknown. Here we show that ATP hydrolysis-driven head disengagement, leading to SMC ring-opening, is essential for replication in human cells. Single-molecule analyses reveal that forced closure of SMC ring suppresses the translocation of cohesin on DNA, as well as the formation of stable DNA loops. We will discuss the mechanisms of how SMC ring-opening modulates both cohesion and genome structure.

[2S4-2](#) ゲノムフォールディングを制御する SMC タンパク質の構造・機能のシミュレーション研究
Computational approach to structures and dynamic functions of SMC proteins that organize genome folding

Shoji Takada (*Kyoto Univ. Grad. Sch. Sci.*)

Structural maintenance of chromosomes (SMC) complexes, such as cohesin and condensin, play major roles in genome structure organization. Recently, single-molecule experiments, cryo-EM studies, and biochemical assays elucidated many key features of SMCs. One common function of SMCs may be to extrude a DNA loop driven by ATP hydrolysis cycles, in addition to some other functions specific to each protein. However, how the DNA loop extrusion is realized by SMCs remains elusive. Using coarse-grained molecular simulation approaches, we address structure dynamics, ATP-dependent conformational changes, and interactions to DNA of SMC proteins including cohesin, condensin, and bacterial SMC proteins.

[2S4-3](#) 一分子ヌクレオソームイメージングによって明らかにする生細胞のクロマチン環境とその外的影響
Chromatin behavior in living cells revealed by single-nucleosome imaging

Kazuhiro Maeshima^{1,2} (¹National Institute of Genetics, ²SOKENDAI)

Using single-nucleosome imaging, we have revealed that chromatin is highly dynamic and locally behaves like a liquid in living human cells. Our single-nucleosome imaging is a powerful tool to detect possible changes in the chromatin state induced by various factors such as chemicals or drugs. Using this advantage, we recently examined the chromatin effect of 1,6-hexanediol (1,6-HD), a chemical widely used for melting cellular liquid droplets/compartments formed by liquid-liquid phase separation. We found that 1,6-HD immobilizes and hyper-condenses chromatin in living human cells. This 1,6-HD action seems distinct from its melting activity of liquid droplets, suggesting that liquid droplet results obtained using 1,6-HD should be carefully interpreted or reconsidered.

[2S4-4](#) DNA 液滴の液-液相分離：ナノ～メソスケールの DNA 物性のゲノムモダリティ
Liquid-liquid phase separation of DNA liquid: Genome modality of DNA physics in nanomesoscopic scale

Masahiro Takinoue^{1,2} (¹Dept. Computer Sci., Tokyo Tech, ²Dept. Life Sci. Tech., Tokyo Tech)

Liquid-liquid phase separation droplets involving nucleic acids, such as nucleoli, are well known. In this presentation, we report on the liquid-liquid phase separation of self-assembled DNA nanostructures, called DNA droplets, which exhibit viscoelastic fluid properties and show interesting dynamic properties such as fission and fusion in response to nucleic acid, protein, and light stimuli. Furthermore, in a microspace with molecular crowding, liquid-liquid phase separation occurs under different conditions than in bulk solutions. Thus, knowing the dynamics of DNA droplets and comparing it with the dynamics of chromatin and chromosomes in cells will be nanotechnology for understanding the genomic modalities of DNA properties at the nano- to meso-scale.

[2S4-5](#) 精子クロマチンの操作と測定
Manipulation and measurement of sperm chromatin

Yuki Okada (*IQB, Univ. Tokyo*)

In mammalian sperm chromatin, more than 90% of histones are replaced by sperm-specific small basic proteins called protamines. The incorporation of protamines into sperm chromatin causes a highly condensed structure, which has impeded biochemical analyses of sperm chromatin. We have been working to establish efficient methods for solubilizing sperm chromatin by using chaperon proteins and chemicals to solve this problem. On the other hand, sperm chromatin condensation is biologically essential for the physical protection of sperm DNA and fertility acquisition. Therefore, we are trying to quantify the sperm chromatin using next-generation sequencing to provide useful knowledge for the diagnosis of male infertility. The detail will be introduced in the presentation.

[2S5-1](#) シアノバクテリアの時計タンパク質 KaiC の 2 つの ATPase ドメインによる概日時計の機械式時計モデル
Mechanical clock model for cyanobacterial circadian clock, based on the activities of two ATPase domains in KaiC

Kumiko Ito-Miwa, Takao Kondo (*Grad. Sch. Sci., Univ. Nagoya*)

The cyanobacterial circadian clock consists of three clock proteins, KaiA, KaiB, and KaiC, which can generate a circadian rhythm *in vitro*. The ATPase activity of KaiC determines the period and temperature compensation, as the pacemaker. Based on the biochemical feature of KaiC, we propose that (i) tension generated by the energy from KaiC ATPase activity generates the harmonic oscillation, and (ii) mechanical loose coupling between two oscillations derived from two ATPase domains in KaiC sustains the harmonic oscillation of KaiC, reminiscent of the mechanical pendulum clock. To elucidate this mechanism, we show some key positions within KaiC that function in the tuning for the 24-h period and temperature compensation, by the biochemical analysis of KaiC point mutants.

2S5-2**KaiABC 振動子における温度補償性と 1 分子レベルのフィードバックループ**
Temperature compensation and single-molecular feedback loops in the KaiABC oscillator**Masaki Sasai** (*Nagoya University*)

Does the KaiABC oscillator share a common principle of temperature compensation (TC) mechanism with other transcription-translation oscillators? We propose that the prominent elongation of the oscillation period in mutant KaiCs (Ito-Miwa et al. PNAS 2020) is a clue to this problem. Mutational perturbation should obscure the KaiC structural transitions, weakening the negative feedback between reactions and structure in a KaiC hexamer to elongate the oscillation period at the single-molecular level. A theoretical model showed that the same mechanism works in higher temperatures, leading to the robust TC in the oscillation. The model suggested that TC in the ATPase activity contributes to but is insufficient for TC in the oscillation rhythm.

2S5-3**連続滴定小角 X 線散乱測定を用いたリン酸化/脱リン酸化 KaiC アンサンブルに対する KaiA の滴定挙動解析**
Binding behavior of KaiA for phosphorylated/dephosphorylated KaiC ensemble using continuous titration small-angle X-ray scattering**Hironari Kamikubo**^{1,2,3}, Yoichi Yamazaki² (¹*CDG, NAIST*, ²*MS, NAIST*, ³*IMSS, KEK*)

Assembly and disassembly of Kai proteins are closely related to the phosphorylation cycle of KaiC. To elucidate the binding behavior of KaiA with KaiC ensembles containing different levels of phosphorylation, we carried out continuous titration SAXS experiments using a μ -fluidics based auto sampling system. Every sample with the different phosphorylation levels showed a noticeable increase in the cross term reflecting KaiA/C complex formation. The titration curves against the KaiC ensembles can be represented by the simple binding of KaiA₂ and KaiC₆, but a KaiC ensemble exhibits a limited number of binding modes (strong/weak) depending on the phosphorylation level.

2S5-4**Exploring ancient origin of circadian oscillation through KaiC evolution****Atsushi Mukaiyama**^{1,2}, Yoshihiko Furuike^{1,2}, Shuji Akiyama^{1,2} (¹*IMS, 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. KaiC and its homologues are widespread in bacteria and archaea, and their evolutionary origin is thought to be older than that of cyanobacteria. We therefore restored amino acid sequences of ancestral KaiCs based on a phylogenetic tree and analyzed those functions. Our results suggest that the circadian rhythm first appeared in the earliest cyanobacteria together with KaiC.

2S5-5**シアノバクテリア時計タンパク質 KaiC の根幹を成すアロステリック制御**
Core Allosteric Regulation in Cyanobacterial Circadian Clock Protein KaiC**Yoshihiko Furuike**^{1,2}, Atsushi Mukaiyama^{1,2}, Dongyan Ouyang¹, Kumiko Ito-Miwa³, Simon Damien^{1,2}, Eiki Yamashita⁴, Takao Kondo³ (¹*Research Center of Integrative Molecular Systems (CIMoS), Institute for Molecular Science*, ²*SOKENDAI (The Graduate University for Advanced Studies)*, ³*Graduate School of Science, Nagoya University*, ⁴*Institute for Protein Research, Osaka University*)

Circadian clock systems are driven by post-translational phosphorylation at multiple sites of clock proteins. A cyanobacterial clock protein, KaiC, experiences cyclic phosphorylation and dephosphorylation at S431 and T432 *in vitro*. The oscillation is reconstituted in the presence of ATP and other clock proteins, KaiA and KaiB. Our crystallography visualizing tertiary and quaternary structural changes during KaiC dephosphorylation reveals that ADP-ATP exchange in N-terminal ATPase (C1) domain is bidirectionally coupled to phospho-state switch in C-terminal (C2) domain. Biochemical assays using a series of mutants suggest that the observed C1-C2 communication constitutes a core of the allostery required for the oscillatability of cyanobacterial clock.

[2S6-1](#) (2-01-1712) Extensive Sampling of Spike protein down, one-up, one-open, and two-up-like Conformations and Transitions in SARS-Cov-2

Hisham Dokainish¹, Suyong Re⁴, Chigusa Kobayashi², Takaharu Mori¹, Jaewoon Jung^{1,2}, Yuji Sugita^{1,2,3} (¹*Theoretical Molecular Science Laboratory, Riken*, ²*Computational Biophysics Research Team, RIKEN*, ³*Laboratory for Biomolecular Function Simulation, RIKEN*, ⁴*Center for Drug Design Research, National Institutes of Biomedical Innovation*)

Spike (S) protein is the primary antigenic target for SARS-Cov-2 vaccine development and neutralization. Its receptor binding domain undergoes (RBD) large conformational change from inactive Down to active Up, allowing for ACE2 binding. Despite the abundance of Down, 1Up, 2Up and 3Up Cryo-EM structures, little is known about Spike transitions. Here, we employed our recently proposed enhanced sampling method (gREST_SSCR) to widely sample Spike conformational space, including the transition from Down to 1Up and 1Up to 2Up conformations. Glycans and salt bridges were found to mediate / register the transitions. Unprecedented cryptic pockets were identified at the RBDs' interface that might be targeted to shift S-protein conformational equilibrium hindering cell entry.

[2S6-2*](#) (2-03-1327) An estimation method for the diffusion coefficient using MD simulations with the basic cell containing only one protein as solute

Tomoya Iwashita¹, Masaaki Nagao¹, Akira Yoshimori², Masahide Terazima³, Ryo Akiyama¹ (¹*Department of Chemistry, Graduate School of Science, Kyushu University*, ²*Department of Physics, Niigata University*, ³*Department of Chemistry, Graduate School of Science, Kyoto University*)

A concise correction proposed by Yeh and Hummer has been used for estimations of the diffusion coefficient in finite concentration systems. Here, we performed MD simulations with systems containing only one solute (protein) to study the diffusivity in a dilute solution. In the systems, the additional correction term proposed by Yeh and Hummer is necessary even for relatively large systems. It seems that the correction term is essential when using huge proteins. The correction term includes the hydrodynamic radius, and it made the use of the term difficult. We show that estimation with the term works when the radius is undetermined. We also reveal that the correction term can explain the effective viscosity of solvent between the proteins located in each replica cell.

[2S6-3](#) Oligomer formation of proteins studied by generalized-ensemble algorithms

Satoru G. Itoh^{1,2,3} (¹*IMS*, ²*ExCELLS*, ³*SOKENDAI*)

More than 40 proteins are known to form aggregates such as amyloid fibrils and oligomers, and these aggregates are thought to be associated with disease. In order to overcome such diseases, it is essential to elucidate the protein aggregation process. However, protein aggregation is a very slow process, and even the formation process of small oligomers is difficult to investigate with conventional molecular dynamics simulations. Enhanced sampling methods such as the generalized-ensemble algorithms are useful for studying the slow process. In my talk, I will show recent research on the oligomerization process of amyloid- β peptides using the generalized-ensemble algorithms.

[2S6-4](#) 大規模タンパク質系への適用を目指した構造サンプリング法の開発
Enhanced sampling methods targeting at large proteins

Kei Moritsugu (*Grad. Sch. Med. Life Sci., Yokohama City Univ.*)

In this talk, we present our recent developments on enhanced sampling methods that are in particular aimed to be efficiently computable for applications to large proteins. These are, multiscale enhanced sampling, that allows all-atom structural sampling by coupling with the accelerated dynamics of coarse-grained model, coupled Nosé-Hoover equation, in which a physical system is simulated at nonequilibrium temperature that is fluctuating in a dynamic manner, and weighted ensemble, that enables to obtain a comprehensive path ensemble of protein structural changes as well as the associated kinetic rate constants. The application studies to such as cyclic peptide and enzyme catalysis are also introduced to illustrate the usefulness of these enhanced sampling methods.

2S6-5 マルチドメインタンパク質のリガンド結合による構造変化の分子機構
Molecular mechanisms underlying ligand-induced conformational changes in multi-domain proteins

Yuji Sugita^{1,2,3} (¹RIKEN CPR, ²RIKEN R-CCS, ³RIKEN BDR)

Recently, we developed gREST by modifying the scheme of REST2, which is one of the generalized-ensemble algorithms [1]. gREST enhances conformational sampling of large biological systems by selecting a solute region and exchanging the solute temperatures between neighboring replicas like T-REMD [2]. Since the number of atoms in solute region is small, gREST is applicable to large systems. Here, we discuss one of the applications of gREST on ligand-induced conformational changes in ribose binding protein (RBP) in apo and holo states [3]. Based on the simulation analysis, we discuss molecular mechanisms for ligand-induced conformational changes in RBP [4]. [1] JCP 149, 072304 (2018), [2] CPL 314, 141-151 (1999), [3] IJMS 22, 270 (2021), [4] JPCB 125, 2898-2909 (2021).

2S6-6 膜に埋もれたヒトエンドセリン受容体に結合するボセンタンの結合メカニズム：スライドする
フライ・キャストイングと配向選択メカニズム
Sliding fly-casting and directional-selection mechanisms of bosentan binding to human endothelin receptor embedded in membrane

Junichi Higo (*Graduate School of Information Science, University of Hyogo*)

We studied the binding mechanism of a ligand, bosentan, to human endothelin receptor (hETB), one of the G protein-coupled receptors (GPCR), using a sampling method, GA-guided multidimensional virtual-system coupled molecular dynamics (GA-guided mD-VcMD). The system, which was expressed by an all-atom model, consisted of bosentan, hETB, membrane (POPC bilayers and cholesterol), and solvent. The initial bosentan's position was distant from hETB, which was 65 Å far from the bosentan's binding position). From the resultant free-energy landscape, the most-thermodynamically stable conformation was the native-like complex structure. We obtained two binding mechanisms: Sliding fly-casting and directional-selection. We explain the mechanism in the presentation.

2S6-7 生体分子シミュレーションのための拡張アンサンブル法
Generalized-ensemble algorithms for biomolecular simulations

Yuko Okamoto (*Graduate School of Science, Nagoya Univ.*)

Biomolecular simulations often result in error because they tend to get trapped in local-minimum energy states. In order to overcome this difficulty, we have been advocating the uses of generalized-ensemble algorithms which are based on non-Boltzmann weight factors (for reviews, see, e.g., Refs. [1-4]). In this talk, I will present the latest results of our applications of generalized-ensemble algorithms to biomolecular systems. [1] U. H. E. Hansmann and Y. Okamoto, *Curr Opin in Struct Biol* **9**, 177 (1999). [2] A. Mitsutake, Y. Sugita, and Y. Okamoto, *Biopolymers* **60**, 96 (2001). [3] H. Okumura, S.G. Itoh, and Y. Okamoto, in *Pract Asp Comput Chem II*, J. Leszczynski and M. K. Shukla (eds.) (Springer, 2012) pp. 69-101. [4] Y. Okamoto, *Biophys Physicobiol* **16**, 344 (2019).

2S7-1 (1-10-1442) Local membrane curvature influences lipid signaling

Marcel Hoernig¹, Torsten Bullmann², Tatsuo Shibata³ (¹Institute of Biomaterials and Biomolecular Systems, University of Stuttgart, 70569 Stuttgart, Germany, ²Carl-Ludwig-Institute for Physiology, University of Leipzig, 04103 Leipzig, Germany, ³Laboratory for Physical Biology, RIKEN Center for Biosystems Dynamics Research, Kobe 650-0047, Japan)

PIP3 dynamics observed in membranes are responsible for the protruding edge formation in cancer and amoeboid cells. There are related to the membrane-protrusive activities and formation of macropinocytic cups in Dictyostelium and mammalian cells. Here, we present new insights in the complex pattern evolution of PIP3 waves, and show evidences on how the spatiotemporal dynamics self-regulate through shape, size and local membrane curvature of the plasma membrane in single Dictyostelium cells. We extract and map the lipid signalling on the entire three-dimensional plasma membrane. By statistical analysis of the PIP3 domain dynamics and local noise-fluctuation dynamics, we reveal the importance of the membrane topology with particular impact on the local membrane curvature.

2S7-2 Chemical tools for manipulating signaling proteins and lipids on organelle membranes**Shinya Tsukiji** (*Grad. Sch. Eng., Nagoya Inst. Tech.*)

Membranes serve as platforms for spatially coordinating biological processes in mammalian cells, and various signaling proteins and lipids are dynamically regulated on specific organelle membranes to control cell decision-making. Recently, it is increasingly evident that lipid metabolism and localization are also regulated via the formation of membrane contacts between different cellular organelles. Therefore, techniques that enable the artificial control of molecular processes involving organelle membranes are valuable tools for cell biology and engineering applications. This presentation will focus on new chemical approaches that we developed to manipulate signaling proteins and lipids on organelle membranes in a reversible manner with small molecules in living cells.

2S7-3 A common oligomer identified using 2D IR spectroscopy in mammals that contract type 2 diabetes**Martin Zanni** (*University of Wisconsin-Madison*)

Humans and some, but not all, mammals exhibit amyloid plaques and type 2 diabetes. In this presentation, I will present results in which we use 2D IR spectroscopy and isotope labeling to identify an amyloid oligomer in humans that has beta-sheet-like structure in residues 20-29 of amylin. Data will also be shown for a series of animal mutants and the presence of the oligomer correlated to aggregation propensity, the cellular toxicity of each polypeptide, and the likelihood for that species to contract type 2 diabetes. The results support the hypothesis that there is a common amyloid oligomer structure across species that is responsible for the toxic effects of amylin.

2S7-4 膜貫通ペプチドを用いたナノポアの新規設計
De novo design of nanopore using transmembrane peptides**Ryuji Kawano** (*Department of Biotechnology and Life Science, Tokyo University of Agriculture and Technology*)

Nanopore technology has recently had attracted attention as protein detection and amino acid sequencing. The selectivity depends on the size matching between the target molecule and the nanopore. Although a wide variety of pore-forming proteins have been investigated for their nanopore capability, the target suitable nanopore, such as amino acid detection, has still been explored. In this presentation, we will present a de novo designed nanopore that consists of a transmembrane peptide with a beta-hairpin structure. The peptides are assembling to form a nanopore structure in a lipid bilayer and it can detect DNA or polyaminoacid at the single molecular level. I will introduce the recent progress of this de novo designed nanopore in this session.

2S7-5 生体膜機能の理解に向けた脂質-膜タンパク質相互作用解析
Interaction analysis between membrane proteins and lipids to understand biological membranes**Nobuaki Matsumori** (*Grad. Sch. Sci., Kyushu Univ.*)

Although the interactions with lipids are known to regulate functions and structures of membrane proteins (MPs), the detailed mechanism remains unclear due to lack of methodology for analyzing their interactions. We recently reported a method for quantitatively evaluating MP-lipid interactions using surface plasmon resonance (SPR) system. In the method, SPR sensor chip surface is modified with a self-assembled monolayer, on which a MP is covalently immobilized, and the interaction between the immobilized MP and solubilized lipids is detected. We applied this method to bacteriorhodopsin and KcsA potassium channel, and consequently not only identified their specific lipids but also demonstrated that the specific lipids regulate the functions of these MPs.

2S7-6 スマートシャペロン高分子による脂質膜の刺激応答性小胞・シート転移
Stimuli-responsive vesicle/sheet transformation of lipid membranes mediated by smart chaperone polymers

Atsushi Maruyama (*School of Life Sci. & Tech., Tokyo Inst. of Tech.*)

Self-assembling property of lipid membranes and its dynamics play pivotal roles in living systems. Among the lipid membrane assemblies, there is a few observations for 2D lipid assembly, lipid sheet, and transformation between sheets and vesicles. We found that cell-sized lipid vesicles were quantitatively converted to self-standing nanosheets with high efficiency by addition of an amphiphilic membrane-disruptive peptide, E5, and a cationic copolymer, which had chaperoning activity to fold E5 to helical structure. We constructed lipid membrane systems that spontaneously transformed between lipid vesicles and sheets in response to a particular stimulus, such as enzyme, temperature, pH and time duration, by designing smart chaperone polymers.

2S7-7 弱毒性カチオン性両親媒性ペプチド存在下の IgG による液滴形成と効率的細胞内移行
Liquid droplet formation and facile cytosolic translocation of IgG in the presence of attenuated cationic amphiphilic lytic peptides

Shiroh Futaki (*Inst. Chem. Res., Kyoto Univ.*)

Fc region binding peptide conjugated with attenuated cationic amphiphilic lytic peptide L17E trimer [FcB(L17E)₃] was designed for immunoglobulin G (IgG) delivery into cells. Particle-like liquid droplets were generated by mixing Alexa Fluor 488 labeled IgG (Alexa488-IgG) with FcB(L17E)₃. Droplet contact with the cellular membrane led to spontaneous influx and distribution of Alexa488-IgG throughout cells in serum containing medium. Involvement of cellular machinery accompanied by actin polymerization and membrane ruffling was suggested for the translocation. In the presence of FcB(L17E)₃, anti-nuclear pore complex antibodies labeled with Alexa Fluor 594 were successfully delivered into the cells and bound to their intracellular targets.

3S1-1 Cyclodextrins increase membrane tension and are universal activators of mechanosensitive channels

Charles David Cox (*Victor Chang Cardiac Research Institute, Sydney*)

The bacterial mechanosensitive channel of small conductance, MscS, has been extensively studied to understand how mechanical forces are converted into the conformational changes that underlie mechanosensitive (MS) channel gating. We showed that lipid removal by β -cyclodextrin can mimic membrane tension. Here, we show that all cyclodextrins (CDs) can activate reconstituted *E. coli* MscS and that MscS activation by CDs depends on CD-mediated lipid removal. Since CDs can also open the least tension-sensitive MS channel, MscL, they should be able to open any MS channel that responds to membrane tension. Thus, CDs emerge as a universal tool for the structural and functional characterization of unrelated MS channels.

3S1-2 Understanding the interaction of phenolic acids with phospholipid bilayers

Sheik Imamul Hossain¹, **Evelyn Deplazes**^{1,2} (¹*School of Life Sciences, University of Technology Sydney, Australia*,
²*School of Chemistry and Molecular Biosciences, University of Queensland, Australia*)

We combine tethered lipid bilayer (tBLM) electrical impedance spectroscopy (EIS) with MD simulations to study the membrane interactions of six phenolic compounds: caffeic acid methyl ester (CAME), caffeic acid (CA), 3,4-dihydroxybenzoic acid (DHBA), chlorogenic acid (CA), syringic acid (SA) and p-coumaric acid (pCA). Experiments showed that CAME, CA and DHBA significantly increase phospholipid bilayer permeability while CGA, SA and pCA show no effect. Simulations show that membrane-altering compounds interact with the phosphate oxygen while inactive compounds primarily interact with interfacial water. The membrane-altering effects are governed by specific interactions at the water-lipid interface and show no correlation with lipophilicity.

3S1-3 Structural analyses on pathogenic RNA viruses**Yukihiko Sugita**^{1,2} (¹*InFront, Kyoto Univ.*, ²*Hakubi Center, Kyoto Univ.*)

There are many important pathogenic RNA viruses for public health in the world, such as influenza, measles, rabies viruses. In addition, many of emerging infectious diseases, such as Ebola virus and novel corona virus diseases, are caused by RNA viruses. In order to elucidate the assembly mechanism of viruses and to develop vaccines and antiviral drugs, it is important to clarify their molecular structure. Cryo-electron microscopy, which has achieved remarkable technological development in recent years, is an indispensable technique for structural analysis of RNA viruses. In this presentation, I will introduce the structural analysis of pathogenic RNA viruses by cryo-electron microscopy being conducted at Kyoto University.

3S1-4 酵母複製とプリオン伝送の多スケール運動・空間モデル
A multi-scale kinetic and spatial model of yeast replication and prion transmission**Damien Hall** (*Kanazawa University WPI-NANO-LSI*)

Yeast cells of a single mating type can acquire an amyloid prion in two ways (i.) Spontaneous nucleation of the prion within the yeast cell, and (ii.) Infection via mother-to-daughter transmission during the cell division cycle. Here I model these two general processes using a multiscale approach. The yeast growth cycle is considered in two stages, a mature yeast that is competent to bud (M) and a distinct daughter yeast (D). Each transition in yeast growth is stochastically regulated. Between the relatively coarse time-points used for the particle level description a set of differential equations, describing the nucleation, growth, fragmentation and clumping of amyloid fibrils, is solved numerically, for each individual yeast cell.

3S1-5 合成小分子を利用した細胞内タンパク質の光操作
Chemo-optogenetic manipulation of protein functions in living cells using synthetic small molecules**Tatsuyuki Yoshii** (*CiRA, Kyoto Univ.*)

Manipulating protein functions using light is a powerful approach for controlling signaling processes with high spatial and temporal resolution. We developed a chemo-optogenetic approach for controlling protein localization using a photoactivatable small molecules. We synthesized chemicals that can recruit tag-fused proteins of interest from the cytoplasm to the plasma membrane within seconds upon light illumination. The present technology enables the spatiotemporal control of signaling processes in living cells. Using the chemical, we were able to implement optically control and visualize molecular processes in a single cell, simultaneously.

3S2-1 A specific eIF4A paralog facilitates LARP1-mediated translation repression during mTORC1 inhibition**Shintaro Iwasaki** (*RIKEN Cluster for Pioneering Research*)

Eukaryotic translation initiation factor (eIF) 4A — a DEAD-box RNA-binding protein — plays an essential role in translation initiation. Two mammalian eIF4A paralogs, eIF4A1 and eIF4A2, have been assumed to be redundant because of their high homology, and the difference in their functions has been poorly understood. Here, we show that eIF4A1, but not eIF4A2, enhances translational repression during the inhibition of mechanistic target of rapamycin complex 1 (mTORC1), which is an essential kinase complex for cell proliferation. Our data show that the distinct protein interactions of these highly homologous translation factor paralogs shape protein synthesis during mTORC1 inhibition and provide a unique example of the repressive role of a universal translation activator.

3S2-2

人工神経回路組織における神経回路とタンパク質合成制御

Organoids-on-a-chip models for understanding neuronal circuits and underlying protein synthesis regulations

Yoshiho Ikeuchi^{1,2,3} (¹*IIS, Univ. Tokyo*, ²*Chem. Bio., Eng., Univ. Tokyo*, ³*Inst. AI and Beyond, Univ. Tokyo*)

Neurons extend axons to establish communications to form macroscopic circuits. Although the complexity of the macroscopic network hindered elucidation of functional mechanisms of the brain, organoid technologies have recently provided novel avenues to investigate human brain function by constructing small segments of the brain *in vitro*. However, neural organoids cannot form macroscopic circuits spontaneously without manipulation. I will introduce our “organoid-on-a-chip” approach to model macroscopic circuits by applying microfluidic technologies. The model provides an ideal platform to experimentally assess both network dynamics and biochemical changes. I will discuss utilization of the model to analyze neuronal regulation of protein synthesis.

3S2-3

生理的体温変化による体内時計のパラメトリック制御

Parametric entrainment of the circadian clock by body temperature change

Takahito Miyake, Yuich Inoue, Masao Doi (*Grad. Sch. Pharm. Sci., Kyoto Univ.*)

The circadian clock is the most fundamental time-keeping system for organisms. Physiologically, diurnal body temperature changes play a key role in synchronizing numerous tissue-clocks across the body (Shimatani et al., 2020; Miyake et al., 2019). However, how the temperature changes regulate the phase or angular velocity of the tissue-clocks is totally unknown. In this research background, we recently found that a mimic body temperature shift accelerates the translational velocity of the core clock gene. We also reported that body temperature decreases during siesta is genetically programmed (Goda et al., 2018). In this talk, we would like to discuss the importance of the parametric circadian clock entrainment via temperature-driven translational velocity regulation.

3S2-4

Fluorescent nanodiamonds for thermal biology

Shingo Sotoma¹, Yoshie Harada^{1,2} (¹*IPR, Osaka Univ.*, ²*QIQB, Osaka Univ.*)

Fluorescent nanodiamonds (FNDs) have recently reported as a novel fluorescent probe with unique optical properties. Fluorescence from nitrogen-vacancy centers (NVCs) in FNDs shows neither photoblinking nor photobleaching, which enables quantitative and long-term imaging *in vitro* and *in vivo*. Besides, a quantum states of the electron spins in NVCs can be read out optically, which render FNDs as a nanoscale temperature sensor. FNDs have drawn a great deal of attention since the invention and their development potential and applications in the thermal biology are proving to be manifold and vast. In my presentation, I will show our recent achievement of the FND-based technologies including surface chemical modification and temperature sensing inside a cell.

3S2-5

細胞内温度シグナリングによる翻訳調節機構

Intracellular thermal signaling facilitates translation control

Kohki Okabe^{1,2} (¹*Grad. Sch. Pharm. Sci., Univ. Tokyo*, ²*PRESTO, JST*)

The translation rate is not constant, but dynamically fluctuates, allowing for complex gene expression. However, the physicochemical mechanisms that drive parametric translation are unknown. Since previous studies have shown that spatiotemporal temperature fluctuations exist in intracellular locations and that translation consumes a large amount of energy, we here focused on the intracellular temperature as a physicochemical mechanism that affects the translation rate. Using our original methods to measure local intracellular temperature and to manipulate the local temperature, we revealed the contribution of thermal signaling on translation. This may be a mechanism to control the translation speed in a fast and continuous manner.

3S3-1 誘電緩和分光法で観測する水和角質層中の水と氷

Water and ices in hydrated stratum corneum observed via dielectric relaxation spectroscopy

Masahiro Nakanishi (*Fac. Eng., Fukuoka Inst. Tech.*)

In the present talk, dielectric spectra of hydrated stratum corneum (SC) below freezing temperature will be discussed. At lower hydration level, only one apparent dielectric process with accompanying excess wing is recognized in the dielectric spectra. With increasing hydration level, these spectra are getting complicated: four apparent processes were observed. Comparing different temperature protocols, such as slow and rapid cooling, these processes are assigned to hydration water and ices at different states. This finding opens the possibility that water at different states can be discerned each other via the electrical method which is more straightforward than other methods.

3S3-2 中性子散乱を用いて明らかとなった水和水の熱活性がタンパク質ダイナミクスに与える影響

Effect of hydration and its thermal energy on protein dynamics monitored by neutron scattering

Naoki Yamamoto (*Sch. Med., Jichi Med. Univ.*)

Protein function is expressed in the thermal fluctuation of solvent, water. Therefore, it is essential to understand how protein dynamics are activated by thermal fluctuation of water molecules in the vicinity of protein molecule, i.e. hydration water. Here, how hydration water affects protein dynamics will be introduced. Using neutron scattering, we have recently suggested that hydration water molecules which strongly interacts with protein surface are crucial for activation of protein dynamics, whereas those loosely interacting with protein surface do not play role for the activation [1]. We will discuss the molecular mechanism of the phenomena and role of these hydration water molecules for function. [1] N. Yamamoto et al., *J. Phys. Chem. Lett.* 2021, 12, 2172-2176

3S3-3 生体分子と水の凍結・融解・ガラス転移

Freezing, Thawing and Glass Transition of Biomolecules and Water

Hiroshi Nakagawa (*Japan Atomic Energy Agency*)

Water activity (A_w) is a thermodynamic quantity defined as the ratio of the water vapor pressure of a sample to that of pure water at the same temperature. This value is known to be a reliable indication of the microbial growth, enzymatic activity, and preservation and quality of foods. The molecular basis of A_w is under debate in the related disciplines. The water activity of glycerol-water mixtures can be controlled by changing its glycerol and water ratio. In this study, the diffusive dynamics of water were investigated with glycerol-water mixtures at various A_w s by incoherent quasi-elastic neutron scattering (IQENS), and then the observed dynamics were compared with the differential scanning analysis (DSC).

3S3-4 Polyampholytes for low-temperature preservation of cells and proteins**Robin Rajan, Kazuaki Matsumura** (*Japan Advanced Institute of Science and Technology*)

Preservation of cells and proteins is crucial for many applications and requires low temperatures, which in turn triggers a myriad of undesirable consequences. The most frequently encountered problem is the osmotic damage caused by the increase in salt concentration in the surrounding medium because of freeze concentration. To this end, we have developed polyampholytes based on poly-L-lysine (PLL) which yielded excellent cryoprotection results and was able to reduce the osmotic damage to decrease the freeze concentration by trapping salt in the molecules, which was established by solid-state NMR studies. Moreover, polyampholyte grafted onto poly-vinyl alcohol could efficiently protect proteins from multiple freeze-thaw cycles as well as during cryopreservation.

3S4-1 KEK クライオ電顕施設の運用と現状について
Operation and recent activities of the cryo-EM facility in KEK

Naruhiko Adachi (*SBRC, IMSS, KEK*)

The cryo-EM network, which was launched in March 2019, is a network for Japanese researchers to perform high-resolution structural analysis using 300 kV and 200 kV cryo-EM, which were introduced by national projects, such as BINDS. In this presentation, we will briefly explain the network and introduce the KEK cryo-EM facility, which is one of the facilities of the network, its operation status, usage, recent activities, and future plans. We also present examples of some trials for large-scale dynamics in protein with single particle analyses.

3S4-2 X線小角散乱データと粗視化分子動力学計算に基づく生体分子の構造ダイナミクスの解明
Modeling structural dynamics of biomolecules using small angle X-ray scattering data and coarse-grained molecular dynamics simulations

Masahiro Shimizu, Aya Okuda, Ken Morishima, Yasuhiro Yunoki, Nobuhiro Sato, Rintaro Inoue, Reiko Urade, Masaaki Sugiyama (*KURNS, Kyoto Univ.*)

Dynamics of a biomolecule is a collection of motion with various spatial and temporal scales. One powerful strategy for identifying the complicated dynamics is to combine molecular dynamics simulations with experimental data containing information on molecular motion in solution. In this study, we combine coarse-grained molecular dynamics simulations with small angle X-ray scattering data to reveal structural dynamics of biomolecules. First, we report dynamics of single-stranded DNAs with various sequences and discuss relationship between their base stacking probability and sequence recognition mechanism by a protein. Second, we discuss domain structure of multi-domain protein ER-60 depending on its redox state of CGHC motif.

3S4-3 NMR と EPR を組み合わせたマルチドメインタンパク質の大規模ダイナミクスの探索
Large-scale conformational distribution of a multi-domain protein enzyme investigated by NMR and EPR

Tomohide Saio (*Inst. of Adv. Med. Sci.*)

Multi-domain proteins often undergo large scale conformational changes that are critical for their functions. However, lack of the efficient strategy for visualizing conformational states and changes impeded the understanding of the mechanism. Here in this study, an integrative structural analysis exploiting NMR, EPR, and paramagnetic lanthanide ions was performed on a 47-kDa protein enzyme MurD. The NMR experiments exploiting paramagnetic probes detected the conformational changes of MurD upon binding to the ligand. The EPR experiments provided the information about conformational variation of MurD. The data visualized ligand-induced changes of the conformational states and variation of MurD that have been obscured in the previous structural studies.

3S4-4 X線/中性子散乱と MD シミュレーションを用いた統合的アプローチによる IDP の動的構造と機能の理解
Integrated approach using X-ray/Neutron scattering and MD simulation for understanding dynamic structure and function of IDP

Takashi Oda^{1,2} (¹*Department of Life Science, Rikkyo University,* ²*Graduate School of Medical Life Science, Yokohama City University*)

Dynamic structure of IDP is closely related to function. However, the methods that can analyze the dynamic structure of IDP are limited. Small-angle X-ray scattering (SAXS) can provide dynamic structural information, but it is low resolution. In addition, in multi-domain proteins with intrinsically disordered regions (IDR), scattering from each domain and IDR is observed as a single scattering curve, which makes interpretation difficult. Small-angle neutron scattering (SANS) using deuterated protein, can provide scattering data from the target region. Molecular dynamics (MD) can simulate dynamic structures with atomic resolution, and it can compensate for the low resolution of SAXS. In this session, we report an integral approach using SAXS, SANS and MD simulation.

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- [3S4-5](#) ストレス刺激により誘起される ATP 枯渇および低 pH 条件における MAPK p38 α の頑強な酵素活性を担う機能的構造平衡の解明
Functional equilibrium underlying the robust kinase activity of MAPK p38 α under the stress-associated ATP-depleted, low pH condition

Yuji Tokunaga¹, Koh Takeuchi¹, Hideo Takahashi², Ichio Shimada³ (¹*CMB, AIST*, ²*Grad. Sch. Med. Life Sci., Yokohama City Univ.*, ³*Tsurumi Inst., Riken*)

Stress-induced reduction of cellular ATP and pH could attenuate the activity of ATP-utilizing proteins, including stress-activated mitogen-activated protein kinases (MAPKs). Nevertheless, even under such a seemingly unfavorable condition, MAPK p38 α phosphorylates its substrates for stress response. We found that weak acidification unexpectedly made the affinity of p38 α for ATP, thereby compensating for the ATP depletion. Solution NMR delineated a pH-sensitive conformational equilibrium of p38 α between the states with distinct affinity for ATP. Two conserved histidine residues were identified as the pH sensor responsible for the equilibrium. These mechanisms would confer robust substrate phosphorylation by p38 α within stressed cells for efficient signal transduction.

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- [3S5-1](#) 遺伝子組換え抗菌ペプチド生産と NMR 解析への応用
Application of novel overexpression systems of recombinant antimicrobial peptides for NMR analysis

Tomoyasu Aizawa (*Grad. Sch. Life Sci., Hokkaido Univ.*)

In general, small peptides are very difficult to produce using recombinant technology because they are easily degraded in their soluble form. However, making large numbers of targets is an important step in the study of peptides. In particular, NMR studies using stable isotope-labeled recombinant peptides are one of the most powerful tools for studying structures and interactions. In this talk, I will describe several methods to facilitate expression levels of recombinant antimicrobial peptides that are toxic to the expressing host and difficult to express in conventional production systems. The application of NMR in research will also be presented.

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- [3S5-2](#) AI で設計した膜貫通ペプチドの分子動力学計算による選択と理解
Using molecular dynamics simulations to prioritize and understand AI-generated cell penetrating peptides

Koji Tsuda (*Grad. Sch. Frontier Sci., Univ. Tokyo*)

Cell-penetrating peptides have important therapeutic applications in drug delivery, but the variety of known cell-penetrating peptides is still limited. With a promise to accelerate peptide development, artificial intelligence (AI) techniques including deep generative models are currently in spotlight. Scientists, however, are often overwhelmed by an excessive number of unannotated sequences generated by AI and find it difficult to obtain insights to prioritize them for experimental validation. To avoid this pitfall, we leverage molecular dynamics (MD) simulations to obtain mechanistic information to prioritize and understand AI-generated peptides.

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- [3S5-3](#) 単一巨大リボソーム法や単一細胞実験から解明された抗菌ペプチドの作用機構
Modes of Action of Antimicrobial Peptides (AMPs) revealed by the Single Giant Unilamellar Vesicle (GUV) Method and Single Cell experiments

Masahito Yamazaki^{1,2,3} (¹*Res. Inst. Ele., Shizuoka Univ.*, ²*Grad. Sch. Sci. Tech., Shizuoka Univ.*, ³*Grad. Sch. Sci., Shizuoka Univ.*)

Most AMPs induce damage of bacterial plasma membranes with consequent significant leakage of internal contents, which is one of the main causes for their bactericidal activities. We have obtained the detailed information on the elementary processes of AMPs-induced damage of lipid bilayers and those of the translocation of AMPs across lipid bilayer using the single GUV method (1). The effect of membrane tension and membrane potential on their action have been revealed. It is important to compare the results of the interaction of AMPs with single bacterial cells and spheroplasts (2) with those obtained using the single GUV method. (1) *PCCP*, 16, 15752, 2014; *Langmuir*, 34, 3349, 2018; *Biophys. Rev.* 11, 431, 2019, (2) *JBC*, 294, 10449, 2019; *J. Bacteriol.*, 203, e00021-21, 2021.

[3S5-4*](#) (2-10-1351) 放射光円二色性・直線二色性・蛍光異方性により明確化された生体膜に誘起されたマガニン 2β 凝集体の特徴
(2-10-1351) Membrane-Induced β-Aggregates of Magainin 2 Characterized by Circular Dichroism, Linear Dichroism, and Fluorescence Anisotropy

Munehiro Kumashiro¹, Shoma Suenaga¹, Koishi Matsuo² (¹*Grad. Sch. Sci., Hiroshima Univ.*, ²*HiSOR, Hiroshima Univ.*)

Synchrotron-radiation circular dichroism spectra of magainin 2 (M2) were measured in DPPG lipid membrane at lipid-to-peptide (L/P) molar ratio from 0 to 26. The results showed that the conformation of M2 changed from random coil to α-helix structures via an intermediate state as the L/P increases. The adsorption model fitting analysis of the spectra indicated that α-helix monomers assembled and transformed to β-sheet oligomers in the intermediate state. Linear dichroism provided the orientation of the β-sheet structure on the membrane surface. Fluorescence anisotropy of liposome showed that the formation of β-aggregates caused the disorder of the membrane, suggesting that the β-aggregates in membranes play a crucial role in the disruption of cell membrane by M2.

[3S5-5](#) Conformational plasticity defines cell permeabilization activity of cyclic peptides

Koh Takeuchi^{1,2} (¹*CMB, AIST*, ²*Grad. Sch. Pharm. Sci., The Univ. of Tokyo*)

Cyclic peptides have emerged as a novel pharmaceutical modality for targeting intracellular protein-protein interactions (PPIs). However, only a subset of the cyclic peptides can enter mammalian cells to inhibit intracellular PPIs with the molecular mechanism that remains largely unknown. By comparing the 3D structures of cyclorasin, a set of 11-mer cyclic peptides that inhibit the Ras-Raf PPI, we found that peptides with cell permeabilization activities can change their conformation in water to a characteristic amphipathic structure in DMSO. However, those that do not permeate cells cannot adopt the amphipathic structure, indicating that conformational plasticity is an important structural element that defines the cell permeabilization activities of cyclic peptides.

[3S5-6](#) アミロイド β ペプチドの凝集と解離の分子動力学シミュレーション
Molecular Dynamics Simulations for Aggregation and Disaggregation of Amyloid-β Peptides

Hisashi Okumura^{1,2,3} (¹*Exploratory Research Center on Life and Living Systems*, ²*Institute for Molecular Science*, ³*SOKENDAI*)

Many proteins aggregate at higher concentrations and form spherical substances called oligomers and needle-like substances called amyloid fibrils. These protein aggregates cause more than 40 kinds of diseases, for example, Alzheimer's disease is thought to be caused by the oligomers and amyloid fibrils formed by amyloid-β (Aβ) peptides. To investigate the aggregation and disaggregation of Aβ, we performed several molecular dynamics (MD) simulations of Aβ peptides. In this talk, I will present the aggregation process of Aβ peptides, conformations of an Aβ peptide at hydrophilic/hydrophobic interface, and disaggregation by supersonic wave and infrared-laser irradiation.

[3S5-7](#) 膜環境におけるアミロイド β の分子集合
Molecular assembly of amyloid-β in membrane environments

Maho Yagi-Utsumi^{1,2} (¹*ExCELLS, NINS*, ²*IMS, NINS*)

The morphology of amyloid fibrils is strongly influenced by solution conditions, e.g. temperature, pressure, and gravity. In addition, the aggregation of various amyloidogenic proteins as exemplified by amyloid β (Aβ) in Alzheimer's disease can be significantly promoted in membranes environments, which induce their conformational changes as crucial steps for amyloid fibril formation. Therefore, for deeper understanding of the molecular mechanism behind the amyloid formation, it is necessary to characterize dynamic structural changes and interactions of Aβ molecules in such complex microenvironments. Here, I present structural insights into Aβ assembly considering the environmental factors, highlighting NMR studies of Aβ molecules situated in glycolipid clusters.

3S6-1 SCOPE-seq: Scalable Technology for Linking Live Cell Imaging and Single-Cell RNA-seq**Peter Sims** (*Columbia University*)

Single-cell RNA-seq (scRNA-seq) has emerged as a powerful tool for uncovering cell types in complex tissues and cell state transitions. However, many cellular phenotypes are dynamic or difficult to infer from the transcriptome alone. Live cell imaging provides access to an orthogonal set of cellular phenotypes. We recently developed SCOPE-seq for linking live cell imaging and scRNA-seq on a large-scale. The technology combines microfluidics with barcoded RNA capture beads that can be decoded both optically and by conventional sequencing. I will describe the evolution of this technology, basic science applications in developmental neuroscience, and translational applications with the potential to impact the treatment of malignant brain tumors.

3S6-2 (2-15-1736) 微小電気穿孔法を用いた細胞膜の機械特性と遺伝子発現の統合解析
(2-15-1736) A combined analysis of membrane-mechanical phenotyping and transcriptomics using nanoelectroporation**Akifumi Shiomi**, Taikopaul Kaneko, Kaori Nishikawa, Hirofumi Shintaku (*Hakubi, CPR, RIKEN*)

Mechanical properties of the cellular membrane are phenotypic expression that are involved in various biological contexts, especially aging. However, these detailed molecular cascade remains to be uncovered due to the complex physiological processes and the unexplained initiation factors. Here, we report an approach that enables a combination analysis on membrane-mechanical phenotype and gene expression in each of thousands of single cells leveraging nanoelectroporation, dubbed ELASTomics (electroporation-based lipid-bilayer assay for stiffness and transcriptomics). Applying ELASTomics to human TIG-1 fibroblasts, we dissect the link between the membrane-mechanical phenotype and gene expression along with the cellular senescence at single-cell resolution.

3S6-3 免疫細胞の活性化の瞬間を見て探って調べる
Analysis of Gene Expression at the Moment of Immune Cell Activation by Live Cell Imaging & Harvesting**Yoshitaka Shirasaki** (*Grad.Sch.Pharm., Univ. Tokyo*)

Immune cells activate upon external stimuli and shift to their inflammatory state through evolving networks of gene expression regulation. Previous studies of live-cell imaging in immune cell activation have revealed that individual cells exhibit not only quantitative and qualitative diversity in their activation, but also large temporal variations. To investigate the transition of gene expression during activation to an inflammatory state, we need to retrieve individual cells according to the timing of their activation. In this study, we have developed a time-dependent cell state selection technique based on live-cell imaging. As a result, we succeeded in determining the stage-dependent gene expression pattern along with the activation of immune cells.

3S6-4 超高速流体制御が拓くオンチップ細胞操作・計測
On-chip cell manipulation and analysis opened up by ultra-high-speed flow control**Shinya Sakuma** (*Dept. of Mechanical Engineering, Kyushu University*)

Since Reynolds number, which is the ratio of inertial force to viscous force, generally takes a small value in microchannels, we can utilize stable environment in on-chip cell manipulation/analysis. Up to the present time, a considerable number of functions represented by cell transportation have been realized by utilizing the stable environment. Under these circumstances, we have integrated on-/off-chip flow control technologies into the microfluidic chip, which enable to utilize wide range of Reynolds number, and achieved new functions and applications; high-resolution cell positioning; high-speed and high-resolution pipetting; high-speed on-chip cell sorting. In this presentation, these examples are introduced as new topics of on-chip cell manipulation and analysis.

Yoshihiro Izumi¹, Kohta Nakatani¹, Kosuke Hata¹, Shohei Yamamura², Masaki Matsumoto³, Takeshi Bamba¹*(¹Medical Institute of Bioregulation, Kyushu University, ²Health and Medical Research Institute, National Institute of Advanced Industrial Science and Technology, ³Graduate School of Medical and Dental Sciences, Niigata University)*

Analytical methods to accurately identify and quantify comprehensive metabolites or proteins from single mammalian cells are still in development. The aim of this study was to develop a single-cell metabolomic and proteomic analytical system based on highly sensitive nano-liquid chromatography tandem mass spectrometry (nano-LC/MS/MS). We firstly developed a method called in-line sample preparation for efficient cellular metabolomics or proteomics (ISPEC). By combining live single-cell sampling, ISPEC, and nano-LC/MS/MS, we successfully detected approximately 100 metabolites or 300 proteins from single cells. Our single-cell proteomic and metabolomic analytical system represents a potentially useful tool for in-depth studies focused on cell metabolism and heterogeneity.

Jianshi Jin, Katsuyuki Shiroguchi (*BDR, RIKEN*)

Predicting molecularly-defined states of biological samples from microscopy images by deep learning has had a great impact on biological studies. However, microscopy image-based prediction of whole transcriptome-defined states of single cells has not been performed due to technical difficulties in data acquisition. 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. Using these datasets, we predicted the transcriptome-defined cell states from the cell images by deep learning. Base on this prediction, we propose Machine-learning Refined Images as an Omics-based cell marker which does not rely on a specific gene(s) or antibody labeling.

[1-01-1330](#) SARS-CoV-2 変異株に有効な中和抗体の理論的設計

Theoretical design of neutralizing antibodies that are effective for SARS-CoV-2 variants

Rina Aoyama¹, Sairi Matsumoto¹, Yuuki Hayashi¹, Munchito Arai^{1,2} (¹*Dept. Life Sci., Univ. Tokyo*, ²*Dept. Phys., Univ. Tokyo*)

The development of therapeutic drugs for COVID-19 caused by the severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2) has rapidly progressed around the world. Several antibody therapeutics that bind the receptor-binding domain (RBD) of the Spike protein of SARS-CoV-2 have been approved for clinical use. However, the antibody therapeutics may reduce or lose their efficacy by mutations in the RBD. In fact, casirivimab has a reduced affinity to the E484K mutant of RBD. Here, we rationally design neutralizing antibodies that can bind RBD mutants, such as E484K. We use the protein modeling software Rosetta to theoretically design the antibodies. We will experimentally validate whether the designed antibodies bind tightly to RBD mutants.

[1-01-1342](#) Relationship between designability of proteins and frustration : A lattice model study

Kazuma Toko, George Chikenji (*Dept. of App. Phys., Nagoya Univ.*)

Designability of protein structure is the number of sequences that can design the structure. What features determine the designability of structures? Here, we hypothesize that local rules of real protein determine designability. We use the HP lattice protein model in order to verify this hypothesis. We found that the relationship between sequences and structures of HP model with penalty on local structure is consistent with that of observed in the database of real proteins: The local structure with penalty does not appear in highly designable structures, and it appears in some of the poorly designable structures. These results suggest that local rules of protein are the determinant of the designability of protein structures.

[1-01-1354](#) アルカン合成酵素の高活性化変異体の合理的設計

Rational design of highly active mutants of an alkane-producing enzyme

Masaaki Isoda¹, Yuuki Hayashi^{1,2}, Munchito Arai^{1,2,3} (¹*Dept. Integ. Sci., Univ. Tokyo*, ²*Dept. Life Sci., Univ. Tokyo*, ³*Dept. Physics, Univ. Tokyo*)

Alkane biosynthesis has attracted much attention as a promising way of producing carbon-neutral, sustainable energy. A key enzyme for alkane biosynthesis in cyanobacteria is aldehyde-deformylating oxygenase (ADO). ADO is a soluble, globular protein and has an activity of converting fatty aldehydes into alkanes/alkenes. However, the alkane-producing activity of ADO is very low, and thus the improvement of the ADO activity is required to put it to practical use. Here, we attempt to create highly active mutants of ADO by rational design using Rosetta. Our strategy is to search for the mutants that destabilize the product-bound form of ADO, while stabilizing the substrate-bound form. The detailed results will be presented at the meeting.

[1-01-1406](#) 緑色蛍光蛋白質由来赤色蛍光蛋白質の開発

Engineering of a coral green fluorescent protein into red

Hiroimi Imamura¹, Shiho Otsubo², Mizuho Nishida¹, Norihiro Takekawa², Katsumi Imada² (¹*Grad. Sch. Biost., Kyoto Univ.*, ²*Dept. Macromol. Sci., Grad. Sch. Sci., Osaka Univ.*)

Fluorescent proteins (FPs) are widely used in biological research as versatile tags for protein/organelle/cell, components of biosensors, and models for studying the molecular evolution of proteins. Red FPs are characterized as their chromophore structure with an extended π -conjugation system, as compared to green FPs. Because natural red FPs have low sequence similarity with green FPs, it has been unclear which amino acids are essential for the auto-catalytic formation of the red chromophore. In this study, we succeeded in the engineering of a coral green fluorescent protein, AzamiGreen, into red by introducing 29 amino acid mutations. The crystal structure of the resultant red FP revealed drastic structural rearrangements around the chromophore due to the mutations.

[1-01-1418](#) 緑色蛍光蛋白質 AzamiGreen 由来赤色蛍光蛋白質の結晶構造解析に基づく赤色蛍光団形成の構造基盤

Structural basis of red chromophore formation based on crystal structures of artificial red fluorescent proteins derived from AzamiGreen

Shiho Otsubo¹, Hiromi Imamura², Norihiro Takekawa¹, Katsumi Imada¹ (¹*Dept. Macromol. Sci., Grad. Sch. Sci., Osaka Univ.*, ²*Grad. Sch. Biost., Kyoto Univ.*)

Red fluorescent protein (RFP) is useful for deep tissue imaging, but fluorescence intensities of existing RFPs are far from satisfaction. To develop a high-performance RFP, various studies on fluorescent proteins with long-wavelength emission have been performed. However, the mechanism of red chromophore formation is still unclear. Recently, we created novel RFPs by introducing dozens of mutations in AzamiGreen, a coral GFP. Back mutation studies of the artificial RFPs suggested residues essential for redification. To clarify the role of the residues, we determined the crystal structures of the artificial RFPs and some back mutant variants. We will discuss possible mechanisms of the stable red chromophore formation based on the structures.

[1-01-1430](#) The register shift rules for $\beta\alpha\beta$ -motifs for de novo protein design: A database analysis and all-atom calculations

Senji Mishima, George Chikenji, Hiroto Murata (*Dept. of App. Phys., 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 (1) register shift rules are important for de novo design of β -sheet proteins; (2) according to the PDB analysis, preferred register shifts in a $\beta\alpha\beta$ -motif strongly depend on the loop torsion types; and (3) 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 $\beta\alpha\beta$ -motifs with another popular loop-type (GBA-loop). Detailed results will be reported in the presentation.

[1-01-1442](#) The Effect of Molecular Weight on the Formation of Fibroin Precursor and Nanofiber

Kok Sim Chan¹, Kento Yonezawa², Takehiro Sato³, Yoichi Yamazaki¹, Sachiko Toma-Fukai¹, Hironari Kamikubo^{1,2,4} (¹*Division 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.*, ⁴*Institute of Materials Structure Science, High Energy Accelerator Research Organization (KEK)*)

Our research group has uncovered precursors responsible for the formation of fibroin protein nanofiber, which may be present in spider silk. However, the structural characteristics of these fibroin precursors remain unclear. To characterize these structures, we prepared two fibroin precursors with different molecular weights, 50 kDa and 200 kDa, and carried out Dynamic Light Scattering and Atomic Force Microscopy. Results of these analyses show that, despite their difference in molecular weight, the precursors are similar in size, suggesting that a large part of the fibroin could be disordered. This presentation presents the detailed structural characterization of these two fibroin precursors.

[1-01-1454](#) ペリプラズム結合蛋白質 AcfC と協働するコレラ菌走化性受容体 Mlp8 のリガンド認識機構
Ligand recognition mechanism of Mlp8, a chemoreceptor protein of *Vibrio cholerae*, with AcfC, a periplasmic binding protein

Yuzuki Yabunaka¹, Yohei Takahashi¹, Yuka Tsuzuki¹, Norihiro Takekawa¹, So-ichiro Nishiyama², Hiroataka Tajima³, Ikuro Kawagishi³, Katsumi Imada¹ (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, Mlp8 is involved in chemotactic response to mucus and galactose-6-sulfate. Mlp8 is thought to recognize ligands together with AcfC, a periplasmic binding protein, because *mlp8* forms an operon with *acfC*. However, the ligand recognition mechanism of Mlp8 and the interaction between Mlp8 and AcfC remain unclear. To understand the mechanisms, we determined the crystal structures of the ligand binding domain of Mlp8 and AcfC and performed pull-down experiments with AcfC under various conditions. We will discuss the ligand recognition mechanism of Mlp8 based on the structures and interactions between these proteins.

1-01-1506 光誘導可能な液滴への閉じ込めによる多酵素反応の活性化
Facilitating a two-step enzymatic reaction by trapping two enzymes in light-inducible droplets

Rihito Okubo¹, Yuuki Hayashi¹, Munchito Arai^{1,2} (¹*Dept. Life Sci., Univ. Tokyo*, ²*Dept. Phys., Univ. Tokyo*)

Protein droplets formed by liquid-liquid phase separation can concentrate specific proteins inside and provide an environment for them to efficiently work. Thus, we hypothesized that trapping two enzymes in droplets may facilitate a two-step enzymatic reaction. Two enzymes essential for alkane biosynthesis are acyl-ACP reductase (AAR) and aldehyde-deformylating oxygenase (ADO). Interaction between them is necessary for efficient delivery of an aldehyde from AAR to ADO. Here, to facilitate alkane biosynthesis in cells, we fused each of AAR and ADO with the disordered region of FUS that forms droplets. Furthermore, we also fused them with optogenetic tools pMag and nMag to control droplet formation by blue light. The result will be presented at the meeting.

1-01-1518 Analysis of differences in the number of β -sheet structures that have different β -strand's connections and orientations

Takumi Nishina, George Chikenji (*Dept. of App. Phys., Nagoya Univ*)

A β -sheet structure is classified by the order of β -strand's connections and orientations of β -strand. It is known that the number of classified β -sheet structures in Protein DataBank (PDB) is different. Among the β -sheet structures, there are reverse structures in which the orientation of the N- and C-term are only reversed. Although the two structures are so similar, the difference in the number of such structures in PDB is remarkable. And, it is still unclear why such a difference is occurring. In order to discover the cause of this difference in the number of structures, we analyzed the PDB. As a result, we found that the frequency of each β -sheet structure may depend on the characteristics of the loop connecting the β -strand.

1-02-1330 Structural analysis of monomeric photosystem II at 2.78 Å resolution using Cryo-electron microscopy

Huaxin Yu^{1,2}, Tasuku Hamaguchi³, Yoshiki Nakajima¹, Keisuke Kawakami³, Fusamichi Akita^{1,4}, Koji Yonekura^{3,5,6}, Jian-Ren Shen¹

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Photosystem II (PSII) functions mainly as a dimer to catalyze the light energy conversion and water oxidation reactions. However, monomeric PSII also exists and functions *in vivo* in some cases. We solved the structure of PSII monomer at 2.78 Å resolution using cryo-electron microscopy, and observed apparent differences in the monomer-monomer interface between the dimer and monomer. One carotenoid and two SQDG molecules were found in the dimer structure but absent in the monomer structure. Additionally, most of PsbO was found to be disordered in the monomer structure. These results indicate that these factors are important for the dimer formation.

1-02-1342 High-resolution single-particle cryo-EM analyses with a CFE electron beam

Tasuku Hamaguchi¹, Keisuke Kawakami¹, Saori Maki-Yonekura¹, Koji Yonekura^{1,2} (¹*RIKEN SPring-8 Center*, ²*IMRAM, Tohoku Univ.*)

Single-particle analysis (SPA) by cryo-electron microscopy (cryo-EM) is a powerful technique for structure determination of protein and protein complexes. In SPA, many structures are now being revealed at an unprecedented speed and resolution, but it is still challenging to obtain the structure beyond 2Å resolution. In 2018, we set up the first JEOL CRYO ARM 300 electron microscope equipped with a cold-field emission (CFE) gun, which produces a highly-coherent electron beam and keeps superior high-resolution signals. The cryo-EM system has been used for SPA of a variety of protein samples. Here, we present these structures obtained so far, as well as latest results including dynamic conformational changes and effects of radiation damage to high-resolution structures.

1-02-1354 Cryo-EM Structure of K⁺-Bound hERG Channel Complexed with the Blocker Astemizole

Tatsuki Asai¹, Naruhiko Adachi², Toshio Moriya², Hideyuki Oki³, Takamitsu Maru³, Masato Kawasaki², Kano Suzuki¹, Sisi Chen¹, Ryohei Ishii⁴, Kazuko Yonemori⁵, Shigeru Igaki⁵, Satoshi Yasuda^{1,6}, Satoshi Ogasawara^{1,6}, Toshiya Senda², Takeshi Murata^{1,6} (¹*Grad. Sch. Sci., Univ. Chiba*, ²*Tsukuba, KEK*, ³*Axcelead Drug Discovery Partners, Inc.*, ⁴*Daiichi Sankyo RD Novare Co., Ltd.*, ⁵*Takeda Pharmaceutical Co., Ltd.*, ⁶*Molecular Chirality Research Center, Univ. Chiba*)

The hERG channel is a voltage-gated potassium channel involved in cardiac repolarization. Off-target hERG inhibition by drugs has become a critical issue in the pharmaceutical industry. The three-dimensional structure of the hERG channel was recently reported using cryogenic electron microscopy (cryo-EM). However, the drug inhibition mechanism remains unclear because of the scarce structural information regarding the drug-bound hERG channels. In this study, we obtained the cryo-EM density map of hERG channel complexed with astemizole, a well-known hERG inhibitor that increases risk of potentially fatal arrhythmia, at 3.5- Å resolution. The structure suggested that astemizole inhibits potassium conduction by binding directly below the selectivity filter.

1-02-1406 クライオ電子顕微鏡単粒子解析と分子動力学シミュレーションを用いた ATP13A2 のポリアミン輸送機構の解明 Cryo-EM structures and MD simulations of ATP13A2 reveal transport mechanism of polyamines

Atsushi Tomita¹, Takashi Daiho², Tomohiro Nishizawa³, Osamu Nreki¹ (¹*Grad. Sch. Sci., Univ. Tokyo*, ²*Dept. of Med., Asahikawa Medical Univ.*, ³*Grad. Sch. Sci., Yokohama City Univ.*)

Polyamines, especially spermine (SPM) are essential for maintaining various biological activities in all eukaryotes. Type VB P-type ATPase ATP13A2 was identified as the lysosomal polyamine exporter that plays a crucial role in the SPM uptake into the cytoplasm. Several mutations in ATP13A2 are also associated with Parkinson's disease. While the mechanisms for ion-pumping and phospholipid-flippase members of the P-type ATPase family have been well investigated, the polyamine transport mechanism by ATP13A2 is still elusive. Here, we report the cryo-EM structures of the human ATP13A2 in its four intermediates. These structures, together with MD simulation and biochemical assays, have revealed the unique mechanism for the recognition and transport of polyamines by ATP13A2.

1-02-1418 鉄硫黄クラスターの構造と酵素活性の相関解析による tRNA 硫黄修飾機構の解明 Reaction mechanism of tRNA thiolation revealed by correlation analysis between the structure of Fe-S clusters and the enzymatic activity

Masato Ishizaka¹, Minghao Chen², Shun Narai¹, Masaki Horitani³, Yoshikazu Tanaka^{2,4}, Min Yao^{1,2} (¹*Grad. Sch. Life Sci., Hokkaido Univ.*, ²*Fac. Adv. Life Sci., Hokkaido Univ.*, ³*Fac. Agri., Saga Univ.*, ⁴*Grad. Sch. Life Sci., Tohoku. Univ.*)

tRNA must undergo thiolation which replaces oxygen in uridine with sulfur to obtain its function. Our recent structural and biochemical analysis of thermophilic tRNA thiolation enzyme TtuA-TtuB suggested that TtuA has an oxygen-sensitive co-factor [4Fe-4S] to receive sulfur from TtuB. On the other hand, human tRNA thiolation enzyme Ncs6 has [4Fe-4S] or [3Fe-4S]. Therefore, the true iron-sulfur (Fe-S) cluster of TtuA/Ncs6 family should be re-examined. Here, we spectroscopically and biochemically analyzed the enzymatic activities of [3Fe-4S]-TtuA and [4Fe-4S]-TtuA, and identified the important residues for the enzymatic activity of TtuA. Taking all results together, we proposed a reaction mechanism of tRNA thiolation based on the accurate structure of the Fe-S cluster.

1-02-1430 Overexpression of stable isotope-labeled cecropin P1 by using calmodulin-fusion protein system and structure analysis by NMR

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Cecropin P1 (CP1), isolated from *Ascaris suum* inhabiting in the intestine of pigs, is a well-studied α -helical antimicrobial peptide (AMP). However, it is difficult to obtain a large amount of recombinant CP1 by using *Escherichia coli* (*E. coli*) system because of high toxicity of CP1 and degradation by endogenous proteases. In this study, we applied calmodulin (CaM), which has many successful cases as a new fusion partner for overexpression of recombinant AMP, to enhance the expression of CP1. As a result, a large amount of stable isotope-labeled CP1 was generated for structural analysis in a membrane-mimic condition by nuclear magnetic resonance (NMR), and the structure of CP1 in a dodecylphosphocholine (DPC) micellar environment was investigated.

[1-02-1442](#) **Structure of a pentameric complex of MotA, a bacterial flagellar stator protein, from *Aquifex aeolicus* by single particle cryo-EM**

Tatsuro Nishikino¹, Norihiro Takekawa², Jun-ichi Kishikawa¹, Mika Hirose¹, Michio Homma³, Takayuki Kato¹, Katsumi Imada² (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, MotA and MotB, and functions as an ion channel. For a long time, the stator complex was thought to be composed of four MotA and two MotB subunits based on biochemical analyses. However, recent structural analyses by single particle cryo-EM revealed that five MotA and two MotB molecules form the single stator complex. In this study, we performed single particle analysis of purified MotA from *Aquifex aeolicus*, a thermophilic bacterium, at 3.42 Å resolution. MotA forms a pentamer even in the absence of MotB. We will discuss structural differences between the MotA pentamer and known MotAB complexes.

[1-02-1454](#) **蛍光寿命測定による脂質二重膜結合状態における α-Synuclein の立体構造解析**
Structural analysis of α-Synuclein in the lipid bilayer bound state by fluorescence lifetime measurements

Ko Sasada, Ryosuke Matsubara, Koichi Fujii, Tetsunari Kimura (*Grad. Sch. Sci., Kobe Univ*)

Parkinson's disease could occur even in the young by A30P mutation in α-synuclein (αsyn). Many experiments for fibrillation in solution have been performed, but less in the native environment where αsyn are bound on the lipid bilayer. In addition, structural analyses of monomers and dimers which are appeared in the early stages of aggregation are necessary to clarify the molecular mechanism. In this study, fluorescence resonance energy transfer measured by fluorescence lifetime and maximum entropy analyses were employed to clarify the distance distribution between fluorescent donors and acceptors along the lipid bilayer binding of WT and A30P. Additional shorter population was observed in A30P, which should be due to the cis-trans isomerization by the proline mutation.

[1-02-1506](#) **(2S2-6) Cryo-EM analysis provides new mechanistic insight into ATP binding to Ca²⁺-ATPase SERCA2b**

Yuxia Zhang¹, Satoshi Watanabe¹, Akihisa Tsutsumi², Hiroshi Kadokura¹, Masahide Kikkawa², Kenji Inaba¹ (¹*Institute of Multidisciplinary Research for Advanced Materials, Tohoku University*, ²*Graduate School of Medicine, The University of Tokyo*)

SERCA2b is a ubiquitous SERCA family member that conducts Ca²⁺ uptake from the cytosol to the ER. Herein, we present a 3.3 Å resolution cryo-EM structure of human SERCA2b in the E1·2Ca²⁺ state, revealing a new conformation for Ca²⁺-bound SERCA2b with a more compact cytosolic domain arrangement than the crystal structure of SERCA1a. Notably, ATP binding residues of SERCA2b in this state are located at similar positions to those in the E1·2Ca²⁺-ATP state, hence the cryo-EM structure likely represents a preformed state prior to ATP binding. With several lines of biochemical evidence, we propose and discuss a novel mechanism of ATP binding to SERCA2b.

[1-02-1518](#) **CW-ESR 分光法によるヌクレオチド結合型 ABC トランスポーターの構造解析**
Structural analyses of ABC transporters in nucleotide bound states investigated by CW-ESR spectroscopy

Ayaka Naka¹, Yasuhiro Kobori^{1,2}, Motonari Tsubaki¹, Yoshitsugu Shiro³, Hiroshi Sugimoto⁴, Tetsunari Kimura¹ (¹*Grad. Sch., Sci., Kobe Univ.*, ²*Mol. Photo. Res. Cent., Kobe Univ.*, ³*Grad. Sch. Sci., Univ. Hyogo*, ⁴*Spring-8, RIKEN*)

ABC transporters are membrane proteins that transport substrates across lipid bilayer. The "alternating access model" has been proposed, in which the transport is realized along the conformational changes in the transmembrane domain (TMD) induced by the binding and hydrolysis of ATP at cellular nucleotide-binding domain. But the correlation between the ATP reaction and conformational changes are still unclear. In this study, spin-labels were doubly introduced into the TMD of the heme importer BhuUV-T, and the spin-spin interactions were observed by CW-ESR spectroscopy with several kinds of nucleotides. AMP-PNP mimicking the ATP bound state increased the open conformer of the TMD toward the periplasmic side compared to the unbound state.

[1-03-1330](#) Implementation of residue level coarse-grained models in GENESIS

Cheng Tan¹, Jaewoon Jung^{1,2}, Chigusa Kobayashi¹, 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*)

We present an implementation of several popular residue-level coarse-grained models for protein and nucleic acid in the molecular dynamics simulation software GENESIS. Our development covers models for both the well-structured biomolecular domains and the intrinsically disordered regions (IDRs). We provide a toolbox, the GENESIS-CG-tools, to generate the various models' input files in a unified format. We implemented the potential functions in atdyn, the atomic decomposition MD programs in GENESIS, and optimized our algorithms for parallelizing the nonbonded interactions and time integrator. With several examples, we demonstrated the usage of GENESIS to study multi-scale biological systems, from a single DNA-binding protein to organelle-sized structures.

[1-03-1342](#) 粗視化シミュレーションと SAXS データに基づくヘテロクロマチンタンパク HP1 α の構造モデリング

Structural modeling of the heterochromatin protein 1 alpha (HP1 α) based on coarse-grained MD simulations and SAXS data

Tatsuki Negami¹, Ayako Furukawa², Kento Yonezawa³, Naruhiko Adachi³, Toshiya Senda³, Nobutaka Shimizu³, Yoshifumi Nishimura^{2,4}, Tohru Terada¹ (¹*Grad. Sch. Agr. Life Sci., Univ. Tokyo*, ²*Grad. Sch. Med. Life Sci., Yokohama city Univ.*, ³*IMSS, KEK*, ⁴*Grad. Sch. Integ. Sci. Life, Hiroshima Univ.*)

Heterochromatin protein 1 alpha (HP1 α) plays an important role for the formation and maintenance of the heterochromatin, which regulates gene expression. Phosphorylation of the N-terminal extension of HP1 α causes phase separation which enables recruitment of repressive factors. In this study, we studied the effect of the phosphorylation on the dynamics by combining coarse-grained molecular dynamics (CGMD) simulations and small-angle X-ray scattering (SAXS) data. We performed CGMD simulations for the unphosphorylated and the phosphorylated HP1 α . Then, structural ensembles that reproduced the SAXS data were extracted from the trajectories. We will discuss the differences in the structure and the dynamics caused by the phosphorylation of HP1 α .

[1-03-1354](#) 深層学習を用いたタンパク質オーダーパラメータの時系列データの予測研究

Application of a deep-learning model for the prediction of the time course of an order parameter of a protein

Renta Sato, Takashi Yoshidome (*Dept. of Appl. Phys., Tohoku Univ.*)

We investigated whether a deep-learning model that enables the treatment of time-series data can predict the time course of an order parameter of a protein. A recurrent neural network (RNN) was employed for the deep-learning model. We applied an RNN to predict the time course of the Q -value of the SH3 protein domain at its thermal denaturation temperature. The SH3 protein domain was modeled by a G \ddot{o} model, and then a molecular dynamics (MD) simulation was performed with the CafeMol program suite. An RNN model was obtained using the MD data for the training data. It was found that, although the time course of the Q -value was not correctly predicted using the RNN model, the distribution of the Q -value was successfully predicted.

[1-03-1406](#) Dynamic Residue Interaction Network Analysis of Secondary Mutations in Protease that Promote Drug Resistance in HIV-1

Ayaka Ojima, Mohini Yadav, Norifumi Yamamoto (*Chiba Tech*)

The human immunodeficiency virus (HIV) is the pathogen of the Acquired Immune Deficiency Syndrome (AIDS). AIDS has become 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 HIV-1 protease promotes development of drug resistance caused by primary mutations, even without directly affecting drug efficacy against anti-HIV drugs. These mutations are referred to as "secondary mutations". In this study, we investigated the dynamic correlation between the drug binding site and its secondary mutation site in HIV-1 protease using dynamic residue interaction network (dRIN) analysis based on molecular dynamics simulations.

[1-03-1418](#) Coarse-grained simulations of multiple intermediates along conformational transition pathways of multi-domain proteins

Ai Shinobu¹, Chigusa Kobayashi², Yasuhiro Matsunaga³, Yuji Sugita^{1,2,4} (¹*RIKEN, BDR*, ²*RIKEN, R-CCS*, ³*Saitama Univ., Grad. Sch. Sci. Eng.*, ⁴*RIKEN, CPR*)

Large-scale motions in multidomain proteins are essential for their function. Coarse grained (CG) molecular dynamics (MD) simulations are an inexpensive and useful tool for studying large-scale motions in proteins, however, they sometime miss possible transition paths and intermediate structures. Moreover, CG potentials often require labour-intensive parametrization. We developed a multi-basin (MB) structure-based Go model for describing conformational motions in proteins. We applied the scheme to the enzyme adenylate kinase and sampled multiple conformational transitions along different pathways and characterized the structures of intermediate states.

[1-03-1430](#) Application of ColDock to docking of cryptic pockets

Ryunosuke Kiuchi, Kazuhiro Takemura, Akio Kitao (*School of Life Science and Technology, Tokyo Institute of Technology*)

Many proteins exert their functions specifically upon binding to ligands. Many docking methods have been developed to predict structures of protein-ligand complexes. Concentrated ligand docking (ColDock) is a simple and accurate method to predict complex structures using MD simulation at high ligand concentration. Some proteins have so-called cryptic pockets, which are accessible only upon ligand binding. The complex structure predictions containing such pockets are challenging because of low accessibility of the pocket in ligand-free structure (apo form). The goal of our study is to make ColDock applicable to proteins with cryptic pockets. This study may contribute to drug discovery by predicting more complex structures.

[1-03-1442](#) 自由エネルギー不等式に基づく Checkpoint kinase1-リガンド系の相対的結合自由エネルギーの推定
 Estimation of relative binding free energy based on a free energy inequality for the Checkpoint kinase1-ligand system

Keita Shibahara, Takeshi Kikuchi (*Dept. Biosci., Col. Life Sci., Ritsumeikan Univ.*)

In a new drug discovery process, the binding free energy between a protein and a ligand is important and there are several computational methods to calculate it. A newly developed technique based on a free energy inequality is applied to the estimation of the relative binding free energies between Checkpoint kinase 1 (Chk1) inhibitor and a ligand. It has been confirmed that our technique requires relatively low computational cost compared with other techniques. The energy minimization, heat treatment, equilibration and 10.2 ns molecular dynamics simulation were performed by Amber18 followed by the calculation of the relative binding free energy based on the free energy inequality process. We currently obtain 0.77 of the correlation coefficient (R^2).

[1-03-1454](#) 自由エネルギー不等式に基づく Cyclin Dependent Kinase2 – リガンド系の相対的結合自由エネルギーの推定
 Estimation of relative binding free energy based on a free energy for the cyclin dependent kinase2 – ligand system

Daiki Atarashi, Takeshi Kikuchi (*Dept. Biosci., Col. Life Sci., Ritsumeikan Univ.*)

A newly developed technique based on a free energy inequality is applied to the estimation of the relative binding free energies between cyclin dependent kinase 2 and a ligand. Our technique does not require sampling of intermediate states as in the free energy perturbation and the thermodynamic integration methods with largely reduced the computational cost. The present technique also does not require the entropy calculation as in the MM-GB(PB) / SA techniques and tuning of parameters as in LIE technique. We currently obtain 0.82 of the correlation coefficient (R^2) and 0.95kcal/mol of average error between calculated and experimentally obtained relative binding free energies. We are trying further improvement of the R^2 and average values.

[1-03-1506](#) ドッキング構造予測のリランキングに向けた蛋白質—ペプチド間相互作用の網羅的解析
Comprehensive analysis of protein-peptide interactions for reranking of docking predictions

Keiichiro Sato¹, Kota Kasahara², Takuya Takahashi² (¹*Grad. Sci. Life Sci., Ritsumeikan Univ.*, ²*Coll. Life. Sci., Ritsumeikan Univ.*)

The molecular principle of protein-peptide binding is still largely unknown. To tackle this, one of promising ways is analyses on structural information accumulated in the Protein Data Bank. Here, we analyzed the relative positions of the peptide atoms with respect to the amino acid residues of the interacting proteins. A three-dimensional Gaussian mixture model was used to capture patterns of atomic interaction. We collected more than a half-million pairs of interacting atoms from the dataset consisting of 5,578 protein-peptide complexes and found 2,771 spatial patterns of interactions. Furthermore, we developed a reranking method for docking predictions based on these patterns of interactions.

[1-03-1518](#) The physical-based criterion for distinguishing superfolds and non-superfolds: the case of pure parallel beta-sheets

Hiroto Murata, George Chikenji (*Dept. of Appl. Phys., Grad. Sch. of Eng., Nagoya Univ.*)

The naturally occurred proteins are classified into folds based on their structures. Some folds are observed in many protein families (superfolds), while others in only a few protein families (non-superfolds). The question is what causes the difference between superfolds and non-superfolds. Here, we propose a criterion for distinguishing them from a physical viewpoint. The criterion demands consistency among a set of physical rules for local structures in a given fold. We show that the criterion well discriminates superfolds and non-superfolds.

[1-04-1330](#) ヌクレオソームから H2A-H2B 量体が脱離する際の自由エネルギープロファイル
Free energy profile of H2A-H2B dimer dissociation from nucleosome

Hisashi Ishida, Hidetoshi Kono (*Quantum Life Science, National Institutes for Quantum and Radiological Science and Technology*)

Nucleosome reconstitution plays an important role in many cellular functions. As the initial step of the H2A-H2B dimer eviction, dimer displacement, which is accompanied by disruption of many of the interactions within the nucleosome, should occur. To understand how H2A/H2B dimer displacement occurs, we carried out all-atom molecular dynamics simulations of wrapped and unwrapped nucleosomes. The free energies for the dimer displacement from these nucleosomes were estimated to be similar, about 30 kcal/mol, but the pathways for the dimer displacement were different. We found that conformational disrupt at the interface between the docking domain of H2A and the adjacent regions of H3 α N-, H3 α C-helices and H4 C-terminal significantly contributed to the free energy.

[1-04-1342](#) 低温条件下での微小管構造動態解析：溶液温度に依存した構造変化における非等方性とヒステリシス
Structural dynamics of native microtubules on cooling: anisotropic and hysteretic structural changes depending on temperature

Shinji Kamimura¹, Toshiaki Yagi², Yusuke Kondo², Juan Estévez-Gallego³, Daniel Lucena-Agell³, J. Fernando Díaz³, Hiroyuki Iwamoto⁴ (¹*Dept. Biol. Sci., Fac. Sci. & Eng., Chuo Univ.*, ²*Dept. Life & Env. Sci., Fac. Bioresource Sci., Pref. Univ. Hiroshima*, ³*El Centro de Investigaciones Biológicas Margarita Salas, CSIC*, ⁴*Res. & Util. Div., JASRI, SPring-8*)

Microtubules (MT) are involved in essential cellular functions. One known characteristic of them is rapid disassembly to tubulin subunits upon cooling, a process whose molecular basis is not yet understood. We hypothesize that the conformational changes in tubulin accumulate strain of MT that triggers disassembly. To test this hypothesis, we analyzed the X-ray fiber diffraction patterns of native MTs during rapid cooling from 37 to 10°C (<20s). We found that shape changes of MT on cooling was anisotropic, i.e., the magnitude of shrinkage was different between longitudinal and diameter directions. Detailed time-course analysis showed that the shrinkage and expansion are hysteretic. The present study would help us to understand how MTs become unstable at low temperatures.

[1-04-1354](#) ファージレセプター結合蛋白質と宿主レセプターの相互作用解析
Interaction analysis of the phage receptor binding protein and the host receptor

Shuji Kanamaru¹, Kazuhiro Takemura¹, Zdravković Aleksandar² (¹*Dep. of Life Sci. and Tech., Tokyo Inst. of Tech.*,
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There are many types of T2-like bacteriophages, which infect a variety of bacteria, including pathogens. They are categorized as T-even phage, represented by T4 phage. However, the major difference between the T2-like phage and the T4 phage is the receptor-binding protein (RBP) at the tip of the tail fiber. The crystal structures of the RBP of the T2-like phage and the host bacterial receptor protein, OmpC, have already been solved, but the detailed interaction between them remains unclear. We have analyzed the detailed interaction of the two proteins by cross-linking them in solution. The results of the MD analysis were in good agreement with the results of the cross-linking experiment. The interaction between phage RBP and host receptor will be discussed.

[1-04-1406](#) 静電相互作用の計算コストを抑えた新規自由エネルギー摂動法の開発
Development of a new free-energy perturbation method for reducing the computational cost of electrostatic interactions

Hiraku Oshima¹, 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 and solubility of ligands in in-silico drug design. Conventional FEP requires additional reciprocal-space calculations in the particle mesh Ewald method, which largely decrease the total computational performance. To overcome this problem, we propose a new FEP method using a REST2-like scaling in the electrostatic interactions, which introduces non-uniform scaling parameters as used in REST2 and reduces the number of reciprocal-space calculations. REST2-like FEP greatly improves the computational performances and would be particularly useful when it is applied to large biomolecular systems.

[1-04-1418](#) 微小管末端標識と高速 AFM による可視化
Visualization of microtubule ends by high-speed AFM

Yuuki Higuchi¹, Noriyuki Kodera², **Ikuko Hayashi**¹ (¹*Yokohama City Univ.*, ²*Kanazawa Univ.*)

Microtubules are polymers of α/β -tubulin dimers and have structural polarity with a fast-growing plus-end and relatively slow-growing minus-end. We have been studying molecular interactions between microtubule and its associated proteins, using purified proteins by high-speed atomic force microscopy (HS-AFM). While HS-AFM is a powerful technique for imaging dynamic biological molecules in solution, the polarity of stabilized microtubule filaments is hard to determine because the filaments consist of a series of tubulin molecules. Recent *in vitro* selection technologies have identified artificial proteins with high affinity for tubulin. By using these proteins, we have developed the labelling method of microtubule ends for the HS-AFM experiments.

[1-04-1430](#) Analysis of Heparin-Induced Tau Oligomer Formation by Dynamic Light Scattering

Ayumi Masui¹, Keisuke Yuzu¹, Keiichi Yamaguchi², Yuji Goto², Yasushi Kawata³, Eri Chatani¹ (¹*Grad. Sch. Sci., Kobe Univ.*, ²*Glob. Ctr. for Med. Engin. and Info., Osaka Univ.*, ³*Grad. Sch. Engin., Tottori Univ.*)

Tau protein, which belongs to the family of microtubule-associated proteins, is involved in neurodegenerative diseases by forming amyloid fibrils in cells. Cytotoxic oligomers are formed as intermediates during the fibril formation of tau, although detailed mechanism of their formation is unclarified. Here, we have used dynamic light scattering to follow the assembly process of molecules in the early stage of the reaction *in vitro*. When tau was co-incubated with heparin, tau aggregation started immediately, and the behavior of the size development changed depending on the concentrations of tau and/or heparin. This suggests that the pathway of oligomer formation is sensitive to reaction conditions.

[1-04-1442](#) 放射光 X線溶液散乱測定における連続濃度変調型 μ 流路自動サンプリングシステムの性能評価
Evaluation of continuous concentration-modulated μ -fluidic auto sampling system for synchrotron SAXS measurements

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Recently, a continuous titration small angle X-ray scattering (SAXS) measurement was developed as one of the methods to analyze the solution structure of molecular complexes and interactions. To achieve accurate titration with high-precision and multipoint measurement, we developed a μ -fluidic auto-sampling system installed in the Photon Factory. However it is necessary to optimize the measurement parameters such as time, and flow rate, and etc., to obtain appropriate results within the limited beam time. To optimize these parameters of this system at beamline (BL-10C), we analyzed the changes in the time of continuous modulation of the concentration and the flow rate, respectively. In addition, we will discuss the change of structure factor depending on the flow rate.

[1-04-1454](#) ホモロガスヘテロオリゴマーの構造的特性解析
Structural characterization of homologous hetero-oligomers

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Many proteins function by forming complexes with other proteins. Homologous hetero-oligomers are protein complexes composed of homologous proteins. It is unclear what structural and functional characteristics were obtained when ancestral homo-oligomers evolved into homologous hetero-oligomers. In this study, we created a data set of homologous hetero-oligomers by using Biological units in the PDB and structural domains of the SCOP database. We will evaluate the structural changes of homologous hetero-oligomers by Motion Tree.

[1-04-1506](#) 溶解性成業ペプチド (SCP) タグによって会合させた BPTI 蛋白質の物性と免疫原性の解析
Biophysical and immunogenic properties of a Bovine Pancreatic Trypsin Inhibitor oligomerized using a Solubility Controlling Peptide tag

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Protein aggregates can cause undesired immunogenicity against therapeutic proteins. Here, we examined the link between the immunogenicity and the size of aggregates of a 6kDa BPTI-19A variant produced by attaching hydrophobic SCP (Solubility Controlling Peptide)-tags to its C-terminus. DLS and SLS measurements indicated that the hydrophobic SCP-tags merely affected the size of BPTI-19A except for the C5I tag, which formed sub-visible aggregates with a hydrodynamic radius (R_h) of ~4 nm. Fluorescence and CD measurements indicated that all variants had native-like structures, except BPTI-C5I, which partially unfolded upon oligomerization. Immunization showed that nanometer-sized aggregates of BPTI-C5I significantly increased the IgG titer (>55 fold), as assessed by ELISA.

[1-04-1518](#) 天然変性タンパク質 p53 液滴内への分子取込と 1 分子ダイナミクス観測
Characterization of molecular uptake and single-molecule dynamics in liquid droplets of p53

Nanako Iwaki^{1,2}, Saori Kanbayashi¹, Trishit Banerjee^{1,2}, Rika Chiba^{1,3}, Michiko Kimura^{1,3}, Hiroyuki Oikawa^{1,2,3}, Satoshi Takahashi^{1,2,3}, Kiyoto Kamagata^{1,2,3} (¹*IMRAM, Tohoku Univ.*, ²*Dep. Chem., Grad. Sch. Sci., Tohoku Univ.*, ³*Grad. Sch. Life Sci., Tohoku Univ.*)

In a living cell, membrane-less organelles are formed by liquid-liquid phase separation of multiple proteins: host proteins forming liquid droplets by themselves and guest proteins recruited into the droplets. Although the droplet formation mechanism of host proteins has been intensively investigated, host-guest proteins interactions and dynamic behavior of guest proteins inside droplets are largely unknown. Here we characterized the localization and dynamic property of guest proteins in liquid droplets using a single-molecule fluorescence microscopy. A variety of guest proteins with different sizes, structures, and oligomeric states were examined in liquid droplets of host p53. Our results provide the localization and dynamic rule of guest proteins in liquid droplets.

[1-05-1330](#) Roles of loop extrusion process in transcription dynamics of target genes of superenhancers

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Superenhancers are localized at the surfaces of transcriptional condensates, which are produced by the phase separation of transcription machineries. The target genes of superenhancers are at the proximity to, but only 20% of them colocalize with, the transcription condensates, implying that the access of the genes to the transcriptional machineries in the condensates limits the transcription dynamics. We here analyze the dynamics of the linker chromatin between a superenhancer and its target gene to predict the transcription dynamics of the gene by taking into account the loop extrusion process. Our theory predicts that with the loop extrusion, the accessibility of the gene to the transcriptional machinery increases with increasing the length of the linker chromatin.

[1-05-1342](#) 粗視化分子シミュレーションによる SMC-kleisin 複合体の構造変化と DNA 結合状態の解明
Coarse-grained Molecular Simulation to Reveal Conformational Change and DNA binding of Bacterial SMC-kleisin Complex

Masataka Yamauchi, Shoji Takada (*Dept. of Biophysics, Grad. of Sci., Kyoto Univ.*)

Structural maintenance of chromosomes (SMC) complexes, such as cohesin and condensin, are ring-shaped ATPase motors that play key roles in chromosome organization, probably by DNA loop extrusion. Opening and closing the ring by ATP hydrolysis is considered essential for the DNA loop extrusion. However, the structural features of the SMC-kleisin complexes in the ATPase cycle remain unclear due to limited structure data. In this study, we examined the conformational changes of a bacterial SMC-kleisin complex by coarse-grained molecular simulation. Our simulations show that engagement of the ATPase domain opens the ring. We also performed DNA binding simulations for the open- and close-ring conformations to obtain insights into the mechanism of DNA loop extrusion.

[1-05-1354](#) 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
Generation of Phase Separated Droplet Induced by Soret Effect and DNA Enrichment by Optical Tweezers

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. Using general known property that DNA prefers Dextran-rich phase, we achieve DNA enrichment at a factor of 10. We find that the generated droplet exists for at least 20 hours and DNA seems to be trapped in the induced droplet, whereas Dextran diffuses from the droplet with time due to equilibration. Surprisingly, DNA enrichment seems to be very stable in the droplet. We will discuss the mechanism of the long time entrapment of DNA.

[1-05-1406](#) Elucidation of nucleosome sliding mechanism in all-atom detail via MD simulations

Syed Hashim Shah, Giovanni Brandani, Shoji Takada (*Department of Biophysics, Graduate School of Science, Kyoto University*)

Chromatin remodeling via nucleosome sliding plays an important role in 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 mechanism and energetics of nucleosome sliding are not clear. In order to better understand this process, we ran microsecond-long simulations, which show the spontaneous formation of stable half-twist defects enabling localized 1-bp sliding. Our ultimate goal is to reconstruct the free energy landscape of the sliding via twist defect propagation by the string method.

[1-05-1418](#) 拡散的ループ形成によるクロマチン相分離
Chromatin phase separation induced by diffusive loop formation

Shin Fujishiro, Masaki Sasai (*Dept. Appl. Phys., Nagoya Univ.*)

In higher eukaryotes, interphase chromatin chains form loop domains organized into active/inactive (A/B) compartments. Recent studies have suggested that phase separation of chromatin in different epigenetic states drives compartmentalization independently of the loop formation. However, a close look at the Hi-C data showed that the A (B) compartment generally bears small (large) loops, suggesting that differently sized loops also account for compartmentalization. We tested this hypothesis by simulating loop formation on a polymer consisting of small and large loop domains. The simulation showed their phase separation, and thus, we propose that compartmentalization is a superposition of two alternative modes: loop-size segregation and epigenetic state segregation.

[1-05-1430](#) 多価相互作用を持つタンパク質の相分離をシミュレーションするためのメソスケール化学量論相互作用モデル
Mesoscale stoichiometric interaction model for simulating phase-separation of multivalent proteins

Yutaka Murata, Toru Niina, Shoji Takada (*Grad. Sch. Sci., Univ. Kyoto*)

Interactions between multivalent proteins control the reversible formation of intracellular membraneless bodies. Recently, the liquid-liquid phase separation (LLPS) of biomolecules has been intensively studied, in which one promising approach is computer simulation. However, to simulate LLPS of multi-domain proteins efficiently, we need mesoscale models, such as one where each domain is modeled as one particle. To date, most of these are based on Monte-Carlo, but not molecular-dynamics simulation. Here, we developed a mesoscale model for molecular dynamics simulation in which stoichiometry of domain interactions are explicitly taken into consideration. We confirmed that this model can represent the characteristic of multivalent protein phase separation.

[1-05-1442](#) 3D DNA nanostructure-based string-like structure for the construction of chromatin-like heterogeneous system

Hong Xuan Chai, Masahiro Takinoue (*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 controlled the degree of aggregation of DNA gel-like structure by controlling the connection between DNA tetrahedral nanostructures.

[1-05-1454](#) Formation of liquid-liquid phase separation droplets based on artificial RNA nanostructures

Minzhi Fan¹, Masahiro Takinoue¹, Hirohide Saito² (*¹Tokyo Institute of Technology, ²Kyoto University*)

This research mainly investigated the difference between DNA and RNA nanostructures with the same sequence and RNA Liquid-liquid phase separation property-dependent behaviour by designing RNA droplets. Design of this research is as following, sticky-end of previously designed DNA X-motif was replaced by the same RNA sequence and RNA kissing-loop sequence to compare. Both numerical simulation and experiment approaches were taken to explore and validate the properties of different RNA nanostructures. Simulation results showed that thermodynamic properties of RNA kissing-loop structure is sequence-dependent. In experiment, observation results of constructed droplets revealed RNA and DNA nanostructures shared some similarities, but the conditions were far altered.

[1-06-1330](#) 鎖長の異なるパーフルオロアルキル基を有する部分フッ素化リン脂質群に再構成したバクテリ
ロドプシンの機能と構造安定性に関する比較研究
Comparison of functionality and structural stability of bR in partially fluorinated DMPC vesicles
with varied perfluoroalkyl chain lengths

Mami Hashimoto¹, Yuka Murai¹, Kohei Morita¹, Takashi Kikukawa², Toshiyuki Takagi³, Hiroshi Takahashi¹, Yasunori Yokoyama⁴, Hideki Amii^{1,5}, Masashi Sonoyama^{1,5,6} (¹Grad. Sch. Sci. Tech., Gunma Univ., ²Fac. Adv. Life Sci., Hokkaido Univ., ³AIST, ⁴Grad. Sch. Eng., Nagoya Univ., ⁵GIAR, Gunma Univ., ⁶GUCFW, Gunma Univ.)

We have developed a partially fluorinated DMPC with a C_nF₉ group in the hydrophobic chain terminal and showed that the lipid is promising for incorporating membrane proteins. Moreover, we have found out that membrane properties of a series of partially fluorinated DMPCs with various Rf (C_nF_{2n+1}) chain lengths (Fn-DMPCs) depend significantly on the Rf chain length. Here, we studied structural and functional properties of a membrane protein bR, a single protein in the purple membrane (PM), in the Fn-DMPC (n = 4, 6, and 8) membranes (bR/Fn-DMPC) using several physicochemical techniques. Regardless of the Rf chain lengths, bR/Fn-DMPCs retain native-like structural and functional properties at 30 °C. Experimental results will be discussed compared to the PM and bR/DMPC.

[1-06-1342](#) ABC トランスポーター MsbA の ATPase 活性に対する機能場の影響
Effect of lipid environments on the ATPase activity of ABC transporter MsbA

Risako Otani¹, Fumio Hayashi², Masashi Sonoyama^{1,3,4} (¹Grad. Sch. Sci. Tech., Gunma Univ., ²Ctr. Inst. Anal. Gunma Univ., ³GIAR, Gunma Univ., ⁴GUCFW, Gunma Univ.)

An ABC transporter MsbA, which localizes in bacterial cell membranes, is known to use ATP hydrolysis energy to transport substances. It is thought that MsbA is homologous to human ABCB1, which confers multidrug resistance to anticancer drugs in cancer cells. In elucidating the substrate transport mechanism, effects of lipid environments on ATPase activity have not been systematically investigated. In this study, we investigated the activity of MsbA reconstituted in bilayer membranes of various phospholipids with different acyl chains. It was clarified that MsbA activity was affected by the differences of composition and physical properties of the phospholipids. We will discuss in detail the experimental results from the viewpoint of lipid-protein interaction.

[1-06-1354](#) ナノディスクに埋め込まれた BamA によって補助される外膜タンパク質のアセンブリ
Assembly of outer membrane proteins assisted by BamA embedded into the nanodisc

Eriko Aoki¹, Kazuo Fujiwara², Masamichi Ikeguchi² (¹GaLSIC, Soka Univ., ²Dept. of 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 outer membrane protein A transmembrane domain (OmpATD) and *Haemophilus Influenzae* adhesin transmembrane domain (HiaTD), using empty nanodiscs and BamA-embedded nanodiscs. The insertion of HiaTD into empty nanodiscs was hardly observed and required the assistance of BamA. In contrast, the insertion of OmpATD into nanodiscs was observed both in the presence and absence of BamA. However, BamA increased the insertion rate of OmpATD into nanodiscs.

[1-06-1406](#) ナノディスクに再構成した鉄還元膜タンパク質 101F6 における電子移動反応の解析
Spectroscopic analysis of electron transfer reaction in iron-reducing membrane protein 101F6
reconstituted into nanodiscs

Aoi Yamaguchi¹, Hamed A Abosharaf², Motonari Tsubaki¹, Tetsunari Kimura¹ (¹Dept. of Chem., Grad Sch. of Sci., Kobe Univ., ²Tanta Univ.)

The tumor suppressor gene, 101F6, is expressed as a membrane protein, which have two b-type hemes, and their electron transfer reaction carry out iron reduction. It has been proposed that these reduced irons and ROS peroxidize unsaturated fatty acids, inducing the cell death called "Ferroptosis," but the experimental evidence that the electron transfer from ascorbic acids to Fe³⁺ through 101F6 causes lipid peroxidation is limited. In this study, purified 101F6 were reconstituted into nanodiscs (101F6-nd) to investigate the lipid peroxidation of reduced 101F6 by MASS spectrometry. Iron reduction activity of 101F6-nd was confirmed by the UV-vis spectroscopy, and the molecular mechanism of ferroptosis will be discussed based on the mass analysis of lipid peroxidation.

[1-06-1418](#) Pressure and temperature phase diagram for liquid–liquid phase separation of the rna-binding protein fused in sarcoma

Shujie Li (*Grad. Sch. Phar., Ritsumei Univ.*)

Liquid-liquid phase separation (LLPS) has been often observed *in vivo* and *in vitro*. The formation of protein condensates, driven by LLPS, is known to be involved in neurodegenerative diseases such as amyotrophic lateral sclerosis (ALS) and frontotemporal lobar degeneration (FTLD). The RNA binding protein fused in sarcoma protein (FUS) play crucial roles in RNA transcription, splicing, and transport. Amyloid fibrils of FUS were observed in the patients of ALS and FTLD. The high-pressure microscopy and high-pressure UV/vis spectroscopy were utilized to investigate the effects of pressure and temperature on the LLPS of FUS. A pressure–temperature phase diagram of the phase separation of FUS was also generated and two types of condensed phases were observed.

[1-06-1430](#) ウシ心筋シトクロム酸化酵素の第二のシトクロム c 結合構造
Second cytochrome c binding structure of the bovine heart cytochrome c oxidase

Kyoko Shinzawa-Itoh¹, Shinpei Aoe², Satoru Shimada¹, Junpei Baba¹, Kouki Fujimoto², Atsuhiko Shimada¹, Eiki Yamashita³, Shinya Yoshikawa¹, Tomitake Tsukihara^{1,3}, **Kazumasa Muramoto**¹ (¹*Grad. Sch. Sci., Univ. Hyogo*, ²*Sch. Sci., Univ. Hyogo*, ³*Inst. Protein Res., Osaka Univ.*)

Respiratory chain generates proton motive force coupled to electron transfer at high energy efficiency. Mitochondrial respiratory terminal O₂ reductase (cytochrome c oxidase: CcO) receives electron from ferrocycytochrome c (Cyt c²⁺) bound to the hydrophilic intermembrane surface of CcO. In previous crystal structure of the Cyt c-CcO complex, Cyt c was bound to the CcO surface near the dicopper Cu_A site in the electron transfer pathway. Here, we report new crystal structure of Cyt c-CcO complex at 2.55 Å resolution, in which two Cyt cs are bound. One of Cyt cs exhibits identical binding geometry to the above. Another Cyt c is weakly bound to the surface near the transmembrane region and distant from the Cu_A site. We discuss possible role of the second Cyt c binding.

[1-06-1442](#) 全長カーゴ受容体 ERGIC-53 と補助因子 MCFD2 との複合体の相関構造解析
Correlative structural analysis of a full-length cargo receptor ERGIC-53 in complex with its partner MCFD2

Satoshi Watanabe¹, Yoshiaki Kise², Kento Yonezawa³, Nobutaka Shimizu³, Osamu Nureki², Kenji Inaba¹ (*1IMRAM, Tohoku Univ.*, ²*Grad. Sch. Sci., Univ. Tokyo*, ³*KEK, IMSS*)

ERGIC-53 transports various glycoproteins such as coagulation factors V/VIII from the ER to the Golgi. ERGIC-53 consists of a carbohydrate recognition domain (CRD), a stalk region and a TM helix. Here we report correlative structural analysis of full length human ERGIC-53 in complex with its partner protein MCFD2. SEC-MALS/SAXS analysis revealed that ERGIC-53 exists as a tetramer, not as a hexamer as previously suggested. Cryo-EM structures revealed its overall structure resembling a four-leaf clover with a long flexible stalk. High-resolution cryo-EM maps of the head region showed that the MCFD2 bound CRD of one protomer interacts with that of another protomer to form putative cargo-binding sites. These results provide insight into the transport mechanism by ERGIC-53.

[1-06-1454](#) ヌクレオソーム DNA 解離の配列依存性
Sequence dependence of nucleosomal DNA unwrapping

Tomoko Sunami, Hidetoshi Kono (*MMS, iQLS, QST*)

The first nucleosomes positioned around the transcription start site, +1 nucleosomes, play critical roles in transcriptional regulation. We previously exhibited that AA/TT is enriched in the entry sites of +1 nucleosomes in yeast, and AA/TT regions in nucleosomes are more susceptible to MNase. To further understand the molecular mechanisms, we performed FRET analysis of nucleosomes reconstituted with and without A-tract at the entry/exit sites. Regardless of the sequences, nucleosomes show similar amount of the wrapped state in low salt concentrations. However, we found salt-induced DNA unwrapping occurs more easily in the A-tract nucleosomes, indicating the transition energy from the wrapped to unwrapped state might be lower for the A-tract nucleosomes.

[1-06-1506](#) Catalytic enhancement of NSD2 following oncogenic mutations E1099K and T1150A is caused by increase in the autoinhibitory loop dynamics

Amarjeet Kumar¹, Ko Sato², Shun Sakuraba¹, Kazuhiro Ogata², Toru Sengoku², Hidetoshi Kono¹ (¹*Mole. Modl. Simu. Grp., Inst. Quant. Life Sci., QST*, ²*Dept. Biochem., YCU Grad. Sch. Med.*)

NSD2 hyperactivity following E1099K and T1150A oncogenic mutations in its SET domain leads to the abnormal distribution of the H3K36 di-methylation, thereby affects transcription. Our nucleosome-bound NSD2 cryo-EM structure revealed a remarkable shift in autoinhibitory loop conformation compared to apo-NSD2. Our MD studies suggest that the oncogenic mutations E1099K and T1150A individually disturb the salt-bridge and the loop-hydrophobic patch interaction network in and around the H3 binding site. Destabilizing these interactions that stably keep the loop closed in the wild type leads to a more frequent opening of the loop. Insights from our study into the regulatory mechanism of NSD2 will help develop the specific inhibitors and treatment of cancer in the future.

[1-06-1518](#) DNA bending enhances the dissociation of tetrameric p53's core domains

Duy Tran, Akio Kitao (*Sch. Life Sci. Tech, TokyoTech*)

p53, a DNA-binding transcription factor, consisting of both intrinsically disordered regions (IDR) and rigid domains, is considered as a protein hub that interacts with a variety of biomolecules to regulate the cellular pathways. The main function of p53 is tumor suppressor. Binding of core domains tetrameric p53s to DNA is crucially important step to exhibit its function. However, how the p53 releases DNA has not been well understood due to flexibility and strong binding of p53. Recently, we carry out the dissociation Parallel Cascade Selection Molecular Dynamics simulation to observe dissociation of the tetrameric p53's core domains out of their complex with DNA, suggesting that the bending of DNA largely contributes to the deformation of p53/DNA complex.

[1-07-1330](#) 細胞分裂に関わるキネシン 5 の頭部間協調におけるネックリンカーの役割の高速一分子観察
High-speed single molecule studies of the role of neck linker on the head-head coordination of kinesin 5

Kentaro Ishizashi (*Grad. Sch. Sci. Eng., Aoyama Gakuin Univ*)

Kinesin 5 is a mitotic motor protein and is known to switch between diffusive and unidirectional mode depending on ionic conditions. We previously showed that during the unidirectional motion two heads of a dimer are less coordinated compared to that of kinesin-1. To investigate the role of neck linker on the coordination, we introduced mutation in a conserved Ile residue on the neck linker and observed its motion using a high-speed dark field microscopy. The mutant heterodimer showed unidirectional motion even under low ionic condition and showed ATP-independent detachment from microtubule less frequently compared to the wild type. These results suggest that the Ile residue suppressed ADP release upon microtubule-binding, explaining impaired head-head coordination.

[1-07-1342](#) 尾部ドメインによるキネシン 1 の運動制御の高速一分子観察
Regulation of kinesin-1 motility by tail domain as studied by high-speed single molecule observation

Motoki Niino¹, Ryo Hashizume¹, Kohei Matsuzaki², Michio Tomishige² (¹*Grad. Sch. Sci. Eng., Aoyama Gakuin Univ.*, ²*Dept. Math. Phys., Col. Sci. Eng., Aoyama Gakuin Univ.*)

Kinesin-1 is a motor protein that transports intracellular cargoes by moving along microtubule. The C-terminal tail domain is known to directly interact with the motor head to suppress the motion in the absence of cargo. However, it is still unclear how the tail interrupts kinesin's motility while it moves along the microtubule. In this study, we used kinesin-1 construct with tail domain and observed its motion using a high-speed dark field microscopy. Kinesin with tail domain frequently stopped the motion for >0.2 s, during which the molecule predominantly took one-head-bound state, and then most of the molecules resumed the motion. These results suggest that the head-tail interaction transiently stops the motion, rather it causes dissociation from microtubule.

[1-07-1354](#) キネシン 1 のネックリンカーの構造変化に伴う熱力学的変化の測定
Measurement of thermodynamic changes associated with conformational changes in the neck linker of kinesin-1

Akemi Tanaka^{1,2}, Takumi Hoashi¹, Michio Tomoshige¹ (¹College of Sci. and Eng., Aoyama Gakuin Univ., ²School of Eng., The Univ. of Tokyo)

Kinesin-1 is a molecular motor protein that move along microtubules by hydrolyzing ATP and by alternately moving two motor domains (heads). The neck linkers that connect two heads play an important role in the unidirectional movement. Previous studies involving single-molecule fluorescence imaging and cryo-EM have revealed the ATP-dependent conformational changes of the heads and neck linkers, although the thermodynamic nature of the neck-linker docking is still unclear. In the current study, we used differential scanning calorimetry to measure the enthalpy of thermal denaturation of kinesin head and to examine the effect of neck-linker docking. The results show that the thermal stability of kinesin head increases as a result of the neck-linker docking.

[1-07-1406](#) マイナスキネシン Kinesin-14 モーターコアの微小管プラス端方向への運動性の実証
Plus-end directionality is present in the catalytic core of kinesin-14 minus-end directed motors

Masahiko Yamagishi, Junichiro Yajima (Dept. Life Sci., Grad. Arts& Sci., Univ. Tokyo)

Molecular motor kinesin-14 moves along microtubules toward the minus end. However, it has long been proposed that the catalytic motor core of this minus-ended kinesin generates movement in the plus-end direction, but this has not yet been directly observed. Here, we designed monomers of kinesin-14 (Ncd, Kar3, KlpA) to be fixed to a surface via either the N- or C-terminus only, and demonstrated that simply switching the anchoring side from N- to C-terminus changes the directionality from minus to plus end. We also showed that KlpA, which was recently reported to have kinesin-density-dependent bidirectional motion, has robust fixation-side-dependent unidirectionality under various densities, indicating that at least a dimeric form is required for bidirectional movement.

[1-07-1418](#) (1S1-1) 1 分子回転観察と操作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 IF₁ の解離機構
(1S1-1) Dissociation mechanism of IF₁ from mitochondrial ATP synthase revealed by single-molecule analysis and manipulation

Ryohei Kobayashi, Hiroshi Ueno, Hiroyuki Noji (Appl. Chem., Grad. Sch. Eng., Univ. Tokyo)

IF₁ is a regulatory protein for mitochondrial ATP synthase, which inhibits ATP hydrolysis by inserting its N-terminus into the $\alpha_3\beta_3$ interface of the F₁ motor. Although biochemical assay and structural analysis have contributed to elucidate how IF₁ blocks catalysis of F₁, the reverse reaction, IF₁ release, has not been well studied. To elucidate how IF₁ is released from F₁, we have performed the single-molecule rotation assay of F₁ with magnetic tweezers, enabling to manipulate rotation of F₁ by applying external force. Our results indicated that ATP synthesis reaction by F₁ promotes IF₁ release. We have also revealed that the probability of IF₁ release strongly correlated with the stall angle, suggesting that it is tightly coupled with the elementary reactions of F₁.

[1-07-1430](#) Direct Observation of Stepping Rotation of V-ATPase Reveals Rigid and Non-integer Coupling between V_o and V₁ Motors

Akihiro Otomo^{1,2}, Tatsuya Iida², Hiroshi Ueno³, Takeshi Murata⁴, Ryota Iino^{1,2} (¹Institute for Molecular Science, ²SOKENDAI, ³Grad. Sch. Eng., The Univ. of Tokyo, ⁴Grad. Sch. Sci., Chiba Univ.)

Enterococcus hirae V-ATPase (EhV_oV₁) is a complex of two rotary motor proteins, EhV_o and EhV₁, and functions as an ATP-driven sodium ion (Na⁺) pump across the cell membrane. To understand how EhV_oV₁ transduces the energy in the presence of structural symmetry mismatch between EhV_o and EhV₁, we directly visualized stepping rotation under the condition that both Na⁺ and ATP bindings are rate-limiting by using a mutant EhV_oV₁(aE634A). We found that EhV_oV₁(aE634A) exhibits 13-pausing positions, reflecting the 10- and 3-fold symmetries of EhV_o and EhV₁, respectively and revealed the kinetics of both substrates binding. These results indicate that coupling between EhV_o and EhV₁ is not elastic but rigid, and ion-to-ATP ratio is not variable (3 or 4) but non-integer (3.3).

[1-07-1442](#) Effect of hinge mutations on F_1 -ATPase energetics

Natsumi Sato¹, Yohei Nakayama¹, Takashi Yoshidome¹, Eiro Muneyuki², Shoichi Toyabe¹ (¹*Grad. Eng., Tohoku Univ.*, ²*Sch. Sci. Eng., Chuo Univ.*)

F_1 -ATPase rotates unidirectionally with exploiting the free energy of ATP hydrolysis. Its energetics is crucially important for understanding their design principles. Previously, we found a unique energetical property of F_1 -ATPase that the internal dissipation during the rotation is negligible, suggesting that the most of the free-energy change is focused on the rotational degree of freedom without loss. However, the mechanism to achieve such a sophisticated control remains to be clarified. Here, we performed experiments using multiple mutants with mutations located near the hinge region of the β subunit. We explored how the mutations affect the energetics using our single-molecule energetics experiments combined with nonequilibrium equality.

[1-07-1454](#) エンジニアリング的アプローチによる F_1 -ATPase 制御因子 IF_1 の分子認識機構の解明
Elucidation of molecular recognition mechanism of IF_1 , a regulator of F_1 -ATPase, studied by an engineering approach

Yuichiro Hatasaki, Ryo Watanabe, Ryohei Kobayashi, Hiroshi Ueno, Hiroyuki Noji (*Appl. Chem., Grad. Sch. Eng., Univ. Tokyo*)

IF_1 is an inhibitor peptide of F_1 motor and regulates ATP synthase. IF_1 is specific to eukaryotes; it inhibits catalysis of mitochondrial F_1 (MF_1) with high affinity but does not inhibit thermophilic *Bacillus* F_1 (TF_1). However, their sequences have high homology and the interaction residues found in crystal structures are quite conserved. Thus, the selective association of IF_1 is unknown. To clarify the molecular basis of this selectivity, we measured IF_1 inhibition against hybrid F_1 s that have subunits from TF_1 and bovine MF_1 . Our result indicated that IF_1 provides species specificity through molecular recognition of β subunit. Based on this finding and structural analysis, we are studying the role of species' specific residues of the β subunit on IF_1 inhibition.

[1-07-1506](#) Simultaneous measurement for the stator-incorporation and the flagellar motor rotation

Tomohiro Teshima, Yumiko Uchida, Yong-Suk Che, Akihiko Ishijima, Hajime Hukuoka (*Grad. Sch. Frontier Biosci. Osaka Univ.*)

In bacterial flagellar motor, stepwise increments of torque is reported and it is thought to reflect the incorporation of stator into the motor. However, the relation between torque and the number of stators has not been directly measured. Therefore, to clarify this relation, we developed mNeonGreen-fusion of Na^+ -driven Chimeric Stator (mNG-stator) because the fluorescence intensity of mNG in a single flagellar motor was about 1.3-fold higher than that of EGFP. We confirmed mNG-stator is incorporated into a motor and generates torque by the observation of tethered cell under TIRF microscopy. Now, we are simultaneously measuring the change in a number of stators and the motor torque when the Na^+ concentration is changed. We will discuss this relation at annual meeting.

[1-07-1518](#) 極べん毛モーターと周べん毛モーターの回転方向制御の協同性の違い
Difference in cooperativity of the rotational control between the motors of polar and peritrichous flagella

Hirotaaka Tajima^{1,2}, Masatoshi Nishikawa^{1,3}, Yuki Miura³, Yoshiyuki Sowa^{1,2,3}, Ikuro Kawagishi^{1,2,3} (¹*Dept. Front. Biosci., Hosei Univ.*, ²*Res. Cent. Micro-Nano Tech., Hosei Univ.*, ³*Grad. Sch. Eng., Hosei Univ.*)

Motors of a polar flagellum of *Vibrio cholerae* and peritrichous flagella of *Escherichia coli* have essentially the same mechanism of rotational control. Binding of the response regulator CheY, in its phosphorylated form, to FliM/FliN of the motor induces clockwise rotation. By enhancing CheY phosphorylation, repellents cause tumbling of *E. coli* cells and incessant back and forth movements of *V. cholerae* cells. We hypothesized that the differential behaviors should be brought about by difference in affinity or cooperativity of CheY action on FliM/FliN. Single-cell analyses of the relation between the abundance of CheY-GFP and the flagellar rotational sense suggest that the CheY-FliM cooperativity of *V. cholerae* is lower than that of *E. coli*.

[1-08-1330](#) ウニにおける H⁺/K⁺イオンポンプ活性は胚の細胞骨格分布極性を高めて原腸形成を促進させる
Sea urchin H⁺/K⁺ ion pump enhances cytoskeletal polarity to drive gastrulation

Kaichi Watanabe¹, Yuhei Yasui¹, Yuta Kurose², Naoaki Sakamoto¹, Akinori Awadu¹ (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.

[1-08-1342](#) Membrane progress and backtracking at the critical condition of engulfment in macrophages

Dan Horonushi¹, Sota Suzuki², Kenji Yasuda^{1,2,3} (¹*Dept. Pure & Appl. Phys., Grad. Sch. Adv. Sci. & Eng., Waseda Univ.*, ²*Dept. Phys., Sch. Adv. Sci. & Eng., Waseda Univ.*, ³*Org. Univ. Res. Initiatives, Waseda Univ.*)

Zipper model explained the driving mechanism of engulfment procedure of macrophages. To confirm the ability and limitation of this model, we tracked the elongation of the cell membrane engulfing IgG-coated polystyrene beads or glass microneedles after the macrophage reached maximum engulfment. The results showed that the irregular membrane backtracking was observed after maximum engulfment. We also evaluated the correlation of the elongation along each needle in two-needle-engulfment and found that each membrane reversed independently. These results indicate that the mechanism of engulfment should imply the function of reverse engulfment after they reach the maximum capacity for their survival and its recovery, however, it is local phenomenon of macrophage membrane.

[1-08-1354](#) 合成ポリペプチドの設計によるコンプレックスコアセルベートの物性制御
Control of Complex Coacervate Physical Properties by Design of Synthetic Polypeptides

Yudai Amami, Akihiro Kishimura, Takeshi Mori, Yoshiki Katayama, Gabrielle Ong, Biplab KC (*Grad. Sch. Systems Life Sciences, Univ. Kyushu*)

Coacervates have attracted much attention as a model system for cytosol-like condensed matter and intracellular phase separation. To understand these phenomena in the biological context and to utilize the obtained knowledge from engineering viewpoint, it is necessary to clarify the correlation between molecular design and physical properties. We have so far investigated various aspects of coacervates using synthetic poly(amino acid)-based polyelectrolytes, poly(aspartic acid) and poly(L-lysine). In this study, correlation between the design of the synthetic polymers and the properties of the resulting coacervates was carefully investigated, particularly focusing on viscosity and interfacial tension of coacervates, and mobility of component polymers of coacervates.

[1-08-1406](#) デザインされたブロック共重合体型合成ポリペプチドからなる複合コアセルベートへのタンパク質取り込みと液滴内相分離挙動
Sequestration of proteins into complex coacervates of designed synthetic polypeptides and phase separation behavior inside the droplet

Akihiro Kishimura^{1,2,3}, Biplab KC¹, Ong Gabrielle Anjani¹, Yudai Amami¹, Takeshi Mori^{1,3}, Yoshiki Katayama^{1,2,3,4} (¹*Department of Applied Chemistry, Faculty of Engineering, Kyushu University*, ²*Center for Molecular Systems, Kyushu University*, ³*Center for Future Chemistry, Kyushu University*, ⁴*Center for Advanced Medical Open Innovation, Kyushu University*)

Intracellular liquid-liquid phase separation (LLPS) can provide a functional membraneless compartment, in which specific biomacromolecules are condensed. From the viewpoint of engineering, we tried to design and fabricate LLPS-mimicking droplets using block-copolymer-based synthetic polypeptides via complex coacervation. We assumed PEGylated-poly(aspartic acids) can work as a synthetic analogue of intrinsically disordered proteins/regions (IDPs/IDRs), and a series of chemically modified poly(aspartic acids) was systematically synthesized. Characteristic protein sequestration behaviors were found for some designed droplets, and, in some cases, clear phase separation took place inside of droplets after protein sequestration.

[1-08-1418](#) 陰圧条件下における金魚ケラトサイト細胞シートの細胞間接着の増強
Cell-cell adhesion increase under the negative pressure conditions in fish keratocytes cell-sheets

Shigeki Ookubo, Hitoshi Tatsumi (*Department of Applied Bioscience, Kanazawa Inst. of Technol., Ishikawa, Japan*)

Vacuum assisted closure is being increasingly used for wound management, which promotes healing by exposing damaged areas to local negative pressure. However, the mechanism of the action of vacuum assisted closure remains unknown especially when applying negative pressure directly to cells. In this experiment, we examined the changes seen in cultured goldfish keratocytes cell-sheets directly exposed to a negative pressure, and analyzed the cell-cell interaction of keratocytes in a cell-sheet. Under the negative pressure conditions, the cell-cell adhesion increased.

[1-08-1430](#) 圧力がミトコンドリア内膜の透過性に及ぼす影響
Effects of pressure on the permeability of the inner mitochondrial membrane

Yoshiki Oie, Yoshihiro Ohta (*Dept. of Life Sci. & Biotech., Grad. Sch. Eng., Tokyo Univ. of Agric. & Tech*)

In a physiological circumstance, cells respond to various mechanical stimuli. Pressure is one of the mechanical stimuli which mainly acts on the membrane. Since mitochondria are organelles that have large surface area, we measured the mitochondrial response to pressure in the present study. To examine the direct effects of pressure on mitochondria, we added +200 mmHg to isolated mitochondria. The permeability was examined by observing the release of fluorescence molecule (calcein) previously entrapped in mitochondria. The addition of pressure increased the permeability of the inner membrane of mitochondria in the presence of calcium ions. These results suggest that mitochondria are would be a pressure sensor. The detailed mechanism will be discussed.

[1-08-1442](#) 細菌の運動性、物性および病原性に与える外膜成分の影響
Effect of the outer membrane components on the bacterial motility, physical property, and pathogenicity

Keigo Abe¹, Shuichi Nakamura¹, Nobuo Koizumi² (¹*Grad. Sch. Eng., Univ. Tohoku*, ²*Department of Bacteriology I, National Institute of Infectious Disease*)

Leptospira is a zoonotic bacterium, infecting various mammalian hosts. The motility of *Leptospira* is a crucial virulence factor. A recent report suggested the contribution of the crawling motility on the host cells to virulence, but the molecular mechanism of how the pathogen uses the motility within the host is unknown. Assuming that the involvement of outer membrane (OM) components in the bacterial dynamics over the host cells, we investigated the leptospiral adhesion and motility on cultured kidney cells by using OM-component-related mutants. The result shows the mutation in LPS affects leptospiral crawling. In addition, we will discuss the OM-component dependence of the rigidity and its effect on the surface dynamics and pathogenicity.

[1-08-1454](#) 細胞膜上の糖タンパク質の立体斥力とウイルス感染抑制効果
Cell membrane glycoproteins facilitate steric repulsive forces to modulate viral infections

Yoshihisa Kaizuka (*National Institute for Materials Science*)

Cell membrane glycocalyx has been suggested to inhibit viral infections with steric repulsive forces, but the inhibitory effect was not fully understood due to its nonspecific and redundant natures. We found that highly glycosylated proteins interfered viral infections in several systems in vitro in molecular-size and -density dependent manners. Such inhibition was reproduced by replacing glycoproteins and viruses with synthetic polymers and nanoparticles. Analysis of single cell transcriptome data of viral infections also revealed the correlation between expression of glycocalyx in cells and viral infection. These data suggest that the steric repulsive forces created by glycocalyx can be a common mechanism to interfere with viral binding and infection in cells.

1-08-1506 化学固定は膜タンパク質を凝集することによって細胞表面にナノスケールのクラスターを形成する
Chemical fixation creates nanoscale clusters on the cell surface by aggregating membrane proteins

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Chemical fixations have been thought to preserve the structures of the cells or tissues. However, given that the fixatives create crosslinks or aggregate proteins, there is a possibility that these fixatives create nanoscale artifacts by aggregation of membrane proteins which move around freely to some extent on the cell surface. In this study, we have developed a new method to observe cell surfaces stably and with high resolution using atomic force microscopy and a microporous silicon nitride membrane. We demonstrate that the size of the protrusions on the cell surface is increased after treatment with three commonly used fixatives and show that these protrusions were created by the aggregation of membrane proteins by fixatives.

1-08-1518 ミトコンドリア電子伝達系のプロトンポンプ活性に及ぼす細胞サイズの影響
Effects of cell size on the activity of the proton pumps in mitochondrial electron transfer chain

Yoshiki Suganuma, Hiroko Kashiwagi, Masato Miura, Yoshihiro Ohta (*Grad. Sch. Eng., Univ. Noko*)

For ATP synthesis in mitochondria, proton translocation through three types of proton pumps and FoF1-ATPase is essential. Since the decrease in ATP synthesis activities of mitochondria are involved in many diseases, it is important to measure the activities of these proteins. We have developed the novel method to measure the activity of each of these proteins in a single cell level by observing mitochondrial membrane potential with fluorescence microscopy. The aim of the present study is comparison of mitochondrial activities of cells with different sizes. Also, we measured the effect of reactive oxygen species (ROS) on proton translocation across the inner membrane of mitochondria. The availability of the present method and the effects of ROS will be discussed.

1-09-1330 アミロイドβ凝集体による神経細胞遊走の抑制
Inhibition of neuronal cell migration by Amyloid-β aggregation

Ryota Kitamura, Masahiro Kuragano, Yusaku Chikai, Kiyotaka Tokuraku (*Muroran Institute of Technology*)

Recently, it was found that newborn neurons produced in the adult brain migrate to the damaged area and promote neuron regeneration. We previously reported that aggregation of Amyloid-β (Aβ), which causes Alzheimer's disease, suppressed the flexibility of the cell membrane. In this study, therefore, we tried to elucidate whether Aβ affects the migration ability by a wound-healing assay using PC12 cells. We demonstrated that Aβ preferentially formed aggregates near the tips of migrating cells, resulting in inhibition of migration ability. Furthermore, the addition of rosmarinic acid, a well-known Aβ aggregation inhibitor, rescued the migration ability. Our findings imply that Aβ aggregates might inhibit the migration of newborn neurons and neuron regeneration.

1-09-1342 Emergence of coordinated migration behavior of isolated single macrophages in confined geometries of microstructures

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The migration behavior of single macrophages in the confined geometries were examined. First, isolated single cells were enclosed in microcapillary tubes, and we discovered their coordinated unidirectional motion contrary to our expectation of random walk-like behavior. We also found the similar unidirectional coordinated migration of single macrophages in the lid-free narrow microchannels etched in the thin agarose layer on the bottom of cultivation dish. However, the random walk-like movement was appeared when the cells moved into the free space until they reached to the wall of the chamber, where the cells began coordinated movement again along the wall, suggesting the confined geometry can trigger the emergence of unidirectional migration of single cells.

[1-09-1354](#) Synaptic anchorage of AMPA receptors mediated by their direct binding to PDZ proteins and dynamic interactions with TARPy-2

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The AMPA subtype of ionotropic glutamate receptor (AMPA) is a key molecule for synaptic plasticity. Our advanced single-molecule imaging found that AMPARs in the neuronal plasma membrane (PM) moved in and out of the synaptic region readily by translational diffusion. ~ 5% of AMPARs entering the synaptic region became immobilized for >100 s. AMPAR's C-terminal PDZ-binding motif was involved in its long-term synapse anchorage. Multiple TARPy-2 molecules might dynamically anchor AMPARs to the synapse. Stimulation increased the AMPAR fraction exhibiting synapse anchorage on the 1000-s scale. These results suggest that the rapid dynamic exchanges of the molecules between the synapse and the dendritic-shaft PM might play important roles in regulating the AMPAR functions.

[1-09-1406](#) High hydrostatic pressure regulate TGF-β signaling pathway in human chondrocytes

Masatoshi Morimatsu¹, Xinxuan Li¹, Masayoshi Nishiyama², Keiji Naruse¹ (¹*Grad. Sch. Med. Dent. Pharma., Okayama Univ.*, ²*Dept. Physics., Kindai Univ.*)

Activities of daily living such as walking and sitting pressurize articular cartilage. However, the effect of pressurization on chondrocytes is poorly understood due to the lack of methods that directly observe cells under high pressure conditions. Here we used our high hydrostatic system to observe human chondrocytes dynamics under high pressure condition. We found that high hydrostatic pressure regulates TGF-β signaling pathway in chondrocytes. High hydrostatic pressure (> 20 MPa) induces the nucleus translocation SMAD 3 proteins. Our results suggest the model of the homeostasis of articular cartilage under high pressure conditions.

[1-09-1418](#) ヒト原腸形成の自己組織化に向けて：iPS細胞の2Dパターン培養
Toward the self-organization of the human gastrulation: 2D pattern culture of iPS cells

Chihiro Takeuchi (*Department of Bioengineering, Graduate School of Engineering, Nagaoka University of Technology*)

Human gastrulation arises from a single discoidal layer (approximately 1 mm in diameter) of epiblast and forms three germ layers (mesoderm, endoderm, and ectoderm). However, little is known about the dynamics of layer formation. We mimic human gastrulation in vitro using human iPS cells and 2D pattern culture. We hypothesized that layer formation can be reproduced by mixing cells in a limited 2D space 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. Mesoderm cells derived from human iPS cells and undifferentiated iPS cells (hypothetical epiblast) were mixed and cultured in a 1 mm discoidal pattern. The ratio of cells was changed and the behavior of cells was observed.

[1-09-1430](#) 試験管内再構成による星状体微小管とアクチン繊維網の相互作用の解析
In vitro reconstitution of microtubule aster interaction with the actin network

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The position of centrosome, the main microtubule organizing center, is instrumental in the definition of cell polarity. It is determined by the balance of pushing and pulling forces along microtubules. Several lines of evidence suggest that these forces depend on the mechanical interplay between microtubules and the actin network. However, the structural complexity of cell interior limits our ability to investigate this mechanism. To elucidate the basic principle of the centrosome positioning, we reconstituted the interaction of an aster of dynamic microtubules with actin networks of various composition and architecture in a cell-sized confinement. Our results suggest that the actin network can contribute to aster positioning depending on its architecture.

[1-09-1442](#) ファロイジン-アクチンとサイトカラシン B-アクチンの相互作用の等温滴定熱測定
Isothermal titration calorimetry of phalloidin-actin and cytochalasin B-actin interactions

Shouron Kure, Riku Kiyonaka, Hideyuki Komatsu (*Dept. of Bioscience and Bioinformatics, Kyushu Inst. Tech.*)

Actin polymerization and depolymerization accompany with changes of thermodynamic parameters (changes of Gibbs energy, enthalpy and entropy). To directly quantify these parameters for the actin polymerization, we have measured heats of phalloidin-binding and the following change of by isothermal titration calorimetry (ITC). When F-actin was titrated by phalloidin, the first and the second gradual peaks were observed. The first peaks are likely to be the phalloidin-binding heats, whereas the second peaks may be associated with the actin-polymerization. The relationship between the second heat peaks and the actin polymerization will be examined. The heat of titration of actin by cytochalasin B of a polymerization inhibitor is also presently being analyzed by ITC.

[1-09-1454](#) 微小管-微小管安定化因子相互作用の等温滴定熱測定
Isothermal titration calorimetry of microtubule-microtubule stabilizing factor interactions

Riku Kiyonaka, Junta Kashima, Hideyuki Komatsu (*Dept. of Bioscience and Bioinformatics, Kyushu Inst. Tech.*)

Microtubule (MT) is stabilized by microtubule binding factors such as a microtubule-binding protein tau and a mitotic inhibitor paclitaxel. Our previous study using isothermal titration calorimetry (ITC) showed that tau-MT interaction exhibited exothermic heat in the presence of paclitaxel. In contrast, we here report that the tau-MT interaction is endothermic in the absence of paclitaxel. In addition, our ITC measurement also shows exothermic heat for MT-paclitaxel interaction. These contrasting results may be due to the high ion concentration in the MT solution, which greatly affects the dilution heat. Therefore, after the ion concentration in the MT solution will be adjusted by dialysis, ITC of MT-tau and MT-paclitaxel interaction will be reevaluated.

[1-09-1506](#) 葉緑体運動に必要な CHUP1 によるアクチンの核形成
Actin nucleation promoted by CHUP1 required for chloroplast movement

Yosuke Yamazaki¹, Sam-Geun Kong², Saku Kijima³, Masamitsu Wada⁴, Taro QP Uyeda¹ (¹*Dep. Phys., Waseda Univ.*, ²*Dep. Biol. Sci., Kongju Natl. Univ.*, ³*Biomed. Res. Inst., AIST*, ⁴*Dep. Biol., Kyushu Univ.*)

Chloroplasts move in response to light intensity for optimizing photosynthesis and preventing photodamage. This movement is inferred to be driven by actin polymerization like *Listeria* movement. CHUP1, whose C-terminal domain (CHUPIC) is structurally similar to the FH2 domain, is shown to be required for the chloroplast movement, and to promote actin polymerization in vitro. But its detailed mechanism is unclear. Here, we observed plant actin polymerization in the presence of profilin and CHUPIC-tagRFP by TIRF microscopy. CHUPIC-tagRFP transiently bound to growing ends of actin filaments without affecting the elongation rate. However, CHUPIC significantly increased the filament density. These results suggest that CHUPIC is an actin nucleator rather than an elongator.

[1-09-1518](#) The amplitude of twisting and bending fluctuations of actin filaments decreased by mechanical stress

Kaoru Okura, Hitoshi Tatsumi (*Department of Applied Bioscience, Kanazawa Inst. of Technol., Ishikawa, Japan*)

It has been proposed that actin filaments sense tension and act as a mechanosensor. In this study, single-molecule fluorescence polarization (SMFP) microscopy was employed to directly measure the torsional and bending fluctuations of a single actin filament under different stresses in order to evaluate the effect of increasing tensile force on the mechanical behavior of actin filaments and protomers. Our results suggest that the angle of torsional fluctuations and local bending and fast fluctuations of a single actin filament decreased under tension increases. The molecular importance of the semiquantitative analysis of the decrease in the fluctuations decrease is discussed.

1-10-1330 気液界面における人工肺サーファクタント膜への負電荷微粒子の影響
Effect of negatively charged particles on a model lung surfactant monolayer at the air-water interface

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Lung surfactant is a complex mixture of lipids and proteins at the air-water interface of the alveolus. Although the study of molecular interactions has been extended to investigate the effects of foreign material on the biophysical behavior of surfactant monolayers, it is difficult to predict the mechanisms by which interactions alter the interfacial character of the surfactants. Here we have used isotherms, surface elastic modulus and fluorescence microscopy to investigate effects of differing concentrations of 200nm polystyrene particles on the ternary monolayer as the monolayer is subject to compression and expansion. The results show that the presence of particles in the subphase at the highest concentration affects the formation and structure of the lipid domains.

1-10-1342 パターン化モデル膜とナノ空間を用いたドーパミン受容体の再構成と機能解析
Functional reconstitution of dopamine D2 receptor into a supported model membrane in a nanometric confinement

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Dopamine D2 receptor (D2R), a G-protein coupled receptor (GPCR), plays essential roles in the neural functions. We developed a methodology to reconstitute and characterize D2R in a supported model membrane in a nanometric confinement. We expressed D2R in CHO cell and transferred it into the model membrane using cell membrane vesicles (blebs). D2R molecules were reconstituted in the nanometric confinement between the supported substrate and PDMS elastomer. The physiological functions of reconstituted D2R were retained as evaluated from its binding to an antagonist and transient dimerization. This nanometric confinement has a new possibility for studying membrane proteins under the quasi-physiological conditions.

1-10-1354 B型肝炎ウイルスのエンベロープのモデリングとシミュレーション
Hepatitis B virus envelope: modeling and simulation

Ryo Urano, Wataru Shinoda (*Grad. Sch. Eng., Nagoya Univ.*)

Hepatitis B virus (HBV) is a cause of world-wide health problem, leading to liver disease. HBV is an envelope virus, and replicative cycle of HBV starts with the interaction between viral membrane protein and host cell receptor. However, molecular mechanism of the interaction remains unclear. One of the reasons is the lack of molecular structure of HBV envelope. Here, we developed a simple envelope model of HBV and performed the molecular dynamics simulation. We will report the procedure of modeling and influence of viral membrane protein into lipid bilayers.

1-10-1406 筋小胞体 Ca ポンプ M2 ヘリックスの Ca 輸送における役割
Role of M2 helix of sarcoplasmic reticulum Ca pump in Ca transport

Takashi Daiho (*Asahikawa Med. Univ.*)

Ca pump catalyzes Ca-transport 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. So, Gly105 functions as a flexible hinge for a critical knee-like joint of M2m/M2c. 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 nearby residues.

[1-10-1418](#) リポソーム再構成系を用いた細菌べん毛モーターのMSリング構築メカニズムの解析
Investigation of the flagellar MS-ring construction mechanism using liposome reconstitution system

Hiroki Kajino¹, Hiroyuki Terashima², Michio Homma¹, Seiji Kojima¹ (¹*Grad. Sch. Sci., Univ. Nagoya*, ²*Trop. Med. Inst., Univ. Nagasaki*)

Vibrio alginolyticus has a single polar flagellum at the cell pole whose formation starts with MS-ring assembly. It is unknown how MS ring, which is composed of 34 molecules of a membrane protein FlIF, is constructed. Here, we used liposome reconstitution system and tried to elucidate MS-ring assembly mechanism. We purified FlIF, reconstituted it into liposome, and then purified FlIG (C-ring component) was added to expect the promotion of MS-ring assembly. FlIF liposome were found to bind FlIG. MS-ring fraction was precipitated by ultracentrifugation of solubilized FlIF liposome and observed with an electron microscope. Unfortunately, we could not observe MS ring in this fraction. Currently, we examine the effect of FlIF, another factor to promote MS-ring formation.

[1-10-1430](#) 両親媒性ペプチドから成るナノディスクを用いたロドプシンのパターン化モデル生体膜への再構成
Reconstitution of rhodopsin into a patterned model membrane using nanodisc formed from amphiphilic peptides

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Model membranes, such as supported lipid bilayers (SLBs), are potentially useful tools for evaluating the physicochemical properties of membrane proteins (MPs). However, it is difficult to reconstitute MPs into a model membrane. In this study, we used nanodisc formed from amphiphilic peptide (peptide-ND) for reconstituting MP. MPs and lipids are wrapped with amphiphilic peptides, and MPs have increased stability compared to solubilized with detergent. Using the peptide-ND, we could reconstitute rhodopsin into a patterned SPBs while preserving its diffusivity. The model system prepared using the peptide-ND has the potential to be a platform for the quantitative analysis of the protein-protein and protein-lipid interactions.

[1-10-1442](#) (2S7-1) Local membrane curvature influences lipid signaling

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PIP3 dynamics observed in membranes are responsible for the protruding edge formation in cancer and amoeboid cells. There are related to the membrane-protrusive activities and formation of macropinocytic cups in Dictyostelium and mammalian cells. Here, we present new insights in the complex pattern evolution of PIP3 waves, and show evidences on how the spatiotemporal dynamics self-regulate through shape, size and local membrane curvature of the plasma membrane in single Dictyostelium cells. We extract and map the lipid signalling on the entire three-dimensional plasma membrane. By statistical analysis of the PIP3 domain dynamics and local noise-fluctuation dynamics, we reveal the importance of the membrane topology with particular impact on the local membrane curvature.

[1-10-1454](#) 脂質スクランブリングペプチドによる細胞貪食誘導
Induction of phagocytosis by phospholipid scrambling peptides

Hiroyuki Nakao, Yusuke Kimura, Keisuke Ikeda, Minoru Nakano (*Fac. Pharm. Sci., Univ. Toyama*)

Phosphatidylserine is mostly localized in the inner leaflet in the plasma membrane. Disruption of the asymmetry, which is mediated by phospholipid scramblases, results in the exposure of phosphatidylserine on the cell surface. The exposed phosphatidylserine is involved in phagocytosis of apoptotic cells. Therefore, control of phospholipid transbilayer movement in the plasma membrane attracts biological and medical interests. We previously developed lipid scrambling peptides in model membrane systems, which can be inserted into lipid bilayers and exhibit phospholipid scrambling activity. In this study, we investigated phosphatidylserine externalization activity of the lipid scrambling peptides and phagocytosis of phosphatidylserine exposed cells with the peptides.

[1-10-1506](#) Bt 菌 Cry46Ab トキシンの小孔形成とその殺蚊活性
Channel-pores formation of *Bacillus thuringiensis* Cry46Ab toxin and its mosquitocidal activity

Midoka Miyazaki, Tohru Hayakawa, Toru Ide (*Grad Schl Interdiscip Sci Engn Health Syst*)

Cry46Ab from *Bacillus thuringiensis* TK-E6 is a new mosquitocidal toxin with an aerolysin-type architecture, and it is expected to be used as a novel bioinsecticide. Cry46Ab acts as a functional pore-forming toxin and characteristics of the resulting channel-pores, including ion selectivity, have been analyzed. In this study, we constructed a variety of Cry46Ab mutants in which an amino acid residue within putative transmembrane β -hairpin region was replaced with other amino acid residue. We also assessed mosquitocidal activity and channel-pore ion-selectivity of Cry46Ab mutants. Considering results obtained, we discuss here about relationship between channel-pore ion selectivity and mosquitocidal activity for Cry46Ab toxin.

[1-10-1518](#) 四量体型ナトリウムチャネルにおける二価カチオンによる活性阻害機構の創出
The generation of the divalent cation blocking on tetrameric sodium channel

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The divalent cation blocking is observed in various tetrameric ion channels, involved in memory formation, muscle contraction. We introduced this divalent cation blocking into a tetrameric sodium channel. The small-side chain mutation of the selectivity filter residue creates a small cavity for an extra water molecule and enables the coordination of divalent cations via a water molecule in the ion pathway. Therefore, the sodium ions were repelled by the giant positive field lying on the bottom of the selectivity filter. It has become possible to know the molecular basis of the divalent cation block of wide-spread biologically important channels. Furthermore, the generation of a new function by single point mutation is reminiscent of the evolutionary process of channels.

[1-11-1330](#) プロトンポンプ型ロドプシンを用いたアポトーシスの光制御
Optical control of apoptotic cell death by light-driven proton pumps

Keiichi Kojima^{1,2}, Shin Nakao², Yuki Sudo^{1,2} (¹*Grad. Sch. of Med. Dent. & Pharm. Sci. Okayama Univ.*, ²*Fac. of Pharm. Sci., Okayama Univ.*)

Photoreceptive membrane protein, microbial rhodopsin, regulates intracellular ion concentrations, leading to various cell responses. Microbial rhodopsin serves as fundamental tools of optogenetics, a technology to control biological phenomena by light. Noteworthy, it is well-known that intracellular pH alkalization is related to apoptosis, a programmed cell death. In this study, we newly demonstrate the optical control of apoptosis by proton pump rhodopsins in human cultured cells and the nematode *Caenorhabditis elegans* [Patent application, 2020-196718]. Based on the results, we discuss the high potential of our developed optical method for precise control of cell death in living cells and animals.

[1-11-1342](#) 1 残基変異による光サイクル型脊椎動物ロドプシンの創製
Construction of photocyclic vertebrate rhodopsin by a single mutation

Kazumi Sakai¹, Yoshinori Shichida², Yasushi Imamoto¹, Takahiro Yamashita¹ (¹*Grad. Sch. Sci., Kyoto Univ.*, ²*Research organization for Sci. and Tech.*)

Opsins are photoreceptive proteins in animals and have diversified photoreaction mechanisms. Vertebrate rhodopsin is a mono-stable opsin which photo-converts to a metastable active state that cannot revert to the dark state. Recently, we identified a unique opsin, Opn5L1, as a photocyclic opsin. Opn5L1 binds all-trans retinal in the dark to form the active state and self-regenerates to the dark state after photo-inactivation. Here, we successfully converted the mono-stable property of vertebrate rhodopsin into the photocyclic property by a single mutation. This opsin photo-converts to the active state and subsequently reverts back to the dark state. We will discuss potential application of this photocyclic opsin to optogenetics by additional mutations.

[1-11-1354](#) 赤色光感受性非視覚オプシンの解析
Characterization of red-sensitive non-visual opsin

Takahiro Yamashita¹, Kengo Fujii¹, Chihiro Fujiyabu¹, Kazumi Sakai¹, Yasuhiro Shiga² (¹*Grad. Sch. Sci., Kyoto Univ.*,
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Opsins are the photoreceptive proteins for visual and non-visual photoreceptions in animals. Analysis of the molecular properties of opsins has identified various opsins whose peak sensitivities range from UV to red. In particular, the diversification of the spectral sensitivities contributes to visual color discrimination. By contrast, many non-visual opsins are sensitive to short wavelength light and there is little information about long wavelength-sensitive non-visual opsins. In this study, we identified a non-visual opsin whose spectral peak is in the red region. We would like to compare the spectral tuning mechanism between this non-visual opsin and vertebrate cone pigments and discuss the physiological relevance of this opsin based on its tissue distributions.

[1-11-1406](#) 無脊椎動物ロドプシンの光構造変化
Light-induced conformational change of invertebrate rhodopsin

Yasushi Imamoto (*Grad. Sch. Sci., Kyoto Univ.*)

Invertebrate rhodopsins are well-characterized bistable opsins which serve as the model of vertebrate non-image-forming opsins. To get the insight into the activation mechanism, light-induced conformational change of octopus rhodopsin was characterized by Fourier transform infrared (FTIR) spectroscopy. Octopus rhodopsin was solubilized by n-dodecyl- β -D-maltoside, highly concentrated, and put in the solution cell (path length, 5-7 μ m). The absorbance change in amide I region in solution was greater than that in hydrated film, and comparable to that of bovine rhodopsin. In addition, multiple bands were observed at ~ 2550 cm^{-1} , possibly derived from the cysteine SH group. Based on these results, conformational change of bistable rhodopsin will be discussed.

[1-11-1418](#) 藍色光にตอบสนองカルシウム透過性が高いチャネルロドプシンの光遺伝学応用へ向けた取り組み
Calcium selectivity and optogenetics application of a deep blue absorbing channelrhodopsin

Satoshi Tsunoda, Rintaro Tashiro, Shoko Hososhima, Hideki Kandori (*Nagoya Institute of Technology*)

Channelrhodopsins (ChRs) are light-gated ion channels extensively applied as optogenetics tools. We previously reported the cation channel properties of KnChR from a filamentous terrestrial alga *Klebsormidium nitens*. Here, we first report ion selectivity of KnChR. By comparison of the permeability ratio ($\text{Ca}^{2+}/\text{Na}^{+}$), KnChR is more Ca^{2+} permeable than ChR2. We succeeded in improving the Ca^{2+} permeability up to 100 times by an amino acid substitution. Secondly, maximal sensitivity was exhibited at 430 nm and 460 nm, the former making KnChR one of the most blue-shifted ChRs. Amino acid substitutions further shifted to 420 nm. We finally demonstrate optical neuronal stimulation by using KnChR to test its applicability for optogenetics for short-wavelength excitation.

[1-11-1430](#) 南極の好冷菌 *Hymenobacter nivis* P3^T 由来プロテオロドプシンの生理学的役割と光化学的特性
Physiological role and photochemical property of the cryophilic *Hymenobacter nivis* P3^T
proteorhodopsin discovered in Antarctica

Kaori Kondo¹, Ryohei Ohtake¹, Mia Terashima², Hisaya Kojima², Manabu Fukui², Makoto Demura³, Takashi Kikukawa³,
Takashi Tsukamoto³ (¹*Graduate school of Life Science, Hokkaido University*, ²*Institute of Low Temperature Science, Hokkaido University*, ³*Faculty of Advanced Life Science, Hokkaido University*)

A cryophilic bacterium *Hymenobacter nivis* P3^T (*H. nivis*) was isolated from red snow in Antarctica. It grows fast under light irradiation without photosynthetic protein. Alternatively, it has a light-driven H^{+} pump proteorhodopsin (PR), which we named HnPR. Here we analyzed the physiological role and photochemical property of HnPR for light utilization in severe condition in Antarctica. The assays of H^{+} pump activity and ATP content in cultured *H. nivis* revealed that *H. nivis* produced ATP using the H^{+} gradient formed by HnPR upon light activation. Through flash photolysis experiments on recombinant HnPR, its photocycle at 5 $^{\circ}\text{C}$ was found out to be as fast as that of other typical PRs at 20 $^{\circ}\text{C}$, indicating the cold adapted photochemical property of HnPR.

[1-11-1442](#) A *Geminigera cryophila* Anion Channelrhodopsin Shows Significantly Slow Photocycle

Hina Kurane¹, Makoto Demura², Takashi Kikukawa², Takashi Tsukamoto² (¹*Graduate School of Life Science, Hokkaido University*, ²*Faculty of Advanced Life Science*)

Anion channelrhodopsins (ACRs) represented by *GtACR1* are light-gated anion-selective channel identified in cryptophyte algae. Here we investigated a *Geminigera cryophila* ACR (*GcACR*), which is a close relative of *GtACR1*. *GcACR* was recombinantly expressed in yeast cells and showed anion (Cl⁻) transport activity under continuous light illumination. However, the activity was far weaker than that of *GtACR1*. To identify the cause of this, we performed spectroscopy measurements using purified *GcACR*. As a result, *GcACR* undergoes a significantly slow photocycle (~300 min) compared to that of *GtACR1* (~2 s). Therefore, a branched photocycle is likely to exist in *GcACR* under the continuous light as same as cation channelrhodopsins, which results in the weak transport activity.

[1-11-1454](#) クリプト藻由来の光受容陽イオンチャネルのキネティクス
Kinetic evaluation of light-gated cation channels from cryptophyte

Shoko Hososhima, Shunta Shigemura, Hideki Kandori, Satoshi Tsunoda (*Life Science and Applied Chemistry, Nagoya Institute of Technology*)

Optogenetics has revolutionized the study of experimental biology, making it possible to optically manipulate various biological functions in high temporal and high special resolutions. Here we report electrophysiological properties and optogenetical application of light-gated cation channels from cryptophyte. One of them, GtCCR4 exhibits powerful channel activity with a high light sensitivity compared to ChR2. Furthermore, GtCCR4 showed higher Na⁺ selectivity, and conducted almost no H⁺ and no Ca²⁺. When GtCCR4 was expressed in cultured neurons, successful neuronal firing was observed even by weaker light than required for ChR2 excitation without loss of temporal resolutions, suggesting a potential of GtCCR4 as an ideal optogenetics tool.

[1-12-1330](#) GroE 基質タンパク質によく見られる構造モチーフ
Small structural patterns common in chaperonin GroE substrate proteins

Shintaro Minami¹, Tatsuya Niwa², Eri Uemura², Ryotaro Koike¹, Hideki Taguchi², **Motonori Ota**¹ (¹*Grad. Sch. Info., Nagoya Univ.*, ²*IIR, Tokyo Tech.*)

Chaperonin GroE, a general chaperone, facilitates the folding of certain proteins. GroE prefers proteins adopting α/β class structures, especially TIM barrels, as substrates. We assumed the presence of clearer common features in substrates by focusing on the local structures. We computationally extracted the substructures that were most exclusively included in substrates, and developed a GroE substrate predictor. The selected substructures are projectable onto a 2-layer $2\alpha4\beta$ sandwich, the most ubiquitous substructure in proteins, which explains the versatile role of GroE in folding. We experimentally examined all false positive predictions by our predictor, and found that over half of them were “true positives”. Together, these results support our hypothesis.

[1-12-1342](#) Disentangling the Effects of Histone Post-Translational Modifications on Nucleosome Packing and Chromatin Structure

Justin Chan, Hidetoshi Kono (*Molecular Modeling and Simulation Group, Institute for Quantum and Life Science (iQLS), QST*)

DNA carries the blueprint of life. The control of when and how much genetic information is expressed in cells is partly governed by epigenetics. Nucleosomes, 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 and change the chromatin's structure. Although experimental data of contact frequency maps between nucleosomes (Hi-CO & Micro-C XL) and the locations of the PTMs (ChIP-seq) are available, we lack a method to disentangle and to study 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.

[1-12-1354](#) A meta-inference approach to modeling the 3d structure of chromatin from Hi-C data

Giovanni Bruno Brandani, Chenyang Gu, Shoji Takada (*Dept Biophysics, Div Biology, Grad School Science, Kyoto University*)

The 3d organization of Eukaryotic genomes influences key biological processes such as gene expression, and can be investigated using Hi-C experiments, which measure the frequency of contacts between pairs of genomic loci in large population of cells. While Hi-C provides many insights into the organization of chromatin, it cannot capture the effect of cell-cell heterogeneity, which is important in many situations such as enhancer-promoter interactions. Using Hi-C data in combination with a polymer model, we reconstruct the full heterogeneous ensemble of 3d chromatin conformations in mouse ES cells using meta-inference, a recently-developed approach to integrate population-averaged experimental data into molecular dynamics simulations within a rigorous Bayesian framework.

[1-12-1406](#) Comparative Scoring Power Assessments of Protein-Ligand Docking Scoring Functions by Considering Protein Functional Groups

Yovita Ardiyani¹, Hafumi Nishi^{1,2,3}, Kengo Kinoshita^{1,3} (¹*Grad. Sch. Info. Sci., Tohoku Univ.*, ²*Fac. Core Res., Ochanomizu Univ.*, ³*ToMMo, Tohoku Univ.*)

In molecular docking, there are many search algorithms produce robust binding pose results with divergent kinds of scoring functions (SFs), but the existing docking research treated divergent kinds of proteins in the same manner. Our study aim was to assess the scoring functions' ability to predict binding affinity on particular groups based on protein molecular function and binding sites' local structural features. The scoring result of 8 SFs were measured with the known binding affinity on the PDBbind core set 2016. Although machine learning based SFs outperformed all classical SFs, each scoring function showed a unique performance profile on particular groups of proteins. In this study, we show the relation between the performance and functional group of proteins.

[1-12-1418](#) ヒトタンパク質データセットを利用した天然変性領域の長さタンパク質の機能の関係
Relationship between Length of Intrinsically Disordered Regions and Protein Function

Haruka Tanimoto, Ryotaro Koike, Motonori Ota (*Grad. Sch. Info., Nagoya Univ.*)

Intrinsically disordered proteins are the ones that have regions do not adopt three-dimensional structure (disordered regions) even under physiological conditions. In this study, we used keywords in human-protein datasets to investigate the relationship between length of disordered regions and protein function. Focusing on each keyword, we tried to divide proteins with a long disordered region and those with a short disordered region, so that the division provides the smallest P-value. We also determined keywords that are sensitive to the length of the disordered regions. Details will be shown in the presentation.

[1-12-1430](#) 慢性歯周炎における血液組織の遺伝子発現データのメタ解析
Meta-analysis for gene expression data of blood tissue in chronic periodontitis

Hideto Koizumi, Takanori Sasaki (*Fac. Adv. Math. Sci., Univ. Meiji*)

Periodontal disease (PD) is known to cause an inflammatory response in the body and exacerbate insulin resistance. In this study, we investigated the differentially expressed genes (DEGs) in the blood of patients with PD and estimated genes that may promote diabetes and its complications. In particular, we selected DEGs ($\text{LogFC} > 0.4$) common to all of three microarray and two RNA-seq datasets for peripheral blood neutrophils / monocytes of patients with PD. As a result of this meta-analysis, genes contribute to diabetes and its complications (ABCG1, CPVL, KLF10) were included in the selected 31 DEGs. This result suggests that the expression level of genes contribute not only to insulin resistance but also diabetic complications is changed in the blood of patients with PD.

[1-12-1442](#) 仮想系共役サンプリング法の開発と応用
Development and Application of the virtual-system coupled canonical sampling method

Kota Kasahara¹, Qilin Xie², Yusuke Sakai², Yuta Nakano², Junichi Higo³, Takuya Takahashi¹ (¹*Coll. Life Sci., Ritsumeikan Univ.*, ²*Grad. Sch. Life. Sci., Ritsumeikan Univ.*, ³*Res. Org. Sci. Tech., Ritsumeikan Univ.*)

Exploring a rugged energy surface by sampling methods, such as molecular dynamics and Monte Carlo, generally requires a huge computational cost because a trajectory is frequently trapped in energy minima. Here, we developed a new extended ensemble approach, termed virtual-system coupled canonical sampling method (VcS). This method splits the phase space along with predefined multiple reaction coordinates into several subregions, and transitions among these subregions are enhanced by controlling transition probability. In this talk, we will present efficiency of this method by using a toy model, which consists of a particle in the double-well potential field. VcS efficiently enhanced the conformational changes and converged to the canonical distribution.

[1-13-1330](#) 結合蛋白質 CARMIL や twinfilin がキャップ蛋白質の構造ゆらぎに与える影響を弾性ネットワークモデルにより解析する
Elastic network model analysis shows distinct flexibilities of capping protein bound to CARMIL or twinfilin

Ryotaro Koike, Motonori Ota (*Grad. Sch. Info., Nagoya Univ.*)

Capping protein (CP) binds to the barbed end of an actin filament and inhibits the further elongation of the filament. CARMIL protein binds CP and dissociates CP from the barbed end. The previous works suggest the CARMIL binding alters the flexibility of CP and facilitates the dissociation. Twinfilin also binds CP through its C-terminal tail. The complex structures of CP/twinfilin tail (TWtail) revealed the binding sites of CARMIL and TWtail are overlapped. However, the TWtail binding does not facilitate the dissociation of CP from the barbed end. Applying elastic network model to CP/TWtail complex structures, we found TWtail binding does not alter the flexibilities of CP. Focusing on the overlapped binding sites, we explore the region affecting the flexibility.

[1-13-1342](#) RNA-seq 発現解析・バスウェイ解析による、腫瘍選択的抗 CD137 アゴニスト抗体 STA551 の癌微小環境および正常組織への効果
RNA-seq based expression analysis of the extracellular ATP 環境 dependent tumor-selective response of the STA551 antibody targeting CD137

Shoichi Metsugi¹, Kazuya Takakuwa¹, Sayuri Horikawa¹, Ryo Uchikawa¹, Kenji Taniguchi¹, Koki Hamada¹, Yoshinori Narita², Mika Sakurai¹ (¹*Chugai Pharmaceutical Co. Ltd.*, ²*Chugai Pharmabody Research Pte. Ltd*)

Agonist antibodies targeting CD137 have been clinically unsuccessful due to systemic toxicity. We exploited extracellular adenosine triphosphate (exATP), which is a hallmark of the tumor microenvironment. We generated a novel anti-CD137 switch antibody, STA551, which exerts agonistic activity only in the presence of exATP. We employed RNA-seq analysis to elucidate the response in the tumor microenvironment and normal tissues in a human CD137 knock-in mouse model. We also identified pathways influenced by STA551. We found that the expression of leucocyte-related genes such as Cd8a and Gzma was changed in tumors but largely unaffected in normal tissues, suggesting that STA551 changes the population or activity of TILs only in tumor tissues.

[1-13-1354](#) 精製因子によるゲノム転写翻訳系の再構成とその網羅的解析
Reconstitution of the *E.coli* genome transcription and translation system with its purified elements

Yukino Matsui¹, Tatsuya Niwa², Hideki Taguchi², Nobuhide Doi¹, Kci Fujiwara¹ (¹*Dept. Biosci. Info., Keio univ.*, ²*Cell Biol. Center IIR, Tokyo Tech.*)

Creating living cells from its biomolecules is one of the grand challenges in synthetic biology. Although our previous study showed the purified bacterial genome can be transcribed and translated by cell extract *in vitro*, it was unknown whether it can be achieved with the purified elements. Here, we report i) the *E.coli* genome can be transcribed and translated by its purified elements, ii) almost 100% gene of the *E.coli* genome can be transcribed by the only RNA polymerase, iii) more than 400 proteins have been identified as newly synthesized proteins from the reconstituted system. These results shed light on the feasibility of creating living cells from biomolecules and a potential of this system to become a novel method for studying the genome expression principle.

[1-13-1406](#) 核スペck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, Hiroshima University*)

Eukaryotes have a nucleus within the cell. The activity of the cell is supported by many proteins. In the process of producing these proteins, nuclear bodies play an important role. There are various types of nuclear bodies. In particular, we focused on “nuclear speckles”. Nuclear speckles are irregularly scattered in the nucleus. Since they contain various components involved in splicing, they are thought to regulate the post-transcriptional regulation of genes. Additionally, when transcription is stopped, nuclear speckles gather to form spherical structures. However, the molecular mechanism of this RNA-dependent change of nuclear speckles haven't been clarified. Then we investigated the dynamics of nuclear speckles by simulating them using a coarse-grained model.

[1-13-1418](#) 転写因子 PC4 の天然変性領域とテグメントタンパク質 VP16 の結合メカニズムの計算科学的検討
Simulation study of binding mechanism between intrinsically disordered region of transcription factor PC4 and tegument protein VP16

Qilin Xie¹, Yuta Nakano¹, Yusuke Sakai¹, Kota Kasahara², Junichi Higo³, Takuya Takahashi² (¹*Grad. Sch. Life Sci., Ritsumeikan Univ.*, ²*Coll. Life Sci., Ritsumeikan Univ.*, ³*Res. Org. Sci. Tech., Ritsumeikan Univ.*)

PC4 is a transcription factor that activates RNA polymerase II by interacting with the transactivation regions of various proteins. Previous studies reported that PC4 binds to herpes simplex virion protein (VP16). Their binding is regulated by the intrinsically disordered region of PC4, the N-terminal domain (PC4ntd), but the molecular mechanism is unknown. Here, we elucidate the interaction between PC4ntd and VP16 by using a sampling method, the virtual-system coupled canonical molecular dynamics. We constructed the simulation model including the PC4-VP16 complex and a truncated peptide of PC4ntd. As a result, we found PC4ntd and VP16 had multiple binding modes including multivalent salt bridges between unspecified pairs of charged residues.

[1-13-1430](#) 出芽酵母の胞子形成関連遺伝子群の各時間クラスへの非階層的クラスタリング
Non-hierarchical clustering of sporulation related genes of budding yeast to each temporal class

Aoi Tani, Takanori Sasaki (*Fac. Adv. Math. Sci., Meiji Univ.*)

Sporulation in *S.cerevisiae* is consisted of at least seven temporal classes, and specific transcription factors(TF) induce expression of many genes in each class. In this study, we attempted clustering of DEGs that function in intra- or inter-temporal classes by using microarray data for the sporulation process of *S.cerevisiae*. 2,937 of DEGs were clustered by k-means++ method, followed by calculation of membership value(m-val) of each gene for each cluster by concept of Fuzzy clustering method. The accuracy for clustering evaluated by using index genes that characterize each temporal class was >90%. On these clusters, major early sporulation TFs, UME6 and IME1 had high m-val for some clusters, suggesting the correlation between m-val and gene regulation network.

[1-13-1442](#) UV_C 照射によるゲノム変異導入は効果的な方法か？
Is the introduction of genomic mutations by UV_C irradiation an effective method?

Kunio Ihara^{1,2}, Keisuke Matsuo², Kazuma Uesaka¹ (¹*Nagoya University, Center for Gene Research*, ²*Nagoya University, Faculty of Science*)

UV_C light (254 nm) is effectively absorbed by the DNA molecule, so it is known to directly modify DNA and excite small molecules such as oxygen to generate radicals, which secondarily affect DNA. Although UV_C has been used for introducing genomic DNA mutations, the efficiency of mutation introduction has been evaluated by the frequency of appearance of drug-resistant mutant. Even now there is a few report on how much mutation is actually introduced into the entire genome as the irradiation dose increases. We performed 36 independent UV_C irradiation experiments (UV does category; 0, 0-3, 3-6, 6-9, 9- mJ/cm²) using the extremely haloalkaliphilic archaea, and analyzed the genomic DNA more than 500 strains. As a result, UVC mutation was NOT as effective as imagined.

[1-13-1454](#) トランスクリプトーム解析による表現型多型の考察
Transcriptome data analysis for phenotype polymorphism

Miko Imada, **Akinori Awazu** (*Dept. Math. and Life Sci., Hiroshima Univ.*)

Large variations of expression levels among biological replications with the same genotype grown under the same condition were often observed in various genes, not only single cell level but also cell populations or multicellular-organism levels. Such variations were known to correlate to various features of genes such as their functions and regulation networks. On the other hand, the relationship between such variations of genes expression levels among biological replications and phenotype polymorphism among individuals was not revealed. We performed transcriptome data analysis in order to clarify the connection from such microscopic variations to macroscopic phenotype variations.

[1-14-1330](#) A log-periodic based model of cell-group repair and failure—cancer

Hiroshi Yoshida (*Math Dept. Kyushu Univ.*)

A log-periodic based model of cell-group repair—regeneration phenomena and repair-failure—cancer in multicellular organisms is proposed here. In this model, each cell is assumed to have a value of a log-periodic curve. A log-periodicity was originally introduced to model destruction phenomena, where cooperative behavior seems important and might be similar to cell motility. In our previous work, it was impossible to explain regeneration across leg segments, namely segment regeneration. In this presentation, on the other hand, each cell is assumed to have a value of a log-periodic curve, which provides an explanation of segment regeneration. I am going to also show and discuss some wound-repair patterns and repair-failure-patterns as cancer.

[1-14-1342](#) Emergent slower synchronous beating behavior in spontaneous beating cardiomyocyte clusters

Yoshitsune Hondo, Kazufumi Sakamoto, Kenji Yasuda (*Dept. Pure & Appl. Phys., Grad. Sch. Adv. Sci. & Eng., Waseda Univ.*)

Conventional faster firing regulation model in cardiomyocyte synchronization predicts the synchronous beating in clusters should follow to the fastest component cells. However, we found the emergence slower beating intervals in the jointed two clusters. In the experiment, we formed two cardiomyocyte clusters having different interbeat intervals (IBIs). When two cardiomyocyte clusters were connected, they synchronized in the longer IBIs than both of those two clusters' original IBIs. Then, we separated them, and their beatings tend to recover to their original shorter IBIs. The results suggest that the connection of clusters has an ability to create slower synchronous beatings as an emergent behavior, which cannot be explained by the conventional models.

[1-14-1354](#) Can overdrive suppression explain the synchronized beating behavior of spontaneous beating cardiomyocyte clusters?

Kazufumi Sakamoto, Yoshitsune Hondo, Kenji Yasuda (*Dept. Pure & Appl. Phys., Grad. Sch. Adv. Sci. & Eng., Waseda Univ.*)

Faster firing regulation model is thought to be a dominant rule of cardiomyocyte synchronization. We investigated the dominant rule of synchronized cardiomyocyte clusters from the viewpoint of component single cells in the clusters. Cardiomyocyte clusters were formed and their beating intervals were compared with isolated single cells acquired from those clusters. Distribution analysis revealed that the clusters' synchronized interbeat intervals (IBIs) were longer than the majority of those of component single cells, which is against the conventional faster firing regulation model or overdrive suppression. The results suggest that emergent slower synchronous beating created in cardiomyocyte clusters as a community effect of spontaneously beating cells.

[1-14-1406](#) Stochastic modeling of the effect of vaccination strategies on the spread of a COVID-19-type virus

Yuki Matsuzawa¹, Shiho Ando¹, Mc Gahan Patricia¹, Hiromichi Tsurui², Hall Damien³, Yutaka Kuroda¹ (¹*Department of Biotechnology and Life Sciences, Tokyo University of Agriculture and Technology*, ²*Department of Immunological Diagnosis, Juntendo University School of Medicine*, ³*W.P.I. Nano Life Science Institute, Kanazawa University*)

Stochastic modeling of viral spread in light of eradication strategies can be advantageous as sophisticated scenarios are modeled without a need for complicated mathematical formulation. Here, we extend our previously reported stochastic model to examine the effect of vaccination strategies on the spread of a virus. Our model contains sets of adjustable parameters characterizing viral transmission, degree of personal mobility and describing the fraction of people being vaccinated, and the protection provided by the vaccine. We used our new model to ask questions: What fraction of the population needs to be immunized, how fast, and how to best couple mass-vaccination and mobility reduction to significantly reduce the total number of infections.

[1-14-1418](#) 曲率誘導タンパク質の反応拡散波による管状膜の変形
Deformation of tubular membranes with excitable reaction-diffusion waves of curvature-inducing proteins

Naoki Tamemoto, Hiroshi Noguchi (*ISSP, Univ. Tokyo*)

It is known that reaction-diffusion waves of proteins on cell membranes play important roles in living cells, such as cell migration and cell division. Curvature-inducing proteins are also involved in reaction-diffusion waves on membranes. Previously, we have shown that the dynamics of curvature-inducing proteins and vesicle shapes affect each other using modified Brusselator models. In this study, we investigate the effect of the mechanochemical feedback on the deformation of a tubular membrane with a traveling wave using the modified Fitz-Hugh Nagumo model.

[1-14-1430](#) 自己駆動粒子の確率的な走化性
Stochastic Chemotaxis Demonstrated by a Self-Propelled Particle

J. Nobuhiko Suematsu¹, Kota Ikeda¹, Kenta Odagiri² (¹*Grad. Sch. Adv. Math. Sci., Meiji Univ.*, ²*Dep. Net. and Info., Senshu Univ.*)

Non-living self-propelled particles have been actively developed and show variety of functionalities. In particular, taxis behavior is one of the important fundamental functions response to environmental gradients. Usually, taxis behavior is realized by sensing the gradient of environmental condition and controlling the direction of motion. On the other hand, bacteria succeeds to chemotaxis without direct sensing the chemical concentration gradient around them. The bacteria only tunes their running period depending on the concentration of attractants around them, as the results, they response to the gentle concentration gradient stochastically. In this study, such a stochastic response to concentration gradient was reproduced by non-living self-propelled object.

[1-14-1442](#) 繊維状粒子凝集の CA タイプ解析
CA-type formal analysis of fibrous assembly of particles

Takashi Konno (*Biomath., Med., Uni. Fukui*)

In the framework of 2D and 3D cellular automata (CA), transition rules leading to fibrously assembled "structures" were constructed and analyzed. The elements could represent proteins in an abstractive form. The analysis in high dimensional CA systems could naturally be unexhaustive, but careful choice of the CA transition rules gave valuable insights into the physical reality. The rules could also be translated into the "energy" term. "Fibrous" pattern of a state in the CA lattice could directly be regarded as "fibers", but more abstractive definitions of "structure" were also challenged. This study is an initial step towards elucidating hidden logics unconsciously employed for recognizing "structures" in daily and/or scientific life.

[1-14-1454](#) Establishment of quantitative mechanical measurements for intracellular structures

Ryota Ori, Hirokazu Tanimoto (*Grad. Sch. Nanobioscience., Univ. Yokohama City*)

Microtubules are very important structures for cellular functions involving cell shape determination, division, and intracellular transport, and it is essential to understand their mechanical properties. However, the mechanical properties of a single microtubule have not been clarified, because its methods have not been established. In this study, we establish an experimental system for mechanical measurements of single microtubule polymers and networks in cultured cells. We device magnetic tweezers that can apply a controlled force of 1-100 pN to probe particles which is introduced into the cell. Using these techniques, we have succeeded in directly deforming single microtubules inside the cell.

[1-14-1506](#) 力学刺激に応じた非石灰化・石灰化線維軟骨の分布を有する腱・靭帯附着部形成の数理モデリング
Mathematical modeling of enthesis formation with mechano-dependent distribution of uncalcified and calcified fibrocartilage

Akiko Fukuda¹, Yoshitaka Kameo^{1,2}, Taiji Adachi^{1,2} (¹*Grad. Sch. Biostudies, Kyoto Univ.*, ²*Inst. Front. Life Med. Sci., Kyoto Univ.*)

Fibrocartilaginous enthesis, connecting tendon/ligament to bone, is known to have characteristic distribution of uncalcified and calcified fibrocartilage (UFC/CFC) that depends on mechanical conditions. The purpose of this study is to understand the mechanism of enthesis formation with such mechano-dependent distribution. We modeled enthesis formation to elucidate the interaction between mechanical stimuli (MS) and biological factors. Using a simple two-dimensional tissue model, computer simulations showed that the mathematical model can express the UFC/CFC distribution in response to MS. Replicating the physiological distribution of UFC/CFC will contribute to clarify the effects of MS on the formation of functional enthesis that plays important roles in load-bearing.

[1-14-1518](#) クサカゲロウの翅の規範とした表面に微細構造を持つフィルムの電場計算
Electric field calculations of a film with surface fine structure inspired by a wing of green lacewing

Yuro Katsurashima¹, Leona Takahashi², Kazunari Yoshida¹ (¹*Grad.Sch.Sci.,Univ.Yamagata*, ²*Grad.Sch.Sci.,Yniv.Ymagata*)

Anti-reflection technology has been studied for a long time. Recently, anti-reflective moth-eye structure has been attracting attention. In this study, we focused on the green lacewing wings. The green lacewing wings have numerous nanometer-ordered protrusions consisting mainly of oil and fat. These nano-protrusions increase the light transmittance of the green lacewing wings. 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 light transmittance of the model with the protrusions was higher than that of the model without the protrusions.

[1-15-1330](#) (2S2-4) 細胞膜中の TRPV1・TRPV4 チャンネルの 1 分子動態の比較解析
(2S2-4) Comparative analysis of single-molecule dynamics of TRPV1 and TRPV4 channels in living cells

Masataka Yanagawa^{1,2}, Yutaro Kuwashima^{1,3}, Mitsuhiro Abe¹, Michio Hiroshima^{1,4}, Masahiro Ueda^{4,5}, Makoto Arita^{3,6,7}, Yasushi Sako¹ (¹*Riken CPR*, ²*JST, PRESTO*, ³*Faculty Pharm., Keio Univ.*, ⁴*Riken BDR*, ⁵*Grad. Sch. Front. Biosci., Osaka University*, ⁶*Riken IMS*, ⁷*Grad. Sch. Med. Life Sci., Yokohama City Univ.*)

TRPV channels are multimodal sensor of various stimuli, including temperature and chemicals. Here we undertook single-molecule time-lapse imaging of TRPV1 and TRPV4 in HEK293 cells. In the resting state, TRPV4 was more likely to form higher-order oligomers within immobile membrane domains than TRPV1. TRPV1 became immobile upon activation, followed by its gradual endocytosis. In contrast, TRPV4 was rapidly internalized after agonist stimulation. The selective loss of immobile higher-order oligomers from the cell surface through endocytosis increased the proportion of the fast-diffusing state for both subtypes. Our results provide a possible mechanism for the different rates of endocytosis of TRPV1 and TRPV4 based on the membrane domain localization.

[1-15-1342](#) Gタンパク質共役型受容体オリゴマーとGタンパク質の結合能に関する生細胞一分子解析
Live-cell single-molecule analysis on the binding affinity of G protein-coupled receptor
oligomers with G protein

Tomoki Nishiguchi¹, Hideaki Yoshimura², Rinshi S. Kasai³, Takahiro K. Fujiwara⁴, Takeaki Ozawa² (¹*Grad. Sch. Med. Dent. Sci., Niigata Univ.*, ²*Grad. Sch. Sci., Univ. Tokyo*, ³*iGCORE, Gifu Univ.*, ⁴*iCeMS, Kyoto Univ.*)

G protein-coupled receptors (GPCRs) transduce extracellular signals by activating cytosolic G-proteins. Although a dynamic equilibrium between monomers and dimers of GPCRs has been reported, the presence of larger oligomers and their functional roles are still unclear. Here, we distinguished small oligomers composed of four or fewer receptors from the other large oligomers using single-molecule live-cell imaging. Full agonist stimulation increased a fraction of the large oligomers within 10 s. G protein-interacting time of the large oligomers was increased from 49.4 ms to 67.2 ms, whereas that of the small oligomers was unchanged. These results suggest that the ligand-binding event and the large oligomer formation cooperatively regulate the signal transduction.

[1-15-1354](#) 0.1℃の温度上昇をオルガネラレベルで可視化する：蛍光タンパク質を用いた高感度温度プローブの開発
A highly sensitive thermosensor using fluorescent proteins to capture temperature change of 0.1℃ at the organelle level

Shun-ichi Fukushima, Takeharu Nagai (*SANKEN, Osaka Univ.*)

Intracellular temperature is an important factor affecting intracellular biochemical reactions. Even trivial temperature changes of as little as 1℃ can induce changes in metabolic responses and intracellular signaling. To understand the mechanisms of thermogenesis that cause changes in the thermal environment, and the associated changes in cellular functions, it is necessary to clearly capture when and where intracellular temperature changes at the subcellular level. Here, we developed a genetically-encoded fluorescent thermosensor that can sensitively detect temperature changes (maximum temperature sensitivity: $51 \pm 6.3\%/^{\circ}\text{C}$) and localize to specific organelles such as mitochondria. This sensor will allow us to proactively approach the unknown thermogenesis events.

[1-15-1406](#) 生体機能多重測定のための最短吸収・発光波長を持つ蛍光タンパク質の開発
Development of a violet fluorescent protein with the shortest absorption/emission wavelengths
for multiplex bioimaging

Kazunori Sugiura, Takeharu Nagai (*Osaka Univ., SANKEN*)

A variety of fluorescent proteins with different fluorescence wavelengths have been created so far by engineering of *Aequorea victoria* green fluorescent protein (avGFP). In this study, we attempted to develop a novel avGFP mutant with a fluorescence peak at 414 nm, which is the shortest wavelength among the existing avGFP-like fluorescent proteins. We named this fluorescent protein “Sumire” after the violet fluorescence color. Sumire can be utilized as a FRET donor in combination with a fluorescent protein with an absorption peak at around 400 nm (e. g. T-Sapphire), as a FRET acceptor. In this conference, we will introduce a successful application of this FRET pair with CFP-YFP pair for multiplex imaging of biological functions

[1-15-1418](#) High throughput genotype-phenotype linkage by Raman microscopy

Yuki Yoshida, Reiko Okura, Kenichiro F. Kamei, Yuichi Wakamoto (*Grad. Sch. Arts Sci., Univ. Tokyo*)

The establishment of comprehensive genetic resources, e.g., single gene knockout collection, has enabled comparative physiological and cell biological studies. Building on this foundation, we hypothesized that simultaneous profiling of such resources would provide further insights on genotype-phenotype linkage. We have previously observed that the Raman spectrum, a profile obtained by detecting cellular Raman scattering, reflects the cellular state in *E. coli*. Thus, we established a time-lapse Raman microscopy system using a quartz glass microfluidic mother machine device and profiled various Keio collection strains combined with FISH-based identification of each strain. In this presentation, we discuss our initial results obtained through this microscopic environment.

1-15-1430 カルマン smoother を用いたノイズに対して頑健な細胞牽引力測定
Kalman smoother traction force microscopy for robust force inference

Aozora Matsuda¹, Toshinori Namba², Shuji Ishihara² (¹Junior Division Science 1 of College of Art and Science, The University of Tokyo, ²Graduate school of Arts and Sciences, The University of Tokyo)

Mechanotransduction is becoming an important research subject in cell and developmental biology, for which traction force microscopy (TFM), methods for measuring traction force of cells, play a crucial role. However, the methods need to solve an ill-posed problem and existing approaches are often not robust to noise. We try to improve the robustness by applying Kalman smoother which exploits temporal continuity of physical quantities in time series data. This method is tested with artificially generated data under noise, and is also applied to experimental data.

1-15-1442 Development of iSCAT Microscopy and Improvement of the Images with Deep Learning

Satori Kowashi¹, Yasushi Okada^{1,2,3} (¹Univ. of Tokyo, Grad. Sch. of Sci., Dept. of Phys., ²RIKEN, BDR, Lab. for Cell Polarity Regulation, ³Univ. of Tokyo, Grad. Sch. of Med., Dept. of Med. Sci.)

Interferometric scattering microscopy (iSCAT), is recently proposed microscopy that can detect a single, unlabeled proteins by the interference of scattering light and reflected light. However, this interference signal is as small as 0.1% of the background reflected light. iSCAT signal is thus low-contrast and suffers from non-uniformity of the background. In this work, I overcame the problem by deep learning based methods. As a proof-of-concept, I used fluorescence microscopic images as the background-free training data. I reconstructed a microscope optics to obtain iSCAT and fluorescence images simultaneously. CARE2D (Content of Aware Image Restoration for 2D) was used for the image processing. More than half of the beads were successfully detected.

1-15-1454 熱揺らぎ一定モード原子間力顕微鏡の開発
Development of constant thermal fluctuation mode atomic force microscopy

Daisuke Yamamoto (*Fac. Sci., Fukuoka Univ.*)

Atomic force microscopy (AFM) enables to visualize the structures and dynamics of proteins in the physiological environments. AFM images are acquired by scanning the probe tip over the sample surface. To obtain reliable AFM images, it is required to minimize the tip-sample interaction force during scanning. Here, I have developed a novel scanning mode of AFM, termed constant thermal fluctuation mode AFM, in which the magnitude of the thermal fluctuation of the cantilever is measured to control the tip-sample distance. The loading force in this mode was significantly lower than in the conventional tapping mode. The operational principle of the constant thermal fluctuation mode AFM and its applications to imaging protein molecules will be presented.

1-15-1506 Development of Damage-free Imaging Cell Sorter Exploiting Alginate Capsules

Toshinosuke Akimoto, Kenji Yasuda (*Dept. Pure & Appl. Phys., Grad. Sch. Adv. Sci. & Eng., Waseda Univ.*)

A damage-free sorting procedure is essential for quality control of cell sorting technology. We developed an imaging cell sorter combining with encapsulation technology of cells into alginate gel beads. As the electrophoretic force of alginate gel beads is neutral to the external electric field, we added samples having surface charges into the alginate beads and confirmed the electrophoretic force reflected entirely to the contents in the alginate beads. When we added the polystyrene nanoparticles into the cell-encapsulated alginate beads as additives, the electrophoretic force was enhanced successfully without any damage on cells in the capsules even though the electric field was applied. The results suggest the potential of alginate capsules for imaging cell sorters.

[1-15-1518](#) A programmable DNA origami nanospring that reports dynamics of single integrin traction forces in living cells

Hitomi Matsubara^{1,2}, Hiroki Fukunaga^{1,2}, Takahiro Saitoh¹, Keigo Ikezaki³, Mitsuhiro Iwaki^{2,4} (¹*Grad. FBS., Univ. Osaka*, ²*BDR., RIKEN*, ³*Grad. Pys. Sci., Univ. Tokyo*, ⁴*IFReC., Univ. Osaka*)

A variety of force sensors have been developed to measure cellular mechanical forces that regulate many biological processes; however, dynamics of forces was elusive. In this study, we developed a DNA-based molecular tension sensor (nanospring) which is a programmable nanostructure with a coil shape and evaluated the force-extension curve using acoustic force spectroscopy. We attached one end of the nanospring to single integrin receptors of human fibroblast through the ligand (RGD peptide) and the other end was attached to bottom of the dish. We successfully observed the dynamics of single integrin traction force and we will discuss the result in this meeting.

[1-16-1330*](#) Analyzing a printable actuator composed of an engineered kinesins by a computer simulation

Yurino Aoyama¹, Yuichi Hiratsuka², Takahiro Nitta³ (¹*Grad. Appl. Math. Phys. Div., Gifu University*, ²*Sch. Materials Sci., JAIST*, ³*Appl. Phys. Course, Faculty of Eng., Gifu University*)

Muscle tissues can be regarded as scalable and highly efficient actuators. Incorporating muscle tissues into engineered systems at will may enable autonomous soft robots without external equipment, and biological computations. In this study, we developed a computer simulation of a printable actuator composed of an engineered biomolecular motor. From this simulation, we investigated contraction forces of the actuators fixed at both ends and with various shapes. From our analysis we found that there was a direct relationship between the maximum tension and breaking time. In addition, the actuator was found to select shorter paths between anchors. These findings may be useful for driving soft robots and performing biological computations using the actuator.

[1-16-1342*](#) 自動振動を利用した羽ばたきロボットの開発
The development of insect-like flapping robot using self-excited vibration

Takahito Fujimori¹, Ryo Wakamoto², Youichi Masuda² (¹*Undergraduate of School of Science of Biology, Osaka university*, ²*Department of Mechanical Engineering, Osaka University*)

Particular types of insects flap their wings at high frequencies, more than 100times per second. This is because they move their muscle, called "indirect muscle", that attaches not to their wings themselves but to their elastic exoskeleton, which acts like a spring, resulting in interaction between the wings and the exoskeleton and making it possible to flap at high frequencies beyond nerve pulses. The objective of this paper is to develop an actuator that can generate such movement by study of insect flight muscle and write down their properties into mathematical model.

[1-16-1354*](#) DNA コンピューティングを用いた分子ロボットの自動制御
Automated control of molecular robots using DNA computing

Kohei Nishiyama¹, Daiki Matsumoto², Jakia Jannat Keya³, Ibuki Kawamata², Shin-ichiro M. Nomura², Akira Kakugo^{1,3} (¹*Grad. Sch. of Chem. Sci. and Eng., Hokkaido Univ.*, ²*Grad. Sch. of Eng., Tohoku Univ.*, ³*Grad. Sch. of Sci., Hokkaido Univ.*)

Social animals are known to form swarms to accomplish complex tasks that cannot be performed by single entities. Recently, great deal of effort has been devoted to developing molecular-sized robots which adopt this strategy. However, the operation of such molecular swarm robots requires external signaling, which relies on human operation hence not a completely automated system. Here, we aim at developing the molecular swarm robots using kinesin/microtubule whose collective motion can be automatically controlled by a DNA-based cascade reaction system. Our preliminary results confirmed that the formation of the swarms of the MTs and dissociation into the discrete MTs can be controlled using the automated outputs of DNA signals by the installed cascade reaction system.

[1-16-1406*](#) 蛍光増大能を指標とした新規蛍光 RNA アプタマー創出法の開発
An efficient method to obtain fluorogenic RNA aptamers based on ability to activate fluorescence

Keisuke Ito, Ryo Iizuka, Sotaro Uemura (*Dept. Biol. Sci., Grad. Sch. Sci., The Univ. Tokyo*)

Fluorogenic RNA aptamers, which specifically bind nonfluorescent dyes and drastically enhance the fluorescence, are useful for imaging RNA in live cells. However, the existing RNA aptamers exhibit weak fluorescence, and then it has been difficult to visualize RNAs with low expression levels. Most of the aptamers were engineered through repeated rounds of *in vitro* selection based on the binding to the target dyes; the selected RNAs do not always display strong fluorescence enhancement upon the binding to the dyes. Here, we have developed an efficient method to obtain fluorogenic RNA aptamers based on ability to activate fluorescence by *in vitro* selection with *in vitro* compartmentalization. In the meeting, details of the method will be discussed.

[1-16-1418*](#) On-chip 無細胞クローニングに向けた 1 分子環状 DNA からの増幅
Amplification from single molecular circular DNA for on-chip cell-free cloning

Kohei Higashi¹, Yoshihiro Minagawa¹, Masayuki Suetsugu², Hiroyuki Noji¹ (¹*Dept. Appl. Chem., Grad. Sch. Eng., Univ. Tokyo*, ²*Dept. Life Sci., Coll. Sci., Rikkyo Univ.*)

Molecular cloning method, although well-established, has several fundamental limitations such as low throughput, low compatibility with automation systems, and difficulties to handle toxic genes or highly repeated sequences. To address these challenges, we aim to develop on-chip cell-free cloning technology, by implementing cell-free biosystems in a femtoliter reactor array device (FRAD). We developed on-chip cell-free system for DNA isolation and amplification by integrating reconstituted replication cycle reaction system on FRAD. In comparison with conventional molecular cloning methods that typically takes one day including cultivation, this method requires only 60 min, that is extremely fast and is expected to improve throughput.

[1-16-1430*](#) 水性二相系液滴を利用した DNA マイクロカプセルの設計
Design of DNA microcapsules using aqueous two-phase system droplets

Mayumi Chano, Marcos Masukawa, Masahiro Takinoue (*Department of Computer Science, School of Computing, Tokyo Institute of Technology*)

Functional microcapsules have attracted much attention for their potential to construct artificial cells and molecular robots. The use of DNA as a functional material has advantages in programmability and designability. In a previous study, functional microcapsules were developed by accumulating DNA origami nanoplates at the interface of water-in-oil droplets. However, for *in vivo* use, the oil needs to be removed and an oil-free method is required. Therefore, we designed the DNA nanoplates to adhere to each other when the linker DNA is added. We proposed a new DNA microcapsule by accumulating the DNA nanoplates at the dextran droplet interface created by the aqueous two-phase system of PEG and dextran. This oil-free method has the advantage of easy *in vivo* application.

[1-16-1442](#) 負のポアソン比をもつ 3 次元 DNA ナノ構造体の設計
Design of 3D DNA nanostructures with negative Poisson's ratio

Nagi Yamashita¹, Masahiro Takinoue² (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.*)

DNA microstructures such as DNA gel which imitate chromatin has been studied to reveal the relationship between dynamic structures of chromatin and transcriptional activity. However, DNA gel composed of unit cells called motifs has not been able to control transcriptional activity yet. This is because the conventional motifs do not shrink the gel enough to turn off transcriptional activity. Therefore, the objective is to design new DNA motifs with negative Poisson's ratio and development DNA gel with it as a component. Our study focused on structures with negative Poisson's ratio which are characterized by superior expansion and shrinkage to cause more dramatic deformation of DNA gel. 3D DNA nanostructures were designed as DNA motifs from polygone data using vHelix.

[1-16-1454](#) 低温条件下で DNA 状態機械が効率的に動作するための状態配列長の短縮
Reduction of the length of state sequences for efficient operation of a DNA state machine under low temperature conditions

Ken Komiya (*JAMSTEC*)

Whiplash PCR (WPCR) is a synthetic biochemical reaction, which implements successive state transitions according to a program encoded by each DNA molecule. WPCR uniquely allows the program-parallel computation, and is capable of various information processing including solution to a graph problem. However, WPCR requires extremely high temperature reaction conditions to overcome its inherent efficiency problem caused by competitive hairpin structure formation. In this work, we investigated the effect of reducing the length of state sequences for increasing the efficiency of the target hairpin structure formation. The thermophilic property of the DNA state machine was evaluated in the statistical thermodynamic model simulation and the biochemical experiment.

[1-16-1506](#) フェリチン 1 分子中の H, L サブユニットの割合制御と鉄ナノ粒子の結晶性の比較
Regulation of H/L subunit content in apoferritin and crystallinity of the iron core

Tomoko Kanamaru¹, Shuji Kanamaru², **Hideyuki Yoshimura**¹ (¹*Meiji Univ.*, ²*Tokyo Inst. Tech.*)

Apoferritin is an iron storage protein, composed of 24 subunits to give a hollow shell with an 8 nm diameter cavity. Two types of subunits, H and L subunits, are known. H-subunit has Fe(II) oxidation site and L-subunit has no oxidation site. We have reported synthesis of single crystal of magnetite (Fe₃O₄) nanoparticle using homo L-subunit apoferritin in slow oxidation process. However, its efficiency was very poor. To improve efficiency and keeping crystallinity, we plan to introduce small number of H-subunit in an apoferritin molecule. To control number of H-subunit in a molecule, we use plasmids with different copy numbers. Relation with number of H-subunit in a molecule and crystallinity of nanoparticle will be reported.

[1-16-1518](#) Screening of agarolytic microbial cells with a deformability-based microfluidic microdroplet sorting device

Mikihisa Muta¹, Kai Saito¹, Ryo Iizuka¹, Wataru Kawakubo², Dong Hyun Yoon³, Tetsushi Sekiguchi³, Shuichi Shoji², Mei Ito⁴, Yuji Hatada⁴, Takashi Funatsu¹ (¹*Grad. Sch. of Pharm. Sci., The Univ. of Tokyo*, ²*Dept. of Nanosci. and Nanoeng., Waseda Univ.*, ³*Res. Org. for Nano & Life Innov., Waseda Univ.*, ⁴*Dept. of Life Sci. and Green Chem., Saitama Inst. of Technol.*)

We have developed a culture-independent method for screening hydrogel-degrading microbial cells using deformability-based microfluidic microdroplet sorting. In this method, microbial cells are encapsulated at the single-cell level in hydrogel-containing water-in-oil (W/O) microdroplets. The W/O microdroplets, where the hydrogel is degraded into smaller molecules, increase the deformability. The screening is achieved by using a microfluidic device that enables the sorting depending on the deformability of W/O microdroplets. Using this method, we successfully isolated single agarose-degrading bacterial cells from seawater.

[2-01-1315*](#) The potential of artificially designed α -helical peptide nanofibers

Minami Kurokawa¹, Mika Hirose², Akihiro Kawamoto², Atsuo Tamura¹ (¹*Grad. Sch. Sci., Univ. Kobe.*, ²*IPR, Osaka Univ.*)

Many synthetic peptides based on α -helix and β -sheet sequence motifs have been reported so far. The potential of designed helical peptides for the construction of well-defined protein fibrils remains largely untapped, despite the fact that prototypes for fibrils derived from α -helical coiled coil motifs occurs widely in native biological systems such as cytoskeleton and extracellular matrix. In this study, we artificially designed α -helical peptide nanofibers, which are consisted of 21 amino acid residues. Then we investigated thermodynamic properties of them and found that they show high cooperativity in response to heat. This may lead to the development of an environmentally friendly liquid-crystal nano-device that can be controlled by external temperature.

2-01-1327* SARS-CoV-2 スパイクタンパク質の受容体結合ドメインに対する中和抗体の合理的設計
Rational design of neutralizing antibodies against the receptor-binding domain of SARS-CoV-2 Spike protein

Sairi Matsumoto¹, Yuuki Hayashi¹, Munechito Arai^{1,2} (¹*Dept. Life Sci., Univ. Tokyo*, ²*Dept. Phys., Univ. Tokyo*)

SARS-CoV-2 is an emerging virus that causes the COVID-19 pandemic. Thus, there is an urgent need to develop therapeutics to inhibit the infection of SARS-CoV-2. Since the infection occurs when the receptor-binding domain (RBD) of the Spike protein binds to human ACE2, here we rationally designed neutralizing antibodies that bind the SARS-CoV-2 RBD using a single-chain variable fragment (scFv) of the antibody against SARS-CoV RBD as a template. We constructed a model of the complex between the scFv and SARS-CoV-2 RBD and performed theoretical saturation mutagenesis for the scFv using Rosetta. Then, RBD and scFv proteins were expressed in *E. coli* and purified. The binding affinity between RBD and the designed scFv proteins will be presented at the meeting.

2-01-1339* 転写活性化に関与する相互作用を標的としたペプチド阻害剤の合理的設計
Rational design of the peptide inhibitor targeting the interactions involved in transcriptional activation

Nao Sato¹, Shunji Suetaka¹, Yuuki Hayashi¹, Munechito Arai^{1,2} (¹*Dept. Life Sci., Univ. Tokyo*, ²*Dept. Phys., Univ. Tokyo*)

Protein-protein interactions (PPI) have attracted much attention in drug discovery. Interactions of the KIX domain of a transcriptional coactivator CBP with various transcriptional activators are involved in leukemia and other diseases. Here, we computationally designed KIX inhibitors using the peptide fragment corresponding to the transactivation domain of a transcriptional activator MLL. Using Rosetta software, we theoretically searched for the mutants of the MLL fragment that may bind KIX tightly. We successfully obtained the mutant that binds KIX two-fold more tightly than the wild type. Experiment to verify that the designed peptide competes out the wild-type MLL in KIX binding is under way. Our strategy may be useful for designing PPI inhibitors.

2-01-1351* α ヘリックスを介したタンパク質間相互作用の阻害に向けた合理的医薬品設計
Rational drug design to inhibit α -helix-mediated protein-protein interactions

Shunji Suetaka¹, Nao Sato¹, Eiji Honda², Hajime Takashima², Yoshiki Oka¹, Tomoko Kunihara¹, Dai Takehara², Atsushi Yoshimori³, Yuuki Hayashi¹, Munechito Arai^{1,4} (¹*Dept. Life Sci., Univ. Tokyo*, ²*PRISM BioLab Co., Ltd.*, ³*Inst. Theor. Med., Inc.*, ⁴*Dept. Phys., Univ. Tokyo*)

Inhibiting protein-protein interactions associated with serious diseases is promising in drug discovery. The KIX domain of CBP interacts with many α -helical transcriptional activators, including c-Myb and MLL, and are involved in leukemia. Here, we rationally designed inhibitors of the KIX-mediated interactions in two ways. First, using a helical fragment of c-Myb, we successfully designed a peptide that binds KIX with nanomolar affinity and inhibits the c-Myb-KIX interaction. Second, from the library of α -helix mimetics, we selected small compounds that mimicked one-turn helix in c-Myb or MLL and obtained four hit compounds that bind KIX with sub-micromolar affinity. These strategies will be useful for designing inhibitors of helix-mediated interactions.

2-01-1403* Magnet のタンパク質間相互作用を強化する変異体の合理的設計
Improving dimer affinity of Magnets photodimerizers by computational design

Masataka Yoshimura¹, Yuki Aono¹, Yuuki Hayashi¹, Moritoshi Sato^{1,2}, Munechito Arai^{1,3} (¹*Dept. Life Sci., Univ. Tokyo*, ²*CREST, JST*, ³*Dept. Phys., Univ. Tokyo*)

Magnets are optogenetic tools for manipulating protein-protein interactions and have been widely used in cell biology. The Magnets consist of pMag and nMag that heterodimerize when exposed to blue light, thereby inducing interactions between proteins fused with them. However, since the binding affinity between pMag and nMag is weak, tandem repeat of pMag is required to enhance the affinity. To overcome this issue, here we computationally designed the pMag/nMag mutants with higher mutual affinity than the original ones by theoretical saturation mutagenesis. Complementation experiments using split-firefly luciferase fused with pMag/nMag mutants demonstrated the improvement of the dimer affinity. These variants may expand the usefulness of the Magnets system.

[2-01-1415*](#) PD-1 受容体を標的とする免疫チェックポイント阻害タンパク質の合理的設計
Rational design of immune checkpoint inhibitory proteins targeting the PD-1 receptor

Hirotao Shimamura¹, Yuuki Hayashi², Munechito Arai^{1,2} (¹Dept. Phys., Univ. Tokyo, ²Dept. Life Sci., Univ. Tokyo)

The PD-1/PD-L1 immune checkpoint is an important target in cancer treatment. PD-1 is a receptor of T cells that evades autoimmunity by binding to PD-L1, which is normally expressed on antigen-presenting cells. PD-L1 is also expressed on cancer cells, thereby suppressing T cell activation against cancer. Thus, inhibitors of the PD-1/PD-L1 interaction, such as antibodies targeting PD-1, have been successfully used in cancer treatment. Here, we rationally design small-protein inhibitors that bind PD-1 more tightly than antibody medicines. We theoretically introduce mutations into the PD-L1 fragment using Rosetta to search for tight binders to PD-1. We will experimentally verify whether the designed small proteins can inhibit the PD-1/PD-L1 interaction.

[2-01-1427*](#) アレルギー性喘息を抑制する interleukin-33/ST2 阻害剤の合理的な設計
Rational design of an interleukin-33/ST2 inhibitor for suppressing allergic asthma

Mizuki Teranishi¹, Mio Sano¹, Yuuki Hayashi¹, Munechito Arai^{1,2} (¹Dept. Life Sci., Univ. Tokyo, ²Dept. Phys., Univ. Tokyo)

Inhibitors of protein-protein interactions (PPIs) have been a major target in drug discovery. The PPI involved in allergic asthma is the interaction between interleukin-33 (IL-33) and its receptor ST2. Here, to develop an inhibitor of its interaction, we used IL-33 as a template for theoretical design of the mutants that has higher affinity to ST2 than the wild type, while avoiding subsequent interaction with an IL-1 receptor accessory protein. We calculated binding energies of various IL-33 mutants to ST2 using the protein design software Rosetta and obtained several mutants that are predicted to enhance ST2 binding. Then, we measured the ST2-binding affinity of the mutants by fluorescence anisotropy. The detailed results will be presented at the meeting.

[2-01-1439*](#) バンドル様相互作用面を用いない多様な回転対称複合体の設計
Toward design of diverse symmetric protein homo-oligomers using non-bundle-like interface

Shingo Kaida¹, Naoya Kobayashi², Takahiro Kosugi^{3,4,5,6}, Nobuyasu Koga^{3,4,5} (¹Dept. Structural Molecular Sci., SOKENDAI, ²Div. Mat. Sci., Grad. Sch. Sci. Tech., NAIST, ³ExCELLS, NINS, ⁴CIMoS, IMS, ⁵SOKENDAI, ⁶JST, PRESTO)

Design of cyclic protein oligomers using α -helical repeat proteins as subunit was reported. However, it is difficult to create oligomers with diverse shapes because of restriction on shape of interfaces. In this study, we focused on design cyclic homo-oligomers with diverse shapes. To this end, we used de novo designed all- α protein with uneven surface which can provide multiple candidates for interface all over the surface. Using computers, input monomeric proteins were rotated randomly, placed in C6 symmetry, then introduced mutations on surface residues to create interfaces contributing to form hexamer. After expression and purification for each designed proteins, **experimental characterizations suggested one designed protein form hexamer** in high concentration.

[2-01-1451*](#) (1S6-6) アデノシン A_{2A} 受容体の不活性型構造を安定化するための all- α 融合パートナータンパク質のゼロからの合理デザイン
(1S6-6) De novo design of an alpha-helical fusion partner protein to stabilize adenosine A_{2A} receptor in the inactive state

Masaya Mitsumoto^{1,2}, Kanna Sugaya³, Kazuki Kazama³, Ryosuke Nakano³, Takahiro Kosugi^{1,2,4}, Takeshi Murata³, Nobuyasu Koga^{1,2,4} (¹SOKENDAI, ²IMS, NINS, ³Grad. Sch. of Sci. and Eng., Chiba Univ., ⁴ExCELLS, NINS)

GPCRs are known for low stability and large conformational changes upon transitions between multiple states. Here, we aim to rationally stabilize one of the class A GPCRs, adenosine A_{2A} receptor (A_{2A}R), in a targeted state. For class A GPCRs, the transmembrane helices 5 and 6 (TM5 and TM6) connected by the intracellular loop 3 (ICL3) exhibit large conformational changes. Therefore, we computationally de novo designed an all- α fusion partner protein FiX1, designed to be fused to the TM5 and TM6 of the inactive-state A_{2A}R without kinks or intervening loops. Experimentally, FiX1 was found to be folded into unique shape and form helical structures even around 100°C, and the fusion of A_{2A}R with FiX1 was found to be stabilized in the inactive state as designed.

[2-01-1503](#) 脂肪酸結合タンパク質 FABP3 と FABP7 におけるリガンド結合特性の比較

A comparative study of ligand-binding properties between fatty acid-binding proteins FABP3 and FABP7

Hazuki Namiki¹, Shun Tokudome¹, Mai Nomura¹, Fumio Hayashi², Yusuke Inoue^{1,3}, Shigeru Sugiyama⁴, Shigeru Matsuoka⁵, Michio Murata⁶, Masashi Sonoyama^{1,3,7} (¹*Grad. Sch. Sci. Tech., Gunma Univ.*, ²*Ctr. Inst. Anal., Gunma Univ.*, ³*GUCFW, Gunma Univ.*, ⁴*Sch. Sci. Tech., Kochi Univ.*, ⁵*Grad. Sch. Med., Oita Univ.*, ⁶*Grad. Sch. Sci., Osaka Univ.*, ⁷*GIAR, Gunma Univ.*)

Ten subtypes of fatty acid-binding protein (FABP) were identified in human. Among them, although FABP3 and FABP7 are highly similar subtypes present in the brain, differences in fatty acid (FA)-binding properties between them are still unknown. In this study, we conducted extensive binding analyses for various saturated and unsaturated FAs to know FA-binding properties in a comprehensive manner. For both FABPs, the binding affinity of short-chain saturated FAs (C7-C12) was highly dependent on the hydrophobicity of FAs, while that of long-chain saturated FAs was not correlated with their hydrophobicity. Experimental results on unsaturated FAs, which are dependent on the degree of unsaturation of FAs, will also be discussed.

[2-01-1515](#) ヒト PTH1 受容体における内因性リガンド認識メカニズムとそのダイナミクス Endogenous ligand recognition and structural transition of a human PTH receptor

Kazuhiro Kobayashi¹, Kouki Kawakami², Tsukasa Kusakizako¹, Hirotake Gono¹, Atsushi Tomita¹, Wataru Shihoya¹, Kan Kobayashi¹, Keitaro Yamashita³, Tomohiro Nishizawa⁴, Hideaki Kato^{1,5}, Asuka Inoue², Osamu Nureki¹ (¹*Department of Biological Sciences Graduate School of Science The University of Tokyo*, ²*Graduate School of Pharmaceutical Sciences, Tohoku University*, ³*MRC Laboratory of Molecular Biology*, ⁴*Graduate School of Medical Life Science, Yokohaya City University*, ⁵*Komaba Institute for Science, The University of Tokyo*)

Parathyroid hormone receptor 1 (PTH1R) is a class B G-protein-coupled receptor (GPCR) that controls calcium homeostasis and bone-turn over. The receptor is activated by two endogenous pleiotropic peptide hormones called PTH and PTHrP. These hormones share similar sequences and activate the stimulatory G-protein (Gs) signaling pathway but show different physiological functions. The difference of the molecular action is presumed to be caused by the differences in the ligand dissociation kinetics, but the structural basis for the ligand recognition and the dynamics of the receptor remains elusive. We report cryo-EM structures of the two endogenous ligand bound PTH1R-Gs, which explains the distinct duration of G_s signaling between the two endogenous ligands.

[2-01-1600](#) Role of the domain 3 of the hemolytic lectin CEL-III in hemolytic activity and oligomerization

Suichiro Goda^{1,2}, Keisuke Fukumoto¹, Yuta Yamawaki¹, Hideaki Unno¹, Tomomitsu Hatakeyama¹ (¹*Grad. Sch. Of Eng., Nagasaki Univ.*, ²*GaLSIC, Soka Univ.*)

Seven monomers of hemolytic lectin CEL-III form heptameric pore in the cell membrane of red blood cell to disrupt it. CEL-III consists of two carbohydrate binding domains (domain 1,2) and pore forming domain (domain 3). In domain 3, α -helix structure in monomer changes to β -strand in β -barrel pore structure, stem region. To elucidate the oligomerization promoting factor, deletion mutants were made. Lack of stem region mutant of CEL-III forms heptamer. Whereas, lack of domain 3 mutant of CEL-III exists as monomer. These results indicate that the domain 3 plays an important role in oligomerization and except stem region also important. These suggest that the monomer of CEL-III associates to heptamer then makes transmembrane pore.

[2-01-1612](#) Mechanistic insights into Bedaquiline inhibition of the mycobacterial ATP synthase

Alexander Krah¹, Peter J. Bond^{1,2} (¹*Bioinformatics Institute (BII), Agency for Science, Technology and Research (A*STAR)*, ²*Department of Biological Sciences, National University of Singapore*)

Mycobacterium tuberculosis causes tuberculosis, a major health problem. The disease is responsible for more than a million deaths per year. Recently, multi-drug resistant strains have been identified. Thus, new targets need to be identified and drugs for these targets need to be developed and the mechanism of drug action is required to be clarified. The mycobacterial ATP synthase has been shown to be targeted by Bedaquiline. We use molecular dynamics simulations to study how Bedaquiline inhibits the mycobacterial ATP synthase.

[2-01-1624](#) タンパク質の熱伝導度
Thermal conductivity of proteins

Takahisa Yamato (*Nagoya Univ.*)

Under physiological conditions in the cell, protein molecules are thermally fluctuating, and tightly packed atoms and amino acid residues are strongly interacting to each other. Such interactions are characterized in terms of heat/energy flow at the atomic level. We have been studying the energy transport network in proteins using our computer program called CURP (CURrent calculations for Proteins). Recently, we extended this program so that it calculates the thermal conductivities of proteins based on linear response theory. As an example, we applied this method to a small globular protein, villin headpiece, and the value of its thermal conductivity was 0.3 ± 0.01 [W/m*K], in good agreement with experimental/computational studies on the other proteins in the literatures.

[2-01-1636](#) フィンブリンのアクチンフィラメントに対する一方方向性の協同的相互作用はフィラメントの短縮を引き起こす
Unidirectional cooperative interaction of fimbrin to actin filaments evokes the filament shortening

Ryosuke Tsunabuchi¹, Naoki Hosokawa¹, Masahiro Kuragano¹, Atsuki Yoshino¹, Keitaro Shibata², Taro Q.P. Uyeda³, Kiyotaka Tokuraku¹ (¹*Muroran Institute of Technology*, ²*Graduate School of Medical Science, Tokushima University*, ³*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 remained unknown. In this study, we focused on the cooperative interaction of fimbrin, one of ABPs, to reveal the formation mechanism of well-ordered parallel FA bundles in filopodia. Real-time imaging of interaction between actin-binding domain 2 of fimbrin and FAs revealed that fimbrin formed low-density clusters, which grew unidirectionally along FAs. Interestingly, the binding of fimbrin shortened the length of FAs. These results suggested that fimbrin-FAs interaction accompanied by unidirectional long-range allostery helps the formation of parallel FAs bundles. Our findings will help understand the mechanism of filopodia formation.

[2-01-1648](#) マグネトソーム鎖の細胞内配置の制御に関わる MamY タンパク質の機能解析
Functional analyses of MamY protein involving in subcellular positioning of magnetosomes chain

Rino Shimoshige¹, Yousuke Kikuchi², Azuma Taoka^{2,3} (¹*Grad. Sch. Nat. Sci. Tech. Kanazawa Univ.*, ²*Inst. Sci. Eng. Kanazawa Univ.*, ³*NanoLSI, Kanazawa Univ.*)

Magnetotactic bacteria produce a membranous organelle called magnetosome. MamY thought to be involved in magnetosome positioning along positive curvature in a spiral shaped cell. Here, we characterized MamY protein using HS-AFM. MamY was expressed in *Escherichia coli*. We purified MamY from solubilized membrane fraction. Then, we observed the purified MamY protein using HS-AFM on bare mica substrates. MamY proteins were observed as globular particles with diameter of 5.3 ± 1.7 nm ($n=516$). We reconstituted purified MamY in liposomes using polar lipids extracted from *E. coli*. At present, we are trying to observe MamY dynamic behavior on positive curvature membrane using HS-AFM.

[2-01-1700](#) バッファー成分が抗体製剤の不溶性異物形成に与える影響について
Impact of Buffer Component on the Formation of Visible Particles in Antibody Preparations

Chihiro Wayu, Hiroyuki Suetomo, Maki Mitani, Toshihito Hosokawa (*Bio Process Research and Development Laboratories, Kyowa Kirin Co., Ltd.*)

Due to the nature of proteins, biopharmaceuticals have a risk of particulate formation under a variety of stresses. Accelerated and stressed stability studies are conducted to minimize quality risk, but it is generally difficult to accurately predict the particle formation that occurs during long-term storage. In this study, several colloidal stability parameters prior to storage and particulate formation after long-term storage were measured in the monoclonal antibody solutions prepared with various additives. It was revealed that the colloidal stability parameters on the non-stress antibody drugs had a slight correlation to particulate formation. The results are expected to be an alternative evaluation method for long-term stability studies of the particulate formation.

[2-01-1712](#) (2S6-1) Extensive Sampling of Spike protein down, one-up, one-open, and two-up-like Conformations and Transitions in SARS-Cov-2

Hisham Dokainish¹, Suyong Re⁴, Chigusa Kobayashi², Takaharu Mori¹, Jaewoon Jung^{1,2}, Yuji Sugita^{1,2,3} (¹*Theoretical Molecular Science Laboratory, Riken*, ²*Computational Biophysics Research Team, RIKEN*, ³*Laboratory for Biomolecular Function Simulation, RIKEN*, ⁴*Center for Drug Design Research, National Institutes of Biomedical Innovation*)

Spike (S) protein is the primary antigenic target for SARS-Cov-2 vaccine development and neutralization. Its receptor binding domain undergoes (RBD) large conformational change from inactive Down to active Up, allowing for ACE2 binding. Despite the abundance of Down, 1Up, 2Up and 3Up Cryo-EM structures, little is known about Spike transitions. Here, we employed our recently proposed enhanced sampling method (gREST_SSCR) to widely sample Spike conformational space, including the transition from Down to 1Up and 1Up to 2Up conformations. Glycans and salt bridges were found to mediate / register the transitions. Unprecedented cryptic pockets were identified at the RBDs' interface that might be targeted to shift S-protein conformational equilibrium hindering cell entry.

[2-01-1724](#) 織毛虫テトラヒメナにおける内腕ダイニン発現系の開発および単頭分子種の運動特性
Development of an expression system in *Tetrahymena* inner arm dynein and motile properties of the single-headed subspecies

Masaki Edamatsu (*Dept. Life Sci., Grad. Sch. Arts Sci., Univ. Tokyo*)

Diverse inner arm dyneins cooperate with outer arm dyneins to produce ciliary beating. This study demonstrates an expression system for inner arm dyneins in *Tetrahymena*. The motor domain of inner arm dynein (Dyh8p or Dyh12p) was fused with the tail of outer arm dynein (Dyh3p) and expressed in viable DYH3-knockout (vKO-DYH3) cells. The chimeric dyneins were observed in the oral apparatus and cilia on the cell bodies, and the motor domains of Dyh8p and Dyh12p moved toward the minus ends of microtubules at 0.8 and 0.3 $\mu\text{m/s}$, respectively. The gliding velocities of Dyh8p and Dyh12p were decreased in 5 mM ATP but not increased in 0.1 or 0.5 mM ADP. This expression system will be useful for molecular studies on diverse inner arm dyneins.

[2-01-1736](#) 発色団および非発色団解離基間の相互作用は、蛍光タンパク質の光学的性質において重要な役割を担う
Interplay of protonations at chromophore and non-chromophore sites plays a key role in the photo-properties of fluorescent proteins

Tetsuichi Wazawa, Ryohei Noma, Kazunori Sugiura, Takeharu Nagai (*SANKEN, Osaka Univ.*)

Photoswitchable fluorescent proteins reversibly switch between the fluorescently-bright and dark states with the photo-induced isomerization of the chromophore. Previously we developed a photoswitchable fluorescent protein Kohinoor 2.0 that is more useful for highly-biocompatible super-resolution imaging than its forerunner, Kohinoor [Wazawa et al (2021) *Microscopy*, **70**, in press]. Here we reveal that Kohinoor 2.0 and Kohinoor are in pH-dependent multiple equilibria, and the anionic phenolate state of chromophore in Kohinoor 2.0 is more stabilized by 1.9-fold at neutral pH than in Kohinoor, leading to higher fluorescence intensity. Thus, the detailed analysis of pH-dependent behavior is likely to be useful for the development of novel fluorescent proteins.

[2-01-1748](#) Measurement on integrated forces of multiple kinesin motors through cross-linked microtubules with a glass microneedle

Naruaki Tsuji¹, Naritaka Kobayashi¹, Seichiro Nakabayashi¹, Hiroshi Yoshikawa², Ryuzo Kawamura¹ (¹*Grad. Sch. Sci. Eng., Saitama Univ.*, ²*Grad. Sch. Eng., Osaka Univ.*)

Nanomeric deformations of motor proteins can be potentially integrated for generation of large forces, as seen in natural cell system. Here, we tried to measure an integrated output force in an artificial system, constructing a multimolecular setup with purified conventional kinesin and microtubules. We simply designed the setup in which microtubules were networked by chemical cross-link and driven by kinesins on a glass substrate accompanied with hydrolysis of adenosine-triphosphate. While the network sways with amplitudes up to several tens of micrometers, output force was measured from bending of a glass microneedle placed on it. It marked a maximum output of 1.0 nN, implying the integration of the kinesin driving forces which are on the order of piconewtons.

2-01-1800 **グルタミン酸脱水素酵素活性クレフト周辺での補酵素結合経路探索**
Search for binding pathway of co-enzyme around the active-site cleft of glutamate dehydrogenase

Taiki Wakabayashi^{1,2}, Mao Oide^{1,2}, Takayuki Kato³, Masayoshi Nakasako^{1,2} (¹*Dept. Phys., Keio Univ.*, ²*RSC, RIKEN, Protein Inst., Osaka Univ.*)

We have two questions on the formation of enzyme-substrate/cofactor complex: (1) Are there indirect pathways to bind their substrate/cofactor molecules? (2) whether does the binding process correlate with the dynamical motions of enzymes? To clarify these questions, we studied the binding modes of NADP to the NAD-binding domains of hexameric glutamate dehydrogenase (GDH) by cryogenic transmission electron microscopy (TEM). By classifying a number of TEM images of GDH, we found that NADP molecules differently bound to the NAD-binding domain, depending on the motion of the NAD-binding domain to open/close the active-site cleft. In the presentation, we will show the details of the structure analysis and discuss the pathway of NADP to complete binding state.

2-01-1812 **Free energy landscape analysis of conformational transition of NtrC by chameleon model**

Taisei Nagata, Masaki Sasai, Tomoki P. Terada (*Dept. Appl. Phys., Grad. Sch. Eng., Nagoya Univ.*)

We study the conformational transition by coarse-grained molecular dynamics simulation. We use chameleon model, an extended model of Go-like model with which we can calculate the free energy landscape of conformational transitions (Terada et al., *J. Phys. Chem. B* 117, 12864 (2013)). We focus on the NtrC receiver domain which exhibits allosteric transition with the register shift of α -helix. The chameleon model was applied to NtrC and the simulation results showed a free energy landscape with two states corresponding to active and inactive states. Therefore, we performed a free energy landscape analysis of conformational transition of NtrC. Free energy landscape analysis shows that the α -helix rotates in the intermediate state between active and inactive states.

2-02-1315* **繊毛虫ヨツヒメゾウリムシ由来アルギニンキナーゼの構造解析**
Structural analysis of arginine kinase from the ciliate *Paramecium tetraurelia*

Junpei Yokota¹, Yumeto Otsuka¹, Yoshino Kojima¹, Daichi Yano², Koji Uda¹, Tomohiko Suzuki¹, Shigeru Sugiyama¹ (¹*Fac. Sci. & Tec., Kochi Univ.*, ²*Dept. Environ. Biol., Chubu Univ.*)

Arginine kinase (AK) is the enzyme that catalyzes the reversible transfer of phosphoryl groups from ATP to arginine, yielding ADP and arginine phosphate. The ciliate *Paramecium tetraurelia* has four AKs (*PtAK1-4*). Recombinant *PtAK1-4* were expressed in *Escherichia coli* and their kinetics parameters determined. Interestingly, AK3 showed typical substrate inhibition toward arginine, and enzymatic activity markedly decreased when arginine concentration increased. This is the first example of substrate inhibition in wild-type AKs. To elucidate the substrate inhibition mechanism of AK3, we performed a crystallographic study of *PtAK3*. Here we report the crystal structure of the apo form of *PtAK3* at 2.0 Å resolution.

2-02-1327* **SSX1 に示唆される新規の DNA 結合ドメインのその溶液中構造解析**
Structural analysis of the C-terminal region of SSX1 harboring a potential DNA-binding site

Kanami Takahashi¹, Noriyuki Kodera², Yohei Miyanoiri³, Miki Senda⁴, Kosuke Kato⁵, Naoki Horikoshi⁶, Satoshi Takenaka⁷, Kenji Iwasaki⁸ (¹*Grad. Sch. Sci. and Tech., Univ. of Tsukuba*, ²*WPI-NanoLSI, Kanazawa Univ.*, ³*IPR, Osaka Univ.*, ⁴*SBRC, KEK*, ⁵*Grad. Sch. of Comprehensive Human Sciences, Univ. of Tsukuba*, ⁶*IQB, Univ. of Tokyo*, ⁷*Osaka International Cancer Inst. Hosp.*, ⁸*TARA, Univ. of Tsukuba*)

Synovial sarcoma (SS) is a rare malignancy that accounts for 8% to 10% of all soft tissue malignancies. In all cases the pathogenic fusion protein SS18-SSX is produced, suggesting that when it binds to the chromatin remodeling complex BAF it forms an aberrant BAF complex. The abnormal BAF complex causes a deviation from the normal pattern of gene expression, leading to the belief that it is the trigger for SS. However, the structure and biochemical characteristics of SS18-SSX remain largely unknown. In this study, first, we succeeded in expressing and purifying SS18-SSX. Secondly, nano-imaging of SS18-SSX revealed the region of intrinsic disorder. To make further progress in the study of this protein we are now focusing on the SSX region, which is the culprit domain.

[2-02-1339*](#) 表面増強赤外分光法を用いた Heliorhodopsin の光誘起構造変化解析
Light-induced structural change of Heliorhodopsin analyzed by using SEIRA spectroscopy

Soichiro Kato¹, Jingyi Tang¹, Insyeeerah Binti Muhammad Jauhari², Masanori Hashimoto¹, 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 the infrared absorption intensity increasing about 100 times by adsorbing molecules on a gold thin film. The closer it is to the gold film, the stronger the enhancement, and the 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. It is thought that more information can be obtained than ordinary infrared spectroscopy. In this study, we applied SEIRA spectroscopy on a membrane protein heliorhodopsin, which is a new rhodopsin family discovered in 2018, in addition to time-resolved FTIR to discuss its structural changes and dynamics.

[2-02-1351*](#) NMR によるシニヨリンとその変異体の立体構造解析
Structure analysis of chignolin and its mutant by NMR

Shumpei Koroku¹, Misaki Imai², Koh Takeuchi², Yutaka Maruyama³, Ayori Mitsutake¹ (¹*Meiji Univ.*, ²*AIST*, ³*RIKEN*)

Chignolin, which was designed by Honda et al., is an artificial mini-protein consisting of 10 amino acids:GYDPETGTWG. Its atomic coordinates were determined by NMR. It is widely used to test new simulation algorithm and analysis methods. Chignolin is characterized by two stable states in molecular dynamics (MD) simulations: a native state and a misfolded state. In our previous works, we proposed several mutations of Thr8 to stabilize the misfolded structure rather than the native structure. Here, we show the results of determination of structures of super-chignolin, chignolin and its mutant by NMR analysis.

[2-02-1403*](#) ヒト由来抗菌ペプチド LL-37 とその霊長類オルソログの大量発現系構築及び NMR 法を用いた構造・機能解析
Construction of an overexpression system for a human antimicrobial peptide LL-37 and its primate orthologs and elucidation by NMR

Mitsuki Shibagaki¹, Waka Ueda¹, Kohei Kano², Hao Gu², Tomoyasu Aizawa^{1,2,3} (¹*Sch. Sci., Hokkaido Univ.*, ²*Grad. Sch. Life Sci., Hokkaido Univ.*, ³*Fac. Adv. Life Sci., Hokkaido Univ.*)

Human LL-37 is a member of the cathelicidin family of antimicrobial peptides (AMPs). While there are several cathelicidin paralogs in many mammalian species, only one cathelicidin gene, LL-37 is found in humans. LL-37 has multifunctional bioactivities, so that it is expected to have medical applications. Primates have orthologs that are highly homologous to LL-37, and further knowledge of the characteristics of these orthologs is important to understand the mode of action of LL-37. In order to produce large amounts of peptides for analyzing them by NMR, recombinant overexpression is advantageous. We overexpressed LL-37 and its primate orthologs by a novel calmodulin fusion expression system that protects them from degradation and exerting toxicity to the host cell.

[2-02-1415*](#) Cryo-EM structure analysis of Secretory Pathway Calcium/Manganese ATPase 1 (SPCA1)

Zhenghao Chen^{1,2}, Satoshi Watanabe^{1,2}, Hironori Hashida^{1,2}, Michio Inoue^{1,2}, Akihisa Tsutsumi³, Masahide Kikkawa³, Kenji Inaba^{1,2} (¹*Dept. of Struc. Biol., Grad. Sch. of Life Sci., Tohoku Univ.*, ²*IMRAM, Tohoku Univ.*, ³*Dept of Cell Biol. and Ana., Grad. Sch. of Med, Univ. Tokyo*)

The calcium ion concentration along the secretory pathway is strictly controlled by several calcium channels and pumps. Secretory Pathway Calcium/Manganese ATPase 1 (SPCA1) is a P-type ATPase that transports calcium/manganese ions (Ca²⁺/Mn²⁺) from the cytosol to the Golgi lumen, and contributes to maintaining the homeostasis of Ca²⁺/Mn²⁺. The deficiency of SPCA1 is known to cause Hailey-Hailey disease, neurodegenerative diseases, and inhibition of viral maturation. However, the structure and mechanism of SPCA1 remain poorly understood. Here we established a human cell expression system for SPCA1 and succeeded in determining the first cryo-electron microscopy structure of human SPCA1a in E2-BeF₃⁻ state at a resolution of 3.3 Å.

[2-02-1427*](#) セイヨウイトスギ GRP (ジベレリン調節タンパク質) アレルゲンの立体構造解析と抗体結合部位予測
NMR Structural Analysis and Epitope Prediction of GRP (Gibberellin Regulated Protein)
Allergen of European Cypress Pollen

Tomona Iizuka, Jingkang Zheng, Hiroyuki Kumeta, Yasuhiro Kumaki, Tomoyasu Aizawa (*Grad. Sci. Life Sci., Hokkaido Univ.*)

Gibberellin Regulated Protein (GRP) is a widely conserved peptide with antimicrobial activity in plants, which causes allergies, especially in pollen and fruits. GRP allergens have cross-reactive and are responsible for Pollen-Fruits Associated Syndrome (PFAS). However, its mechanism of allergenicity is not revealed, partly because GRP has a complex 3D structure with six disulfide bonds. In this study, we analyzed the 3D structure and epitope sites of GRP allergen in European cypress (*Cupressus sempervirens*). A *Pichia pastoris* expression system was constructed, and the 3D structure of ¹⁵N-labeled GRP was analyzed by NMR. Epitope sites of GRP allergens were predicted using DiscoTope2.0. The results suggest that the GRP allergen acts as a multivalent antigen.

[2-02-1439](#) *Porphyromonas gingivalis* における主要 Mfa1 線毛バリエーションである Mfa53 の構造
Structure of Mfa53, a major fimbriin variant of Mfa1 fimbriae, of *Porphyromonas gingivalis*

Rei Kojima¹, Satoshi Shibata², Norihiro Takekawa¹, Mikio Shoji³, Katsumi Imada¹ (¹*Dept. Macromol. Sci., Grad. Sch. Sci., Osaka Univ.*, ²*Fac. Med., Tottori Univ.*, ³*Grad. Sch. Biomed Sci., Nagasaki Univ.*)

Porphyromonas gingivalis, a major periodontal pathogen, express at least two types of Type V fimbriae, FimA and Mfa1 fimbriae, for biofilm formation and adhesion to host cells. Mfa53 is identified as a major fimbriin variant of the Mfa1 fimbriae. However, Mfa53 is 65 residues shorter than Mfa1 and shows only 30% amino acid sequence identity to mature Mfa1. To characterize the Mfa53 fimbriae and elucidate the mechanism of fimbriae formation, we determined the crystal structure of Mfa53 at 1.5 Å resolution and compared it with the low resolution cryo-EM structure of the Mfa53 fimbriae. The structures suggest that the growth mechanism of the Mfa53 fimbriae is identical to that of FimA fimbriae, and that Mfa53 is easy to form fimbriae than the FimA and Mfa1 fimbriae.

[2-02-1451](#) Cryo-CLEM 法を用いた糸状仮足観察に関する研究
A study on the observation of Filopodia using the Cryo-CLEM method

Miho Nakafukasako, Tomoya Higo, Yuki Gomibuchi, Yusuke V. Morimoto, Takuo Yasunaga (*Grad. Sch. Comp. Sci. Syst. Eng., KIT*)

Cells move using the filopodia as an antenna. We found that there are two types of the filopodial structure in moving cells, i.e. "Round structure" with a rounded tip and "Sharp structure" like an arrow formed up by F-actin bundles. Thus, we have investigated dynamical changes in conformation by cryo-CLEM methods, but it is challenging to search good targets of elongating/regressing filopodia before imaging by cryo-EM. Here we tried to develop suitable grids for cryo-EM, which bind fluorescent beads as location markers. Three types of fluorescent beads, which are different in size, were scattered on the grids for NG108-15 cell observation, and we will report on the current problems in the observation of filopodia using the Cryo-CLEM method.

[2-02-1503](#) Cryo-EM flexible fitting refinement with automatic error fixing for de novo protein structure modeling

Takaharu Mori¹, Genki Terashi², Daisuke Matsuoka¹, Daisuke Kihara², Yuji Sugita^{1,3,4} (¹*RIKEN CPR*, ²*Purdue Univ.*, ³*RIKEN BDR*, ⁴*RIKEN R-CCS*)

De novo modeling combined with flexible fitting refinement (FFR) has been widely used to build a cryo-EM structure of new proteins. In de novo prediction, artificial conformations containing local structural errors such as chirality errors, cis peptide bonds, and ring penetrations are frequently generated, but cannot be easily removed in the subsequent FFR. We propose an efficient scheme for FFR, in which the local structural errors are fixed first, followed by FFR using an iterative simulated annealing (SA) molecular dynamics (MD) protocol with the united atom (UA) model in an implicit solvent model; we call this scheme "SAUA-FFR". The SAUA-FFR scheme realizes efficient and accurate protein structure modeling from medium-resolution maps with less overfitting.

[2-02-1600*](#) マイクロ波および中赤外誘電分光法が示すグリセロールの保水様式：強い水素結合と弱い水素結合の共存

The water-holding mechanism of glycerol revealed by microwave and mid-infrared spectroscopy: coexistence of strong and weak hydrogen bonds

Miho Morita¹, Toshiyuki Shikata², Yuichi Ogawa¹, Tetsuhito Suzuki¹, Naoshi Kondo¹, Keiichiro Shiraga¹ (¹Grad. Sch. Agriculture., Kyoto Univ., ²Grad. Sch. Agriculture., Tokyo Univ. of Agriculture and Tech.)

The molecular origin of glycerol's water-holding capacity is not fully understood. We measured complex dielectric spectra of glycerol aqueous solutions over a wide concentration range in the microwave and mid-infrared regions. With the amount of bulk water estimated from the dielectric relaxation in the microwave region, the infrared spectra of water in the hydration shell were analytically determined. As a result, the coexistence of water molecules with weak and strong hydrogen bonds became noticeable as increasing glycerol concentration. We speculate that the weakly hydrogen bonded species is originated from confined water molecules in the glycerol network, which may contribute to the water-holding capacity of glycerol as well as formation of strong hydrogen bonds.

[2-02-1612*](#) 機械学習による蛋白質の水和構造予測

Prediction of hydration structures of proteins by using machine learning

Kochi Sato^{1,2}, Mao Oide^{1,2}, Masayoshi Nakasako^{1,2} (¹Dept. Phys., Keio Univ., ²RSC, RIKEN)

Hydration is indispensable for the structure and function of proteins. In recent years, cryogenic transmission electron microscopy has enabled us to visualize the atomic structures of proteins, but the technique is difficult to identify hydration water molecules because of the small scattering cross section of oxygen atom in water molecules. To overcome this problem, we developed a neural network to predict hydration structures of proteins. The network was constructed by machine learning on the distribution of protein atoms around water molecules in high-resolution X-ray structure models. The constructed network predicts hydration structures in the cavities, protein interfaces and on the first-layer hydration shell including hydrophobic surfaces.

[2-02-1624*](#) (1S8-3) 水和水の OH 伸縮振動バンドに基づく生体保護作用を持つ小分子の水素結合強化作用の評価

(1S8-3) Hydrogen bond strengthening effect of stabilizing osmolytes investigated by OH stretching band of hydration water

Fumiki Matsumura¹, Toshiyuki Shikata², Yuichi Ogawa¹, Tetsuhito Suzuki¹, Naoshi Kondo¹, Keiichiro Shiraga¹ (¹Grad. Sch. Agri., Kyoto Univ., ²Grad. Sch. Agri., Tokyo Univ. of Agriculture and Technology)

Although number of studies have addressed its importance, general understanding of the protein-stabilizing effects of osmolytes on water hydrogen bond strength is yet to be reached. In this study, with the aid of dielectric relaxation spectroscopy in the microwave region, we determined the OH stretching band of water molecules around stabilizing osmolytes: trehalose and Trimethylamine-N-oxide (TMAO). We found that these stabilizing osmolytes let surrounding water molecules enhance the red-side of the OH stretching intensity, which clearly shows that both trehalose and TMAO strengthen hydrogen bonds of water surrounding them. This result indicates that water molecules with strong hydrogen bond can be an essential characteristic of stabilizing osmolytes.

[2-02-1636](#) 深層学習と溶液理論のハイブリッドアプローチによるタンパク質水和水分布予測

A hybrid approach of deep learning and solvation theory for predicting the hydration structures around proteins

Kosuke Kawama¹, Yusaku Fukushima¹, Takashi Yoshidome¹, Mitsunori Ikeguchi^{2,3}, Masateru Ohta³ (¹Dep. of Appl. Phys., Tohoku Univ., ²Grad. Sch. of Med. Life Sci., Yokohama City Univ., ³Riken)

Hydration is an important factor in understanding a variety of biological processes, such as protein folding and ligand binding. With the use of all-atom molecular dynamics simulation, the three-dimensional distribution function of water molecules around a protein can be obtained as a hydration structure. However, its high computational cost hinders its application to a large number of proteins. In the present paper, we propose that a hybrid of the 3D-RISM theory and a deep-learning technique can resolve this issue. The hybrid enables us to successfully reproduce the hydration structures around proteins and at ligand-binding sites, and to reduce the computational time for each protein to approximately 10 s.

[2-02-1648](#) 深層学習による GIST の高速計算法の研究
A Fast Calculation Method for the Grid Inhomogeneous Solvation Theory via Deep Learning

Yusaku Fukushima, Takashi Yoshidome (*Dept. of Appl. Phys., Tohoku Univ.*)

Hydration plays an important role in various biological processes, such as protein folding and ligand binding. The grid inhomogeneous solvation theory (GIST) has successfully computed the spatial distribution of hydration energy and entropy. However, although GIST provides detailed thermodynamic information about the solvent, its applications are still few, such as in docking algorithms, owing to its long computation time (a few days). In this study, we aimed to develop a deep learning model for calculating the GIST with a short computation time. Our model generates thermodynamic information within a few tens of seconds, and the information is close to that obtained by GIST-based methods. This result indicated that GIST calculation using deep learning is effective.

[2-02-1700](#) Analysis of urea effect for binding free energy of lysozyme-(GlcNac)₃

Simon Hikiri, Nobuyuki Matubayasi (*Osaka Univ. Grad. Sch. Eng. Sci.*)

In order to elucidate physical origin of the urea effect on the lysozyme-(GlcNac)₃ binding at atomic level, we employ all-atom molecular dynamics and calculate the change in the binding free energy ($\Delta\Delta F$) with the solution environment through the energy-representation method. In a thermodynamic cycle, $\Delta\Delta F$ can be calculated from the free energy change of transfer of the solute consisting of the lysozyme and ligand from pure-water environment to a water-urea mixture and the explicit estimation of the conformational entropy of solute is unnecessary due to the variational principle. Therefore, we focus on solvation free energy (SFE) of the solute. SEF is decomposed into the electrostatic, van der Waals, and excluded-volume components to identify the key component.

[2-02-1712](#) 分子動力学シミュレーションによるタンパク質の水和ダイナミクスと構造の相関解析
Analysis of relationship between the hydration dynamics and the structures of model proteins with MD simulations

Takuya Takahashi¹, Takuya Fujisawa², Shingo Nobunaga², Ryutaro Inou¹, Yui Nakamura¹, Kei Sakamoto¹, Kouta Kasahara¹ (¹*Coll. Life Sci., Ritsumeikan Univ.*, ²*Grad. Sch. Life Sci., Ritsumeikan Univ.*)

MD simulations were performed on various peptides with different conformations, and the effects of their physicochemical properties and structure on the hydration dynamics were analyzed from the obtained MD data. Specifically, we used alpha helical peptides, beta-sheet peptide, and some other hydrophobic polypeptides as the protein models. In order to elucidate the hydration water dynamics, several indices such as the translational movement, the number of hydrogen bonds, accessible surface area, root mean square fluctuation, and approximation functions to the time correlation function of rotational movement were chosen. We also evaluated the effect of water models, solvent ions and force fields on hydration dynamics.

[2-02-1724](#) 蛋白質水と自由エネルギーの十分な精度および超高速での計算
Calculation of hydration free energy of a protein with sufficient accuracy and remarkably high speed

Masato Kawamura¹, Syunsuke Miyamoto¹, Tomohiko Hayashi¹, Masahiro Kinoshita² (¹*Grad. Sch. Eng., Niigata Univ.*, ²*Grad. Sch. Sci., Chiba Univ.*)

We recently developed an accurate and rapid statistical-mechanical method enabling us to calculate not only the hydration free energy (HFE) but also a variety of physically insightful, energetic and entropic components of the HFE for diverse solutes including proteins. A solute with a significantly large total charge can be handled without difficulty. When the HFE of a very large protein is to be calculated for considerably many different structures, however, it is desired that the method be further accelerated. Here we achieve drastic acceleration of the method with its sufficient accuracy being retained. We demonstrate for a protein possessing over 100 residues with a prescribed structure that the calculation is finished in a few seconds on a standard workstation.

[2-02-1736](#) 統計力学に基づくタンパク質-ペプチド複合体の天然構造予測法の開発
Theoretical study based on statistical mechanics for predicting native-like poses of a protein-peptide complex

Shunsuke Miyamoto, Masato Kawamura, Tomohiko Hayashi (*Grad. Sch. Eng., Niigata Univ.*)

Designing a peptide with high affinity for a protein is a difficult task yet crucial in establishing the pharmacotherapeutics for intractable diseases. A clue to the effective design of the protein-binding peptide is the rapid identification of the native-like poses of a protein-peptide complex. In this study, we tackle this issue using our recently developed method by which the microscopic structural information is rapidly correlated with thermodynamic properties through statistical mechanics. We prepare the structures of a native complex and a number of the decoy complexes with a wide variety of binding poses. Then, we apply our physics-based free-energy function (FEF) to the structures and the protein-peptide complex giving the lowest value to FEF is identified.

[2-02-1748](#) 分子シミュレーションベースの機械学習アプローチによる水分子低温ダイナミクス
Simulation-based machine-learning approach for the low-temperature water dynamics

Taku Mizukami¹, Nguyen Viet Cuong³, Dam Hieu Chi² (¹*Materials Sci. JAIST*, ²*Knowledge Sci. JAIST*, ³*HPC systems Inc.*)

Water plays an important role in biological systems. The functions of biomolecule express in a hydrated environment that have mechanisms tightly influenced by water interaction. A simulation-based machine-learning approach is presented that quantitatively analyzes the hydration water. We focus on the motive behavior of all water molecules observed in the classical MD simulations especially in low-temperature that relates to the protein hydration water dynamics. Our approach consists of 1) The clustering technique that categorizes the atomistic configuration to create descriptors, and 2) The machine-learning technique that predict a physicochemical feature on the feature space. By means of the methodology, we will report the low-temperature water diffusional motion.

[2-02-1800](#) 蛋白質の機能的動きに沿った溶媒和自由エネルギー変化の評価法開発
Changes in solvation free energy along protein functional motion: analyses using restraint-free grid-based inhomogeneous solvation theory

Tomotaka Oroguchi^{1,2} (¹*Fact. Sci. Tech., Keio Univ.*, ²*RIKEN SPring-8 Center*)

To quantitatively investigate the role of water molecules in a protein functional motion in MD simulation, it is necessary to calculate changes in solvation free energy along the motion. However, most of analysis methods for solvation free energy require restraints on a protein structure, and therefore only representative conformations along a motion are often selected and analyzed. Here I develop an analysis method that calculates solvation free energy without restraints, called as restraint-free grid-based inhomogeneous solvation theory (rf-GIST). The rf-GIST also enables us to estimate a contribution of each amino-acid residue to total solvation free energy. The method is applied to the free-energy analysis of a functional domain motion of guanylate kinase.

[2-03-1315*](#) HSP70 と HSP40 の複合体のダイナミクスと HSP70 の Lid ドメインの役割に関するシミュレーション研究
Simulation study of the dynamics of Heat Shock Protein (HSP) 70 and HSP40 complex and the role of the Lid domain in HSP70

Lisa Matsukura¹, Kira Fukuoka², Naoyuki Miyashita^{1,2} (¹*Grad. Sch. BOST., KINDAI University*, ²*Faculty of BOST., KINDAI University*)

HSP70 is one of the chaperon proteins, assists in folding proteins. HSP70 consists of a nucleotide-binding domain, a substrate-binding site, and a Lid domain. In the HSP70 chaperone cycle, a substrate binds to HSP70 in the Lid open conformation with ATP-bound, and the J-domain of HSP40 stimulates ATP hydrolysis in HSP70. It induces the structural change to the Lid closed conformation. At present, little is known about the detailed process of the HSP70 chaperone cycle. In this study, to investigate the detailed interaction between the Lid and the substrate-binding site, the interaction of HSP70 and HSP40, and pathway from the Lid close to Lid open conformations, we performed molecular dynamics simulations of the HSP40 and the open and close conformations of HSP70.

[2-03-1327*](#) (2S6-2) An estimation method for the diffusion coefficient using MD simulations with the basic cell containing only one protein as solute

Tomoya Iwashita¹, Masaaki Nagao¹, Akira Yoshimori², Masahide Terazima³, Ryo Akiyama¹ (¹*Department of Chemistry, Graduate School of Science, Kyushu University*, ²*Department of Physics, Niigata University*, ³*Department of Chemistry, Graduate School of Science, Kyoto University*)

A concise correction proposed by Yeh and Hummer has been used for estimations of the diffusion coefficient in finite concentration systems. Here, we performed MD simulations with systems containing only one solute (protein) to study the diffusivity in a dilute solution. In the systems, the additional correction term proposed by Yeh and Hummer is necessary even for relatively large systems. It seems that the correction term is essential when using huge proteins. The correction term includes the hydrodynamic radius, and it made the use of the term difficult. We show that estimation with the term works when the radius is undetermined. We also reveal that the correction term can explain the effective viscosity of solvent between the proteins located in each replica cell.

[2-03-1339*](#) 18 残基チオエーテル結合環状ペプチドと humanPlexinB1 の複合体のシミュレーション
Simulation of complex of 18-residue thioether-bonded cyclic peptide and human PlexinB1

Daiki Noguchi, Ayori Mitsutake (*Graduate School of Meiji, University of Meiji*)

Peptide drugs, which are placed at the "middle point" between micro- and macro-molecular drugs, have been noted in recent years. They can be specifically applied to the target protein and reduce development costs. The thioether-bonded cyclic peptides have a bond between the N-terminal carbon atom and the sulfur atom of cysteine at the 15th or 16th residue. In addition, experimental results reported that each of them has a different affinity for human PlexinB1. In order to elucidate the mechanism, it is important to investigate the difference in the stability of these peptides. Therefore, we performed molecular dynamics simulations of a complex of each peptide and human PlexinB1. This poster shows the simulation results.

[2-03-1351*](#) 統計力学モデルによるタンパク質のフォールディング反応機構の解析
Predicting mechanism and kinetics of protein folding reactions by an extended statistical mechanical model

Koji Ooka¹, Munehito Arai^{1,2} (¹*Dept. Phys., Univ. Tokyo*, ²*Dept. Life Sci., Univ. Tokyo*)

Wako-Saitô-Muñoz-Eaton (WSME) model is a coarse-grained, structure-based model and can calculate free energy landscapes of protein folding. Here, to calculate free energy landscapes of multi-domain proteins, we extended the WSME model by introducing non-local interaction terms. We applied our model to lysozymes and α -lactalbumins and successfully predicted the free energy landscapes that are consistent with experimentally observed folding pathways. Remarkably, we also succeeded in obtaining the detailed kinetics of the folding reaction of hen egg-white lysozyme, fully consistent with the experimental results. We will further extend this model to predict the folding reactions involving disulfide-bond formation based on statistical mechanics.

[2-03-1403*](#) 統計力学モデルへの厳密なコンタクト計算の導入によるタンパク質フォールディング経路予測の改善
Improving the statistical mechanical model of protein folding by accurate contact calculation

Runjing Liu¹, Koji Ooka², Munehito Arai^{1,2,3} (¹*Dept. Integ. Sci., Univ. Tokyo*, ²*Dept. Phys., Univ. Tokyo*, ³*Dept. Life Sci., Univ. Tokyo*)

While protein structure prediction has made a remarkable leap, challenges still remain in computational prediction of protein folding pathways. Wako-Saitô-Muñoz-Eaton (WSME) model is a statistical mechanical model whose calculation is consistent with experimental results on the folding of protein A. However, this still fails to predict the temperature dependence of its folding pathway. To overcome this problem, here we introduce accurate contact calculation in the WSME model. When the contact energies are calculated using the AMBER force field, the model successfully reproduces the temperature dependence of the folding pathway of protein A. Our results suggest that the simple statistical mechanical model can accurately predict protein folding mechanisms.

[2-03-1415*](#) 分子動力学計算による肝細胞増殖因子受容体 MET のアロステリック機構解析
Allosteric mechanism of hepatocyte growth factor receptor MET analyzed by molecular dynamics simulation

Tatsuki Namba, Mikuru Iijima, Jun Ohnuki, Mitsunori Takano (*Dept. of Pure & Appl. Phys., Grad. Sch. Adv. Sci. & Eng., Waseda Univ.*)

The hepatocyte growth factor (HGF) receptor, MET, is activated by binding of HGF, which causes dimerization of MET and juxtaposition of the kinase domains. Because of limited structural information, it remains unclear how the binding of HGF causes the dimerization of MET. In this study, by molecular dynamics simulation using the X-ray structure of MET in complex with the serine protease-like (SP) domain of HGF, we investigated how MET responds to the binding of HGF. Considering the Coulomb interactions between MET and HGF, we analyzed the dielectric response of MET to the binding of HGF and its long-range propagation within the molecule, i.e., the dielectric allostery. We also examine the effect of other domains of HGF which are necessary for MET activation.

[2-03-1427](#) 分子動力学シミュレーションによる繊維形成に関与する FUS-LC タンパク質の天然変性領域の特性評価
Characterization of the Intrinsically Disordered Region of FUS-LC protein involved in fibril formation with molecular dynamics simulations

Maud Chan-Yao-Chong, Justin Chan, Amarjeet Kumar, Shun Sakuraba, Hidetoshi Kono (*National Institutes for Quantum and Radiological Science and Technology; Quantum Life and Medicine Department, Quantum Life Science Institute; Biomolecule simulation group*)

In the cell nucleus, liquid-liquid phase separation (LLPS) caused by proteins is thought to be the key mechanism that produces non-membrane compartments which segregate sets of DNA and proteins. In some diseases such as amyotrophic lateral sclerosis (ALS) and Alzheimer, it is observed that proteins that separate into LLPS can aggregate and form insoluble fibrils. In ALS patients, mutations have been found in the low-complexity (LC) regions of the FUS protein. LC domains, do not have a stable conformation, are classified as Intrinsically Disordered Proteins and could self-aggregate and form fibrils. Using all-atom molecular dynamics simulations, we study the fibril structures of FUS-LC domain and the impact of the mutations to understand the aggregation mechanism.

[2-03-1439](#) Quantum chemistry analysis of the high-resolution crystal structure of GFP in the A state

Hoang Anh Dao, Kazuki Takeda (*Kyoto University, Graduate School of Science*)

Conventional crystallographic analyses usually cannot provide the electronic structure of the active site of proteins whilst the multipolar atom model (MAM) refinement at ultra-high resolution can derive proteins's experimental electron density distribution with fine view. Here we report an examination of a MAM refinement result of green fluorescent protein (GFP) in the A state by means of the quantum theory of atoms in molecules (QTAIM) and natural bond orbital (NBO) frameworks. The nature of hydrogen bonding (HB), the weaker CH- π HB and lone-pair- π interactions around the chromophore were analyzed to understand the spectroscopic properties of GFP. We will discuss about the energy of these interactions and their effect on the chromophore's electronic structure.

[2-03-1451](#) 細胞スケール分子動力学シミュレーションのためのトラジェクトリ解析プログラムの開発
Development of Trajectory Analyzer for Cellular-Scale Molecular Dynamics Simulations

Isseki Yu¹, Daisuke Matsuoka², Yuji Sugita² (¹*Dep. Bioinformatics*, ²*Theoret. Mol. Sci. Lab.*)

Computational power with the latest supercomputers have enabled atomistic molecular dynamics (MD) simulations of cytoplasm, and other cellular environments. They often contain vast number of biomolecules, resulting in more than a million or greater number of atoms. This suggests that their trajectory analyses become heavy computations, which could be another bottleneck in a simulation study. We have developed SPANA (SPatial decomposition ANALysis) to carry out trajectory analyses of such large-scale simulations using multiple CPU cores in parallel. SPANA employs a spatial decomposition of a large biological system to distribute structural and dynamical analyses into the individual CPU core and allows us to reduce the computational time for the analysis significantly.

[2-03-1503](#) VAEによる機械学習を用いた MSES 法の拡張
VAE-driven multiscale enhanced sampling

Kei Moritsugu (*Grad. Sch. Med. Life Sci., Yokohama City Univ.*)

Multiscale enhanced sampling (MSES) allows an enhanced sampling of all-atom structure (MM) by coupling with the accelerated dynamics of coarse-grained (CG) model. Here, we propose an extension to replace the CG model with variational autoencoder (VAE). VAE is a machine learning method that designs complex generative model of data through latent space as a representation of compressed data. VAE can then generate the structural information (such as residua-residue distances as features) that interpolates two different structures by use of the simulation trajectories of the two structures, which is adopted to drive the MM sampling. The present method has been applied to the structural change of ribose binding protein with observing the dynamics on the latent space of VAE.

[2-03-1515](#) Unguided Binding MD of Protein-Protein Complexes by PPI-ColDock

Kazuhiro Takemura, Akio Kitao (*SLST, TokyoTech*)

We recently proposed a simple but efficient and accurate method, Concentrated ligand Docking (ColDock), for predicting protein-ligand complex structures using MD simulation at high ligand concentration. In ColDock, many ligands are randomly distributed around a target protein to induce spontaneous binding of the ligand to the correct binding site. To apply ColDock to protein-protein interactions (PPI), multiple molecules of two kinds of proteins that make complex are distributed to increase the number of encounter events. We successfully observed the formations of near-native complexes. Since time to form complexes and their similarity to the native complexes depends on the target complexes, we explore suitable conditions for efficient sampling of binding events.

[2-03-1527](#) Molecular dynamics simulation of phosphorylated and unmodified intrinsically disordered region of TGIF-1 with its homeodomain

Yuta Nakano¹, Qilin Xie¹, Yusuke Sakai¹, Kota Kasahara², Toru Sengoku⁴, Junichi Higo³, Kazuhiro Ogata⁴, Takuya Takahashi² (¹*Grad. Sch. Life Sci., Ritsumeikan Univ.*, ²*Coll. Life. Sci., Ritsumeikan Univ.*, ³*Res. Org. Sci. Tech., Ritsumeikan Univ.*, ⁴*Grad. Sch. Med., Yokohama City Univ*)

TGIF1 is a multifunctional protein that represses the transcriptional activation of TGF- β . TGIF1 has an intrinsically disordered region (IDR), whose phosphorylation is thought to inhibit TGIF1-HD binding to DNA. In addition, the molecular mechanism of the inhibition by IDR is not known because of the difficulty in analyzing their three-dimensional structure. In this study, we applied our original simulation method, the virtual system coupled canonical molecular dynamics (VcMD) method to analyze structures of phosphorylated and non-phosphorylated IDR form. The results showed that IDRs were attracted to the homeodomain in the phosphorylation form. Contrarily, in the non-phosphorylation form, IDR was not attracted to the homeodomain.

[2-03-1600](#) Analysis of interactions at protein-protein interfaces in protein structure database

Wataru Sagawa (*Dept. of Appl. Phys., Grad. Sch. Eng., Nagoya Univ.*)

Protein-Protein Interactions (PPIs) play an important role for molecular functions in biology. Understanding the mechanism is necessary for designing proteins that interact with other proteins, but it is not fully understood. To reveal it, we performed a database analysis of protein-protein interfaces, especially focusing on water molecules. The reason why we focused on water molecules is that water molecules are often neglected in protein interaction studies even though water remains caught at the interfaces. We show results that suggest the importance of water molecules for PPIs.

[2-03-1612](#) Tau 断片が C 末端領域を含むチューブリンヘテロ二量体の構造に及ぼす効果を分子動力学計算で解明する
Tau Segment Affecting Conformations of Tubulin Heterodimers Including C-Terminal Tails Revealed by Molecular Dynamics Simulation

Naoyuki Furuta¹, Takuma Todoroki¹, Koji Umezawa^{1,2} (¹*Grad. Sch. Of Sci. & Tech., Shinshu Univ.*, ²*IBS, Shinshu Univ.*)

Tau is a microtubule (MT)-binding protein, which stabilizes MT. The second MT-binding site (R2) of Tau forms a complex structure with MT (PDB ID: 6cvn). Tau R2 binds in the vicinity of the intrinsically disordered region, the C-terminal tails (CTTs), of $\alpha\beta$ -tubulins. The conformations of CTTs seem to be affected by Tau R2 binding. However, as the CTTs are disordered, their conformational differences induced by Tau have not been investigated. Then, we performed molecular dynamics (MD) simulation to clarify effects of Tau R2 on $\alpha\beta$ -tubulins including CTTs. The GDP- and GTP-bound $\alpha\beta$ -tubulins were computed in the absence or presence of Tau R2. The results suggested that Tau R2 spatially attract the β -tubulin CTT and that Tau R2 reduce fluctuation of α -tubulin.

[2-03-1624](#) Molecular dynamics simulation of loop capturing during cohesin-mediated DNA loop extrusion mechanism

Chenyang Gu, Shoji Takada, Tsuyoshi Terakawa, Giovanni Brandani (*Grad. Sch. Sci., Univ. Kyoto*)

The non-random 3D folding of the eukaryotic genome into a small nucleus is important for many biological processes such as the regulation of gene expression. Topologically-associated domains (TADs) are key components of such organization in interphase, and are established mainly by the cohesin complex through the process of loop extrusion. However, the molecular details of this mechanism are still unclear. Using coarse-grained molecular dynamics simulations, we study how the essential components of human cohesin interact with DNA, focusing on the DNA loop-capturing step of the loop extrusion process. Our results provide insights into the mechanism that would be difficult to achieve with experiments alone.

[2-03-1636](#) Conformations and distributions of Cryptdin-4, lipids, and water observed in membrane self-assembly molecular dynamics simulations

Takao Yoda (*Nagahama Institute of Bio-Science and Technology*)

Cryptdin-4 (Crp4) is an antimicrobial peptide that permeabilizes negatively charged membrane. It also goes across the membrane during its action. Fourteen years ago, an experimental study suggested that Crp4 oligomerization takes place just before the translocation. Here we performed molecular dynamics simulations to visualize Crp4 conformations within a membrane. Since Crp4 bactericidal action takes ~100 seconds, we cannot do a brute-force simulation of the translocation process. Thus, we tried to observe Crp4 interactions by membrane self-assembly simulations. Our results show that (1) Crp4 oligomer tends to be within the membrane in comparison to monomer and (2) Crp4 oligomers are highly interacting with lipid head groups, ions, and water even within the membrane.

[2-03-1648](#) タンパク質フォールディングにおける動的協同性
Dynamic Cooperativity in Protein Folding

Song-Ho Chong (*Kobe, Riken*)

Protein folding is considered to be cooperative, but elucidating underlying molecular processes remains as a challenge. Here, we address how and when the folding process is cooperative on a molecular scale. To this end, we analyze multipoint time-correlation functions probing time-dependent cooperativity between multiple amino acids, which were computed from long folding simulation trajectories. We find that the simultaneous multiple amino-acid contact formation starts to develop only upon entering the folding transition path and attains a maximum at the transition state. Thus, our work not only provides a new mechanistic view on the folding cooperativity, but also offers a conceptually novel characterization of the folding transition state.

[2-03-1700](#) gmfit による単一および複数サブユニットの 3D 密度マップの重ね合わせの改良: ラプラシアン演算と CSS 探索の適用
An improvement of gmfit for single and multiple subunit fitting on 3D density map : Laplacian operator and CSS search

Takeshi Kawabata¹, Haruki Nakamura², Genji Kurisu² (¹*Protein Research Foundation*, ²*Inst. Prot. Res., Osaka Univ.*)

The *gmfit* program has been developed for fitting of atomic models into a 3D density map using Gaussian mixture model (GMM). We have improved the algorithm both for single and multiple subunit fitting. For the single subunit fitting, a grid-layout is introduced to generate initial poses comprehensively. Laplacian edge detecting operator has a better sensitivity especially for a local fitting into a low-resolution 3D map. We newly introduced the Laplacian operator to 3D density represented by GMM in an analytical form. For the multiple subunit fitting, we have introduced a CSS (Combination of Single subunit Searches), which provide poses of multiple subunits by combining poses of single subunit searches. This is effective for relatively small number of subunits (<10).

[2-03-1712](#) 分子動力学シミュレーションに基づいた環状ペプチドの膜透過率の大規模予測
Large-scale membrane permeability prediction of cyclic peptides crossing a lipid bilayer based on molecular dynamics simulations

Masatake Sugita, Satoshi Sugiyama, Takuya Fujie, Yasushi Yoshikawa, Keisuke Yanagisawa, Masahito Ohue, Yutaka Akiyama (*Dept. Comput. Sci., Tokyo Inst. Tech.*)

Membrane permeability is a significant obstacle facing the development of cyclic peptide drugs. To investigate common features of permeable peptides, it is necessary to reproduce the membrane permeation process of cyclic peptides through the lipid bilayer. In this study, we simulated the membrane permeation process of 156 cyclic peptides (6-8 aa) with diverse chemical structures across the lipid bilayer based on steered molecular dynamics (MD) and replica-exchange umbrella sampling (REUS) simulations. As a result, a reasonable correlation between experimentally assessed and calculated membrane permeability was observed for the peptides, except for strongly hydrophobic peptides. The relevance between the desolvation and membrane permeability was also demonstrated.

[2-03-1724](#) タンパク質における連続 3 残基 Loop-Closure 問題の解の個数に関するロボット工学的解析
Robotics-based Analysis of the Number of Solutions for Loop-Closure Problem of Three Consecutive Residues in a Protein

Keisuke Arikawa (*Fcl. Eng., Kanagawa Inst. of Tech.*)

Three consecutive residue units in a protein contain six movable backbone bond axes. Calculating the conformations of a unit maintaining a relative position and orientation between its ends is a type of loop closure problem. The problem is equivalent to the inverse kinematics problem of a robotic arm with six revolute joints. Based on the methods in robotics, we have solved the loop closure problems for three consecutive residue units randomly sampled from PDB. All the real solutions for each unit were calculated, and the feasibility of the solutions was evaluated based on the Ramachandran plot. Focusing on the number of solutions, we calculated the feature values, such as the average and maximum, and the dependency on the secondary structures.

[2-03-1736](#) Verification of simulations using Virtual system coupled canonical molecular dynamics for the small protein inhibitor

Yusuke Sakai¹, Yuuta Nakano¹, Qilin Xie¹, Kota Kasahara², Junichi Higo³, Takuya Takahashi² (¹*Grad. Sch. Life Sci., Ritsumeikan Univ.*, ²*Coll. Life. Sci., Ritsumeikan Univ.*, ³*Res. Org. Sci. Tech., Ritsumeikan Univ.*)

We have developed Virtual system coupled canonical molecular dynamics (VcMD), which is extended ensemble simulation method. In this method, conformational changes of the system (real system) along arbitrarily defined reaction coordinates are enhanced by coupling the real system with a non-physical (virtual) system. The VcMD method has been applied various biophysical phenomena including peptide-peptide and peptide-protein interactions. However, a prediction performance for specific recognition of small ligands by a deep pocket on the protein surface is not well validated so far. Therefore, in this study, we investigated the free-energy landscape of protein-small ligand interactions using the VcMD method.

[2-03-1748](#) 粗視化分子シミュレーションで探る ABC トランスポーター ABCG2 の構造ダイナミクス
Structural dynamics of the ABC transporter ABCG2 explored by coarse-grained molecular simulations

Ryosuke Hirano, Minoru Sakurai, **Tadaomi Furuta** (*Sch. Life Sci. Tech., Tokyo Tech*)

ABCG2 is one of the human ABC transporters and is intensely investigated focused on the multidrug resistance. However, the transport mechanism of ABCG2 is still unclear at the atomic level. Here, we investigated the structural dynamics of ABCG2 by coarse-grained molecular simulations using our recently developed ATP force field (Hirano et al., *J. Comput. Chem.* **40**, 2096-2102 (2019)). As a result, we observed the dimerization of the nucleotide-binding domains induce by the ATP binding and a conformational transition from the inward-facing to outward-facing structure in the holo system. On the other hand, these phenomena were not observed in the apo system. In the presentation, based on these results, we will discuss the structure-function relationship of ABC transporters.

[2-03-1800](#) 粗視化モデルによる転写因子 Nanog のオリゴマー化と相分離についてのシミュレーション研究
Coarse-grained molecular simulations on oligomerization and condensate formation of transcription factor Nanog

Azuki Mizutani, Shoji Takada (*Grad. Sch. Sci., Univ. Kyoto*)

Nanog is one of the master transcription factors for the maintenance of pluripotency in mammals. Biochemically, Nanog is known to form homodimers in solution, and to form a condensate via phase-separation *in vitro* at high concentration. The tryptophan repeat (WR) in the C-terminal region of Nanog is responsible for its dimerization. Nanog contains N- and C-terminal disordered tails, in addition to a small DNA binding domain, making it difficult to study this protein by X-ray crystallography or cryo-EM. To characterize its structural details, we performed coarse-grained molecular simulations of mouse Nanog. Comparing the dynamics of WT-Nanog and WR-mutated one, we investigated the importance of WR in the dimerization and the formation of condensates.

[2-03-1812](#) ヘリックス傾向の異なる 9 種類のペプチド周囲における水和ダイナミクスの分子動力学的研究
Molecular dynamics study of hydrated water dynamics around 9 peptides with different helix propensity

Shingo Nobunaga, Takuya Takahashi, Kota Kasahara (*Grad. Sch. Life Sci., Ritsumeikan Univ.*)

Proteins exhibit unique physicochemical properties, structures, dynamics, functions depending on their sequence. In addition, solvent is the other key factor to determine the protein properties. In this study, we investigated effects of sequence on peptide and solvent dynamics by using nine variants of a model peptide whose helix tendency have been experimentally solved. We discuss the effects of solvent in terms of correlation among measurements describing dynamics and structures of solvent and solute, such as secondary structure content, solvent accessible surface area, root-mean-square displacement, root-mean-square fluctuation, the number of hydrogen bonds, diffusion coefficient of solvent, rotational relaxation time of solvent.

[2-03-1824](#) ディープニューラルネットワークと分子動力学シミュレーションを用いた 3 次元反応座標上のタンパク質構造変化モーフィングプログラムの開発
Development of the Morphing Program for Protein Structural Changes on 3D Reaction Coordinates Using DNN and MD Simulations

Ryota Kiyooka¹, Lisa Matsukura¹, Masaki Ottawa¹, Kira Fukuoka², Naoyuki Miyashita^{1,2} (¹*Grad. Sch. BOST, KINDAI Univ.*, ²*BOST, KINDAI Univ.*)

The structure change of the protein and the dynamics are essential in a living cell. Molecular dynamics (MD) simulations have been known as promising tools to elucidate detailed protein dynamics. However, it is difficult to trace the protein structure changes by MD simulations because the time-scale of the structural changes is too long for MD simulations. Thus, to observe the structural changes, light and easy ways have been desired. In this study, to obtain the morphing movies for the pathway of protein structure changes easily, we developed the morphing program of the protein structure changes on three-dimensional (3D) reaction coordinates using the deep neural network (DNN) and MD simulations. Here we investigated the structure changes by several proteins using it.

[2-04-1315*](#) 抗体表面への正荷電残基変異導入による抗体の pH 非依存的な熱安定性獲得機構

The mechanism by which positive supercharging mutations confer pH-independent thermal stability of an antibody

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Supercharging is a method to improve physicochemical properties of proteins by mutating surface with charged amino acids. We explored how supercharging affects antibody Fabs. We computationally designed a supercharged Fab with the net charge of +10 (pos10) compared to -4 of the wild-type (WT) Fab. **pos10 showed preserved thermal stability at pH 6 and 8**, while the WT denatured at lower temperature at pH 8 than at pH 6. Here, the secondary structure and the binding affinity to the antigen were preserved. Moreover, **molecular dynamics simulations revealed preferential solvation of phosphate ions to the pos10 surface relative to the WT surface**. It was suggested that supercharging would be a useful approach to preserving thermal stability of antibodies in a wide range of pH.

[2-04-1327*](#) Dynamic residue interaction network analysis of the H274Y mutant in neuraminidase conferring drug resistance in influenza virus

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One of the major oseltamivir (OTV) resistant strain of influenza virus exhibits His-to-Tyr mutation at position 274 (H274Y) in neuraminidase (NA). In this study, we investigated the dynamic correlation between the OTV binding site of NA and its H274Y mutation site using molecular dynamics simulations and dynamic residue interaction network (dRIN) analysis. The dRIN analysis revealed that the OTV binding and its H274Y mutation sites interacts via three interface residues. The H274Y mutation enhanced the interaction between the residue 274 and the three interface residues, resulting in significant decrease in interaction between OTV and its surrounding 150-loop residues. We concluded that such changes in residue interactions could reduce the binding affinity of OTV to NA.

[2-04-1339*](#) Investigation of pore diameter conversion of β -barrel nanopore-forming protein by changing number of β -strands

Toshiyuki Tosaka, Koki Kamiya (*Grad. Sci. & Tech., Univ. Gunma*)

Nanopore-forming protein in cell membranes allows a permeation of substances such as ions, nutrients, and small molecules. β -barrel nanopore-forming proteins have stable structures and constant pore diameters. OmpG with 14 β -strands, which is one of the β -barrel nanopore-forming protein, transports ion and trisaccharide. In this study, to create OmpG with the controllable precise nanopores for transportation various size of biomolecule, we prepare mutant OmpG with different number of β -strands. The amount of ions through single-molecule OmpG mutants was measured using a patch clamp method of the artificial lipid bilayer. A change of ion permeability and pore size depends on the region of β -strands which were inserted or deleted into the OmpG.

[2-04-1351*](#) インスリンの由来種に依存したアミロイド核形成メカニズム

Early aggregation kinetics upon the amyloid nucleation of bovine and human insulin

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Protein misfolding often results in the formation of amyloid fibrils, which are protein aggregates associated with serious amyloidoses. Amyloid nucleation is a key molecular event because the amyloid nuclei rapidly induce the subsequent growth of amyloid fibrils, although much remains unclear how the nucleation occurs. Here, we investigated the early aggregation mechanism of bovine and human insulin, the amino acid sequence of which are slightly different. Dynamic and static light scattering analyses revealed that bovine insulin exhibits explosive aggregation with a monomodal distribution, in contrast to quite slow development of human insulin. Based on further analyses and modeling of aggregation, the detailed amyloid nucleation mechanism will be discussed.

[2-04-1403*](#) チャンネルロドプシン C1C2 の光中間状態におけるレチナール発色団の構造ダイナミクス
Structural Dynamics of the Retinal Chromophore in the Photo-Intermediate States of
Channelrhodopsin C1C2

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Channelrhodopsins (ChRs) are crucial light-gated ion channels in optogenetics. To reveal their gating mechanism, we measured time-resolved resonance Raman spectra of the retinal in ChR C1C2. We observed large changes in Raman bands in the P₁-P₃ states compared to the dark state. Especially, whereas widths of C=N stretching band of the retinal Schiff base (RSB) in H₂O and D₂O were 16-17 cm⁻¹ in the dark, P₁ and P₂ states, they changed to 22 and 12 cm⁻¹ in the P₃ state, respectively. The broader bandwidth in H₂O than D₂O indicates a hydrogen bonding of water to the RSB. Since no water exists near the RSB in the dark state and bulk water flows into the protein in the P₃ state, the influx water binds to the RSB in the P₃ state, and the ion pathway extends to near the RSB.

[2-04-1415*](#) 線維前駆中間体の成長を防ぐ αB-クリスタリンのアミロイド線維化阻害: 安定な複合体の形成
Inhibition of amyloid fibrillation by αB-crystallin by preventing the growth of prefibrillar
intermediates: Formation of a stable complex

Yuki Kokubo¹, Keisuke Yuzu¹, Junna Hayashi², John A. Carver², Eri Chatani¹ (¹*Grad. Sch. Sci., Kobe Univ.*, ²*Res. Sch. Chem., The Austral. Natl. Univ.*)

Amyloid fibrils are abnormal aggregates of proteins associated with various serious diseases. Small heat shock proteins (sHsps) have been reported to inhibit fibrillation of various disease-related proteins such as α-synuclein and amyloid-β; however, the detailed mechanism of inhibition is not fully understood. In this study, we have investigated the chaperone activity of αB-crystallin (αB-C), the most representative mammalian sHsp, on insulin B-chain by dynamic light scattering and other methods. As a result, it was proposed that αB-C prevents nucleation stage, especially the growth of prefibrillar intermediates. αB-C forms a more stable αB-C-B-chain complex than the B-chain intermediates, resulting in the suppression of fibrillation.

[2-04-1427*](#) 大腸菌フェリチンの構造・機能に及ぼす正味電荷の効果
Effects of net charge on the structure and function of *Escherichia coli* ferritin

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Ferritin (Ftn) is a protein cage capable of storing up to 4500 iron atoms. Electrostatic potential is speculated to be important to attract iron ions. However, it is not clarified how a net charge associates with its function in detail. In this research, we made *Escherichia coli* ferritin (EcFtnA) mutants having different net charges by substituting Glu/Gln on the surface of Ftn to Gln/Glu residues (QE and EQ mutants). These mutants were characterized structurally and functionally by analytical ultracentrifugation, small-angle X-ray scattering and native-PAGE. Surprisingly, it was found that the net charges of QE mutants were unchanged from the net charge of EcFtnA while those of EQ mutants changed depending on the number of substitutions.

[2-04-1439*](#) ラン藻でのアルカン合成に関わる 2 つの酵素の親和性を理論的に向上させる
Improving bioalkane production by computationally enhancing the affinity between two enzymes
for cyanobacterial alkane synthesis

Katsuhisa Iwaya¹, Yuuki Hayashi², Munchito Arai^{1,2} (¹*Dept. Phys., Univ. Tokyo*, ²*Dept. Life Sci., Univ. Tokyo*)

Two enzymes essential for cyanobacterial alkane synthesis are acyl-(acyl carrier protein (ACP)) reductase (AAR) and aldehyde-deformylating oxygenase (ADO). Previous studies showed that fatty aldehyde produced by AAR is efficiently delivered to ADO through the interaction between them. However, since the affinity between AAR and ADO is weak, we hypothesized that enhancement of the AAR-ADO interaction may improve bioalkane production. Here, we computationally designed the ADO mutants that have higher affinity to AAR using Rosetta software. We successfully obtained the ADO mutants that improved alkane production in *Escherichia coli* coexpressing AAR. Our results suggest an important role of the AAR-ADO interaction in alkane biosynthesis.

[2-04-1451*](#) アクチンとA β の相互作用特性はアクチンの重合状態で異なる

The interaction behavior between actin and A β differs depending on the polymerization state of actin

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(¹Muroran Institute of Technology, ²Al-Farahidi University)

Amyloid β (A β) aggregation induces neuronal cell death, but the mechanism remains unclear. Since various proteins coexist with A β in the body, in this study, we first evaluated the effects of various proteins for A β aggregation using the quantum dot imaging we previously reported. The result revealed monomeric actin has the highest inhibitory activity for A β aggregation among tested proteins. Interestingly, polymerized actin showed significantly lower inhibitory activity than monomeric actin, and aggregated A β adhered to the actin filaments. Furthermore, we found that A β promoted the formation of abnormal aggregates of actin *in vitro* and *in vivo*. These results suggest that the interaction of A β and actin is involved in neuronal cell death.

[2-04-1503*](#) 酵素一分子の活性ゆらぎと進化能の関係

Correlation between the fluctuation of single enzyme activity and evolvability

Takahito Iida, Hiroshi Ueno, Hiroyuki Noji (*Grad. App. Chem., Univ. Tokyo*)

This study aims to understand the correlation between the fluctuation of single enzyme activity and evolvability. For this purpose, we have developed a method to correctly synthesize many mutant enzymes from each single DNA enclosed in micro-reactor and quantitatively analyze their activities. The template DNA was enclosed in micro-reactor device and the model enzyme, alkaline phosphatase, was synthesized in cell-free condition. After recovering the enzymes from the device, the catalytic activity from single enzymes was measured. Single enzyme activity showed the fluctuation even they are synthesized from the same DNA. Furthermore, there was a positive relationship between the mutation rate and the fluctuation of single enzyme activity from mutant library.

[2-04-1515*](#) 新規スコアによる相分離関連 IDR の分類

Classification of Intrinsically Disordered Regions involved in Liquid-Liquid Phase Separation Using the Novel Score

Hayato Aida^{1,2,3}, Ryuhei Harada², Yasuteru Shigeta², Kentaro Tomii¹ (¹AIRC, AIST., ²CCS, Univ. of Tsukuba., ³Master's Program in Biol., Univ. of Tsukuba.)

Intrinsically Disordered Regions (IDRs) in proteins are often necessary for modulating intracellular liquid-liquid phase separation (LLPS). A recent study showed that the valence and patterning of aromatic residues in IDRs can modulate LLPS. Based on that study, we proposed a novel score with no dependence on amino acid composition to represent the distribution of aromatic residues in IDRs. To calculate the score, which we call BS-score, we regarded the sequence of IDRs as sticks broken by aromatic residues and applied the statistical model called Broken Stick model. Here, we present clustering results of IDRs in LLPS related proteins based on BS-score and amino acid composition to characterize them.

[2-04-1527](#) 粒径に関する非加算性を取り入れた朝倉一大沢理論：生体高分子の壁面への吸着物性に関する検討
Asakura-Oosawa theory incorporating non-additivities of particle sizes: Study of adsorption properties of biopolymers on a wall

Ken-ichi Amano, Masahiro Maebayashi (*Fac. Agric., Meijo Univ.*)

Understanding the adsorption properties of biopolymers on walls is important for the development of nanotechnology. In this study, the adsorption properties of biopolymers on a wall surface were investigated from the viewpoint of Asakura-Oosawa theory in the environment where multiple species of biopolymer exist. Here, we incorporated non-additivities of the particle sizes into the theory. From the new theory, an adsorption equation for the walls that is independent of non-additivity was found. In the presentation, we show the adsorption properties of biopolymers under various conditions and explain possible mechanism of the incomprehensible behaviors possibly resulted from commonly performed numerical calculations.

[2-04-1600*](#) ラマン分光法を用いた液-液相分離による液滴内のタンパク質濃度変化のラベルフリー観測
Label-free observation of protein concentration change in a droplet formed by liquid-liquid phase separation using Raman spectroscopy

Kohei Yokosawa¹, Daiki Shibata¹, Shinji Kajimoto^{1,2}, Takakazu Nakabayashi¹ (¹*Grad. Sch. Pharm. Sci., Tohoku Univ.*, ²*JST PRESTO*)

Liquid-liquid phase separation (LLPS) of protein solution has been widely studied in cell biology. LLPS results in the formation of small protein-rich liquid droplets, which are involved in a variety of biological reactions. However, the properties of the droplets have not been well understood because a label-free measurement method for a single droplet has not been developed. We thus propose Raman microscopy as the promising method and show that the quantification of a single droplet can be performed using the Raman band of water as an intensity standard. Using Raman microscopy, we could detect changes in protein concentration in a droplet with changing condition such as pH and initial concentration, and the change was discussed based on a two-component phase diagram.

[2-04-1612*](#) 静水圧印加時における in vitro Ras 活性測定系の確立
Establishment of in vitro system to measure Ras activity under hydrostatic pressure

Teruhiko Matsuda¹, Minki Chang², Katsuko Furukawa², Takashi Ushida³, Taro Uyeda¹ (¹*Dept. Physics / Applied Physics, School of Advanced Science and Engineering, Waseda Univ.*, ²*Dept. Bio Eng, Faculty of Engineering, Univ of Tokyo*, ³*Dept. Mech Eng, Faculty of Engineering, Univ of Tokyo*)

Ras in cultured chondrocytes is activated by hydrostatic pressure (HP) and this has been implicated in signal transduction in chondrocytes in joints. It was thus speculated that Ras itself, regulators of the Ras cycle such as GAP and GEF, and/or the upstream regulator of Ras have the HP sensitivity. To identify which factor has the HP sensitivity, we established an in vitro system to measure relative content of active Ras with or without HP using the FRET-based Ras activity probe Raichu (Mochizuki et al., 2005). Current preliminary results suggested that physiological HP (25~30 MPa) increase active Ras in the presence of either GAP or GEF.

[2-04-1624*](#) 疾患関連タンパク質の液-液相分離とラマン分光法を用いたその定量
Liquid-liquid phase separation of disease-associated protein and its quantification using Raman spectroscopy

Kazuki Murakami¹, Shinji Kajimoto¹, Daiki Shibata¹, Kunisato Kuroi², Takakazu Nakabayashi¹ (¹*Grad. Sch. Pharm. Sci., Tohoku Univ.*, ²*Fac. Pharm. Sci., Kobe Gakuin Univ.*)

Liquid-liquid phase separation (LLPS) is associated with protein aggregation in neurodegenerative diseases. Although LLPS has extensively studied, current methods have several difficulties. In this presentation, we show that ataxin-3, associated with Machado-Joseph disease, exhibits LLPS in an intracellular crowded state and propose that a single droplet can be quantified using Raman microscopy in a label-free manner. We succeeded in quantifying the concentration of ataxin-3 in a droplet using the O-H stretching band of water as an internal intensity standard and revealed that the protein concentration in a droplet was dependent on the outside state. We therefore propose that Raman microscopy will become a powerful technique for studying LLPS.

[2-04-1636*](#) 自家蛍光寿命イメージングを用いた液-液相分離におけるタンパク質の構造変化のラベルフリー観測
Label-free observation of protein structural changes in liquid-liquid phase separation using autofluorescence lifetime imaging

Uchu Matsuura¹, Shinya Tahara¹, Shinji Kajimoto^{1,2}, Takakazu Nakabayashi¹ (¹*Faculty of Pharmaceutical Sciences, Tohoku University.*, ²*JST PRESTO, Japan.*)

Liquid-liquid phase separation is a phenomenon where proteins form highly concentrated liquid droplets in solution. While droplets control various functions in cells, it also promotes protein aggregation. Understanding the aggregation mechanism via droplets needs to clarify the changes in structure and physical properties of the proteins forming droplets. In this study, we demonstrated that autofluorescence lifetime imaging enables label-free analysis of proteins in a single droplet. We measured the fluorescence lifetime of the tryptophan residues of ataxin-3, a causative protein of neurodegenerative disease. It is shown that the protein structure in the droplet is different from that in the dispersed solution and gradually changes with time.

[2-04-1648*](#) ナノポア内におけるβヘアピンペプチドの段階的なトランスロケーション過程の観察
Observing a stepwise translocation of β-hairpin peptides through a nanopore

Miyu Fukuda, Masataka Usami, Ryuji Kawano (*Department of Biotechnology and Life Science, Tokyo University of Agriculture and Technology.*)

The structural information of proteins and peptides is the essential information for their functions. The conventional evaluation of the structure is based on their freezing structure such as the crystal or cryo-structure; therefore, it is difficult to obtain the dynamic structural information on individual proteins. We have attempted to acquire the dynamic structural information using a nanopore measurement, which can perform electrical detection of the structural information at the single molecule level. The nanopore measurement of a β-hairpin peptide used in this study showed that current signals with multiple states were observed when peptides passed through the nanopore. This may reflect a stepwise translocation for a peptide with the unfolding.

[2-04-1700*](#) 異なるカチオン存在下でのウイルスロドプシン OLPVRI の時間分解光誘起赤外分光研究
Time-dependent light-induced ATR-FTIR study of viral rhodopsin OLPVRI in the presence of different cations

Mako Aoyama, Kota Katayama, Hideki Kandori (*Grad. Sch. Eng., Nagoya Inst. Tech.*)

OLPVRI is one of microbial rhodopsins from Organic Lake phycodnavirus. To date, it has been suggested that OLPVRI functions light-gated Na⁺/K⁺ selective cation channel and its channel activity is blocked by Ca²⁺. However, the molecular mechanisms of channel gating and blocking are not well understood. To study light-gated structural changes in the presence of different cations, we performed time-dependent ATR-FTIR difference spectroscopy upon light illumination. OLPVRI was successfully prepared by *E. coli* expression system. From the results, we found that the light-induced structural change and the kinetics of return to the original state of OLPVRI differed depending on the cation species. Spectral basis for channel gating and blocking mechanism will be discussed.

[2-04-1712*](#) Amino acid side chain parameters on phase separation of protein

Akira Nomoto, Suguru Nishinami, Kentaro Shiraki (*Pure and Appl. Sci., Univ. Tsukuba*)

Evaluating the interactions of amino acids is necessary to understand the propensity of protein folding, aggregation, and liquid-liquid phase separation (LLPS). Here, we investigate the solubility of amino acid side chain (SASC) in 20 kinds of amino acid solvents by subtracting the solubility of glycine from that of each amino acid. The SASC represented soluble and insoluble interactions depending on the type of amino acid and the pH of the solvent. Interestingly, the SASC showed a different propensity from the hydrophobicity of the side chain of each amino acid. These findings indicate that the SASC can distinguish the interactions of amino acids that contribute to LLPS and aggregation of proteins.

[2-04-1724](#) 高速原子間力顕微鏡を用いたアミロイドβ線維に対するダイナミックフォースマッピング
Dynamic Force Mapping to Amyloid-Beta Fibrils Using High-Speed Atomic Force Microscopy

Shogo Miyajima¹, Maho Yagi-Utsumi², Christian Ganser², Takayuki Uchihashi^{1,2}, Koichi Kato² (¹*Grad. Sch. Sci., Univ. Nagoya*, ²*ExCELLS*)

Amyloid fibrils are self-assembled aggregates of misfolded insoluble proteins that have been implicated in neurodegenerative diseases such as Alzheimer's disease. Amyloid-β (Aβ) oligomers are highly neurotoxic and play an important role in tip of fibrils during elongation but the detailed mechanism of its supramolecular structure construction has not been elucidated before. In this study, we have applied dynamic force mapping, which enables us to evaluate the stiffness of a sample deduced from force curves obtained at each pixel, of Aβ fibrils in solution using high-speed atomic force microscopy (HS-AFM). In this presentation, we will discuss the relationship mechanical properties along the fibril and the fibril elongation.

2-04-1736 糖ガラスに包埋されたタンパク質の構造と安定性
Structure and stability of proteins embedded in sugar glass

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In extreme environments such as desiccation and freezing, for survival, organisms accumulate sugar as a "compatible solute" that protects biological components and cell membranes instead of water and stops or reduces metabolic activity. As such a mechanism of environmental resistance, the "glass state theory" (protection of higher-order structures by vitrification of sugar) or the "water substitution theory" (hydrogen bonding with sugar as a substitute for water) has been considered. However, little is known about the effects of sugar due to a lack of relevant experimental studies. Using X-ray scattering and neutron scattering in a complementary way, we investigated the protein structures embedded in various sugar glasses and/or rubber states.

2-04-1748 VHH における CDR3-Framework region 間分子内相互作用に着目した Framework region 変異体の物理化学的解析
Physicochemical studies of mutations in framework regions of VHH focusing on intramolecular interactions with CDR3

Seisho Kinoshita¹, Makoto Nakakido^{1,2}, Daisuke Kuroda^{1,2}, Jose Caaveiro³, Kouhei Tsumoto^{1,2,4} (¹*Dept. of Bioeng., Sch. of Eng., Univ. of Tokyo*, ²*Dept. of Chem. Biotech., Sch. of Eng., Univ. of Tokyo*, ³*Grad. Sch. of Pharm. Sci., Kyushu Univ.*, ⁴*Inst. of Med. Sci., Univ. of Tokyo*)

VHhs are useful tools in biotechnological and medical applications. Compared to other antibodies, VHhs have longer CDR3, and some VHhs have a conformation in which a long CDR3 loop covers the framework region (FR). By employing MD simulations, the residues of FR that exhibited intramolecular interactions with CDR3 were identified. Mutational analysis of these residues showed a decrease in thermal stability and affinity. Subsequently we performed mutational analyses on a synthetic VHH, which was generated by exchanging the CDRs of the VHH for those from another humanized VHH. The results showed an increase in thermal stability and affinity. In the light of these data, we discuss an important role of intramolecular interactions between the CDR3 and the framework region.

2-04-1800 フィブロインの剪断応力解析
Shear Stress Analysis of Fibroin

Kento Tsutsumi¹, Satoru Onishi¹, Muneya Daidai¹, Kento Yonezawa³, Takehiro Satou³, Yoichi Yamazaki¹, Sachiko Toma¹, Hironari Kamikubo^{1,2,4} (¹*NAIST,MS*, ²*NAIST,CDG*, ³*Supiber inc.*, ⁴*KEK,IMSS*)

Fibroin is a structural protein that constructs spider silk, which exhibits high mechanical strength. We discovered that a precursor is required for the elongation reaction of fibroin nanofibers. This reaction is similar to the nuclear-demanding elongation reaction of proteins found in amyloid fibrils. The nucleation-elongation reaction of amyloid is known to be induced by mechanical stimuli, such as shear stress. We speculate that shear stress induces fibrillar elongation in fibroin as well. In this study, we measured the elongation response of fibroin nanofibers when subjected to shear stress. In the results, the formation of precursors and the elongation of nanofibers were confirmed when shear stress was applied.

2-04-1812 光誘起フォールディング反応および分子シャペロン SecB との相互作用カイネティクス
Kinetic analyses of photoinduced protein folding and interaction with molecular chaperone SecB

Ikuya Nakaoka¹, Yusuke Nakasone¹, Honoka Ota², Soichiro Kawagoe^{2,3}, Koichiro Ishimori², Tomohide Saio^{3,4}, Masahide Terazima¹ (¹*Graduate School of Science, Kyoto University.*, ²*Hokkaido University Graduate School of Chemical Sciences and Engineering.*, ³*Graduate School of Medical Sciences, Tokushima University Faculty of Medicine.*, ⁴*Institute of Advanced Medical Sciences Tokushima University*)

To understand molecular mechanisms of protein folding, we investigate the light-induced structural change of AzoGB1, a B1 domain of protein G containing an azobenzene in its helical structure. Utilizing the photoisomerization of azobenzene, folding of AzoGB1 is triggered by light and we measured the conformation change by the transient grating method. We found that the diffusion coefficient (D) of AzoGB1 increased with a time constant of 1 ms upon photoexcitation, which is attributed to the folding reaction. In the presence of SecB (a molecular chaperone from bacteria), D changed in two phases (slight decrease (200 μ s) and significant increase (17 ms)). SecB may bind unfolded AzoGB1 to prevent aggregation and the folding requires the dissociation from SecB.

[2-04-1824](#) MSDC-MD によるカルシウム結合タンパク質の自由エネルギー解析
Free-energy analysis of Calmodulin (calcium ion binding protein) using MSDC-MD

Hiroimitsu Shimoyama, Yasuteru Shigeta (*CCS, Univ. Tsukuba*)

Calmodulin (CaM) is a multifunctional calcium-binding protein, which regulates various biochemical processes. CaM acts via structural changes and complex forming with its target enzymes. CaM has two globular domains (N-lobe and C-lobe) connected by a long linker region. Upon calcium binding, the N-lobe and C-lobe undergo local conformational changes, after that, entire CaM wraps the target enzyme through a large conformational change. However, the regulation mechanism is still unclear. In order to clarify the allosteric interactions, in this study, multi-scale divide-and-conquer molecular dynamics (MSDC-MD) was used to analyze the free energy landscape of CaM. The analysis showed the thermodynamics of CaM.

[2-05-1315*](#) 長鎖 DNA では発現活性が増大する・無細胞系発現系での検証
Longer DNA enhances the efficiency of cell free-gene expression

Takashi Nishio¹, Yuko Yoshikawa¹, Kenichi Yoshikawa¹, Shin-ichi Sato² (¹*Faculty of Life and Medical Sci., Doshisha Univ.*, ²*Institute for Chem. Res., Kyoto Univ.*)

We will report our experimental observation concerning the length dependence on the activity of cell-free gene expression. It is found that longer DNA molecules exhibit significantly greater potency in gene expression; for example, the expression level for DNA with 25.7 kbp is 1,000-times higher than that for DNA of 1.7 kbp. AFM observation indicates that longer DNA takes shrunken conformation with a higher segment density in the reaction mixture for gene expression, in contrast to the stiff conformation of shorter DNA. We will discuss the mechanism for the favorable effect of longer DNA on gene expression in terms of the enhancement of access of RNA polymerase to the shrunken conformation. Reference T. Nishio, et al., *Sci. Rep.* **11**, 11739 (2021).

[2-05-1327*](#) DNA 演算とナノポア計測による癌特異的 microRNA 発現上昇・低下のパターン認識
Nanopore decoding for DNA-computed microRNA patterns involving over and under-expression

Sotaro Takiguchi, Ryuji Kawano (*Dep. of Biotech. and Life Sci., Tokyo Univ. of Agri. and Tech.*)

DNA computing has been expected to expand the research field from mathematical computation to diagnostic application. However, the conventional approach to decode the output information from molecules to a human-recognizable signal required time consuming processes or fluorescence detection. We have recently proposed the method for rapid and label-free decoding of oligonucleotides in mathematical DNA computation using nanopore technology. Here, as a real-life application of our proposed methodology, we describe the pattern recognition of microRNA, which is a promising biomarker with cancer type-specificity. We were successful in simultaneous monitoring of over and under-expression of 2 individual microRNAs, showing feasibility as a tool for rapid cancer diagnosis.

[2-05-1339*](#) レーンスイッチメカニズム：DNA トランスロケースによるヌクレオソームリポジショニング
The lane switch mechanism: Nucleosome repositioning induced by a DNA translocase

Fritz Nagae, Giovanni Brandani, Shoji Takada, Tsuyoshi Terakawa (*Grad. Sch. Sci, Kyoto Univ.*)

During eukaryotic DNA transactions such as transcription, DNA replication, and DNA repair, various translocases inevitably encounter a nucleosome. Previous single-molecule experiments have shown that a translocase causes downstream nucleosome repositioning after the collision. However, its molecular mechanism has not been identified. Thus, we performed coarse-grained molecular dynamics simulations of the collision between a model translocase and a nucleosome. Based on the results of the simulations, we propose that the translocase induces downstream nucleosome repositioning by a lane-switch mechanism. Biochemical experiments further support the simulation results. This novel mechanism improves the molecular understanding of DNA transaction on nucleosomal DNA.

[2-05-1351*](#) 真核生物の転写開始複合体における DNA 開裂過程の調査
Investigation of DNA opening process in eukaryotic transcription initiation complexes

Genki Shino, Shoji Takada (*Div. of Bio. Sci., Grad. Sch. of Sci., Kyoto Univ.*)

The molecular mechanism of transcription initiation process has been actively studied by using cryo-electron microscopy and biochemical experiments. The transcription of eukaryotic protein-coding genes results from forming transcription initiation complex on the promoter DNA, consisting of RNA polymerase II and the six general transcription factors (TFIIA, B, D, E, F, and H), and DNA opening mainly by TFIIF including ATP-dependent translocase. However, the details of DNA opening are unclear. To address this problem, we performed multiscale (coarse-grained and all-atom) molecular dynamics simulations, and investigated how DNA in transcription initiation complex opens.

[2-05-1403*](#) DNA ハイブリダイゼーションのキネティックな制御
Kinetic control of DNA hybridization

Hiroyuki Aoyanagi¹, Shinji Ono¹, Simone Pigolotti², Shoichi Toyabe¹ (*¹Grad. Sch. Eng., Univ. Tohoku, ²OIST*)

Accurate binding between molecules is crucial in biotechnology. For example, in PCR, the binding of mismatched primer results in false-positive. The mismatch has lower stability than the complementary binding. A standard way to improve the hybridization fidelity is to slow down the irreversible reaction after the binding so that the binding equilibration proceeds. However, this approach reduces the performance. Here, we propose a novel kinetic approach that circumvents this trade-off between speed and fidelity. We demonstrate that a simple mechanism, which just adds a third blocker strand, drastically reduces the hybridization error without performance loss. We also apply the method to the COVID-19 assay.

[2-05-1415*](#) DNA-polymer emulsions: self-assembly and purification of DNA structures

Marcos Masukawa¹, Fujio Yu¹, Yusuke Sato², Kanta Tsumoto³, Kenichi Yoshikawa⁴, Masahiro Takinoue¹
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The cell nucleus is characterized by the confinement of DNA in the presence of proteins which yield tertiary and quaternary structures to the genome. The structures are associated with transcription regulation and are therefore an important part of cell biology. Confinement and crowding effects can be modeled by DNA-polymer systems. We observed that DNA self-assembled structures, depending on their size and shape, partition into specific portions of aqueous-aqueous emulsions formed by polymers dextran and polyethylene glycol(PEG). The preferential partition of DNA demonstrates a simple model of DNA organization based on phase separation and was applied for self-assembly and purification of DNA structures.

[2-05-1427*](#) Cancer diagnosis based on identifying miRNAs with DNA computing droplets

Jing Gong¹, Nozomi Tsumura², Yusuke Sato³, Masahiro Takinoue² (*¹School of Life Science and Technology, Tokyo Institute of Technology, ²School of Computing, Tokyo Institute of Technology, ³Frontier Research Institute for Interdisciplinary Sciences, Tohoku University*)

Nucleic acid-sensing plays an essential role in the diagnosis of a variety of diseases. It has shown that biopolymer assemblies such as liquid-liquid phase separation (LLPS) are crucial for intracellular sensing and activation/inactivation of reactions. In addition, DNA nanotechnology has led to the discovery of DNA droplets and the ability to control dynamics such as phase separation by sequence design. Here, we developed a DNA computing droplet with a nucleic acid-sensing function that recognizes miRNAs, which are expected to be applied to cancer diagnosis. The DNA droplets were modified with nucleic acids. As a result, reactions with the target molecules cause phase separation of the DNA droplets, and the presence or absence of the target can be determined.

[2-05-1439*](#) 分子ネットワークのボトムアップ構築のための RNP 分子集合体の設計と制御技術の研究
Development of design and control techniques of RNP molecular assemblies for bottom-up construction of molecular networks

Kazuya Ankai¹, Shin-ichiro M. Nomura¹, Hirohisa Ohno², Hirohide Saito² (¹*Dept. Robotics, Tohoku Univ.*, ²*CiRA, Kyoto Univ.*)

Recently, live cells are gradually known they use compartments not only separated by membrane but also the molecular droplets, such as P granules. These structures have accessibility between external and internal environment and make local nonuniform state in cells. In addition, it is reported that some proteins and nucleic acids self-assembly to form droplets via multipoint interactions. However, it is unclear what molecular properties and structural requirements of assembled structure are needed to decide a property in detail. Here, we study RNA and Protein's molecular design to identify parameters to decide such properties and establish the technique for control the droplet. We will report about the result of molecular self-assembly with the designed molecules.

[2-05-1451*](#) クライオ電子顕微鏡単粒子解析を用いたリボソームを標的としたアミノ配糖体抗菌薬の新規作用機序の解明
Elucidation of new action mechanism of aminoglycoside antibiotics on ribosomes using single particle cryo-electron microscopy

Junta Tomono¹, Kosuke Asano¹, Masato Suzuki², Takeshi Yokoyama¹, Yoshikazu Tanaka¹ (¹*Grad. Sch. Life Sci., Tohoku Univ.*, ²*AMR Research Center, National Institute of Infectious Diseases*)

Aminoglycoside antibiotics (AGs) are one of the most major clinically used antibiotics. In general, AGs bind to the decoding center of 16S ribosomal RNA and lead to the misreading of mRNA to cause bactericidal action. In the clinical site, some semi-synthetic AGs show high antimicrobial activities. However, the reason why these antibiotics show high activities have remained unexplained. We investigated the effects of these semi-synthetic AGs to the translation system using cell-free translation system. Interestingly, one of these AGs inhibited translation strongly. Therefore, we visualized how this AG inhibits translation of ribosome using cryo-electron microscopy (cryo-EM). Cryo-EM structure revealed that tRNA stalled at the new position.

[2-05-1503](#) 側方相分離が誘起するカプセル様 DNA ハイドロゲル表面のパターン形成
Lateral phase separation of DNA nanostructures that induces pattern formation on capsule-like DNA hydrogels

Sato Yusuke^{1,2}, Masahiro Takinoue² (¹*FRIS, Tohoku Univ.*, ²*Dept. Comput. Sci., TokyoTech*)

Phase separation is a key phenomenon in artificial cell studies. As a compartmental capsule is an essential cell structure, many studies have focused on the lateral phase separation of lipid vesicles. Here, we report the lateral liquid-liquid phase separation of DNA nanostructures that leads to the pattern formation on capsule-like DNA hydrogels. The hydrogels formed on a water-in-oil droplet interface exhibited various patterns by the phase separation. The appearance frequency of the patterns was altered by changing the mixing ratio of the nanostructures. We envision that by incorporating various DNA nanodevices into DNA hydrogel capsules, the capsules can be used as a chassis for functional artificial molecular systems.

[2-05-1515](#) Gold nanoparticle modification of DNA gel for remote control with radiofrequency magnetic field

Yoshiaki Sano (*Department of Life Science and Technology, School of Life Science and Technology, Tokyo Institute of Technology*.)

Numerous techniques for creating molecular robots have already been reported. However, the molecular robots fabricated so far are only capable of performing one or two steps of a chemical reaction. One of the reasons for this is that the rate of biochemical reactions is too slow to be controlled by molecular robots alone. In this study, we will construct and evaluate a remote-control system that can change the morphology of a DNA gel modified with gold nanoparticles (GNPs) by externally irradiating it with the radiofrequency magnetic field (RFMF). This technology is expected to serve as a bridge between the chemical field, which deals with soft matter such as DNA, and engineering fields such as electricity, information, and control.

[2-05-1527](#) DNA 反応拡散系によるパターン形成のカスケード化
DNA-based reaction-diffusion system for cascaded pattern formation

Keita Abe¹, Satoshi Murata¹, Ibuki Kawamata^{1,2} (¹*Grad. Sch. Eng., Univ. Tohoku*, ²*Univ. Ochanomizu*)

Inspired by pattern formation in nature, we propose a DNA-based reaction-diffusion system for cascaded pattern formation. In this system, two types of DNA molecules diffusing from two sources meet at the midpoint and polymerize there. This process is used to accumulate molecules there (bisector formation). The position where the bisector appears can be varied by adjusting the length of the DNA, and multiple bisector formations can be superimposed using orthogonal sequences. Furthermore, by making it so that another molecule is released as two molecules polymerize, it is possible to make the pattern formation cascaded. We will report the results of experiments and reaction-diffusion simulations demonstrating pattern formation in hydrogels and highly viscous media.

[2-05-1600](#) アミノ酸のアロマフィリシティ・インデックス：芳香族表面に対するタンパク質の親和性の予測
Aromaphilicity index of amino acids: Prediction of protein binding affinity for aromatic surfaces

Atsushi Hirano¹, Tomoshi Kameda² (¹*NMRI, AIST*, ²*AIRC, AIST*)

Conventionally, hydrophilicity and hydrophobicity have been used as indices for describing characteristics of amino acids. This study introduces a new index—aromaphilicity (aromatic-loving nature) index—of amino acids. This index reflects the affinity of the amino acid side chains for aromatic carbon surfaces, such as graphene and carbon nanotubes, which was quantified by molecular dynamics simulations. This index was successfully correlated with the experimentally determined affinities of amino acids for aromatic carbon surfaces ($R^2 = 0.8$). It appeared that aromatic amino acids and arginine have especially high aromaphilicity index values. This index is used as a tool for visualizing and predicting the affinity hot spots of protein surfaces for the aromatic surfaces.

[2-05-1612](#) アミロイド凝集反応におけるダイナミクスと凝集形態に及ぼす超音波キャビテーション効果について
Ultrasonic-cavitation effects on morphology and kinetics of amyloidogenic aggregation reaction

Hajime Toda¹, Kichitaro Nakajima², Keiichi Yamaguchi², Hirotsugu Ogi¹, Yuji Goto² (¹*Grad. School Eng., Osaka Univ.*, ²*Global Center for Med. Eng. Info., Osaka Univ.*)

Experimental studies on amyloid-fibril formation have been limited by a long reaction time resulted from the high-energy barrier for nucleation. Ultrasonication to protein solutions is an effective method to accelerate the fibril-formation reaction. However, ultrasonic effects on the fibril-formation reaction remain unclear in detail. In this study, we systematically investigated the aggregation reaction of b2-microglobulin, which is related to dialysis-related amyloidosis, using a laboratory-built ultrasonic instrument. Comparing the results under ultrasonic and traditional shaking agitations revealed that ultrasonication highly accelerated the fibril formation, especially for dilute monomer solutions, and improved the detection limit of the amyloid-fibril seeds.

[2-05-1624](#) Helix nucleation facilitated by the closed loop structure

Yuki Yanagida, Kiyomi Yoshida, Kazuo Fujiwara, Masamichi Ikeguchi (*Dept. Biosci., Soka Univ.*)

CHIBLAF is a fragment of β -lactoglobulin corresponding to the residue 97-142. It has a disulfide bond (Cys106-Cys119) and forms α -helices in the 98-107 and 114-135 regions. It has been shown that the helices are destabilized when the disulfide bond is cleaved. From this result, we assumed that the loop formation reduces the conformations that can be taken by the residues in the loop and facilitates the nucleation of the helix. To prove this hypothesis, we constructed the three derivatives in which 1, 3, or 7 Gly residue(s) was (were) inserted between the residues 109 and 110. The CD spectrum showed that the helix content decreased as the number of inserted Gly. NMR showed that the helix regions were identical with those of CHIBLAF, supporting our hypothesis.

[2-05-1636](#) Photocontrol of the small G-protein H-Ras GTPase activity using thiol reactive photochromic compounds incorporated into the HVR domain

Nahar Rufiat, Shinsaku Maruta (*Department of Bioinformatics, Soka University, Japan*)

Ras superfamily functions as biomolecular switches in cellular signal transduction. Ras forms nanocluster on the plasma membrane by the HVR at C-terminal which provides site for effectors. First, we have observed the GTPase activity of NBB modified HVR domain of Ras which shows lower GTPase activity. Simultaneously, we tried to photocontrol HVR domain by incorporating the azobenzene derivatives (PAM) which reversibly regulate the GTPase activity by photoirradiation. Interestingly, Cis state of PAM modified H-Ras showed lower GTPase activity and multimer formation which is consistent with NBB modified H-Ras. In this study, we have demonstrated the photocontrol of HVR domain using azobenzene derivatives in the presence of GEF and GAP.

[2-05-1648](#) タンパク質のローカルな静電ポテンシャルを用いたプロトンの濃度勾配調節機能
Regulation of proton concentration gradient by local electrostatic potential of proteins

Kaori Chiba (*Natl Inst. Tech, Ibaraki Col.*)

The planarity of peptide bonds connecting the main chain of a protein is an essential constraint for structural analysis. We have conducted several experimental approaches using proteins to show that the physical properties of peptide bonds in a protein molecule may change individually depending on the intramolecular electrostatic potential. On the other hand, using small molecule, kinetic experiments have shown that the planarity of peptide bonds relaxes in environments with high proton concentrations. Based on these findings, we propose a new model in which a single peptide bond at the entrance of the mitochondrial proton pump regulates the opening and closing of the channel depending on the proton concentration at the intermembrane site.

[2-05-1700](#) 海洋性ビブリオ菌極べん毛遺伝子のマスターレギュレーター FlaK の機能と生化学的性質
Functional and biochemical characterization of FlaK, a master regulator for the polar flagellar genes of *Vibrio alginolyticus*

Tomoya Kobayakawa, Seiji Kojima, Michio Homma (*Grad. Sch. Sci., Univ. Nagoya*)

Vibrio alginolyticus has a single polar flagellum, whose genes are encoded in a regulon with four transcriptional hierarchies. FlaK, which belongs to the first hierarchy and an ATPase, works as the master regulator. However, how FlaK regulates the synthesis of a single polar flagellum has remain unclear. Here, we made six mutants based on the insight from *Pseudomonas* FleQ, an ortholog of FlaK, and analyzed their motilities. We also purified FlaK, and their ATPase activities and multimeric structures were examined. As a result, we found that FlaK mutants that abolished motility lost their ATPase activity and hexamer formation. Consistent with those, an ATPase activity of wild-type FlaK was reduced in the presence of FlhG, a negative regulator for flagellar biogenesis.

[2-05-1712](#) Molecular mechanism of glycolytic flux control intrinsic to human phosphoglycerate kinase

Hiromasa Yagi¹, Takuma Kasai¹, Elisa Rioual¹, Teppei Ikeya², Takanori Kigawa¹ (¹*BDR, RIKEN*, ²*Grad. Sch. Sci., Tokyo Metropolitan Univ.*)

Control of glycolytic flux plays an important role in the energy production and metabolic homeostasis in cells. Phosphoglycerate kinase (PGK) catalyzes the reversible phosphotransfer to generate 3-phosphoglycerate (3PG) and ATP in glycolysis. PGK controls glycolytic flux according to the intracellular [ATP]/[ADP] ratio; however, its molecular mechanism remains unknown. Herein, we report a protein-level regulation of human PGK reaction by switching ligand-binding cooperativities between adenine nucleotides and 3PG, which is finely tuned to appropriately respond to the changes in the intracellular [ATP]/[ADP] ratio. Our findings reveal a molecular mechanism intrinsic to human PGK controlling glycolytic flux by rapid adaptation to changes in the intracellular environment.

[2-05-1724](#) SARS-CoV-2 の RNA 依存性 RNA ポリメラーゼにおけるリジン残基による「バケツリレー」リガンド輸送
"Bucket brigade" ligand transportation by lysine residues in RNA-dependent RNA polymerase of SARS-CoV-2

Shoichi Tanimoto¹, Satoru Itoh^{1,2,3}, Hisashi Okumura^{1,2,3} (*¹IMS, ²EXCELLS, ³SOKENDAI*)

The RNA-dependent RNA polymerase (RdRp) of SARS-CoV-2 is a promising drug target for COVID-19 because it plays an important role in the RNA replication. Remdesivir and favipiravir are expected to be recognized by RdRp and inhibit the RNA replication. However, the recognition process of these compounds remains unknown. To clarify the recognition mechanism, we performed molecular dynamics simulations for RdRp with these compounds and adenosine triphosphate located far away. We identified three recognition paths commonly found in all ligands. It was also observed that lysine residues of RdRp carried the ligands to the binding site like a "bucket brigade". Our findings contribute to the understanding of the efficient ligand recognition by RdRp at the atomic level.

[2-05-1736](#) カメレオンモデルによるアデニル酸キナーゼの構造転移の研究
A study on the conformational transition of adenylate kinase by the chameleon model

Itsuki Yoshida, Masaki Sasai, Tomoki P. Terada (*Dept. Appl. Phys., Grad. Sch. Eng., Nagoya Univ.*)

Chameleon model is the model for description of two-state conformational transition of proteins. In the model, the interaction between residues changes depending on how similar the environment around the residues is to one state and the other state. We applied the model to the conformational transition of adenylate kinase. We calculated the rates of conformational transition from the free energy difference between fully closed state and transition state which is the rate-limiting step of the enzymatic activity. We found that the temperature dependence of calculated conformational transition rates is similar to that of experimental enzymatic activity, showing that chameleon model gives a good approximation of free energy landscape of conformational transition.

[2-05-1748](#) ローダミンファロイジン標識アクチンフィラメントにおける蛍光強度の時空間的ゆらぎ
Spatiotemporal fluctuations in fluorescence intensity of rhodamine phalloidin-labeled actin filaments

Kenta Toshino, Yosuke Yamazaki, Taro Q.P. Uyeda (*Dept. Physics, School of Advanced Science and Engineering, Waseda Univ.*)

Actin filaments have multiple semi-stable conformations (Kozuka et al., 2005). We found that actin filaments labeled with rhodamine phalloidin have bright and dark regions on the micrometer order along the length, and the fluorescence intensity changes reversibly on the sub-second order. This phenomenon requires intense illumination and observation in a solution containing glucose, glucose oxidase and catalase. Similar fluorescence fluctuation was not observed when NHS-rhodamine was directly attached to aminosilane on the glass surface. Thus, this spatiotemporal fluorescence fluctuation may be caused by changes in the surrounding environment of rhodamine due to the cooperative structural polymorphism of actin filaments and the transition among the structures.

[2-05-1800](#) コレステロールと γ 切断酵素の基質結合部位との相互作用
Interaction Between Cholesterol and Substrate Binding Sites of γ -secretase

Chika Minami, Naoyuki Miyashita (*Grad. Sch. BOST, KINDAI Univ.*)

A γ -secretase (γ -s) has been known as one of the aspartic proteases. It cleaves various membrane proteins such as amyloid precursor protein (APP) and Notch related to signal transduction. The γ -s and these proteins make heterodimerization. Our recent research has suggested that lipids and cholesterol assist the dimerization of several membrane proteins in the membrane. To understand the mechanism of the lipids assisting the heterodimerization of APP/Notch and γ -s, we performed the coarse-grained molecular dynamics simulations of the γ -s, the complex of the γ -s and APP, and the complex of the γ -s and Notch. We found a cholesterol bind to the substrate-binding site of γ -s, and it might induce the interaction between the γ -s and APP/Notch.

[2-05-1812](#) Expression and purification of the antimicrobial peptide cryptdin family in *Escherichia coli* by enhancing inclusion body formation

Yuchi Song, Shaonan Yan, Yi Wang, Wendian Yang, Weiming Geng, Tomoyasu Aizawa (*Grad. Sch. of Life Sci, Hokkaido Univ*)

The cryptdin (crp) is an antimicrobial peptide found in mouse small intestine and there are six isoforms. For production of recombinant crp by *E. coli* with avoiding undesirable degradation, co-expression with an aggregation prone partner protein were used for accelerating the formation of stable inclusion body. For improving the expression efficiency of all crps, OrigamiB strain was used to enhance the formation of inter-molecular disulfide bridges between the partner and target protein. By this method we could obtain inclusion bodies contain large amount of crps. After separation from the partner protein by using cIEX crps were successfully refolded in vitro. In conclusion, we developed a method for the expression and purification of the crps in *E. coli*.

[2-05-1824](#) Multiple bactericidal actions of cryptdin-4 and its reduced form via oxidative stress and membrane disruption

Yi Wang, Yuchi Song, Rina Hiramane, Tomoyasu Aizawa (*Grad. Sci. Life Sci., Hokkaido Univ.*)

Cryptidin-4 (crp4) is an enteric α -defensin, the main effector of oral infections, and defines the ileal microbiota composition. In this study, the role of reactive oxygen species in the antibacterial action of crp4 was studied by the effects of antioxidants on crp4 susceptibility of *E. coli*. Among the antioxidants checked, all provided substantial protection against oxidized crp4 (crp4oxi) only. Membrane permeabilization assay demonstrated that reduced crp4 (crp4red) killed bacteria by the formation of pores or channels for ion losing without affecting the integrity of bacteria through deep insertion into or integration with the cell membrane. Our results confirmed the multiple actions involved in the actions of crp4 on bacteria killing.

[2-06-1315*](#) リン脂質二重膜に再構成したアーキロドプシン-3(AR3)の四次構造と光サイクル
Quaternary structure and photocycle of archaerhodopsin-3 (AR3) reconstituted in phospholipid bilayer membrane

Rio Kikuchi¹, Fumio Hayashi², Kiiichi Inoue³, Masashi Sonoyama^{1,4,5} (¹*Grad. Sch. Sci. Tech., Gunma Univ.*, ²*Ctr. Inst. Anal. Gunma Univ.*, ³*ISSP, Univ. Tokyo*, ⁴*GLAR, Gunma Univ.*, ⁵*GUCFW, Gunma Univ.*)

Archaerhodopsin-3 (AR3) is a membrane protein closely related to bacteriorhodopsin (bR). Few previous studies on AR3 reconstituted in phospholipid bilayer have been reported so far. In this study, structural and functional properties of AR3 reconstituted in ester-linked DMPC vesicles were investigated with visible CD and transient absorption spectroscopies. A biphasic CD pattern of reconstituted AR3 remained unchanged even after the gel-to-liquid crystalline phase transition, indicating that AR3 molecules retain their oligomeric structures even in the fluid phase, which strikingly contrasts with the phase transition-induced disassembly of bR trimers. We will all so report experimental results on reconstituted AR3 in ether-linked and partially fluorinated phospholipids.

[2-06-1327*](#) リン脂質二分子膜及び可溶性状態におけるプロテオロドプシンの多量体構造や光サイクルの比較研究

A comparative study of oligomeric states and photocycle of proteorhodopsin in phospholipid bilayer membranes and detergent micelles

Yuka Shinohara¹, Airi Yamamoto¹, Fumio Hayashi², Takashi Kikukawa³, 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*GLAR, Gunma Univ.*, ⁵*GUCFW, Gunma Univ.*)

Proteorhodopsin (PR) is an outward light-driven proton pump, similar to bacteriorhodopsin (bR), a well-studied microbial rhodopsin. A limited number of previous works on oligomeric states and photocycle of PR in phospholipid membranes have been reported. In this study, effects of lipid environments on structural and functional properties were investigated for PR in POPC and DMPC liposomes and DDM micelles using CD and laser flash photolysis measurements. Analogous visible CD patterns were observed for every sample, showing a similar quaternary structure, irrespective of lipid environments. On the other hand, transient absorption changes differ depending on lipid environments, including the phase behaviors of phospholipid bilayers.

[2-06-1339*](#) Effect of acidity and salt concentration on functional properties of Na⁺ pump rhodopsin from *Indibacter alkaliphilus*

Shingo Yoshizawa¹, Takashi Kikukawa², Fumio Hayashi³, Masashi Sonoyama^{4,5} (¹*Grad. Sch. Sci. Tech., Gunma Univ.*, ²*Fac. Adv. Life Sci., Hokkaido Univ.*, ³*Inst. Anal. Cent., Gunma Univ.*, ⁴*GIAR, Gunma Univ.*, ⁵*GUCFW, Gunma Univ.*)

Na⁺ pump rhodopsin (NaR), a recently identified microbial rhodopsin, has the function of outward Na⁺ transport. Because of its unique properties, NaR is now attracting much more attention as a tool for optogenetics, and detailed analyses of its function have been extensively performed. In the present study, we examined functional properties of NaR from *Indibacter alkaliphilus* (IaNaR) under various pH/salt concentrations using circular dichroism and transient absorption measurements. It was elucidated that the oligomeric state of IaNaR, which is dependent on the acidity and salt concentration, affects the ion transport function. Furthermore, the structural stability of IaNaR depending on the oligomeric state will also be discussed.

[2-06-1351*](#) 擬環状エーテル型脂質の部分フッ素化が膜物性に及ぼす影響
Effects of partial fluorination of phospholipids bearing a single membrane-spanning chain on membrane properties

Kanako Shimamoto¹, Rui Kawahara¹, Naoyuki Tsuchida¹, Toshiyuki Takagi², Hiroshi Takahashi¹, Hideki Amii^{1,3}, Masashi Sonoyama^{1,3,4} (¹*Grad. Sch. Sci. Tech., Gunma Univ.*, ²*AIST, GIAR, Gunma Univ.*, ⁴*GUCFW, Gunma Univ.*)

Double-stranded macrocyclic tetraether lipids are major components of the plasma membranes of archaea. We have developed an amacrocyclic tetraether phospholipid AC-(di-*O*-C14PC)₂ as a biomimetic material, which exhibited significant membrane properties different from ordinary bilayers. In this study, a partially fluorinated phospholipid AC-(F4-di-*O*-C14PC)₂ was developed by introducing a perfluorobutyl group into the terminal of the tetradecyl chain in AC-(di-*O*-C14PC)₂. The novel AC-(F4-di-*O*-C14PC)₂ membrane showed remarkably lower T_m than AC-(di-*O*-C14PC)₂. Experimental results on another novel partially fluorinated phospholipid, in which the perfluoroethyl group is introduced in the central part of the cross-linked chain, will also be discussed.

[2-06-1403*](#) 全反射赤外分光法による kappa-オピオイド受容体のリガンド認識機構研究
ATR-FTIR study of ligand recognition on kappa opioid receptor

Seiya Iwata¹, Kohei Suzuki¹, Kota Katayama¹, Ryoji Suno², Chiyo Suno², Takuya Kobayashi², Koichi Tsujimoto³, So Iwata³, Hideki Kandori¹ (¹*Grad. Sch. Eng., Tech. Inst. Nagoya*, ²*Grad. Sch. Med., Univ. Med. Kansai*, ³*Grad. Sch. Med., Univ. Kyoto*)

Perfusion-induced difference attenuated total reflection-Fourier transform infrared (ATR-FTIR) spectroscopy is a promising approach for investigating ligand recognition of G protein-coupled receptors (GPCRs). We have recently employed this technique on muscarinic receptor to reveal its ligand binding mechanism. Here, we apply for kappa opioid receptor (KOR) that is an important drug target for diseases involving mood and reward because some KOR ligands offer the potential to overcome negative side effect. Our FTIR study of KOR-ligand interaction provides different conformational changes between KOR selective antagonist (JDTic) and agonist (U-50488). By measuring and comparing of other important ligands, we will discuss the molecular mechanism of ligand recognition.

[2-06-1415*](#) アクチノバクテリア門の細菌がもつ新規ロドプシン群
A novel cluster of microbial rhodopsin present in terrestrial *Actinobacteria*

Mako Ueno¹, Fumio Hayashi², Takashi Kikukawa³, 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 recent 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 novel rhodopsins encoded in terrestrial bacteria. As a result, we identified 90 sequences, all of which are included in a novel cluster distinct from already-known microbial rhodopsins in the phylogenetic tree. The identified sequences are mainly encoded in terrestrial *Actinobacteria* and commonly have longer C-terminus. Clarified functions and structures of the identified sequences would broaden our knowledge of bacterial habitat and adaptability.

[2-06-1427*](#) Heterotrimer formation of MdtB and MdtC, transporter components of the bacterial xenobiotic efflux complex

Kenichiro Kashihara¹, Hirotaka Tajima^{2,3}, Masatoshi Nishikawa³, Yoshiyuki Sowa^{1,2,3}, Ikuro Kawagishi^{1,2,3} (¹*Grad. Sch. Eng., Hosei Univ.*, ²*Res. Cent. Micro-Nano Tech.*, ³*Dept. Front. Biosci.*)

Among the five RND-type xenobiotic efflux systems of *Escherichia coli*, TolC-MdtABC is unique in that it has two inner membrane transporter (IMT) components, MdtB and MdtC. Although IMT generally exists as homotrimers, they are supposed to form heterotrimers because among genetically manipulated tandem-linked trimers, only MdtBBC is active in drug efflux. Here we visualized freely diffusible MdtB and MdtC by tagging them with GFP and tagRFP. When expressed alone, MdtB forms a homotrimer but MdtC does not. When expressed together, heterotrimers, MdtBBC and MdtBCC, were preferentially formed, in addition to the MdtBBB homotrimer. These results are consistent with the previous study, but the detection of MdtBBB raises the possibility that it has some physiological role.

[2-06-1439*](#) 非天然基質の触媒を実現するシトクロム P450BM3 の酸化型中間体の構造解析
Structure of a heme-oxy intermediate of cytochrome P450BM3 catalyzing a non-natural substrate

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P450BM3 is known as a biocatalyst that can activate C-H bonds of various non-natural substrates by incorporating inert dummy substrates ("decoy"). To expand its biotechnological application, it is desirable to achieve efficient molecular design of decoy molecules based on dynamic protein structures. Here, we determined a structure of the initial intermediate, a heme-oxy species with a decoy and styrene (non-natural substrate). Microcrystals were used for freeze-trapping the intermediate under air atmosphere. We found that O₂ binding causes rearrangement of styrene to an optimal orientation, though the electron density of O₂ was somewhat distorted due to X-ray radiation damage. The damage-free structural analysis of the intermediate using SACLA is currently underway.

[2-06-1451*](#) Conformational dynamics of *E. coli* Cytidine Repressor DNA Binding domain studied by Single-molecule Fluorescence Spectroscopy

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E. coli cytidine repressor (CytR) regulates multiple operons and has very broad DNA specificity. Albeit earlier ensemble level studies revealed multiple conformations for its DNA binding domain (CytR-DBD), properties both in DNA-free and bound conditions are still unclear. Here by single-molecule FRET, we studied CytR-DBD conformational dynamics at the single-molecule level. Results at various ionic strengths and denaturant conditions prove both tertiary structural interactions and positively charged amino acids control its conformational dimensions. Single-molecule binding assays with a broad range of DNA sequences indicate that DNA's negative surface potential screens unfavorable electrostatic repulsions and changes its conformational landscape non-specifically.

[2-06-1503*](#) 全原子分子動力学シミュレーションによるヒト L 型アミノ酸トランスポーター LAT1-CD98hc 複合体の構造変化と輸送機序の解明
Transport mechanism of human LAT1-CD98hc complex studied by all-atom MD

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The L-type amino acid transporter 1 (LAT1) transports large neutral amino acids across the membrane. Because LAT1 is overexpressed in tumor cells and contributes to the supply of essential amino acids, LAT1 is a pharmaceutical target of cancers. Upon the substrate transport, LAT1 is considered to undergo conformational changes between the outward-facing (OF) and the inward-facing (IF) states. Recently, both the OF and IF conformations have been solved using cryo-EM, and however, the detailed mechanism underlying the transport has not been understood. To elucidate the transport mechanism coupled with the conformational changes, substrate transport simulations were performed using all-atom molecular dynamics (MD) simulations.

[2-06-1515*](#) (1S6-4) 分子シミュレーションによるオレキシン 2 受容体-G タンパク質複合体の動的性質の研究 (1S6-4) Dynamics of Orexin2 Receptor and G-protein Complex with Molecular Dynamics Simulations

Shun Yokoi, Ayori Mitsutake (*Department of Physics, School of Science and Technology, Meiji University*)

Orexin2 receptor (OX2R) is classified as a class A G-protein-coupled receptor (GPCR) and belongs to the group of orexinergic systems. The OX2R is involved in the regulation of feeding behavior and sleep-wake rhythm to give some examples. Such kinds of neurological processes are caused by GPCR activation. Although the structure of the OX2R has been clarified, the atomic-level mechanisms of GPCR and G-protein activation remain unknown. Here, we performed and analyzed several microsecond-scale molecular dynamics (MD) simulations. In this poster, we first show the results of the MD simulations and investigate the dynamics of OX2R and G-protein complex. Then, we discuss implications for the activation mechanism of OX2R and for the binding mechanism of G-protein.

[2-06-1600](#) 大腸菌 UvrD C 末端アミノ酸欠損変異体の DNA 巻き戻しダイナミクス
DNA-unwinding dynamics of *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 which plays a crucial role in nucleotide excision repair and methyl-directed mismatch repair. 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 already reported in the past annual meetings 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 report that a UvrD mutant lacking longer C-terminal amino acids can still oligomerize and unwind DNA.

[2-06-1612](#) 悪性高熱症を引き起こす RyR1 チャンネル中間領域変異による細胞の高熱感受性
Cellular heat hypersensitivities caused by mutation in the middle region of the RyR1 channel implicated in malignant hyperthermia

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Malignant hyperthermia (MH) is a life-threatening disease triggered by, e.g., inhalant of anesthetic gases. Mutations in Ca²⁺ release channels ryanodine-receptor-type-1 (RyR1) causes MH, leading to uncontrollable Ca²⁺ release and thermogenesis in skeletal muscles. However, it is still unknown how only one mutation changes the whole protein function. We have recently found the variety of heat hypersensitivities in the RyR1 mutants of MH overexpressed in HEK293 cells using an optically controlled local heat pulse method [Oyama, bioRxiv (2020)]. Here, to explore the influence of mutations at the middle region that a mouse model has been established [Yamazawa, Nat. Commun. (2021)], we examined the heat hypersensitivities of those RyR1 mutants in the HEK293 cell system.

[2-06-1624](#) 一分子蛍光測定を用いた SARS-CoV-2 N タンパク質と RNA の結合様式
Structural characterization of RNA upon the binding with SARS-CoV-2 N protein by single molecule fluorescence measurements

Leo Suzuki^{1,2}, Hiroyuki Oikawa^{1,2}, Satoshi Takahashi^{1,2} (¹*IMRAM, Tohoku Univ.*, ²*Grad. Sch. Life Sci., Tohoku Univ.*)

Nucleocapsid (N) protein of SARS-CoV-2 binds to the viral genomic RNA (gRNA), forms RNA-protein complex and helps the packaging of gRNA inside of the virus. However, the detailed structural changes of N as well as gRNA upon the complex formation are largely unknown. In this investigation, we attempted to observe structural changes of a 40-base adenylic acid (polyA) upon the mixing with N. We utilized single-molecule fluorescence resonance energy transfer (sm-FRET) measurements to detect the structural transitions of the labeled polyA and the fluorescence correlation spectroscopy (FCS) to observe assembly of N protein with polyA. We observed that the shrinking of polyA by sm-FRET measurement and the association of a limited number of N to polyA by FCS.

[2-06-1636](#) Molecular mechanism of MutS sliding on DNA explored by coarse-grained molecular dynamics simulations

Keisuke Inoue, Shoji Takada, Tsuyoshi Terakawa (*Department of Biophysics, Graduate School of Science, Kyoto University*)

MutS is a protein that recognizes a DNA base-pair mismatch as the first step of the mismatch repair molecular process. MutS has ATP hydrolysis activity and changes its conformation depending on its nucleotide state. Previous experiments showed that MutS slides along DNA and searches a mismatch. However, the detailed molecular mechanism of the sliding has remained elusive. In this study, we performed coarse-grained molecular dynamics simulations of MutS sliding on DNA using experimentally solved structures of MutS bound to ATP and ADP, respectively. The simulation results shed light on the molecular mechanism of the mismatch search dynamics and its dependency on the nucleotide states of MutS.

[2-06-1648](#) Processive Motion of Lambda Exonuclease revealed by Reactive Coarse-Grained Molecular Dynamics Simulation

Toru Niina, Shoji Takada (*Grad. Sch. Sci., Univ. Kyoto*)

Biomolecular machines largely require chemical reactions as their energy source. To investigate the underlying mechanisms of their processive motion, it is inevitable to take reactions into account. Although molecular dynamics (MD) simulation is powerful tool to investigate structural dynamics at residue level, it is practically difficult to carry out a long-time MD simulation coupled with chemical reactions because of the computational cost. Here we extended a well-established coarse-grained model of DNA and protein to run MD coupled with successive chemical reactions of nucleic acid. Employing hybrid Monte Carlo/MD approach, we reproduced a processive motion of lambda exonuclease degrading a DNA strand and investigated the mechanism of its dynamics.

[2-06-1700](#) DNA 結合に伴うヘテロクロマチンタンパク質 HP1 の天然変性領域の ESR 動的構造解析
Structural Dynamics of Intrinsically Disordered Region of HP1 upon DNA Binding Studied by Spin Labeling ESR Spectroscopy

Isoa Suetake^{2,3,4}, Kazunobu Sato⁵, Risa Mutoh⁶, Yuichi Mishima², Takeji Takui⁵, Tohru Kawakami², Hironobu Hojo², Toshimichi Fujiwara², Makoto Miyata¹, **Toshiaki Arata**^{1,2} (¹*Dept. Biol., Grad. Sch. Sci., Osaka City Univ.*, ²*IPR, Osaka Univ.*, ³*Grad. Sch. Nutrition, Nakamura Gakuen Univ.*, ⁴*Twin Res. Ctr., Osaka Univ.*, ⁵*Dept. Chem., Grad. Sch. Sci., Osaka City Univ.*, ⁶*Dept. Phys., Fac. Sci., Fukuoka Univ.*)

HP1 forms a dimer of Ntail-CD-HR-CSD-Ctail *via* CSD-CSD¹. To extend our previous study², the side-chain rotational dynamics of nitroxide spin label³ at the residues of Ntail and HR IDRs in HP1 was examined and found to be extremely high and unchanged with DNA on sub-nsec time scale, but Ntail and specific region of HR were immobilized by DNA on nsec time scale in glycerol where protein-DNA affinity was strengthened. These results suggest that without glycerol Ntail and HR bind to DNA *via* only few side chains and diffuse translationally on DNA. We now determine Ctail dynamics and try IDR geometry from interspin distances 1.5-8 nm using pulsed ESR^{2,3}. 1. Mishima *et al.* NAR **43**, 10200 (2015). 2. Suetake *et al.* BBRC **567**, 42-48 (2021). 3. Arata, IJMS **21**, E672 (2020).

[2-06-1712](#) 高速原子間力顕微鏡による膜中 TRPV1 チャンネルの動態観察
Dynamics of transient receptor potential vanilloid1 (TRPV1) in lipid bilayer observed by high speed atomic force microscopy (HS-AFM)

Daichi Mukai¹, Zhao Yimeng⁴, Mikihiro Shibata^{2,3}, Motoyuki Hattori⁴, Ayumi Sumino^{2,3} (¹*Dept. of Nano Life Sci., Grad. Sch. of Frontier Sci. Initiative, Univ. Kanazawa*, ²*WPI-NanoLSI, Univ. Kanazawa*, ³*Institute for Frontier Sci. Initiative, Univ. Kanazawa*, ⁴*Sch. of Life Sci., Univ. Fudan*)

TRPV1 is a tetrameric cation channel that opens by binding of vanilloid compounds. The structure of TRPV1 in detergent has been solved by cryo-electron microscopy (cryo-EM), however, the structure of its cytoplasmic domains (CPD) in the lipid bilayer environment are still unknown. Here, we reconstituted the TRPV1 into lipid bilayer with the CPD facing upward and observed by HS-AFM. HS-AFM showed tetrameric structure of the CPD whose height from the bilayer surface was about 3.5 nm. This is smaller than the height imaged in detergent by previous cryo-EM study (~5 nm), suggesting that structure of the CPD changed by interaction with lipid bilayer. In addition, the agonist, capsazepine, suppressed the fluctuation of the CPD in both rotational and radial directions.

[2-06-1724](#) カリウムチャネル KcsA の開閉にともなう構造変化
Conformational Changes of KcsA K⁺ Channel upon Gating

Hiroko Takazaki¹, Hirofumi Shimizu², Takuo Yasunaga³ (¹*IPR, Univ. Osaka*, ²*Fac. Med. Sci., Univ. Fukui*, ³*Grad. Sch. Comp. Sci. Syst. Eng., KIT*)

KcsA is a proton-activated, voltage-modulated K⁺ channel. It has open and closed conformations under acidic and neutral conditions, respectively. KcsA structures have been solved by X-ray crystallography, but the structural changes between the two conformations were smaller than those predicted by diffracted X-ray tracking. Here, we try to elucidate the structures of KcsA under acidic and neutral conditions with suitable detergents by cryo-EM and single particle analysis. For K⁺ flow, C4 symmetry is considered to be required from the previous researches. As a result, almost all structures have C2 symmetry, whereas only one class in acidic condition adopts C4 symmetry. These changes would occur by “twisting” and/or “sliding” of transmembrane alpha-helices.

[2-06-1736](#) チトクロム酸化酵素を活性化する Higd1a の作用機序に関する分光学的研究
Spectroscopic study on the action mechanism of Higd1a for activating cytochrome c oxidase

Waka Matsumura¹, Sachiko Yanagisawa¹, Kyoko Shinzawa-Itoh¹, Yuya Nishida², Takemasa Nagao², Yasunori Shintani², Minoru Kubo¹ (¹*Grad. Sch. Life Sci., Univ. Hyogo, Japan*, ²*Molecular Pharmacology, NCVC, Japan*)

Cytochrome c oxidase (CcO) is the terminal enzyme in the mitochondrial electron transport chain, and its activity is under control through multiple mechanisms for cellular respiration. Higd1a (hypoxia-inducible domain family member 1A), a 12-kDa membrane protein, was recently identified as one of the allosteric activators of CcO in response to hypoxia; however, its action mechanism is not yet understood. Here, we applied visible absorption and resonance Raman spectroscopies to assess the structural effect of Higd1a binding on the CcO active centers. We found that Higd1a perturbed the Soret band of CcO, and it was attributable to structural alteration around heme a₃, the oxygen reduction site. Based on these results, possible action mechanism of Higd1a will be presented.

[2-06-1748](#) ストップフローラマン・吸収分光計を用いたインドールアミン 2,3 ジオキシゲナーゼの反応中間体の研究
Investigation of reaction intermediates of indoleamine 2,3-dioxygenase by using a stopped-flow Raman/absorption spectrometer

Mina Kawamura, Kaho Nasada, Sachiko Yanagisawa, Minoru Kubo (*Grad. Sch. Life Sci., Univ. Hyogo, Japan*)

Indoleamine 2,3-dioxygenase (IDO) is a heme enzyme for Trp degradation using molecular oxygen, and has been attracting attention in terms of cancer drug discovery due to the involvement in immunosuppression. However, the reaction mechanism of IDO is still unclear, because key intermediates following the binding of Trp and O₂ remain elusive on the single turnover condition. Here, we have attempted to capture the intermediates using a stopped-flow spectrometer on various reaction conditions using Trp derivatives and an effector molecule to control rate-limiting steps. Notably, a distinctive Soret change was observed when 5-Br-L-Trp was used as a substrate. To get insights into structural details of the intermediates, stopped-flow Raman measurements are currently underway.

[2-07-1315*](#) キネシン・ダイニンによる軸索輸送速度の極値統計解析
Extreme value analysis of the velocity of axonal transport by kinesin and dynein

Takuma Naoi¹, Yuki Kagawa¹, Kimiko Nagino¹, Shinsuke Niwa², Kumiko Hayashi^{1,3} (¹*Dep. Appl. Phys., Grad. Sch. Eng., Tohoku Univ.*, ²*FRIS, Tohoku Univ.*, ³*JST, PRESTO*)

Although previous studies have investigated motor differences in *in vitro* single-molecule experiments, this study aimed to discover motor differences *in vivo* as well. In particular, we focused on the synaptic cargo transport in DA9 motor neurons of *Caenorhabditis elegans*. The motion of synaptic cargos was observed by fluorescence microscopy, and the velocity was measured using kymograph analysis. Kinesin and dynein differ in structure, ATP-hydrolysis mechanism, and dynamics. Although the average velocity is sensitive to the cargo size, we consider that the results of extreme value analysis (EVA) are independent of it. We expected that EVA would reveal the characteristics of molecular motors *in vivo*.

2-07-1327* 野生型と疾患変異型から構成されるヘテロダイマー KIF1A の 1 分子解析

Single molecule analysis of heterodimers composed of wild-type KIF1A and disease-associated KIF1A

Tomoki Kita¹, Yuzu Anazawa², Kumiko Hayashi^{1,3}, Shinsuke Niwa^{2,4} (¹*Grad. Eng., Tohoku Univ.*, ²*Grad. Life. Sci., Tohoku Univ.*, ³*PRESTO., JST*, ⁴*FRIS., Tohoku Univ.*)

KIF1A is a kinesin superfamily molecular motor that transports synaptic vesicle precursors in axons. KIF1A mutations lead to a group of neuronal diseases called KIF1A-associated neuronal disorder (KAND). KIF1A forms a homodimer and KAND mutations are mostly *de novo* and autosomal dominant; however, it is not known whether the function of wild-type KIF1A is inhibited by disease-associated KIF1A. Here, we developed *in vitro* assays to analyze the motility of single heterodimers composed of wild-type KIF1A and disease-associated KIF1A. Our results demonstrate that disease-associated KIF1A significantly inhibits the motility of wild-type KIF1A when heterodimers are formed. These data indicate the molecular mechanism underlying the dominant nature of *de novo* KAND mutations.

2-07-1339* キネシンとチューブリン C 末端との間の長距離引力

Long-range attraction between kinesin and C-terminal tail of tubulin

Yuta Taguchi, Kyohei Shoji, Jun Ohnuki, Mitsunori Takano (*Dept. of Pure & Appl. Phys., Grad. Sch. Adv. Sci. & Eng., Waseda Univ.*)

Monomeric kinesin, KIF1A, moves toward the plus-end of microtubule (MT). We previously showed by coarse-grained molecular dynamics simulation that KIF1A exhibits Brownian motion along MT, which is based toward the plus-end, and found that the C-terminal tail (CTT) of tubulin plays a crucial role in generating the bias. To fully model CTT, we here used the all-atom model and investigated the free energy profile for the KIF1A-tubulin binding. We found the attraction between KIF1A and tubulin is rather long-ranged due to the fly-casting-like extension of CTT. This long-range attraction should help the long-distance Brownian motion of KIF1A and other MT-binding proteins. We also investigate how the difference of CTT between α and β tubulins affects the binding.

2-07-1351* A novel photochromic compound inhibits mitotic kinesin Eg5 in three isomerization states

Md Alrazi Islam, Shinsaku Maruta (*Grad.Sch.Eng., Soka University*)

Kinesin Eg5 is an ATP-driven motor protein that moves along microtubules. It plays a crucial role in the formation of the bipolar spindle in eukaryotic cell divisions. Therefore, kinesin Eg5 is a target for cancer therapy. It has been suggested that if small chemical compounds inhibit the activity of Eg5, it may induce an antiproliferative effect in cancerous cells. In this study, we developed a novel photochromic Eg5 inhibitor spiropyran-azobenzene derivative (SPSAB). Our experimental data demonstrated that Eg5 activity was controlled by SPSAB in three isomerization states such as SP-Trans (VIS), MC- Cis(UV), and MC- Trans (In the dark), respectively. Subsequently, we analyzed which step in the ATPase cycle is inhibited by SPSAB using mixed motor motility assay.

2-07-1403* ネガティブ染色電子顕微鏡法により明らかにされた繊毛ダイニンの新規構造

Novel isolated ciliary dynein structure revealed by negative stain EM

Yici Lei¹, Hiroshi Imai¹, Ryosuke Yamamoto¹, Rieko Shimo¹, Shinji Kamimura², Toshiaki Yagi³, Naoko Kajimura⁵, Mika Hirose⁴, Takayuki Kato⁴, Kaoru Mitsuoka⁵, Takahide Kon¹ (¹*Dept. Biol. Sci., Grad. Sch. Of Sci., Osaka Univ.*, ²*Dept. Biol. Sci., Chuo Univ.*, ³*Dept. Life Sci., Prefect. Univ. Hiroshima*, ⁴*Inst. Of Protein Res., Osaka Univ.*, ⁵*Res. Ctr. UHVEM, Osaka Univ.*)

Dyneins are phylogenetically classified into three subfamilies, ciliary, cytoplasmic and intraflagellar transport (IFT) dyneins. It is widely known that cytoplasmic and IFT dyneins adopt an inactivated conformation called the phi structure. In contrast, such a distinct inactivation state was not evident for ciliary dynein. Here we report that one of the ciliary dynein species has a novel structure that is very similar to the phi structure. Based on the structural analysis, we propose a novel shutdown mechanism common to all three subfamilies of dynein.

[2-07-1415*](#) 細菌アクチン MreB の ATP 加水分解機構
ATP hydrolysis mechanism of bacterial actin MreB

Daichi Takahashi¹, Ikuko Fujiwara^{1,2,3}, Katsumi Imada⁴, Makoto Miyata^{1,2} (¹Grad. Sch. Sci., Osaka City Univ., ²OCARINA, Osaka City Univ., ³Dept. Bioeng., Nagaoka Univ. Tech., ⁴Grad. Sch. Sci., Osaka Univ.)

MreB is a bacterial actin homologue conserved over the bacterial kingdom. MreB possesses ATPase activity to regulate the polymerization dynamics, which is involved in various cellular processes. However, its ATP hydrolysis mechanism remains unclear. Recently, we found that MreB3, which is one of five MreB isoforms of *Spiroplasma*, shows an extremely low ATPase activity. To elucidate the ATP hydrolysis mechanism of MreB, we determined the crystal structure of MreB3 and conducted mutation analyses based on the structure. The results of these studies suggested that two residues conserved in MreBs but not in MreB3 play essential roles for ATP hydrolysis by forming a proton transfer pathway with a putative nucleophilic water.

[2-07-1427*](#) ミオシン 1c が駆動する F-アクチン回転運動の 3 次元観察
Corkscrew motion of F-actin driven by myosin-1c observed via three-dimensional optical tracking microscope

Yusei Sato¹, Kohei Yoshimura², Kyohei Matsuda¹, Takeshi Haraguchi³, Msahiko Yamagishi¹, Mitsuhiro Sugawa¹, Kohji Ito^{2,3}, Junichiro Yajima¹ (¹Dep. of Life Sciences, Graduate School of Arts and Sciences, The University of Tokyo, ²Dep. of Biology, Chiba Uni., ³Dep. of Biology, Chiba Uni.)

Myosin-1c, a membrane-bound single-headed myosin, shows chiral motility in *in vitro* gliding assays and is closely related to the organization of the left-right axis in organisms. In this study, we evaluated whether *Drosophila melanogaster* myosin-1c drives the longitudinal corkscrew motion of F-actin, as observed in several other dimeric myosin families, by three-dimensional tracking of quantum dots bound to F-actin moving on a surface coated with myosin-1c. Our technique showed that myosin-1c molecules drove a left-handed corkscrewing motion of F-actin in the direction of its long axis. Our findings indicate that myosin-1c generates force not only in axial direction but also in vertical direction to F-actin.

[2-07-1439*](#) 滑らかに回転するバクテリアべん毛モーターの軸-軸受け相互作用を立体構造から紐解く
Structural and functional analysis of the molecular bushing of the bacterial flagellar motor and the interactions with the rod

Tomoko Yamaguchi^{1,2}, Fumiaki Makino^{1,3}, Tomoko Miyata¹, Tohru Minamino¹, Takayuki Kato^{1,4}, Keiichi Namba^{1,2,5,6} (¹Grad. Sch. Frontier Biosci., Osaka Univ., ²RIKEN BDR, ³JEOL Ltd., ⁴IPR, Osaka Univ., ⁵RIKEN Spring-8, ⁶JEOL YOKOGUSHI Res. Alliance Lab., Osaka Univ.)

The basal body of the bacterial flagellum is a rotary motor consisting of several rings and the rod. The LP ring acts as a bushing supporting the distal rod for its rapid and stable rotation without much friction. Here, we used electron cryomicroscopy to solve the LP ring structure from *Salmonella* around the rod at 3.5 Å resolution. The structure shows 26-fold rotational symmetry and intricate intersubunit interactions of each subunit with up to six partners, which explains its extremely high structural stability. The inner surface is charged both positively and negatively. Positive charges on the P ring (part of the LP ring embedded within the peptidoglycan layer) presumably play important roles in its initial assembly around the rod with a negatively charged surface.

[2-07-1451*](#) IV型線毛収縮マシナリーは回転運動を生み出すか？
Does the machinery of type IV pili retraction work as a rotary motor?

Daisuke Sakuma¹, Daisuke Nakane², Azusa Kage¹, Takayuki Nishizaka¹ (¹Dept. Phys., Gakushuin Univ., ²Dept. Eng. Sci., Univ. of Electro-Communications)

Type IV pili (TFP) machinery is bacterial surface appendage and have multiple biological functions. The extension and retraction of TFP are controlled by two ATPases, PilB and PilT, which polymerizes and depolymerizes, respectively, pilin monomers. To understand the detailed mechanism of these processes, we here performed three-dimensional tracking and high-speed recording of fluorescent beads attached to TFP of *Synechocystis* sp. PCC6803. Notably, small fraction of TFP retraction accompanied clear corkscrewing motion, and its handedness was left with no exception. This new finding is the first evidence indicating that PilT drives rotational motion during TFP retraction, and gives a new insight into how the bacterial TFP machinery evolved to the archaeal rotary motor.

[2-07-1503*](#) Cell-free スクリーニングに向けた F_1 -ATPase の *in vitro* 合成及び 1 分子回転観察系の構築
In vitro synthesis of F_1 -ATPase and construction of single molecule rotation assay system for cell-free screening

Mai Taguchi, Hiroshi Ueno, Hiroyuki Noji (*Appl. Chem., 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 such as rotation rate and stepping rotation have been revealed by single molecule studies. However, the design principles of F_1 are still unknown and it is difficult to create F_1 with the desired functions. Here, we aim to create fast-rotating F_1 by cell-free directed evolution and clarify what determines the rotation rate of F_1 . In order to construct cell-free screening system, we examined the conditions for synthesis/biotinylation of F_1 *in vitro*. After adding the molecular chaperone DnaK, Biotin ligase and DNA to the PURE system and incubating for 3 h, we succeeded in one-pot synthesis/biotinylation of F_1 and observing the rotation of *in-vitro* synthesized F_1 .

[2-07-1515*](#) 人工回転分子モーターの設計とその自律的運動のシミュレーション
Novel design of artificial molecular rotary motor and simulation of its autonomous motion

Kenta Ito¹, Yusuke Sato², Sho Toyabe¹ (¹*Grad. Sch. Eng., Tohoku Univ.*, ²*FRIS, Tohoku Univ.*)

Biomolecular motors are autonomous nanomachines that convert energy to mechanical motion. It is a big challenge to develop an autonomous artificial molecular motor because of the difficulty of controlling fuel consumption and movement. For autonomous motion, two characteristics are required; (i) a unidirectional motion driven by steady fuel consumption and (ii) the directional control based on structural asymmetry. Here, we propose a novel mechanism that possesses the above features. We designed a DNA origami-based system and conducted a chemo-mechanical simulation of the motor motion for validating the mechanism. The core mechanisms are an asymmetric steric hindrance and the allosteric reaction of fuel consumption. We plan to proceed with the experiment in the future.

[2-07-1527](#) Insight into cooperative structural remodeling of the flagellar rotor ring complex responsible for directional switching

Tohru Minamino¹, Miki Kinoshita¹, Keiichi Namba^{1,2,3} (¹*Grad. Sch. Frontier Biosci, Osaka Univ.*, ²*RIKEN SPring-8*, ³*RIKEN BDR*)

The C ring of the flagellar motor acts not only as a rotor but also as a switching device that enables the motor to rotate in both counterclockwise and clockwise directions. FliG is the C ring protein consisting of three domains, FliG_N, FliG_M and FliG_C, and two helical domain linkers connecting them: Helix_{NM} connecting FliG_N with FliG_M and Helix_{MC} connecting FliG_M with FliG_C. These two linkers are involved in directional switching of the flagellar motor, but it remains unknown how. Here, we provide evidence suggesting that a change in intramolecular interactions between Helix_{NM} and Helix_{MC} induces a remodeling of hydrophobic interaction networks in the entire C ring structure responsible for directional switching of the motor in a highly cooperative manner.

[2-07-1600](#) 筋節長ナノ計測と電子顕微鏡ライブイメージングで捉えた心筋細胞の筋節振動の力学特性
Mechanical properties of cardiomyocyte sarcomeric oscillations captured by sarcomere length nanometry and electron microscope live imaging

Seine Shintani (*Dept. of Biomedical Sciences., Chubu Univ.*)

Fluorescence microscopic observation, which measures the movement of sarcomere by expressing actinin-GFP, revealed that warming cardiomyocytes causes sarcomere to enter an oscillation state in which it repeatedly contracts and relaxes. This phenomenon was named Hyperthermal Sarcomeric Oscillations (HSOs). It was found that HSOs have Contraction Rhythm Homeostasis, which keeps the oscillation period constant even though the oscillation waveform changes depending on the change in intracellular calcium concentration. The electron microscope live imaging method developed by the presenter also confirmed that the excised heart was in a sarcomeric oscillation state. Mathematical analysis suggests that this property supports the diastolic movement of the heart.

2-07-1612 高圧力により誘発される心筋細胞の非典型的収縮

High hydrostatic pressure induces unconventional cardiomyocyte contraction

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Transient increases in intracellular Ca²⁺ regulate cardiomyocytes contractions in the heart, which is subject to hydrostatic pressure during the contraction. However, the effect of high hydrostatic pressure in cardiomyocytes has not been investigated due to the lack of a quantitative measurement system under high pressure at the cellular level. In the present study, we used two different types of high-pressure techniques. The high pressure shortened the cell length, although it did not change the [Ca²⁺]_i in cardiomyocytes. Furthermore, a non-selective myosin ATPase inhibitor blocked the high pressure-induced contractions. Thus, our data suggest that high pressure can be a novel trigger for cardiomyocyte contraction, with direct modulation of actomyosin interactions.

2-07-1624 演題取り消し

2-07-1636 Dynamics and coordination of the lever-arm swing of muscle myosin in the artificial myosin filament

Hiroki Fukunaga^{1,2}, Masashi Ohmachi², Takumi Washio^{4,5}, Keisuke Fujita^{1,2}, Hiroaki Takagi⁶, Keigo Ikezaki⁷, Toshio Yanagida^{1,2,8}, Mitsuhiro Iwaki^{2,3} (¹FBS, Univ. Osaka, ²Riken, BDR, ³IFReC, Univ. Osaka, ⁴UT-Heart Inc., ⁵FC, Univ. Tokyo, ⁶Nara Med. Univ., ⁷Univ. Tokyo, ⁸NICT)

Muscle contraction is generated by a coordinated motion of myosin motors in thick filaments. However, how individual myosins in an assembly are coordinated together is unclear. Previously we have developed artificial myosin filaments composed of DNA origami and recombinant human muscle myosins, which gives us an analytical platform to clarify single myosin dynamics in the assembly. Here, we used high-speed atomic force microscopy to directly visualize the dynamics of the lever-arm swing of individual human skeletal myosins and the coordination. In this meeting, we will present the current progress of our experiments.

2-07-1648 Trimethylamine-N-oxide (TMAO)がミオシンの熱安定性に与える効果
Effects of trimethylamine-N-oxide (TMAO) on the thermal stability of myosin

Shigeru Chaen (*Department of Biosciences, College of Humanities and Sciences, Nihon University*)

Trimethylamine-N-oxide (TMAO), one of osmolytes, has been shown to enhance protein stability. It has been reported that TMAO protects the interaction between microtubules and kinesin from thermal degradation. We examined here how much TMAO protects the actomyosin motility from thermal denaturation. To assay the effects of TMAO on the thermal stability of myosin, we measured the velocity of actin filament sliding along the heat-treated myosin with TMAO. Myosin incubated for 20 min at 40°C didn't cause the actin filament sliding, but the myosin with above 600 mM TMAO caused the sliding. These results indicate that TMAO protects the actomyosin motility from thermal denaturation. Activation energy of actin filament sliding didn't show any dependence on TMAO concentration.

2-07-1700 再構築したダイニン-微小管複合体の屈曲運動
Active beating of a reconstituted dynein-microtubule complexes

Isabella Guido¹, Kenta Ishibashi², Eberhard Bodenschatz¹, Andrej Vilfan³, Ramin Golestanian¹, Hitoshi Sakakibara², **Kazuhiro Oiwa**^{2,4} (¹MPI. Dynamics Self-Organization, ²Nat. Inst. Info. Commun. Technol., Adv. ICT Res. Inst., ³Jozef Stefan Inst., ⁴Grad. Sch. Sci., Univ. Hyogo)

To fully understand the mechanism of propagating and switching of bend in eukaryotic cilia and flagella requires an understanding of the mechanism of dynein activation and inhibition in the 3D lattice under strict constraints. We constructed a system with a certain constraint on the three-dimensional structure mimicking the axoneme and dynein arm arrays. The system with the same polarity of microtubules and self-organized arrays of outer arm dyneins showed repetitive buckling in the presence of ATP. The minimal synthetic biomolecular structures mimicking the repetitive dynamics of intrinsic axonemes are called “synthoneme”. The synthoneme will be used as a tool for study on the activation process of force generation and the suppression process of switching.

2-07-1712 細胞質ダイニンとその制御タンパク質が紡錘体形成時に示す集積動態の時空間的定量
Spatiotemporal quantification of mitotic accumulation of cytoplasmic dynein I and its regulators at the spindle region

Takayuki Torisawa^{1,2}, Akatsuki Kimura^{1,2} (¹Cell Arch. Lab., Natl. Inst. Genet., ²Dept. Genet., SOKENDAI)

Cytoplasmic dynein is responsible for various cellular processes, and its activity is regulated by various regulatory proteins spatially and temporally. To characterize the spatiotemporal dynamics of regulatory proteins will contribute to understanding the regulation of dynein. Here we focused on the spindle formation in the *C. elegans* early embryo where dynein and its regulatory proteins have to be translocated from cytoplasm to the spindle region. We found that (i) a limited set of regulatory proteins accumulated in the spindle region, (ii) the spatial localization patterns were distinct among the regulators, (iii) the accumulation did not occur at once but sequentially. These findings suggested a fine temporal control of subcellular localization of dynein regulators.

2-07-1724 クライオ電顕で明らかになった外腕ダイニンの構造変化と活性化機構
Cryo-EM reveals remodeling and activation mechanisms of the outer arm dynein complex

Shintaro Kubo¹, Shun Kai Yang¹, Corbin S Black¹, Daniel Dai¹, Melissa Valente-Paterno¹, Jacek Gaetrig², **Muneyoshi Ichikawa**³, Khanh Huy Bui¹ (¹McGill University, ²University of Georgia, ³Nara Institute of Science and Technology)

Outer dynein arm (ODA) complex is a motor protein that drives the ciliary/flagellar beating. Recently, the structure of inhibited Tetrahymena ODA complex before transported into cilia was solved by cryo-electron microscopy (cryo-EM) (Mali, G. R. et al., 2021). To understand how the ODA complex changes its conformation and activates upon binding to the doublet microtubule of the cilia, we obtained the ODA complex structure bound natively to the doublet microtubule by cryo-EM. Our structure provides insights into how the ODA complex is tethered firmly to the ODA complex. By comparing inactive and active forms of the ODA complex, the conformational change that ODA complex undergoes and its activation mechanisms will be discussed.

2-07-1736 クラミドモナスにおける軸糸ダイニンの活性調節
Regulation of axonemal dynein motor activity in Chlamydomonas

Yusuke Kondo, Toshiki Yagi (*Grad. bio. sci., Prefect. Univ. Hiroshima*)

Chlamydomonas outer-arm dynein (OAD) is composed of three heavy chains (HCs), two intermediate chains (ICs), and 11 light chains (LCs). Previous mutant studies demonstrated the importance of OAD for ciliary beating at high beat frequency. Recently, we isolated a novel OAD mutant that retains the normal amount of OAD but swims at ~60% velocity of that of wild type. It has a point mutation in IC2, an IC that anchors OAD to the outer-doublet microtubule. Here, we examined the effect of this mutation on the motility of mutants lacking each one of the three HCs ($\alpha\beta\gamma$). The IC2 mutation was found to lower the motility of mutants lacking either the α or γ HC, but not that of a mutant lacking the β HC, indicating that IC2 functions in combination with β HC.

2-07-1748 翻訳後修飾によるダイニンの運動制御に関する粗視化 MD 計算

Regulating dynein motility controlled by post-translational modification revealed by coarse-grained MD simulation

Shintaroh Kubo^{1,2}, Bui Khanh Huy¹ (¹*Dept. of Anatomy and Cell Biol., McGill Univ.*, ²*Grad. Sch. of Med., The Univ. of Tokyo*)

The microtubules (MTs) that form the cytoskeletons 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 and flagella, walk on A-tubules and B-tubules, respectively. However, it is unknown how dynein-2 and kinesin-2 select A-tubules and B-tubules, respectively, while both A- and B-tubules are composed of the same alpha- and beta-tubulin dimer. 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 simulation to reveal how the movement of dynein-2 changes depending on the PTMs.

2-07-1800 Noise-induced acceleration of a molecular motor, kinesin-1

Takayuki Ariga¹, Keito Tateishi¹, Michio Tomishige², Daisuke Mizuno³ (¹*Grad. Sch. Med., Yamaguchi Univ.*, ²*Dept. Phys. Sci., Aoyama Gakuin Univ.*, ³*Dept. Phys., Kyushu Univ.*)

Kinesin-1 transports vesicles in cells. It has been revealed that nonthermal fluctuations are actively produced in the cells. However, these fluctuations have not been considered in conventional in vitro motility assays. Here, we observed kinesin movement under artificial external force fluctuations that mimic intracellular fluctuations, finding that kinesin accelerates in response to the fluctuations, especially under high loads. The acceleration is reproduced by using mathematical model simulations. The universality of theories behind the model suggests that general enzymes acting in cells share a similar noise-induced acceleration mechanism. In other words, active fluctuations in cells are not just noise but may be used to promote various physiological functions.

2-07-1812 Cytoskeletal component microtubules function as mechano-sensor to regulate intracellular transport

Syeda Rubaiya Nasrin¹, Christian Ganser², Arif Md. Rashedul Kabir¹, Kazuki Sada^{1,3}, Takefumi Yamashita⁴, Mitsunori Ikeguchi⁵, Takayuki Uchihashi^{3,6}, Akira Kakugo^{1,3} (¹*Fac. Sci., Hokkaido Univ., Hokkaido.*, ²*Dept. Creative Res., Nat. Inst. Nat. Sci., Okazaki, Aichi.*, ³*Grad. Sch. Chem. Sci. Engg., Hokkaido Univ., Hokkaido.*, ⁴*Res. Cent. Adv. Sci. Tech., Univ. Tokyo, Tokyo.*, ⁵*Grad. Sch. Med. Life Sci., Yokohama City Univ., Yokohama.*, ⁶*Dept. Phys. Struc. Biol. Res. Cent., Nagoya Univ., Nagoya.*)

Microtubules (MT) have long been regarded as mechanoregulator in cells. However, concrete evidence to specify it has been lacking. This work reports the first evidence to confirm such a claim. MT-based transport by kinesin and dynein was regulated by the MT deformation as observed under fluorescence microscope. High-speed atomic force microscopy imaged single kinesin movement on MT at nanometer-level. Tensional, compressive, and flexural deformation of MT protofilaments slowed down the kinesins. An increase in the interaction energy between kinesin and deformed tubulin, elucidated by molecular dynamic simulation, gave molecular-level understanding of the altered dynamics. This work provides important insight into the role of microtubules to regulate cellular activities.

2-07-1824 神経疾患を引き起こす KIF1A/UNC-104 変異体の軸索輸送とシナプス分布異常の関係

Axonal transport by pathogenic KIF1A/UNC-104 mutants cause abnormal synapse distributions

Yuki Kagawa¹, Ryo Sasaki¹, Yuzu Anazawa², Shinsuke Niwa³, Kumiko Hayashi^{1,4} (¹*Grad. Sch. Eng., Tohoku Univ.*, ²*Grad. Life Sci., Tohoku Univ.*, ³*FRIS, Tohoku Univ.*, ⁴*JST, PRESTO*)

KIF1A/UNC-104 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 mutant. Specifically, we investigated the capture and dissociation events of SVPs at the SVP pools, considered immature synapses. We found the SVP pool sizes and intervals depended on the KIF1A/UNC-104 dynamics. We aim to reproduce the dependence by using the mathematical model of axonal transport and understand the abnormal synapse distributions.

2-08-1315* 損傷した細胞を用いて計測する細胞内粒子動態と細胞死の関係
Relations between Motions of Intracellular Particles and Cell Death in Damaged Cells

Hideaki Ota, Hideo Higuchi (*Grad. Sch. Sci., The Univ. of Tokyo*)

Differences between damaged cells which will die and which will be alive may come from differences in intracellular states, and the differences in intracellular states can be the key about how cells are alive. Our laboratory found intracellular mobility decreased in damaged cells. Other research reported cytoplasmic viscosity drastically increased at ATP depletion in various cellular species. Then, in this research, we measured intracellular mobility and diffusion constants at the same time using cells damaged by reactive oxygen species. Cellular survival probabilities were also measured. As a result, intracellular mobility and survival probabilities had a clear correlation, and diffusion constants had a decreasing trend as survival probabilities decreased.

2-08-1327* 興奮系 Ras の制御に関わる GEF の網羅的解析
Comprehensive analysis of GEFs involved in the regulation of a Ras excitable system

Koji Iwamoto¹, Satomi Matsuoka^{1,2,3}, Masahiro Ueda^{1,2,3} (¹*Dept. of Biol. Sci., Grad. Sch. of Sci., Univ. of Osaka*,
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An excitability of Ras is a core mechanism to self-organize an anterior-posterior polarity for cell migration. We constructed a systematic analysis method to elucidate the individual contribution of 25 GEF isoforms to Ras activation dynamics in *Dictyostelium discoideum*. Live-cell imaging of a fluorescent reporter of activated Ras revealed how the excitable dynamics was modulated by an overexpression of each isoform. A hierarchical clustering showed that the GEF isoforms can be grouped into 5 based on the extent of the spatial and temporal modulation. We identified the group showing the largest modulation without external stimulation as responsible for the excitability. Our method provides a powerful tool to investigate how Ras excitability is regulated by multiple GEFs.

2-08-1339* フォロワー細胞の先端端への割り込みによる上皮細胞集団の拡大
Leading Edge Expansion in Migrating Cell Sheet by Follower Cell's Interruption

Misaki Iwanaga¹, Chika Okimura¹, Tatsunari Sakurai², Yoshiaki Iwade¹ (¹*Grad. Sch. Sci. Tech., Yamaguchi Univ.*,
²*Dept. Math. Eng., Musashino Univ.*)

When a fish body is wounded, epithelial keratocytes migrate collectively as a sheet to close the wound. During the migration, leading edge of the cell sheet expands regardless of the tight cell-cell connections with actomyosin cables. How the leading edge expands is an interesting question. We found the cause is interruption of single follower cells into the leading edge. When the interruption took place, traction forces reflecting the forces that the follower cell pulls two adjacent leader cells were detected at the interruption area. Moreover, the follower cells that have advanced to the leading edge, newly built the cell-cell connection to the adjacent leader cells with actomyosin cables, indicating the follower cells transformed to the leader cells.

2-08-1351* Oligomerization of neuronal receptors is essential for assembly and function of the synapse

Saahil Acharya¹, Taka A. Tsunoyama¹, Irina Meshcheryakova¹, Aya Nakamura¹, Hiroko Hijikata¹, Yuri Nemoto¹, Takahiro K. Fujiwara², Akihiro Kusumi¹ (¹*Membrane Cooperativity Unit, Okinawa Institute of Science and Technology Graduate University (OIST), Okinawa, Japan*, ²*Institute for Integrated Cell-Material Sciences (WPI-iCeMS), Kyoto University, Kyoto, Japan*)

The synapse structures in both the post- and pre-synaptic plasma membranes consist of multiple nano-scale domains, precisely apposed to each other. Synaptic receptors in the post-synapse need to be assembled in the nano-scale domains, precisely opposite from the presynaptic neurotransmitter release sites, for proper synaptic function. We found oligomerization of Neuroligin and AMPA receptors is essential for anchoring the receptors in the synapse. Functional dimeric Neuroligin and tetrameric TARP2 (linked to GluA1 subunits) can be captured as they diffuse through phase-separated condensates containing PSD95, while monomeric Neuroligin and TARP2 cannot. We also revealed that the receptor oligomers enhance condensation, which in turn further recruit receptor oligomers.

[2-08-1403*](#) Investigating the contribution of nuclear size on chromatin dynamics in interphase during *C. elegans* embryogenesis

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The dynamic nature of chromatin is associated with a variety of biological functions, such as transcription and DNA recombination. During *Caenorhabditis elegans* embryogenesis both chromatin mobility and nuclear size decreases, though the relationship between them is unknown. Combining experimental approaches and by establishing new method for tracking chromatin loci movement, we found nuclear size affects chromatin mobility. Moreover, we propose new model based on polymer physics theories to explain the reduction of chromatin movement during *C. elegans* embryogenesis by the transition from unentangled to entangled state. Understanding the sole effect of nuclear size change on the reduction of chromatin dynamics facilitate our knowledge on nuclear and genome organization.

[2-08-1415](#) アクティブな界面摩擦と流体抵抗の幾何学的バランスが決めるアクトミオン液滴の自発運動
Geometric trade-off between interfacial active friction and passive fluid drag determines the motility of actomyosin droplets

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One of the distinctive abilities of migratory cells is force transmission: intracellular contractile forces of actomyosin networks are transmitted to the external environments, which propels the cell body forward. However, physical factors driving efficient force transmission are poorly understood due to the cellular complexity. Here, we develop an *in vitro* migratory cell model encapsulating actomyosin networks in water-in-oil droplets. We find that membrane-bound actin flow can generate *active friction* at the droplet-substrate interface, transmitting the contractility and propels the droplet. Combining microfluidic experiments and active gel theory, we show how the confinement geometry-dependent balance between active friction and fluid drag determines droplet motility.

[2-08-1427*](#) アクトミオン収縮力の光操作による細胞質分裂中の表層張力の機能解析
Optogenetic relaxation of actomyosin contractility uncovers mechanistic roles of cortical tension during cytokinesis

Kei Yamamoto^{1,2,3}, Haruko Miura^{2,3}, Yohei Kondo^{1,2,3}, Kazuhiro Aoki^{1,2,3} (¹*SOKENDAI*, ²*NIBB*, ³*ExCELLS*)

During cytokinesis of animal cells, a contractile ring transiently forms and generates tension to divide a cell. The ring tension is counteracted by the cortical tension; however, the importance of cortical tension is still unclear, because it is difficult to estimate the strength of cortical tension relative to the ring tension. To this end, we developed a new optogenetic tool, named OptoMYPT, enabling the relaxation of contractile force by light. Using OptoMYPT, we found that the relaxation of cortical tension accelerated the furrow ingression. Based on the experimental data and coarse-grained model, we estimated the cortical tension corresponds to at least 14~31% of the ring tension. This balance may achieve both morphological maintenance and timely cytokinesis.

[2-08-1439*](#) 原子間力顕微鏡によるホヤ神経期胚の力学マッピング
Mapping mechanical properties of ascidian embryo during neurulation by atomic force microscopy

Yosuke Tsuboyama, Tomohiro Matsuo, Takaharu Okajima (*Grad. Info. Sci. & Tech. Univ. Hokkaido*)

Neural tube closure (NTC) is a dynamic embryonic process, in which the plate neural progenitor cells form neural tube that grow the brain and nerve chord. Studies reported that the unidirectional zippering in NTC is driven by tensile forces (Hashimoto and Munro, *Dev. Cell* 2019). However, it is unknown about how the stiffness of embryonic cells are temporally changed during neurulation. In this study, we investigated the spatiotemporal dynamics of stiffness of ascidian embryonic cells in neurula period by atomic force microscopy (AFM) (Fujii et al. *Commun. Biol.* 2021). We observed that a characteristic spatial pattern of cell stiffness emerged around the zipper region in the vegetal pole while the cell stiffening asymmetrically occurs in the animal pole.

[2-08-1451*](#) 高速イメージングで明らかにする *Volvox carteri* の鞭毛メタクロナル波による力発生機構
Mechanism of Force Generation by Flagellar Metachronal Waves in *Volvox carteri* Revealed
by High-speed Imaging

Naoki Uemura, Katsuya Shimabukuro (*Chem. Bio. Eng., NIT Ube College*)

We report the relationship between the swimming pattern of *Volvox carteri* and its flagellar metachronal waves. Previous studies have shown that the force produced by *V. carteri* oscillates at 30 Hz. Based on this finding, we performed high-speed imaging of a swimming *V. carteri* spheroid and detected the same 30 Hz oscillation in the velocity. To clarify the origin of the oscillation, we related the velocity change to the waveform transformations of the individual flagellum along a spheroid and found that the velocity reached the maximum when the flagella at the equatorial position completed their effective strokes, whereas lowest at their recovery strokes. Our results clearly demonstrate that flagella at equator play an essential role for *Volvox* swimming.

[2-08-1503*](#) 細胞外小胞の標的細胞への選択的結合機構：1粒子追跡法による解明
Mechanisms of selective binding of small extracellular vesicles to recipient cells as revealed by
single-particle tracking

Tatsuki Isogai¹, Koichiro M. Hiroasawa², Ayano Sho³, Yasuhiko Kizuka^{2,4}, Yasunari Yokota⁵, Kenichi G. N. Suzuki^{2,4} (¹Grad. Sch. Nat Sci Tech., Gifu Univ., ²GCORE, Gifu Univ., ³Dept. App Bio Sci., Gifu Univ., ⁴CREST, JST, ⁵Dept. Eng., Gifu Univ.)

Small extracellular vesicles (sEV) have been drawing an extensive attention as a carrier for cell-cell communication, and sEV studies may resolve the issue of metastatic organotropism. Recent studies suggested that tumor-derived sEV binds to the recipient cells by specific interaction of integrin subunits with extracellular matrix (ECM). However, the mechanisms at the molecular level are unknown. Here, we tried to unravel the mechanisms by single-particle tracking of integrin subunit-knockout sEV. We found that several integrin subunits, N-glycans and sialic acid on sEV regulate the binding affinity of sEV to ECM. Combined with the results by super-resolution microscopy, we will discuss the mechanisms of selective binding of sEV to the recipient cells.

[2-08-1515](#) Effect of a sudden change of confined environments in collective cell migration of epithelial cells

Masaharu Endo¹, Mitsuru Sentoku², Kenji Yasuda^{1,2,3} (¹Dept. Phys., Sch. Adv. Sci. & Eng., Waseda Univ., ²Dept. Pure & Appl. Phys., Grad. Sch. Adv. Sci. & Eng., Waseda Univ., ³Org. Univ. Res. Initiatives, Waseda Univ.)

Collective cell migration is an interactive behavior of cell populations. Using the advantage of agarose photothermal microfabrication technology, we observed the collective migration behavior of vascular epithelial cells by the sudden change of their confined geometry. Cells filled in the reservoir area on the chip were guided into a one-sided agarose channel (20 μm width x 600 μm length). When the cells reached the end of the channel and stopped, we melted an agarose layer to guide those cells into a wide free space. Cells exited from the channel were isolated from their sheet and migrated spontaneously. The results indicate agarose stepwise fabrication can mimic the circulating tumor cell formation or healing from a sudden wound formation.

[2-08-1527](#) A suppressor mutation of a *Chlamydomonas* cilia-less mutant suggests a novel role of Bld10p, an essential protein for centriole assembly

Yuki Nakazawa¹, Masafumi Hirono² (¹STG, OIST, ²Dept. Frontier Biosci., Hosei Univ.)

Centrioles are essential organelles for assembling cilia by serving as their bases. A *Chlamydomonas* mutant *bld10*, which totally lacks centrioles and cilia, has a mutation in the gene for Bld10p, the homolog of mammalian centrosomal protein Cep135. Here, we isolated an extragenic suppressor mutant of an allele of *bld10*. The suppression of the cilia-less phenotype is almost complete except that a small population of the cells has a single cilium. Interestingly, electron microscopy of the suppressed *bld10* cells showed that ciliary axonemes are ectopically assembled in the cytoplasm without the membrane, probably because of aberrant orientation and position of centrioles. These observations suggest that Bld10p has a role in fixing centriole orientation.

2-08-1600 ストレスファイバの直動回転変換モデル

Conversion of linear contraction of stress fibers into rotation in migrating cells

Chika Okimura¹, Shu Akiyama¹, Tatsunari Sakurai², Yoshiaki Iwadate¹ (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 SF is arranged around the nucleus and it is rotating, although they should only linearly contract like myofibrils. Here, we confirmed that the stress fiber rotation is accompanied by the rotation of membrane and nucleus. In addition, we constructed a “soft” mechanical model that mimics the cell body of a keratocyte from a silicone gel and a contractile coil. From the motion analysis of the soft robot, a torque generation principle of the stress fibers was predicted.

2-08-1612 海洋性ビブリオ菌において細胞極の目印タンパク質 HubP がべん毛本数制御因子 FlhG の ATPase 活性に与える影響Effect of the polar landmark protein HubP on ATPase activity of FlhG, a flagellar number regulator of *Vibrio alginolyticus***Yuxi Hao**¹, Norihiro Takekawa², Michio Homma¹, Seiji Kojima¹ (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. Previously, we found that the FlhG mutant with high ATPase activity strongly localized to the cell pole, and severely inhibited cell motility and flagellation. However, the mechanism of ATP-dependent FlhG action at the pole is still unknown. HubP is a single-transmembrane protein localized at the cell pole with a large cytoplasmic region. In *V. cholerae*, it has been shown that FlhG localizes to the pole by interacting with the C-terminus of HubP. In this study, we made some HubP truncation mutants and purified HubP C-terminal fragments. We found that a HubP fragment with C-terminal region enhanced FlhG ATPase activity.

2-08-1624 細菌べん毛のフック-フィラメント連結部にフィラメントキャップが結合した複合体の構造
Structure of the hook-filament junction with the filament cap in the bacterial flagellum**Norihiro Takekawa**¹, Atsushi Ikeda¹, Tomoko Miyata², Fumiaki Makino^{2,3}, Keiichi Namba^{4,5,6}, Katsumi Imada¹ (¹*Dept. Macromol. Sci., Grad. Sch. Sci., Osaka Univ.*, ²*Grad. Sch. Frontier Biosci., Osaka Univ.*, ³*JEOL Ltd.*, ⁴*BDR, RIKEN*, ⁵*SPRING-8, RIKEN*, ⁶*JEOL YOKOGUSHI Res. Alliance. Lab., Osaka Univ.*)

Many bacteria swim by rotating the flagellum. The flagellum consists of three parts: basal body, hook, and filament. Between the hook and the filament, there is a junction that acts as a mechanical adaptor connecting the flexible hook with the rigid filament. The filament cap is attached on the junction to start filament formation by helping flagellin assembly. Here we determined the structure of the junction with the hook and the filament cap by using cryo-electron microscopy at 7.0 Å resolution from 14,939 particle images and built its atomic model. We classified the subunits in the complex into several groups based on their conformations and discuss their interactions and conformational changes.

2-08-1636 蛍光染色法による大腸菌べん毛の挙動の観察Observation of behavior of flagella in *Escherichia coli* by using fluorescence staining**Tatsuya Nakaue**, Yong-Suk Che, Akihiko Ishijima, Hajime Fukuoka (*Grad. Sch. Frontier Biosci. Osaka Univ.*)

E. coli cell has 6-8 flagella and swims in liquid by using this organelle. The shape of flagellum is known to change according to the rotational direction of flagellar motor. In this study, the flagellum is stained with a fluorescent dye and the shape transition of flagellum was observed with a fluorescence microscope. We investigated the origin of transition in flagellar filament and found that shape transition, which were previously thought to propagate from the base of flagellum, frequently occur from the tip of flagellum. In addition, we confirmed whether coordination of the switching between multiple motors that we have been demonstrated by tethered bead assay occurs at the flagellar filament level. We want to discuss obtained results at the meeting.

[2-08-1648](#) 織毛基部と軸系の位相板を用いたクライオ電顕法による構造解析

3D structure of the basal body and the axoneme from motile cilia reconstructed by cryo-electron tomography with the phase plate

Takashi Ishikawa, Akira Noga, Noemi Zimmermann (*Paul Scherrer Institute*)

Our group has been investigating molecular mechanism of ciliary motility and formation, by analyzing 3D structure using cryo-electron tomography (cryo-ET) (summarized in Ishikawa (2017) Cold Spring Harb. Perspect. Biol. 9 (1)). While cryo-ET has been successful to analyze the axoneme, the distal motile part of cilia, utilizing pseudo-nine fold symmetry and 96nm periodicity, structural analysis of the proximal part of cilia was challenging due to lack of periodicity. However, recent progress of cryo-EM provided insight of this part. We will present detailed structure of the basal body, the transition zone and the proximal region of the axoneme, revealed by cryo-ET with enhanced contrast using the Volta phase plate and deep-learning based denoising algorithms.

[2-08-1700](#) フックキャップ蛋白質の輸送はフック蛋白質の輸送を促進する

Secretion of the hook cap protein enhances secretion of the hook protein

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 the construction of the flagellar axial structure, including the rod, the hook and the filament. The hook construction requires the hook cap complex composed of FlgD. The hook protein, FlgE, exported by fT3SS assembles just beneath the hook cap. Thus, secretion of FlgE should be activated after secretion of FlgD. In this study, we analyzed the secretion of FlgD and FlgE using inverted membrane vesicles (IMVs). We found that the FlgE export was drastically enhanced in the presence of very small amount of FlgD. Moreover, the FlgE export was enhanced using IMVs that had exported FlgD before. These results suggest that the FlgD secretion changes the conformation of fT3SS suitable for the FlgE secretion.

[2-08-1712](#) Search for domain in chemoreceptor to cause coordination of rotational switching between flagellar motors

Hiroto Kozono, Yong-Suk Che, Hajime Fukuoka, Akihiko Ishizima (*Grad. Sch. Frontier Bio Sci., Osaka Univ.*)

It has been suggested that spontaneous oscillation of the receptor cluster activity is responsible for the synchronization of switching. Therefore, I aim to clarify which part of the receptor Tar is responsible for the switching entrainment. The method is to create a partial deletion strain of the receptor and a mutant of the ligand binding site and examine the presence of entrainment. The results showed that total and partial deletions of the periplasmic region did not produce switching entrainment. In addition, point mutations in the ligand binding site caused switching entrainment, although the response to aspartate was lost. This suggests that the interaction between the periplasmic regions of the receptors is important for switching entrainment.

[2-08-1724](#) 鞭毛内構造のラセン配置は鞭毛上の場所に依存する

The Helical Arrangement of Axonemal Structures Depends on the Region of the Flagellum

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The 9 peripheral microtubules (PMTs) of *Chlamydomonas* axonemes are arranged so that their associated structures are arranged helically. At the BPJ2020, we reported that the helical arrangement was not observed at the base of the flagella but observed outside. Here, we analyzed the arrangement of the internal structures of the axoneme in detail using electron tomography. The 3D structures were reconstructed from tilt-series of negative-staining electron micrographs of the axonemes. Images of 9 PMTs were extracted and the arrangement of structures on them was compared. At the base, the structures on the PMTs were arranged almost side by side between adjacent PMTs. Other than the base, these structures were arranged so as to be offset by about 32 nm in one direction.

[2-08-1736](#) 受容体アレイのメチル化レベルの変化は大腸菌べん毛モーター間の回転方向転換の同調を引き起こす
 Change in methylation level in receptor array causes coordinated reversal of flagellar motors on a single *Escherichia coli* cell

Yumiko Uchida¹, Tatsuki Hamamoto², Yong-Suk Che¹, Akihiko Ishijima¹, Hajime Fukuoka¹ (¹*Grad. Sch. Frontier Biosci. Osaka Univ.*, ²*OIST Grad. Univ.*)

E. coli cell coordinately controls the rotational switching among flagellar motors without stimuli and this coordination is regulated by the change in CheYp concentration. Here we investigated whether the change of methylation level in receptor array involves in the switching coordination. Both the cells producing Tsr-mutants with fixed methylation level and the cells producing CheB/CheR-mutants lacking demethylation/methylation activities showed no coordination. Trg, natively lacks CheR tether-site (NWETF), conferred no coordination, but Trg+NWETF chimera conferred. We suggest the change of methylation level in receptor array through CheB/CheR fluctuates array's activity to cause the change in CheYp concentration, and this change induces the switching coordination.

[2-08-1748](#) 受容体の協調性を崩す変異型/野生型受容体の比率の定量化とべん毛モーターの協調性
 Quantification for mutant/WT receptors ratio that collapses receptor cooperativity and switching coordination between flagellar motors

Shiori Awa, Yumiko Uchida, Hajime Fukuoka, Akihiko Ishijima, Yong-Suk Che (*Grad. Sch. Frontier Biosci. Osaka Univ.*)

In *E. coli* under steady-state, the rotational switching of two flagellar motors on a cell is highly coordinated. We proposed this coordination is regulated by the fluctuation of CheYp concentration derived from spontaneous activity of receptor array caused by the cooperative manner in the array. To evaluate our suggestion, we measured switching coordination in the cell co-expressing receptor mutant (mTsr) lacking the cooperative response to serine and wild-type receptor (Tar). The coordination was inhibited in dose-dependent manner of the mTsr inducer. Next, we try to quantify relationship between the expression ratio of mTsr and Tar and the degree of coordination. We will discuss the spontaneous activity of receptor array in steady-state in terms of this relation.

[2-08-1800](#) *Bacillus subtilis* 由来べん毛固定子蛋白質 MotS のナトリウム依存的構造変化
 Sodium-dependent conformational change of flagellar stator protein MotS from *Bacillus subtilis*

Maria Uehori¹, Ayaka Yamaguchi¹, Norihiro Takekawa¹, Tohru Minamino², Katsumi Imada¹ (¹*Dept. Macromol. Sci., Grad. Sch. Sci., Osaka Univ.*, ²*Grad. Sch. Frontier Biosci., Osaka Univ.*)

The flagellar motor consists of the rotor and the stator, and torque is generated by the interaction between the rotor and the stator coupled with the specific ion flow. The stator of *Bacillus subtilis* consists of MotP and MotS and functions as a sodium ion channel. BsMotS changes its structure depending on the sodium concentration, but the mechanism is unknown. Here, we determined the crystal structures of a C-terminal fragment of BsMotS (BsMotS_C) under various sodium concentrations. We also performed Far-UV CD spectroscopy under low and high sodium concentrations and found that the N-terminal region of BsMotS_C shows sodium dependent helix-coil transition. We will discuss the mechanism of sodium dependent conformational change of the flagellar stator.

[2-09-1315](#) 線虫 *C. elegans* の低温馴化多様性を制御する神経回路の解析
 Neural circuit regulating the diversity of cold acclimation in *C. elegans*

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We are studying cold acclimation of natural variants in *C. elegans* to reveal how animal response rapid temperature change. We have identified VH15N14R.1 encoding novel protein as a responsible gene which determine the difference of cold acclimation between Hawaiian strain and Australian strain by NGS analysis and SNP analysis. VH15N14R.1 expresses in head neurons including BAG oxygen sensory neuron. Because oxygen signaling modulates ADL thermo-responsivity, we measured ADL thermo-responsivity of VH15N14R.1 mutant. VH15N14R.1 mutant showed the decrement of ADL thermo-responsivity compared wild-type. These imply that oxygen information from BAG via VH15N14R.1 affect ADL thermo responsivity, resulting in regulation of cold acclimation.

[2-09-1327](#) 海馬で合成される男性・女性ホルモンやストレスホルモンによる記憶シナプスの早い non-genomic な制御
Rapid non-genomic modulation of synapses by hippocampus-synthesized androgen, estrogen and stress steroid

Suguru Kawato^{1,2}, Mika Soma^{1,2}, Mari Ikeda^{1,2}, Minoru Saito² (¹Grad. Sch. Med, Juntendo Univ., ²Dept. Bio, Nihon Univ.)

Neurosteroids (sex steroids and stress steroids) are synthesized in the hippocampus, center for learning and memory. Rapid 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 trigger synaptic (membrane) steroid receptors, then inducing kinase signaling (non-genomic), leading to rapid modulation of dendritic spines in 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 synapses.

[2-09-1339](#) *C. elegans* homologue of HADH involved in human mitochondrial fatty acid metabolism regulates neural function in temperature acclimation

Akihisa Fukumoto¹, Misaki Okahata¹, Yohei Minakuchi², Atsushi Toyoda², Akane Ohta¹, Atsushi Kuhara^{1,3} (¹Grad. Sch. Sci., Konan Univ., ²Natl. Inst. of Genetics, Japan, ³PRIME, AMED)

Temperature acclimation of nematode *C. elegans* is dynamically changed within only three hours by altering cultivated temperature conditions (Ohta et al., *Nature commun*, 2014; Okahata et al., *Science advances*, 2019). In this study, we demonstrate that the temperature acclimation is regulated by 3-hydroxy acyl-CoA dehydrogenase (HADH), which is known to be involved in mitochondrial fatty acid β -oxidation in human. Abnormal temperature acclimation of HADH mutant was rescued by expressing wild-type HADH in neurons, suggesting that neuronal HADH is essential for temperature acclimation.

[2-09-1351](#) 神経回路をステップワイズに構築するためのアガロース微細加工技術の開発
Stepwise neuronal network pattern formation in agarose during cultivation using non-destructive microneedle photothermal microfabrication

Haruki Watanabe, Kenji Simoda, Yuhei Tanaka, Kenji Yasuda (*Dept. Pure & Appl. Phys., Grad. Sch. Adv. Sci. & Eng., Waseda Univ*)

Fully direction-control of neurites is essential to form desired neuronal network patterns. We developed a stepwise agarose microfabrication method that can modify microchannel patterns to guide neurites to desired directions during their elongation. Micropatterns with 2 μ m-resolution were formed in the agarose layer using the absorption heat at the tip of 0.7 μ m-diameter platinum-coated glass needle with the permeable 1064-nm wavelength infrared laser. The elongated neurite was guided successfully to another neuron through the stepwise formed microchannel during cultivation. Apoptosis was not observed even the additional microchannel was formed at the edge of the neurite. The results show the potential of this method for non-destructive direction-control of neurites.

[2-09-1403](#) 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, Masashi Fujii, Akinori Awazu (*Graduate School of Integrated Sciences for Life, 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.

[2-09-1415](#) Development of agarose microfabrication technology using Joule heat of micrometer-sized ionic current

Kenji Shimoda, Haruki Watanabe, Kenji Yasuda (*Dept. Pure & Appl. Phys., Grad. Sch. Adv. Sci. & Eng., Waseda Univ.*)

Our previously developed photothermal etching technology enabled us to form desired agarose microstructures during cell cultivation. However, it still has some limitations, such as the unexpected etching caused by the absorption of permeable ITO wiring patterns on the multielectrode array chip. Hence, we have developed a new method exploiting a Joule heat of ion current. The focused ion current was formed at the micrometer hole of the microcapillary tube in which sodium buffer was filled. When the AC voltage was applied between the inside and the outside of the capillary tube, we discovered the formed micrometer-sized spot of Joule heat by the impedance of ion current at the capillary tip can fabricate agarose microstructures successfully.

[2-09-1427](#) 自己学習型ニューロロボットののための、培養神経回路網における連想学習再現の試み
An attempt to reproduce associative learning on a cultured neuronal network for development of a self-learning neurobots

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In previous study, we developed a neurobot system controlled by neuronal activity evoked by electrical stimulation linked to locations of obstacles. In the neurobot system, we applied 2 different inputs to a cultured neuronal network, such as “warming” and “avoiding” input. After simultaneous and repeatedly applying the two inputs, these two inputs were associated with the other input. Sometimes “avoiding” input changed to evoke the activity pattern for “warming”. However, the learning results was not always suitable for perform purposive behavior such as crisis avoidance. Thus, we are investigating the relationship between the network structure in the neuronal network and learning direction.

[2-09-1439](#) ミミズ非連合学習におけるセロトニンの関与
Serotonin-dependent mechanism of non-associative learning in earthworm *Eisenia fetida*

Yoshihiro Kitamura, Toshiaki Nakahara, Hikaru Takahashi (*Dept Math Sci Phys, Col Sci Eng, Kanto Gakuin Univ*)

Molecular mechanism of non-associative learning (habituation) in the earthworm *Eisenia fetida* was investigated. Extracellular recordings showed that number of action potentials decrease by repeated tactile stimulus to same region of the body wall. It is likely that this habituation 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, it is revealed that several 5-HT receptor antagonists inhibit and tryptophan hydroxylase inhibitor delay establishment of habituation. 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.

[2-09-1451](#) マウススライス標本で電位感受性色素を用いてイメージングされた嗅周囲皮質 (PC)と嗅内野 (EC)との皮質神経振動
Cortical oscillations in entorhinal and perirhinal cortices imaged with voltage-sensitive dye in slice preparations of mice

Takashi Tominaga¹, Yoko Tominaga¹, Riichi Kajiwara² (¹Inst. Neurosci., Tokushima Bunri Univ., ²Dept. Electro. Bioinfo., Sch. Sci. Tech., Meiji Univ.)

The voltage-sensitive dye (VSD) imaging enables us to visualize the dynamics of neural activity spread across cortices. Recently we have overcome the poor signal-to-noise ratio and can use the method to see one-time events like neuronal oscillation. Here, we report the neuronal oscillations in a horizontal slice of the medial temporal lobe of a mouse brain. The slice consists of the perirhinal cortex (PC) and the entorhinal cortex (EC), the critical brain area for higher cognitive function. We have successfully imaged the shift of the center of the oscillatory activity starting from surface layers of the EC to deep layers of the PC. We will argue the physiological meaning of the oscillatory activity and the advantages of the wide-field VSD imaging method.

[2-09-1600*](#) Bull's eye 型プラズモニクチップによる神経細胞表面グルタミン酸受容体分子の光捕捉
Optical trapping of glutamate receptors on neuronal cells with a bull's eye-type plasmonic chip

Takashi Koizumi¹, Tomoya Nagasue², Keiko Tawa², Chie Hosokawa¹ (¹*Grad. Sch. Sci., Osaka City Univ.*, ²*Grad. Sch. Sci. Tech., Kwansai Gakuin Univ.*)

Neuronal cells form complex networks and communicate with each other via synaptic connections. For realizing optical control of synaptic transmission between neurons, we have applied optical trapping of AMPAR-type glutamate receptors (AMPARs) on neurons. Here we demonstrate surface plasmon resonance (SPR) based optical trapping of quantum-dot (QD) conjugated AMPARs with a bull's eye-type plasmonic chip. The receptors dynamics in an optical trap was evaluated by fluorescence correlation spectroscopy. The average transit times at the laser focus of QD-AMPARs on neurons cultured on the plasmonic chip increased than that cultured on the coverslip, suggesting that the QD-AMPARs was more constrained at the focal spot due to optical trapping forces enhanced with SPR.

[2-09-1612*](#) モノアラガイの味覚嫌悪学習に対する緑茶由来カテキン混合物の影響
The combined effect of green tea-derived catechins on taste aversive conditioning in *Lymnaea*

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Green tea mainly contains four catechins. One of them, epicatechin (EpiC), has the enhancing effect on long-term memory (LTM) formation for classical conditioning in *Lymnaea*. It is also reported that exposure to green tea during training exhibits the LTM enhancement similarly to pure EpiC experiments. Here, we confirmed whether exposure to a mixture of catechins derived from green tea during taste aversive conditioning elicited similar effects to a pure EpiC. We found that the mixture of catechins did not enhance the LTM formation. Next, we demonstrated that exposure to 3.8 mg / L EpiC, which is the equal level of the catechin mixture, during training enhanced the LTM formation. These results suggest that the combination of catechin may have competitive effects on LTM.

[2-09-1624*](#) 開放系空間における脂質膜上のアミロイドβ凝集挙動の単分子観察
Single Molecule Observation of Amyloid β on Lipid Membrane under Open Space

Akane Iida¹, Hideki Nabika² (¹*Grad. Sch. Sci. Eng., Yamagata Univ.*, ²*Fac. Sci., Yamagata Univ.*)

Alzheimer's disease (AD) is characterized by the aggregation and accumulation of amyloid β (Aβ) peptides that causes cellular damage. Elucidation of the initial aggregation process is important to propose the suppression of AD, whereas it remains partially unknown. One reason is that the interstitial fluid supplies and removes Aβ, making the brain an open system. However, most previous studies were conducted under closed system. Thus, we have investigated the aggregation process of Aβ on the lipid membrane under open system, especially focusing the initial aggregation behavior using single molecule observation. As a result, we proposed a new mechanism that leads to an equilibrium steady state under closed space and a non-equilibrium steady state under open space.

[2-09-1636*](#) クロストリジウム属細菌走化性システムの大腸菌再構成系の確立
Reconstitution of a *Clostridium* chemosensory system in *Escherichia coli*

Shohei Koike, Shota Manabe, Susumu Ogoshi, So-ichiro Nishiyama, Hiroshi Urakami (*Fac. App. Life Sci., Niigata Univ. Pharm. App. Life Sci.*)

Clostridium spp. are spore-forming Gram-positive anaerobic bacteria, some of which are known to be pathogenic. *C. botulinum*, a causative agent of food poisoning, and its non-toxicogenic surrogate, *C. sporogenes*, are motile and possess more than 30 chemoreceptor homologs, which we call MCP-like proteins (MLPs). However, their functions have not been elucidated thus far. Our previous studies revealed that *C. sporogenes* shows a chemotactic response to l-arginine (hereafter referred as "Arg"). In this study, we have inspected the genome of *C. sporogenes* and cloned some *mlp* genes which share high homology with an Arg chemoreceptor, Mlp24 of *Vibrio cholerae*. Functional assays of the candidates are currently underway to identify a novel Arg receptor for *Clostridium* spp.

2-09-1648* 大腸菌細胞側面膜領域における走化性受容体クラスター形成
Chemotaxis receptor clusters in the lateral membrane region of *Escherichia coli* cells

Ayano Inoue¹, Nana Ito¹, Hiroataka Tajjima³, Nishikawa Masatoshi², Yoshiyuki Sowa^{1,2,3}, Ikuro Kawagishi^{1,2,3} (¹Grad. Sch. Sci. & Eng., Hosei Univ., ²Dept. Frontier Biosci., Hosei Univ., ³Res. Cen. Micro-Nano Tech., Hosei Univ.)

Chemoreceptors of *Escherichia coli* form a cluster at a cell pole with a trimer of homodimers as a building unit. Previous studies have revealed that chemoreceptors first inserted into lateral regions of the cytoplasmic membrane and then diffuses toward the cell pole. It has also been shown that homodimers of the chemoreceptors for aspartate (Tar) and serine (Tsr) form mixed trimers of dimers. Here we found via single-molecule imaging that Tar and Tsr form mixed clusters even in lateral membrane regions. The deletion of *aer*, which encodes the low-abundance redox taxis sensor, affected the cluster size of Tar, suggesting Aer forms clusters with the high-abundance ones in lateral membrane regions.

2-09-1700* 神経細胞における早期遺伝子制御の定量的解析
Quantitative analysis of immediate early genes regulation in neuron

Kaho Itoh, Mariko Okada (*Institute for Protein Research, Osaka University*)

Neurons rapidly change the expression of immediately early genes (IEGs) regulating neuronal activity in response to external stimuli. To clarify the mechanism regulating stimuli-induced gene expression, we analyzed RNA-seq data obtained from mouse cortical neuron briefly or sustainably stimulated by KCl. From the analysis, we identified 144 IEGs. We also noticed that IEGs had different expression levels in response to brief and sustained KCl stimuli. The result was further experimentally validated using PC12 cells. Some of IEGs (e.g. *Arc*, *Fos*, *Nr4a1*) showed different time-course expression patterns in response to brief and sustained NGF stimuli in PC12 cells, indicating that these IEGs are differently regulated by positive or negative feedback loops.

2-09-1712 蟻の蟻道合流時における意思決定とその意義について
A movement strategy of a single ant when entering a pheromone trail

Tomoko Sakiyama, Yuta Sakamoto (*Soka University*)

It is well known that ants use pheromones as a navigational tool. However, it seems that ants are not necessarily to rely on pheromone concentrations. Recently, we found that ant foragers moved against an ant flow when entering a pheromone trail at a right angle. This result suggests that ants orient themselves towards a certain direction by interacting with other nest-mates. In this paper, we developed an agent-based model to investigate an adaptivity of this behaviour. In our proposed model, a single agent entering an artificial pheromone trail obeyed two different strategies (the reverse/normal strategy). We found that foragers well-performed when they adopted the reverse strategy, suggesting that they reached a certain goal within a short time using this strategy.

2-09-1724 ボルボックスの鞭毛停止確率の照度依存性
Light intensity dependence of flagellar stop probability of *Volvox*

Keigo Harada, Yoshihiro Murayama (*Applied Physics, Tokyo Univ. of Agri. and Tech.*)

Multicellular organism consisting of simple elements often show higher functions. Green algae *Volvox* consists of two-four thousands of somatic cells, and each somatic cell has two flagella. Flagella stop their beatings when the somatic cell is exposed from dark to bright circumstance, which enable a *Volvox* colony to realize phototaxis. Moreover, a *Volvox* colony can change its sensitivity depending on the total light intensity. To reveal the mechanism of the variable sensitivity, we investigated the light intensity dependence of flagellar stop probability. Experimental results suggest that each somatic cell sense only light intensity difference, and the variable sensitivity could be realized in a colony level.

[2-09-1736](#) 緑藻 *Volvox* 目における細胞数と走光性の関係
Relationship between cell number and phototaxis in green algae *Volvox*

Masaki Tsubouchi, Yoshihiro Murayama (*Applied Physics, Tokyo Univ. of Agri. and Tech.*)

In this study, we investigated the effect of cell number on phototaxis of green algae *Volvox*. We used two species of *Volvox*, *V. carteri* consisting of 2000-4000 cells, and *pleodorina* consisting of 100-250 cells. The somatic cells are uniformly placed on the surface of their spherical shape, and each somatic cell has two flagella. A *Volvox* colony can sense the light intensity difference, and it swims toward the brighter side. We observed the phototactic motion of *Volvox*, and obtained the dependence of velocity and angular distributions on the light intensity difference. The two species showed different types of velocity distributions, and we will discuss the accuracy of phototaxis based on the cell number difference.

[2-09-1748](#) 単細胞緑藻クラミドモナスの負の重力走性メカニズム
Mechanisms of negative gravitaxis in the unicellular green alga *Chlamydomonas reinhardtii*

Azusa Kage¹, Toshihiro Omori², Kenji Kikuchi², Takuji Ishikawa², Takayuki Nishizaka¹ (¹*Dept. Physics, Gakushuin Univ.*, ²*Dept. Finemechanics, Tohoku Univ.*)

Like many other aquatic protists, the unicellular green alga *Chlamydomonas reinhardtii*, a model organism for studying flagellar motility and structure, shows negative gravitaxis, a tendency to swim upward. Density asymmetry and fore-aft shape asymmetry of the body could be involved in negative gravitaxis of *Chlamydomonas*, of which contributions are unknown. When we experimentally compared the rotation of the deflagellated and the flagellated, immobilized cells, the flagellated cells rotated about three times faster. This indicates that the contribution of shape asymmetry is significant. Furthermore, comparison of the simulation and the real trajectory of swimming cells suggested that physiological regulation might be involved in gravitaxis of *Chlamydomonas*.

[2-09-1800](#) 線虫 *C. elegans* の低温順化を司る神経回路における温度受容情報伝達
Thermosensory signaling in neural circuit underlying cold acclimation of *C. elegans*

Akane Ohta¹, Haruka Motomura¹, Atsushi Kuhara^{1,2} (¹*Dept. of Biology, Inst. of Integral Neurobio, Konan Univ.*, ²*PRIME, AMED*)

Temperature is an essential environmental stimulus with affecting animal's biochemistry and biophysics. Animals can respond to temperature changes through altered physiology. Yet, how animals habituate to ambient temperature is poorly known. Nematode *C. elegans* stores temperature experience that induces temperature acclimation-linked cold tolerance. We show here that (1) only three pairs of temperature-sensing neuron regulates cold tolerance through insulin signaling (Ohta et al., *Nature commun*, 2014; Ujisawa Ohta et al., *PNAS*, 2018), and (2) a DEG/ENAC-type mechanoreceptor functions as a temperature receptor (Takagaki, Ohta et al., *EMBO rep.*, 2020). Besides, (3) head-to-tail neural circuit controls cold acclimation via neuropeptide signaling (submitted).

[2-10-1315*](#) 両親媒性タンパク質とリン脂質から構成された非対称小胞の形成
Formation of asymmetric vesicles composed of amphiphilic protein and phospholipid

Masato Suzuki, Koki Kamiya (*Facut. Sci. Tech., Univ. Gunma*)

Liposome membranes have same biochemical and biophysical properties of the cell membranes. Liposomes and lipid vesicles have been used as artificial cell models and drug delivery systems. However, they have problems such as mechanical fragility and complexity in functionalization. Recently, vesicles formed by amphiphilic proteins have been reported. These vesicles have advantages of mechanical fragilities and bifunctionalities. To generate complex artificial cell models, we generate asymmetric lipid-amphiphilic protein vesicles by a droplet transfer method. We confirmed an asymmetry of the lipid-protein vesicles and retention of size and inner solution. Insertion and function of membrane proteins into the asymmetric lipid-protein vesicles were investigated.

2-10-1327* ホスファチジルコリン二重膜特性におよぼす疎水鎖結合様式の影響
Effect of hydrophobic chain-linkage type of phosphatidylcholines on their bilayer membranes

Toshiki Nakao¹, Masaki Goto², Masashi Kurashina², Nobutake Tamai², Mikito Yasuzawa², Hitoshi Matsuki² (¹*Grad. Sch. Advan. Tech. & Sci, Tokushima Univ.*, ²*Grad. Sch. Tech. Indus. & Soc. Sci, Tokushima Univ.*)

An unnatural glycerophospholipid with two amide linkages, dipalmitoylamidodeoxy-phosphatidylcholine (DPADPC), was synthesized and the bilayer phase transitions were observed by methods of differential scanning calorimetry under atmospheric pressure and light-transmittance measurements under high pressure. The temperature–pressure phase diagram and thermodynamic quantities of the phase transitions of the DPADPC bilayer membrane were compared with those of bilayer membranes of hydrophobic chain-linkage isomers, ester-linked dipalmitoyl-PC (DPPC) and ether-linked dihexasadecanoyl-PC (DHPC). We revealed that the molecular interaction in the PC bilayer membranes increases in the order of ether-, ester- and amide-linkage isomers.

2-10-1339* 浸透圧下における粘弾性ベシクルの構造変化解析
Morphological deformation of viscoelastic vesicle under osmotic stress

Tomoki Maruyama¹, Takeshi Mori^{2,3}, Yoshiki Katayama^{2,3,4}, Akihiro Kishimura^{2,4} (¹*Fac. of System Life Science, Kyushu Univ.*, ²*Dept. of Applied Chem., Fac. of Eng., Kyushu Univ.*, ³*Ctr. for Future Chem., Kyushu Univ.*, ⁴*Ctr. for Molecular Systems, Kyushu Univ.*)

Polyion complex vesicle (PICsome) is usually obtained as a unilamellar vesicle, formed from electrostatic interaction between oppositely charged polyelectrolytes. Unlike vesicles composed of a hydrophobic membrane, the PICsome membrane shows high water content due to its hydrophilic nature, resulting in its viscoelasticity and semi-permeability. In this study, we aimed to investigate the morphological deformation of PICsome under osmotic stress, and analyze its relevant behavior. By introducing osmotic stress on PICsome membrane, unilamellar PICsome uniformly deformed into vesicle-in-vesicle structure, which might be achieved via inward budding of its membrane. Finally, several factors related to the deformation behavior of PICsome was clarified.

2-10-1351* (3S5-4) 放射光円二色性・直線二色性・蛍光異方性により明確化された生体膜に誘起されたマガイニン 2 β 凝集体の特徴
(3S5-4) Membrane-Induced β -Aggregates of Magainin 2 Characterized by Circular Dichroism, Linear Dichroism, and Fluorescence Anisotropy

Munehiro Kumashiro¹, Shoma Suenaga¹, Koishi Matsuo² (¹*Grad. Sch. Sci., Hiroshima Univ.*, ²*HiSOR, Hiroshima Univ.*)

Synchrotron-radiation circular dichroism spectra of magainin 2 (M2) were measured in DPPG lipid membrane at lipid-to-peptide (L/P) molar ratio from 0 to 26. The results showed that the conformation of M2 changed from random coil to α -helix structures via an intermediate state as the L/P increases. The adsorption model fitting analysis of the spectra indicated that α -helix monomers assembled and transformed to β -sheet oligomers in the intermediate state. Linear dichroism provided the orientation of the β -sheet structure on the membrane surface. Fluorescence anisotropy of liposome showed that the formation of β -aggregates caused the disorder of the membrane, suggesting that the β -aggregates in membranes play a crucial role in the disruption of cell membrane by M2.

2-10-1403* クラミドモナス封入巨大リポソームの光応答性運動
Motion response of *Chlamydomonas*-containing giant liposomes to optical signal

Shunsuke Shiomi, Masahito Hayashi, Tomoyuki Kaneko (*LaRC, FB, Grad. Sch. Sci. & Eng., Hosei Univ.*)

We are developing an autonomous delivery system using *Chlamydomonas*-containing Giant Liposomes (ChGLs). We have demonstrated that ChGLs can move straight longer than 100 μm at about 10 $\mu\text{m/s}$. In this study, we investigated the motion response of ChGLs to optical stimuli. Under negative-phototactic conditions, ChGLs moved away from the green LED light (525 nm). Furthermore, when the light source direction was changed repeatedly, ChGLs turned away from the light within 10 s each time. The results indicate that we can direct ChGLs to desired positions using optical stimuli. At the next step, we will provide ChGLs with signal integration functions between the optical and other signals, e.g. chemical, thermal, and gravitational ones.

2-10-1415 Membrane viscosity of heterogeneous multi component liposome

Yuka Sakuma (*Grad. Sch. Sci., Tohoku Univ.*)

In cell membranes, the functional constituents such as peptides, proteins, and polysaccharides diffuse in a sea of lipids as single molecules and molecular aggregates. Thus, the fluidity of the membrane is important for understanding the roles of the cell functionality. Therefore, the membrane viscosity which is a measure of the membrane fluidity has been investigated with model biomembrane (liposome). Recently we established a method to estimate the membrane viscosity of heterogeneous multicomponent liposomes by means of microinjection technique. Using this method the membrane viscosity of ternary lipid liposome was measured. By varying the composition of the liposome, the observed membrane viscosity changed more than three orders of magnitude.

2-10-1427 膜相転移への影響からクロロゲン酸のリン脂質ホスファチジルコリン膜表面結合様式を探る Binding mode of chlorogenic acid to phosphatidylcholine bilayer revealed by its effect on the lipid bilayer phase transition

Eri Kumagawa, Yoshiki Yajima, **Hiroshi Takahashi** (*Grad Sci Sci.&Tech., Gunma Univ.*)

Chlorogenic acid (CGA) is the main component of coffee and an antioxidant. CGA has been reported to bear various good health effects. At the same time, it has been found that the addition of CGA induces an undesirable deformation of red blood cells. This fact indicates that CGA may bind to the proteins or/and membrane lipids of red blood cells. In this study, we examine how CGA binds the bilayers of phosphatidylcholine (PC), which is one of the primary lipids of red blood cells, by investigating the effect of CGA on the phase behavior and the structure of dipalmitoyl-PC (DPPC) bilayers. Based on the results obtained from calorimetry, dilatometry, and X-ray diffraction measurements, we will discuss the binding mode of CGA to DPPC bilayers.

2-10-1439 コレステロールが支持脂質二重膜の単層膜特異的な脂質拡散に与える影響 Leaflet-specific lipid diffusion of a supported lipid bilayer in the presence of cholesterol

Masaki Sato, Miyuki Sakaguchi, Shoichi Yamaguchi, Takuhiro Otsu (*Grad. Sch. Sci. Eng., Saitama Univ.*)

Lipid mobility in biological membranes is inevitable for the unique biological functions of the membranes. To quantitatively understand the lipid diffusion, we have recently developed leaflet-specific lipid diffusion analysis based on fluorescence lifetime correlation spectroscopy, which enables us to analyze the lipid diffusion in two leaflets (monolayers) of a lipid bilayer in a leaflet-selective manner. With this analysis, we have found that the lipid diffusion in a glass-side leaflet of a lipid bilayer supported on a glass (SLB) can be modulated by solution pH whereas that in the opposite leaflet is not. To further explore the pH- and leaflet-dependent lipid diffusion in SLB, here, we examine the effect of cholesterol on the leaflet-specific lipid diffusion.

2-10-1451 部分フッ素化ジエーテル型リン脂質の膜物性の解析 Analysis of membrane properties of partially fluorinated diether phospholipid membrane

Chika Arisaka¹, Masaya Miyazaki¹, Toshiyuki Takagi², Hiroshi Takahashi¹, Hideki Amii^{1,3}, Masashi Sonoyama^{1,2,4}
(¹*Grad. Sch. Sci. Tech., Gunma Univ.*, ²*AIST*, ³*GIAR, Gunma Univ.*, ⁴*GUCFW, Gunma Univ.*)

It is highly desirable to develop amphiphilic molecules that can retain the original structure and function of membrane proteins, which often undergo denaturation in various experimental process. Recently, it has been reported that amphiphiles with perfluoroalkyl groups are useful for biophysical studies of membrane proteins. In this study, a perfluorobutyl group was introduced into the terminal of an alkyl chain with varied lengths (C14, C16 and C18) of diether phospholipids, and their membrane properties were investigated with physicochemical methods. DSC measurements for the suspensions showed a significant decrease in T_m compared to their corresponding nonfluorinated phospholipids. The experimental results will be discussed with WAXD and Laurdan fluorescence data.

[2-10-1503](#) Theoretical Study of GM1 gangliosides assembly caused by Cholesterol: Structural Analysis by Coarse-grained Model

Daiki Shibata, Hidemi Nagao, Kazutomo Kawaguchi (*Graduate School of Natural Science and Technology, Kanazawa University*)

GM1 ganglioside is a kind of sphingoglycolipid which contains a sialic acid. All-atom molecular dynamics simulations for a planar lipid bilayer have suggested that cholesterol (Chol) induces accumulation of GM1 [Mori, et al., *J. Phys. Chem. B*, 2012]. In this study, we develop a coarse-grained model for GM1, Chol, and sphingomyelin (SM) to investigate accumulation of GM1 in mixture vesicles. In the coarse-grained model, GM1 is represented by 2 hydrophilic and 2 hydrophobic particles, SM is represented by 1 hydrophilic and 2 hydrophobic particles, and Chol is represented by 1 particle. We performed the Langevin dynamics simulations for GM1/SM and GM1/SM/Chol mixtures. We discuss the effects of Chol on GM1 assembly.

[2-10-1600](#) 抗菌ペプチド・マガイニン 2 の巨大リポソーム中のポア形成に対する浸透圧の効果
Effect of osmotic pressure (Π) on antimicrobial peptide magainin 2 (Mag)-induced pore formation in giant unilamellar vesicles (GUVs)

Md. Masum Billah¹, Samiron Kumar Saha¹, Md. Mamun Or Rashid¹, Masahito Yamazaki^{1,2,3} (¹*Grad. Sch. Sci. Tech., Shizuoka Univ.*, ²*Res. Inst. Ele., Shizuoka Univ.*, ³*Grad. Sch. Sci., Shizuoka Univ.*)

Membrane tension of GUVs due to Π under physiological conditions can be estimated quantitatively (1). Using this method, we investigated the effect of Π on Mag-induced pore formation in single GUVs. Under low Π , Mag generated formation of small pores in GUVs which cannot be observed using optical microscopy. The rate constant of pore formation increased with increasing Π . We estimated theoretically the values of k_p based on the total membrane tension, which are a little larger than those obtained experimentally. We also found the Mag-induced area change of GUVs decreased with increasing Π , which can explain the above difference in the theoretical and experimental k_p values. The mechanisms of these results are discussed. [1] *J. Phys. Chem. B* 124, 5588, 2020.

[2-10-1612](#) 蛍光ラベルされていない抗菌ペプチド PGLa の巨大リポソーム内へのポア形成なしの侵入
Entry of nonlabeled Antimicrobial Peptide PGLa into giant unilamellar vesicle (GUV) lumens without Pore Formation

Md. Hazrat Ali¹, Madhab Lata Shuma¹, Hideo Dohra², Masahito Yamazaki^{1,3,4} (¹*Grad. Sch. Sci. Tech., Shizuoka Univ.*, ²*Res. Inst. Green Sci. Tech.*, ³*Res. Inst. Ele., Shizuoka Univ.*, ⁴*Grad. Sch. Sci., Shizuoka Univ.*)

To eliminate the effect of fluorescent probe labeling, we investigated the entry of nonlabeled PGLa into the lumen of single GUVs using the method developed recently (1). During the interaction of PGLa with single GUVs containing AF647 and LUVs encapsulating the self-quenched calcein, the fluorescence intensity due to calcein in the GUV lumen increased without leakage of AF647, indicating that PGLa enters the GUV lumen without pore formation. The entry of PGLa occurs only during the second increase in the GUV area, indicating that PGLa enters the lumen during its translocation from the outer leaflet to the inner leaflet (2). The fraction of entry of PGLa increases with increasing membrane tension. (1) *Biochemistry*, 59, 1780, 2020, (2) *BBA Biomembrane*, 1863, 183680, 2021

[2-10-1624](#) 抗菌ペプチドの殺菌活性のための最小相互作用時間
Minimum Interaction Time for Bactericidal Activity of Antimicrobial Peptides (AMPs)

Farzana Hossain¹, Masahito Yamazaki^{1,2,3} (¹*Grad. Sch. Sci. Tech., Shizuoka Univ.*, ²*Res. Inst. Ele., Shizuoka Univ.*, ³*Grad. Sch. Sci., Shizuoka Univ.*)

Recently, the interaction of AMPs with single bacterial cells has been examined using confocal laser scanning microscopy (CLSM) (1). After a short time of the interaction, all the fluorescent probes leak out, indicating that bacterial plasma membrane is rapidly damaged. Here we examined the relationships between the interaction time of AMPs (e.g., magainin 2) with bacterial cells (e.g., *E. coli* cells) and their bactericidal activity using the time-kill assay and another new method. We compared these relationships with the results of the interaction of AMPs with single *E. coli* cells obtained using CLSM. On the basis of these results, we discuss the minimum interaction time required for their bactericidal activity. 1. *J. Biol. Chem.* 294, 10449, 2019.

2-10-1636 抗菌ペプチドを模倣した膜活性抗菌剤の設計と作用機構

Design of membrane-active antimicrobial agent by mimicking natural antimicrobial peptides and its action mechanism

Kazuma Yasuhara, Mizuki Kaji, Hideto Kibata, Takuto Nakano, Gwenaël Rapenne (*Div. Mat. Sci., Nara Inst. Sci. Tech.*)

There is a great demand for new antimicrobial agents that do not induce the development of antibiotic resistance. In nature, there is a class of antimicrobial peptides (AMPs) that is effective against a wide variety of pathogens with a small risk of resistance development. AMPs are known to act by disrupting membranes that contrast protein-targeting conventional antibiotics. We have previously designed and synthesized an antimicrobial agent using a calixarene molecular framework to mimic the amphiphilic structure of natural AMPs. In this presentation, we will discuss the structure-activity relationship of the calixarene derivatives as well as their action mechanism investigated using model membranes.

2-10-1648 脂質分子の特性に依存するマガイニン2の膜結合構造

Membrane-Bound Conformations of Magainin 2 depending on the Inherent Characteristics of Lipid Molecules

Ryoga Tsuji¹, Munchiro Kumashiro², Koichi Matsuo³ (¹*Grad. Sch. Adv. Sci. Eng., Hiroshima Univ.*, ²*Grad. Sch. Sci., Hiroshima Univ.*, ³*HiSOR., Hiroshima Univ.*)

Magainin 2 (M2) is an attractive target for understanding the mechanism of membrane interaction of antimicrobial peptides. The membrane-bound conformations of M2 were characterized in the four types of PC membranes with different acyl-chain length by a synchrotron-radiation circular-dichroism spectroscopy. The results showed that the helix structure was formed in the membrane with short acyl chain and in the gel phase, but not in the liquid-crystalline phase. This phase dependence was also confirmed by the fluorescence anisotropy of liposome. In the membrane with long acyl chain, no structural change was observed in either phase, indicating that the helical formations due to the membrane interaction are sensitive to the fluidity and acyl-chain length of lipid molecules.

2-10-1700 抗菌ペプチドのダブル・コオペラティブ効果

Antimicrobial peptide double cooperativity

Kaori Sugihara¹, Ewa Drab² (¹*IIS, Univ. Tokyo*, ²*Univ. Geneva*)

A mixture of different types of biomolecules sometimes boosts or suppresses their activities, or even generates a new function, known as cooperativity. We report a unique cooperative function between two well-known antimicrobial peptides (LL-37/HNP1) that kills bacteria more efficiently, whereas minimizing the host damage by suppressing mammalian cell membrane lysis. Such a “double cooperativity” may be used in our immune system and may help with developing efficient and safe antimicrobial agents in future. In this presentation, we will report our recent efforts in understanding its molecular mechanism by biophysical assays using supported and pore-spanning bilayers such as fluorescence recovery after photobleaching and electrochemical impedance spectroscopy.

2-10-1712 Crowding conditions induce clustering of diffusive molecules inside artificial cells

Yuki Kanakubo¹, Chiho Watanabe², Miho Yanagisawa¹ (¹*Univ. Tokyo*, ²*Hiroshima Univ.*)

Under molecular crowding conditions such as cytoplasm, not only normal molecular diffusion (The mean square displacement (MSD) is proportional to time, $\langle \text{MSD} \rangle = 6Dt^\alpha$, $\alpha = 1$) but also anomalous diffusion ($\alpha < 1$) occurs. We mimic this situation by using artificial cells densely packed with linear or globular molecules and analyze the molecular diffusion inside. For linear molecules, the diffusion behavior is normal, but inside small artificial cells, the diffusion rate D decreases. The value of D varies discretely depending on the cell size and the membrane property, suggesting clustering of the diffusing molecules. For the globular molecules, no clustering is observed. We will discuss the mechanism of clustering in our presentation.

2-10-1724 細胞サイズのミクロな膜閉じ込めによる相分離と分子拡散の制御

Phase separation and molecular diffusion modulated by cell-size micrometric membrane confinement

Chiho Watanabe^{1,2}, Miho Yanagisawa² (¹Hiroshima Univ., ²Univ. Tokyo)

Recent studies suggest that micrometric cell-size confinement can alter molecular behaviors. Here, we aim to investigate the origin of the so-called “cell-size effect” using polymer droplets that mimics cytosolic macromolecular crowding and cell size confinement. By measuring the molecular diffusion inside the cell-size droplets, the diffusion is slower than the bulk solution. Further, the diffusion is slower in droplets with a larger surface-to-volume ratio under the same volume condition, suggesting membrane is a key factor of the cell-size effect. Hence, we examined the membrane properties effect and found that it can modulate diffusion. We shall also discuss the “cell-size effect” on liquid-liquid phase separation (LLPS), which we have been working on recently.

2-10-1736 流れ環境下で生じる非対称脂質膜が引き起こす細胞サイズのリポソームへの分子濃縮

Abiotic molecular transport against a concentration gradient caused by flow-induced membrane asymmetry of cell-sized liposomes

Hironori Sugiyama¹, Toshihisa Osaki^{2,3}, Shoji Takeuchi^{2,4}, Taro Toyota^{5,6} (¹ExCELLS, NIBB, ²IIS, UTokyo, ³KISTEC, ⁴Grad. Sch. Info Sci. Tech., UTokyo, ⁵Grad. Sch. Arts and Sci., UTokyo, ⁶UBI, UTokyo)

Liposome, a closed lipid bilayer of phospholipids, is a promising scaffold for a minimal cell-like system. However, the low membrane permeability makes it difficult to implement long-lasting chemical systems in liposomes. In this presentation, we discuss the unique molecular transport against a concentration gradient across the lipid bilayer that emerged under the flow environment. We clarified that the external flow induces a compositional asymmetry between the inner and outer leaflets, and the asymmetry causes the anomalous molecular transport. The current findings suggest a potential role of the lipid compartment for the abiotic emergence of the functional chemical system in a cell-like compartment, which has been regarded as a mystery at the origin of life.

2-10-1748 環境酸素濃度による大腸菌封入巨大リポソームの形態制御

Motion control of *E. coli*-containing giant liposome using environmental oxygen concentration

Masahito Hayashi, Mai Hayakawa, Tomoyuki Kaneko (*Dept. Frontier Biosci., Hosei Univ.*)

Swarm of self-propelled particles, e.g. condensed culture of swimming bacteria, show unique patterns of mass movement. We demonstrated that a dense *E. coli*-containing Giant Liposome (EcGL) continuously changes its shape like an amoeba cell. In this report, we investigated the motion response of EcGLs to environmental O₂ concentration. A droplet (1 μl) of EcGL suspension was sandwiched between glass slips 80 μm apart. The shape change of EcGL stopped within 1 min after gas around the droplet was exchanged from air (20% O₂) to N₂ (0% O₂). When the gas was exchanged from N₂ to air, EcGLs resumed the continuous shape change. The results indicate that membrane-permeable signal, O₂, can control the deformation mode of BLs.

2-11-1315 *Arthrospira platensis* の red Chl について

The red chlorophyll of *Arthrospira platensis*

Kyoko Matsunaga¹, Miku Honda¹, Ryo Nagao², Jian-Ren Shen², Seiji Akimoto³, Tatsuya Tomo⁴ (¹Faculty of Science, Tokyo University of Science, Tokyo, Japan, ²Research Institute for Interdisciplinary Science and Graduate School of Natural Science and Technology, Okayama University, Okayama, Japan, ³Graduate School of Science, Kobe University, Hyogo, Japan, ⁴Graduate School of Science, Tokyo University of Science, Tokyo, Japan)

Chlorophylls (Chls) play roles in light harvesting, energy transfer, and electron transfer during photosynthesis. Photosystem I bind 7–10 molecules of Chl with absorption maxima at longer wavelengths than the primary electron donor. They are called red-Chl. The 77-K fluorescence spectrum of photosystem I has an emission maximum at 730–740 nm derived from red-Chl, but some cyanobacteria have a fluorescence band at even longer wavelengths. *Arthrospira platensis* has an additional fluorescence band around 760 nm. We isolated and characterized the monomer and trimer complexes of photosystem I in this species. The intensity of fluorescence band at 760 nm varied depending on aggregates. In this meeting, we will report on the reason for red-Chl formation and its function.

[2-11-1327](#) In-vitro reconstruction of light-harvesting complexes of siphonous green alga, *Codium fragile*

Chiari Akiyama¹, Naoko Norioka², Naohiro Oka³, Yumiko Yamano⁴, Tetsuko Nakaniwa², Hideaki Tanaka^{2,5}, Genji Kurisu^{2,5}, Ritsuko Fujii^{1,6} (¹*Grad. Sch. Sci., Osaka City Univ.*, ²*Inst. Protein Res., Osaka Univ.*, ³*BIRC, Tokushima Univ.*, ⁴*Lab. Org. Chem. Life Sci., Kobe Pharm. Univ.*, ⁵*Grad. Sch. Sci., Osaka Univ.*, ⁶*ReCAP, Osaka City Univ.*)

Light-harvesting complexes (LHC) play the crucial role of absorbing sunlight and transferring the energy to photoreaction center. Compared to the well-studied higher plant LHCII, the LHCII from a siphonous green alga, *Codium fragile*, binds the unique pigment siphonaxanthin (Sx) and more chlorophyll (Chl) *b*, allowing it to absorb blue-green region of light. Due to the high sequence identity of both LHC proteins, little is known about the key factors for regulating the absorption band. In this study, LHCII was prepared by in-vitro reconstitution of the siphonous LHCII protein overexpressed in *E. Coli*, with a set of pigments in different compositions and/or components. The biochemical and functional binding of pigments was assessed by spectroscopic measurements.

[2-11-1339](#) フィコビリソームのフィコシアニン 6 量体内のエネルギー移動におけるリンカータンパク質の役割
The role of the linker protein in energy transfer within the phycocyanin hexamer of phycobilisome

Hiroto Kikuchi (*Dept. of Phys. Nippon Med. Sch.*)

Phycobilisome (PBS) is a highly ordered and large peripheral light-harvesting protein complex present on the cytoplasmic side of the thylakoid membrane in cyanobacteria and red algae. The electronic states of the chromophores within PBS are modulated by their environment. Recently the 3-dimensional structure including the linker proteins of PBS from *Porphyridium purpureum* was determined by cryo-electron microscopy at 2.82 Å resolution. In this research we discuss how the light absorption wavelength of the chromophores in phycocyanin hexamer of PBS from *Porphyridium purpureum* are affected by the linker protein or their surrounding environment, using quantum chemical calculation.

[2-11-1351*](#) 励起スペクトル顕微鏡と超解像イメージングで明らかになったステート遷移におけるチラコイド膜の不規則な構造変化
Irregular Transformation of Thylakoid upon State Transition as Revealed by Excitation Spectral and Super-Resolution Microscopy

XianJun Zhang¹, Yuki Fujita¹, Naoya Kaneda¹, Ryutaro Tokutsu², Jun Minagawa², Shen Ye², Yutaka Shibata² (¹*Grad. Sci. Uni. Tohoku*, ²*National Institute for Basic Biology*)

State transition (ST) mechanism plays a crucial role to improve photosynthetic efficiency by redistributing the excitation energy between Photosystems. It is known that the fine thylakoid morphology changes reversibly during ST in higher plants. These morphological changes of thylakoid have been considered important for the ST. However, in a green alga *Chlamydomonas*, it remains unclear how ST is related to the dynamic and elaborate transformation of thylakoid. To clarify this, we conducted the noninvasive imaging of cells with the excitation spectral and super-resolution microscopy. The study revealed that the fine thylakoid transformation by ST did not recover the initial morphology by the reversed ST, indicating random-fluctuation-based transformation of thylakoid.

[2-11-1403*](#) 光合成電子伝達経路の鉄硫黄錯体における電子アクセプター／ドナー鉄サイト
Electron Acceptor–Donor Iron Sites in the Iron–Sulfur Cluster of Photosynthetic Electron–Transfer Pathways

Tomoki Kanda¹, Keisuke Saito^{1,2}, Hiroshi Ishikita^{1,2} (¹*Grad. Eng., Univ. Tokyo*, ²*RCAST, Univ. Tokyo*)

In photosystem I, two electron-transfer pathways via quinones (A_{1A} and A_{1B}) are merged at the iron–sulfur Fe_2S_4 cluster F_X into a single pathway toward the other two Fe_2S_4 clusters F_A and F_B . Using a quantum mechanical/molecular mechanical approach, we identify the redox-active Fe sites in the clusters. In F_A and F_B , the Fe site, which does not belong to the $CxxCxxCxxxCP$ motif, serves as an electron acceptor/donor. F_X has two independent electron acceptor Fe sites for A- and B-branch electron transfers. The two asymmetric electron-transfer pathways from A_1 to F_X and the separation of the electron acceptor and donor Fe sites are likely associated with the specific role of F_X in merging the two electron transfer pathways into the single pathway.

2-11-1415* 光合成反応中心における複数のプロトン移動経路の同定と各経路の機能解明
Mechanism of the formation of proton transfer pathways in photosynthetic

Yu Sugo¹, Keisuke Saito^{1,2}, Hiroshi Ishikita^{1,2} (¹*Department of Applied Chemistry, Univ. Tokyo.*, ²*Research Center for Advanced Science and Technology, Univ. Tokyo.*)

In photosynthetic reaction centers from purple bacteria from *Rhodobacter sphaeroides*, the secondary quinone Q_B accepts two electrons and two protons. Here, we identify proton transfer (PT) pathways that proceed towards the Q_B binding site, using a quantum mechanical/molecular mechanical approach. As the first electron is transferred to Q_B, the formation of the Grothuss-like H-bond network is observed along Asp-L213, Ser-L223, and the distal Q_B carbonyl O site. As the second electron is transferred, the formation of a low-barrier H-bond is observed between His-L190 at Fe and the proximal Q_B O site, which facilitates the second PT. Glu-L212 was assumed to be a direct proton donor for Q_BH⁻, but it facilitates proton transfer toward His-L190 after Q_BH₂ leaves the site.

2-11-1427* 低温ラマン分光法による Photoactive Yellow Protein の初期中間体の構造決定
Structural determination of initial intermediate of Photoactive Yellow Protein by low-temperature Raman spectroscopy

Daisuke Shiga¹, Tomotsumi Fujisawa², Wouter D Hoff³, Masasi Unno² (¹*Grad. Sch. Adv. Health Sci., Saga Univ.*, ²*Fac. Sci. Eng., Saga. Univ.*, ³*Oklahoma State Univ.*)

Photoactive Yellow Protein (PYP) is a blue light sensor of photosynthetic bacteria. This protein covalently binds the p-coumaric acid (pCA) chromophore, and photoreaction of pCA, which starts from the trans-to-cis isomerization, induces the protein structural change to transmit the light sensing signal. To understand the reaction mechanism of PYP, it is important to clarify the structures of its photointermediates. However, the structure of the initial intermediate is, particularly, not well-understood because several different structures have been reported for the initial intermediate. In this study, we used low-temperature Raman spectroscopy to measure the initial intermediate of PYP and determine the chromophore structure.

2-11-1439* bZIP 型転写因子 Photozipper における光誘起二量体形成過程の高速 AFM 観察
High-speed AFM observation on the light-induced dimerization of a bZIP transcription factor, Photozipper

Akihiro Tsuji¹, Hayato Yamashita¹, Osamu Hisatomi², Masayuki Abe¹ (¹*Grad. Sch. of Eng. Sci., Osaka Univ.*, ²*Grad. Sch. of Sci., Osaka Univ.*)

Photozipper (PZ) is a transcription factor containing a basic leucine zipper DNA binding (bZIP) domain and a light-oxygen-voltage-sensing domain. Biochemical studies suggested that blue light (BL) induces PZ dimerization and enhances its affinity for the target DNA. To clarify the single molecular mechanism of PZ dimerization, we observed PZ molecules in the dark and light states by high-speed AFM (HS-AFM). The dimerization process of PZ was visualized, and its kinetics were analyzed. Interestingly, lifetimes of the dimers under light were longer than that in the dark. Further HS-AFM analysis revealed that the bZIP domain is entangled in the dark, but loosens up by BL. Such structural change might allow bZIP-bZIP interaction and contribute to stabilize the PZ dimer.

2-11-1451* AUREO1 の二量体における水素結合の役割
The role of hydrogen bonds in stabilization of AUREO1 dimer

Yumiko Adachi, Hiroto Nakajima, Yuta Nagano, Osamu Hisatomi (*Grad. Sch. Sci., Univ. Osaka*)

Photozipper protein (PZ) consists of functional regions of the *Vaucheria* AUREO1. It is monomeric in the dark state, and undergoes dimerization upon illumination and increases its affinity for DNA. We have reported that blue light induces the deformation of the hydrophobic region on the β -sheet and detaches the A' α helix from LOV core. Here, we prepared PZ mutants with amino acid substitutions in the hydrophobic region and the hydrogen-bonding sites hypothesized in diatom AUREO1a, and measured their size and affinity for DNA. Our data suggested that the hydrophobic region contributes to stabilize both the monomer and dimer forms, and that the latter is further stabilized by hydrogen bonds. These interactions probably enable the conformational switching of AUREO1.

[2-11-1503](#) AUREO1 における発色団 FMN のリビトールリン酸の役割
The role of ribitol-phosphate of the chromophore (FMN) in AUREO1

Osamu Hisatomi, Yuta Nagano (*Grad. Sch. Sci., Osaka Univ.*)

Photozipper (PZ) consists of a bZIP domain and a LOV domain of *Vaucheria* AUREO1, and undergoes dimerization upon illumination and increases its affinity for the target DNA. We prepared apoPZ lacking the chromophore, flavin monophosphate (FMN). Size exclusion chromatography indicated the existence of monomeric and dimeric forms of apoPZ. Reconstituted PZs with FAD, FMN, riboflavin (RF) and lumiflavin (LF) showed absorption spectra typical of a LOV domain, which decreased upon illumination and regenerated in the dark. However, PZs reconstituted with FAD, RF and LF released the chromophore at lower denaturant concentrations than PZ reconstituted with FMN, suggesting that the ribitol-phosphate moiety contributes essentially to the rigid containment of the chromophore.

[2-11-1515](#) 褐藻類シオミドロ Aureochrome – 3 の光反応
Photoreaction of Aureochrome-3 in a brown alga, *E. siliculosus*

Yuta Nagano, Yumiko Adachi, Osamu Hisatomi (*Grad. Sch. of Sci., Osaka Univ.*)

Aureochromes in stramenopiles are blue light (BL) receptor proteins containing a bZIP domain and a LOV domain. Although many sequences are deposited in DNA databases, only a few aureochromes have been analyzed so far. In this study, we made a synthetic gene encoding aureochrome 3 (*Es_Au3*) of a brown alga, *Ectocarpus siliculosus*. Recombinant *Es_Au3* expressed in *E. coli* cells shows an absorption band at around 450 nm with a triplet vibrational structure, which decreases upon BL illumination and is regenerated in the dark. Size exclusion chromatography indicates that the apparent molecular weight (particle size) of *Es_Au3* is larger in the light state than that in the dark state, suggesting that BL induces a conformational change of *Es_Au3*, as well as other aureochromes.

[2-11-1527](#) 光誘起電子移動反応を引き起こす LOV ドメイン変異体
Photoreaction of mutated LOV domain that causes light-induced electron transfer

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LOV domain is a light sensor domain that binds a flavin (FMN). When a cysteine nearby FMN is mutated, the mutant does not show normal photoreaction. Instead, FMN is photoreduced in the presence of reducing agents. In this study, we investigated the photoreduction of LOV mutants. When $[\text{Fe}^{\text{II}}(\text{CN})_6]^{4-}$ was used as an electron donor, the quantum efficiency of a neutral semiquinoid (FMNH[•]) formation was less than 1%. The half time of FMNH[•] oxidation was not influenced between the presence/absence of $[\text{Fe}^{\text{III}}(\text{CN})_6]^{3-}$. If the electron transfer had been completed between iron and LOV, the LOV mutant could not function as an electron-transfer device, which was not the case. The LOV mutant has the potential for a light-induced electron-transfer device.

[2-11-1600](#) 光合成水分解系における翻訳後アミノ酸変換のメカニズム
Mechanism of post-translational amino-acid conversion in the photosynthetic water-oxidizing complex

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The water-oxidizing Mn_4CaO_5 cluster is bound to the PSII proteins through six carboxylate ligands. We recently found that a His mutant at the D1-D170 ligand was converted to the original Asp residue after transcription during phototrophic growth. Here, we investigated the mechanism of this novel amino-acid conversion using FTIR and LC-MS analyses. It was shown that PSII from D1-D170H incorporated with ¹³C-His had ¹³C-Asp at D1-170, whereas photoconversion of D1-H170 did not take place in a Mn²⁺-deficient medium. In addition, D1-E189Q and D1-D342N mutants at other ligand sites also showed similar photoconversion. It is thus proposed that conversions of the mutants of the carboxylate ligands occurred at the protein level by oxidation through a photo-oxidized Mn ion.

[2-11-1612](#) 光化学系 II における第二キノン電子受容体 Q_B への 2 段階プロトン移動の時間分解赤外分光検出
Time-resolved infrared detection of two-step proton transfer to the secondary quinone electron acceptor Q_B in photosystem II

Honami Ito, Yuki Kato, Takumi Noguchi (*Grad. Sch. Sci, Univ. Nagoya*)

In PSII, the secondary quinone electron acceptor Q_B accept two protons to become quinol upon its double reduction. Although theoretical calculations have suggested a two-step mechanism for the proton transfer to Q_B , it has not been proved experimentally. Here, we investigated proton transfer reactions of Q_B in PSII using time-resolved infrared spectroscopy. An infrared absorption change at the CO vibration of Q_B upon the 2nd-flash illumination showed two distinct phases with rates of ~ 5 and ~ 50 ms. The 1st and 2nd phases were attributed to proton transfer to the distal oxygen through D1-S264 and that to the proximal oxygen from the D1-H215 ligand to Fe^{2+} , respectively. This is the first direct observation of two-step proton transfer to Q_B upon double reduction in PSII.

[2-11-1624](#) 光合成光化学系 II 酸素発生系中間状態 $g = 5$ S_2 状態の熱的安定性
Thermodynamically stability of the $g = 5$ S_2 states in the Oxygen Evolving Complex of Photosystem II

Hiroyuki Mino (*Grad. School Sci., Nagoya Univ.*)

The Mn_4CaO_5 cluster, located in the photosystem II protein complex, is the core machinery for photosynthetic oxygen evolution. In the intermediate S_2 state, two kinds of EPR signals, the $g \sim 2$ multiline and $g \sim 4.1$ signal, have been observed. Upon depletion of the extrinsic proteins, another S_2 -state EPR signal was detected at $g \sim 5$. The thermal stability of the $g \sim 5$ state was observed. The half-inhibition temperature for the S_1 - S_2 ($g \sim 5$) transition was about 230 K, which is close to the S_2 - S_3 states transition. The activation energy is 47 kJ/mol. Based on these results, the thermal stability of the three S_2 states was evaluated. The S_1 - S_2 ($g \sim 5$) transition needs to provide a large structure modification, as seen in S_2 - S_3 transition.

[2-11-1636](#) 嫌気性緑色硫黄光合成細菌における Rieske/cytb 複合体と c 型シトクロム間の構造機能相関の解析
Structure-function relationships between the Rieske/cytb complex and c-type cytochromes in anaerobic photosynthetic green sulfur bacteria

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Cytochrome (cyt) *bc* complexes functioning in photosynthetic electron transport chain contain three transmembrane proteins, cyt *b*, cyt *c*₁ or cyt *f*, and Rieske ISP. They conduct electron transport reactions coupled with proton translocation across membranes, resulting in the production of proton motive force to synthesize ATP. Green sulfur bacteria were suggested to contain the most primitive Rieske/cytb complex. We tried to purify this complex under anaerobic conditions to explore the structure-function relationships. We also observed the interaction between the Rieske ISP and cyt *c*-556 by NMR measurements and identified the interaction sites on the Rieske ISP. Based on the results, the electron transfer model of the Rieske/cytb complex and cyt *c*-556 would be proposed.

[2-11-1648](#) プラストシアニンとシトクロム f の複合体形成に関する理論的研究
Theoretical study of complex formation of Plastocyanin and Cytochrome f

Kazutomo Kawaguchi, Hidemi Nagao (*Institute of Science and Engineering, Kanazawa University*)

In photosynthesis, an electron is transferred from Cytochrome f (Cyt f) anchored to cell membrane to water-soluble Plastocyanin (Pc). We have succeeded in estimating a rate constant of electron transfer from Cyt f to Pc by using the Langevin dynamics simulation with our coarse-grained model. However, cell membrane has not been included in our model. In this work, our coarse-grained model is developed for membrane-anchored protein and applied to Cyt f-Pc complex formation. Langevin dynamics simulations were performed for complex system of Cyt f and Pc with Rieske protein and model membrane. We show the effect of Rieske protein and model membrane on conformation of Cyt f-Pc complex. We concluded that cell membrane promoted Cyt f-Pc binding.

[2-11-1700](#) **A. marina** の光化学系 I の光捕集機構 : *T. elongatus* の光化学系 I との比較
The light harvesting mechanism of *A. marina* Photosystem I reaction center: comparison with *T. elongatus* Photosystem I

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A structure of the photosystem I reaction center of *A. marina* (AmPSI) using far-red light has been reported, which has 70 chlorophyll *d* (Chl-*d*), 1 Chl-*d'*, 2 pheophytin *a* (Pheo-*a*) and 12 carotenoids. In this study, we numerically analyzed the light harvesting mechanisms in AmPSI, and compared the functions with those on *T. elongatus* PSI (TePSI). Excitonic couplings and site energy shifts in exciton Hamiltonian were obtained by P-TrESP and CDC methods respectively. Reproducing the experimental absorption/CD spectra, we calculated the transient absorption spectra on AmPSI for the analysis of the light harvesting processes. Pigment replacement analysis *in silico* was also performed to find out the functional/evolutional differences between AmPSI and TePSI.

[2-11-1712](#) Quantitative measurements of the redox chemistry of a flavin cofactor in photolyases and cryptochromes

Yuhei Hosokawa, Hiroyoshi Morita, Mai Nakamura, Shigenori Iwai, Junpei Yamamoto (*Grad. Sch. Eng. Sci., Osaka Univ.*)

Photolyase/cryptochrome superfamily (PCSF) is a flavoprotein family composed of photolyases (PLs) repairing DNA lesions and cryptochromes (CRYs) involved in signal transductions such as circadian rhythm entrainment. It is interesting how PCSF proteins sharing a similar sequence and architecture can play diverse functions. To address the question, we focused on their activation and inactivation processes, in which a flavin adenine dinucleotide (FAD) cofactor is reduced or oxidized. The kinetic and electrochemical measurements of the redox reactions in PCSF proteins from various organisms revealed that both activation and inactivation processes were modulated to achieve their functions. The study would be helpful to understand how photoreceptive CRYs evolved from PLs.

[2-11-1724](#) Light-induced movements of amino acid residues in *Chlamydomonas reinhardtii* animal-like cryptochrome and their roles in photoreduction

Mai Nakamura, Yuhei Hosokawa, Shigenori Iwai, Junpei Yamamoto (*Grad. Sch. Eng. Sci., Univ. Osaka*)

Cryptochrome (CRY) is a blue photoreceptor protein and is involved in a wide range of biological functions. CRY also possesses a flavin adenine dinucleotide (FAD) and form a one-electron reduced flavin in a light-dependent manner. In the recent time-resolved crystal structural analysis of CRY from animal-like *Chlamydomonas reinhardtii* (CrCRY) performed at SACLA, it was found that the movement of some amino acid residues was observed during the photoreduction, suggesting that these residues are functionally important. To identify the roles of the amino acids in the photoreduction, we prepared mutants of the amino acids and performed the photoreduction assay. We will discuss the relationship between the movements and their role of the amino acid residues.

[2-11-1736](#) 時間分解赤外分光法による(6-4)光修復酵素の光修復中間体の計測
Time-resolved IR spectroscopic detection of a photorepair intermediate in (6-4) photolyase

Ai Kadono¹, Daichi Yamada¹, Junpei Yamamoto², Minoru Kubo¹ (¹*Grad. Sch. Sci., Univ. Hyogo, Japan*, ²*Grad. Sch. Eng. Sci., Osaka Univ., Japan*)

(6-4) photolyases are the photorepair flavoenzymes that specifically revert UV-induced DNA photoproducts into normal bases. So far, a photoproduct repair model via sequential two-photon processes has been proposed, but it remains to be examined by direct observation of the reaction processes. Here, we performed TR-IR microspectroscopy to track the photorepair reaction. Although the photorepair was achieved by successive laser flashes, it was not completed upon one-photon illumination. Notably, the spectrum of an intermediate that appeared after one-photon illumination gradually vanished under dark conditions. These results strongly support the successive two-photon mechanism. Now, we are trying to assign the TR-IR spectrum of the intermediate by isotope labeling.

2-11-1748 クリプトクロムが触媒する DNA 光修復反応のマイクロフロー・フラッシュ紫外可視分光解析
Microflow-flash UV-vis spectroscopic analysis of DNA photorepair reaction catalyzed by
cryptochrome

Tatsumi Maeno¹, Daichi Yamada¹, Junpei Yamamoto², Minoru Kubo¹ (¹*Grad. Sch. Sci., Univ. Hyogo*, ²*Grad. Sch. Eng. Sci., Osaka Univ.*)

CraCRY is animal-like cryptochrome from *Chlamydomonas reinhardtii*, but is also known to work as DNA photolyase to photorepair UV-damaged DNA ((6-4) photoproduct) using blue light. This bi-functionality of CraCRY garners attention, but its molecular mechanism is still mystery. Here, we focused on the DNA photolyase activity of CraCRY, and performed microflow-flash, time-resolved UV-vis spectroscopy to understand its photorepair dynamics. We observed that, upon blue light illumination, a photorepair intermediate occurs in 1 ms, via electron transfer and back-electron transfer between CraCRY and (6-4) photoproduct. In the presentation, we will discuss the photolyase mechanism of CraCRY in relation to the two-photon mechanism of well-studied *Xenopus laevis* (6-4) photolyase.

2-11-1800 Molecular insight into photoactivation of BLUF photoreceptor from QM/MM free energy calculation

Masahiko Taguchi, Shun Sakuraba, Chan Justin, Hidetoshi Kono (*Inst. Quant. Life Sci., QST*)

OaPAC is a photoactivated enzyme that forms a homodimer. It has two BLUF photoreceptor domains with long coiled-coil C-terminal helices connecting to the catalytic domains. It is thought that during photoactivation, hydrogen bonding network between Tyr6, Gln48, and chromophore is disrupted, and keto-enol tautomerization of Gln48 occurs in the BLUF domain. However, it remains to be solved how the structural change in the BLUF domain propagates towards the catalytic domain. To investigate the mechanism, we performed QM/MM free energy calculations of the BLUF domain at dark and light states. In the light state, we observed a distinct flip of Trp90 nearby the C-terminal helix, causing the subsequent structural changes in the BLUF core and the C-terminal helix.

2-11-1812 可視光照射下での DNA 二重鎖切断に対する水素分子の保護効果
Effect of molecular hydrogen on DNA double-strand breaks under irradiation of visible light

Tatsuya Asano¹, Yuji Hatano², Hiroto Shimoyachi¹ (¹*Grad. Sch. Sci., Univ. Toyama*, ²*Hydrogen Isotope Research, Univ. Toyama*)

Molecular hydrogen (H₂) has a variety of medical effects. To clarify the role of H₂ in the medical effects, it needs to be revealed how H₂ protects biomolecules. The aim of this study is to examine the protective effect of H₂ for double-strand breaks (DSBs) of genome-sized DNA induced by irradiation of visible light (VL). An aqueous solution containing DNA molecules of bacteriophage T4 GT7 with intercalated fluorescence dye YOYO-1 was irradiated with VL (470-495 nm) under Ar or H₂ gas atmosphere. The rate of DSBs was evaluated with a single molecule observation method using a fluorescence microscope. Based on the quantitative observation of DSBs, we revealed that H₂ molecules serve as a scavenger and reduce the rate of DSBs caused by the irradiation of VL.

2-12-1315 レチナール光異性化酵素として働く動物ロドプシンの分光学的解析
UV-Vis spectroscopic analysis of animal rhodopsins acting as a retinal photoisomerase

Naoya Morimoto¹, Takashi Nagata^{1,2}, Keiichi Inoue¹ (¹*Inst. Solid State Phys., Univ. Tokyo*, ²*JST, PRESTO*)

Retinal G-protein-coupled Receptor (RGR) is a sub-group of animal rhodopsin family found in many vertebrates. Mammalian RGRs are known to serve as a retinal photoisomerase, which regenerates 11-*cis*-retinal from all-*trans*-retinal by photoisomerization to supply it to visual rhodopsins. However, RGRs other than bovine RGR have not been characterized so far. To understand the diversity of RGRs, we investigated the absorption spectra of RGRs from several mammalian and non-mammalian species in the UV-visible region. Most of the RGRs showed similar absorption maxima in the blue region, while a non-mammalian RGR exhibited different characteristics from bovine RGR upon light absorption. We will discuss relationships between absorption characteristics and the function of RGRs.

[2-12-1327](#) 高温環境由来のアーキアから発見されたシゾロドプシンの熱安定性研究
Thermal stability of schizorhodopsin discovered from archaea derived from high-temperature environment

Yuma Kawasaki¹, Masae Konno^{1,2}, Keiichi Inoue¹ (¹*ISSP, Univ. Tokyo*, ²*PRESTO, JST*)

Schizorhodopsins (SzRs) are light-driven inward H⁺ pumps. We focused on novel SzRs, *MtSzR* and *MsSzR*, derived from *Methanoculleus* archaea. They are expected to have high thermal stability, because of thermophilic habitats of the host species. The thermal stabilities of *MsSzR* and *MtSzR* were investigated by measuring the temperature dependence of the denaturation rates and compared with that of SzR1 derived from non-high temperature environment. The denaturation rates of *MtSzR* and *MsSzR* were 15 and 150 times slower than that of SzR1 at 85 °C, respectively. This means that *MtSzR* and *MsSzR* are more stable than SzR1 at high temperature. The different mechanism of high thermal stability was suggested between *MtSzR* and *MsSzR* by the Eyring plots of the denaturation rates.

[2-12-1339](#) シグナルペプチドを持つ Marine group II 古細菌由来 Clade-C ロドプシンの分子特性
Molecular properties of Clade-C rhodopsins with signal peptides derived from Marine Group II archaea (*Ca. Poseidoniales*)

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Marine Group II (MGII) archaea (*Ca. Poseidoniales*) is a globally abundant group of archaea in surface waters. A new rhodopsin clade, named Clade-C, was identified in estuarine MGII archaea. We focused on three Clade-C rhodopsins which have N-terminus signal peptides. *E. coli* cells expressing the Clade-C rhodopsins with their signal peptides showed pigmentation of the cell indicating the expression of properly folded proteins. While, the removal of signal peptides resulted in no pigmentation, indicating that the signal peptide is essential for the expression and/or folding of the proteins. Immunoblot analysis revealed that the signal peptides were removed from the folded protein in *E. coli* cells. The detailed molecular properties of Clade-C rhodopsins will be discussed.

[2-12-1351](#) バクテリアロドプシンの光反応サイクルにおける 2 種類の O 中間体の存在
Existence of two substates in the O intermediate of the bacteriorhodopsin photocycle

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The proton pumping cycle of bacteriorhodopsin is initiated when the retinal chromophore with the 13-*trans* configuration is photo-isomerized into the 13-*cis* configuration. To understand the recovery processes of the initial retinal configuration that occur in the late stage of the photocycle, we analyze absorption kinetics data collected under various conditions. The following features of the *trans* photocycle were revealed. *i*) Two substates of the O intermediate occur. *ii*) The visible absorption band of the first substate (O1) appears at a much shorter wavelength than that of the late substate (O2). *iii*) O1 is in rapid equilibrium with the preceding state (N). We suspect that the retinal chromophore in O1 takes on a distorted 13-*cis* configuration.

[2-12-1403](#) 固体 NMR による暗順応状態ミドルロドプシンのレチナル発色団の構造解析
Structure of a retinal chromophore of dark-adapted middle rhodopsin as studied by solid-state NMR spectroscopy

Izuru Kawamura^{1,2}, Hayto Seki², Seiya Tajima¹, Yoshiteru Makino², Arisu Shigeta², Takashi Okitsu³, Akimori Wada³, Akira Naito², Yuki Sudo⁴ (¹*Grad. Sch. Eng. Sci., Yokohama Natl. Univ.*, ²*Grad. Sch. Eng., Yokohama Natl. Univ.*, ³*Kobe Pharm. Univ.*, ⁴*Grad. Sch. Med. Dent. Pharm. Sci., Okayama Univ.*)

Some isomers of the retinal and the photochemical reaction of middle rhodopsin (MR) found from the *H. walsbyi* are markedly different from those of bacteriorhodopsin and sensory rhodopsin II. Here, the analysis of the ¹³C NMR signals of the retinal chromophore revealed the presence of three types of retinal configurations of dark-adapted MR: all-*trans*, 13-*cis*, and 11-*cis* isomers. The higher field resonance of the 20-¹³C in the all-*trans* form suggested that W182 in MR has an orientation that is different from that in other microbial rhodopsins. Further, ¹⁵N NMR analysis of the protonated Schiff base corresponding to the all-*trans* and 13-*cis*, 15-*syn* isomers in MR showed a strong electrostatic interaction with counter ion. I. Kawamura et al. (2021) *BPPB*, in press.

[2-12-1415](#) 天然アニオンチャネルロドプシン GtACR1 のイオン輸送過程に関する理論的研究
Theoretical study on ion conduction of natural anion channel rhodopsin GtACR1

Takafumi Shikakura, Cheng Cheng, Shigehiko Hayashi (*Grad. Sch. Sci., Kyoto Univ.*)

Channelrhodopsins are photo-sensitive channel proteins with a retinal chromophore. Light absorption causes isomerization of retinal, resulting in ion conduction. Recently a structure of an anion-conducting channelrhodopsin, GtACR1, was determined by X-ray crystallography. However, protonation states of the counterion groups (Glu68 and Asp234) are still under debate, and the mechanism of ion conduction is unknown. Here we examined distributions of water molecules and a Cl⁻ anion in a putative channel with different protonation states by molecular simulations. Ab initio QM/MM free energy geometry optimizations revealed tight coupling of the protonation states and distributions of water molecules and a Cl⁻ anion, providing a molecular insight into the anion-conduction.

[2-12-1427](#) チャネルロドプシンのカチオン伝導の分子動力学研究
Molecular dynamics study of cation conduction in channelrhodopsin

Jun Ohnuki, Takuto Hayashida, Takuma Hiramoto, Mitsunori Takano (*Dept. of Pure & Appl. Phys., Grad. Sch. Adv. Sci. & Eng., Waseda Univ.*)

Channelrhodopsin-2 (ChR2) is a light-induced cation channel in which the photoisomerization of retinal opens the channel gates. Although the previous studies have given insights into the photoisomerization-induced response of the ionic bonds that form the channel gates, the cation-conducting dynamics and the effect of the electric field remain unclear. Therefore, we conducted molecular dynamics simulation of ChR2 in the presence of the applied electric field across membrane and investigated the sodium conduction in ChR2. We here focus on the role of not only the photoisomerization but also the change in the protonation state of the gate-forming residues and discuss the physical mechanism of the gate opening and the cation conduction in ChR2.

[2-12-1439](#) Sodium-ion transportation mechanism of a light-driven sodium pump rhodopsin investigated by step-scan time-resolved FTIR spectroscopy

Sahoko Tomida¹, Akimori Wada², Hideki Kandori^{1,3}, Yuji Furutani^{1,3} (¹*Nagoya Institute of Technology*, ²*Kobe Pharmaceutical University*, ³*OptoBio Technology Research Center, Nagoya Institute of Technology*)

KR2 is a light-driven sodium pump rhodopsin which covalently binds an all-*trans* retinal and light illumination causes retinal isomerization inducing the photocyclic reaction. During the photocycle, K, L/M, and O intermediates are formed. Uptake and release of sodium ion take place with the formation and decay of the O intermediate, respectively. Here, we applied light-induced time-resolved FTIR spectroscopy to study temporal structural changes of KR2. We found spectrally distinct two O intermediates in the photocycle. We also revealed that sodium binding to the extracellular side seems to facilitate a sodium ion release from KR2. From our spectroscopic analysis, model of the structural changes during the photocycle of KR2 will be discussed.

[2-12-1451](#) Color Tuning of Microbial Rhodopsin Proteins: Combined Spectroscopic and QM/MM Modeling Studies

Maria del Carmen Marin Perez¹, Konno Masae^{1,2}, Laura Pedraza-Gonzalez³, Luca De Vico³, Massimo Olivucci^{3,4}, Keiichi Inoue¹ (¹*Univ. Tokyo / ISSP*, ²*Japan Sci. Tech. Agency / PRESTO*, ³*Univ. Siena / Biotech., Chem. and Phar. Depart.*, ⁴*BGSU / Chem. Depart.*)

Color tuning effect in microbial rhodopsins has attracted the interest of researchers as the color of their common retinal chromophores is modulated by their surrounding residues. Here, we combine spectroscopic and QM/MM modeling studies to perform two related color tuning studies: i) two asymmetric color tuning rhodopsins are employed to explore the challenging and partial-conversion achievement of blue-shifted rhodopsin into red-shifted one; and ii) the opposite color tuning rule observe when a conservative hydrophobic residue around the retinylidene β -ionone ring is replaced with an OH-group. A brand-new information about the modification in the electrostatic interaction between protein-chromophore and the structural differences in their chromophores is released.

[2-12-1503](#) Swing motion of Arg108 residue as a gating mechanism of *Indibacter alkaliphilus* Na⁺ pump rhodopsin

Yukino Sato¹, Tsubasa Hashimoto¹, Koji Kato², Yoshikazu Tanaka³, Yoshiaki Tanaka⁴, Tomoya Tsukazaki⁴, Takashi Tsukamoto^{1,5}, Makoto Demura^{1,5}, Min Yao^{1,5}, Takashi Kikukawa^{1,5} (¹*Grad. Sch. Life Sci., Hokkaido Univ.*, ²*RIIS, Okayama Univ.*, ³*Grad. Sch. Life Sci., Tohoku Univ.*, ⁴*Grad. Sch. Biol. Sci., NAIST*, ⁵*Fac. Adv. Life Sci., Hokkaido Univ.*)

R108 corresponds to the R109 in *Krokinobacter eikastus* Na⁺ pump rhodopsin (NaR) and seems to be a "gate" for Na⁺ release. Here we present the data for *Indibacter alkaliphilus* NaR suggesting that the conformational change at extracellular (EC) surface induces the swing motion of R108 residue and resultantly opens the gate. Crystallographic analysis yielded a unique structure that seemed to mimic an open-gate state, where the R108 residue pointed to the EC surface due to the outward movement of the E159-R242 pair. In the dark state, this pair is known to form a complex with E10 at the EC surface. Thus, the light-induced disruption of the complex seems to lead the swing motion of R108 residue. We will discuss this model based on other experimental results.

[2-12-1515](#) DTG ロドプシンの X 線結晶構造解析
X-ray crystallographic analysis on DTG rhodopsin

Keiichi Inoue¹, Kano Suzuki², Masae Konno^{1,3}, Reza Bagherzadeh¹, Andrey Rozenberg⁴, Maria del Carmen Marin¹, Oded Bějá⁴, Takeshi Murata^{2,5} (*Inst. Solid State Phys., Univ. Tokyo*, ²*Grad. Sch. Sci., Chiba Univ.*, ³*PRESTO, JST*, ⁴*Technion*, ⁵*Mol. Chirality Res. Cntr, Chiba Univ.*)

Microbial rhodopsins are a large family of photoreceptive membrane proteins. While they exhibit a wide variety of functions with light energy, the most abundant microbial rhodopsins are outward H⁺ pumps which have conserved extracellular H⁺ acceptor and cytoplasmic H⁺ donor. Recently, a new type of H⁺ pump, DTG rhodopsin, which does not have the cytoplasmic proton donor, was reported. DTG rhodopsin directly takes up an H⁺ from the cytoplasmic side. However, its detailed mechanism was not understood. Here, we revealed the X-ray crystallographic structure of DTG rhodopsin. The cytoplasmic structure and the hydrogen bonding network are considerably different from those of typical H⁺ pumping rhodopsins, and they would be related to the characteristic H⁺ uptake process.

[2-12-1600*](#) 表面増強赤外吸収分光解析によるセンサーロドプシン II—トランスドューサータンパク質融合タンパク質の光誘起構造変化
Light-induced conformational change of pSRII-pHtrII fusion protein analyzed by surface-enhanced infrared spectroscopy

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Sensory rhodopsin 2 (SRII) is a seven-transmembrane protein possessing an all-*trans* retinal chromophore and absorbing blue-green light (498 nm). It forms a 2:2 complex with a transducer protein (pHtrII) to transduce the light signal for negative phototactic response. To discuss the signal transduction mechanism, differences in the light-induced structural changes of pSRII with and without pHtrII were analyzed by surface-enhanced infrared absorption spectroscopy (SEIRA). We produced pSRII-pHtrII fusion protein and checked delay of the M-intermediate to make sure formation of the functional complex. We also found that SEIRA spectra of pSRII only and pSRII-pHtrII complex were different in response to different concentration of the proteins.

[2-12-1612*](#) LED システムを用いたロドプシン蛍光の観察と膜電位の長時間イメージングへの適用
Detection of membrane potential-dependent rhodopsin fluorescence with LED system for long-term imaging

Shiho Kawanishi¹, Keiichi Kojima^{1,2}, Atsushi Shibukawa¹, Masayuki Sakamoto³, Yuki Sudo^{1,2} (¹*Grad. Sch., Med. Dent. & Pharm. Sci., Okayama Univ.*, ²*Grad. Sch., Med. Dent. & Pharm. Sci., Okayama Univ.*, ³*Grad. Sch., Biostudies, Kyoto Univ.*)

Microbial rhodopsin is a seven-transmembrane photoreceptive protein containing chromophore retinal. Among rhodopsins, archaerhodopsin-3 (AR3) and its mutants show voltage-sensitive fluorescence changes. The unique characters as a genetically encoded voltage indicator (GEVI) enable to monitor membrane potential with high spatiotemporal resolution although intense laser excitation (~ 100 W/cm²) is required. Here, we replaced the light source with LED (0.15 W/cm²) and successfully detected voltage-sensitive fluorescence of AR3 and its mutant Archon1 in HEK293 cells. Of note, the LED excitation was less harmful to HEK293 cells than the intense laser excitation. Our results suggest that the system is useful for long-term voltage imaging of living cells with harmlessness.

2-12-1624* 内向きプロトンポンプ型ロドプシン *RmXeR* を用いた光誘起崩壊リポソーム (LiDL) の開発
Development of light-induced disruptive liposome (LiDL) with an inward proton pump rhodopsin *RmXeR*

Taichi Tsuneishi¹, Keiichi Kojima^{1,2}, Fumika Kubota³, Yuma Yamada³, Yuki Sudo^{1,2} (¹*Grad. Sch. of Med., Dent. & Pharm. Sci., Okayama Univ.*, ²*Grad. Sch. of Med., Dent. & Pharm. Sci., Okayama Univ.*, ³*Grad. Sch. of Pharm. Sci., Hokkaido Univ.*)

Liposome is a sphere-shaped lipid bilayer vesicle and is utilized as a carrier for drug delivery system (DDS). For the DDS, it is essential to deliver compounds to the target organs. In addition, the liposome should be promptly disrupted at the target. Microbial rhodopsin is a photoactive membrane protein, and its function can be regulated by light with high spatiotemporal resolution. In this study, we inserted an inward proton pump rhodopsin *RmXeR* into pH-sensitive liposome to develop the light-induced disruptive liposome (LiDL). Fluorescent dye calcein was also incorporated into the liposome and its fluorescence change was observed upon illumination, suggesting the disruption of the liposome followed by calcein release. Its implication would be discussed.

2-12-1636* 青色吸収型プロテオロドプシンにおける異常な pH 依存的長波長シフトの解明
Mechanism of anomalous pH-dependent color change in blue-proteorhodopsin from *Vibrio caribbeanus*

Mizuki Sumikawa¹, Rei Abe-Yoshizumi¹, Takayuki Uchihashi², Hideki Kandori¹ (¹*Nagoya Inst. Tech.*, ²*Dept of phys, Nagoya univ*)

Proteorhodopsins (PRs) are light driven proton pumps found in marine bacteria, which are classified into blue-absorbing (BPR) and green-absorbing (GPR) forms. Previously, we converted a BPR into green-absorbing type by changing pH into 2, whose mechanism was fully unknown. In this study, we found that VcBPR, which also exhibits anomalous pH effect, is converted from an oligomer to a monomer by such pH changes, which was monitored by size-exclusion chromatography and atomic force microscope. We thus hypothesized a positive correlation between oligomer state and color in VcBPR. This hypothesis was examined by site-directed mutagenesis of VcBPR. We will present a structural model to explain the anomalous pH-dependent color change in VcBPR.

2-12-1648* 様々な内向きおよび外向きプロトンポンプロドプシンの電気生理学的解析
Electrophysiological analysis 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 upon light absorption. In addition to an enormous number of outward proton pumps, inward proton pumps such as xenorhodopsins and schizorhodopsins have been discovered recently. It is thus intriguing to compare the molecular mechanism of inward and outward proton pumps. Which is a superior molecular machine? In this study, we determined driving forces of various inward and outward proton pumps by patch clamp recordings, where the driving forces were estimated from the I-V plots. Effect of pH gradient was also studied. We will discuss molecular origin of driving forces in inward and outward proton pump rhodopsins based on the present electrophysiological measurements.

2-12-1700* TAT ロドプシンの Ca²⁺ センサー機能
Ca²⁺ sensing function of TAT rhodopsin

Tepei Sugimoto, Kota Katayama, Hideki Kandori (*Grad. Sch. Univ. Nagoya Institute of Technology*)

TAT rhodopsin in marine bacteria contains protonated (visible-absorbing) and unprotonated (ultraviolet-absorbing) forms at physiological pH, and we recently suggested that TAT rhodopsin is an ultraviolet (UV)-dependent environmental pH sensor. Here we report Ca²⁺ binding activity to TAT rhodopsin, which has never been observed for other microbial rhodopsins. UV-visible spectroscopy showed that population between visible and ultraviolet forms altered depending on the Ca²⁺ concentration, from which we determined the affinity of the Ca²⁺ binding. We also applied ATR-FTIR spectroscopy of Ca²⁺ binding to the wild-type and mutant proteins, from which molecular mechanism and physiological role of Ca²⁺ binding to TAT rhodopsin will be discussed.

[2-12-1712*](#) 光と苦味のセンサーとしてはたらくキイロシヨウジョウバエ Rh7 の赤外分光研究
FTIR study of *Drosophila* Rh7, a light and bitter taste sensor

Kohei Watanabe, Kota Katayama, Hideki Kandori (*Grad. Sch. Eng., Nagoya Inst. Tech.*)

The fruit fly, *Drosophila melanogaster*, senses light and bitter taste using three opsins, Rh1, Rh4, and Rh7. 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 Sf9 insect cells for structural analysis using FTIR spectroscopy. After optimizing the sample preparation conditions, we successfully purified *Drosophila* Rh7. With this sample, we measured light-induced difference ATR-FTIR spectroscopy to elucidate structural changes of the protein moiety and retinal chromophore upon illumination. Based on the obtained data, activation mechanism of *Drosophila* Rh7 will be discussed.

[2-12-1724*](#) 全長型アニオンチャンネルロドプシンの機能解析
Functional Characterization of *Guillardia theta* Anion Channelrhodopsin 1 with its Full-Length Sequence

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Guillardia theta anion channelrhodopsin 1 (*GtACR1*) is composed of a transmembrane domain (rhodopsin domain) and an extended C-terminal domain (CTD). However, the functional role of the CTD and the characteristic of full-length *GtACR1* (*GtACR1_full*) have been unidentified. In this study, we identified that the CTD affected the ion channel function. The anion transport activities of *GtACR1_full* were generally smaller than those of *GtACR1* with only the rhodopsin domain (*GtACR1_295*). In addition, the *GtACR1_full* preferably transported NO₃⁻ to the other anions. Flash-photolysis measurements revealed that *GtACR1_full* had longer photocycle than *GtACR1_295*, indicating the interaction between the rhodopsin domain and the CTD.

[2-12-1736*](#) ラマン光学活性による微生物型ロドプシン単量体と多量体におけるレチナルシッフ塩基の構造解析
Conformational analysis of retinal Schiff base of a microbial rhodopsin in monomeric and oligomeric forms using Raman optical activity

Kohei Nishikawa¹, Tomotsumi Fujisawa², Masashi Unno², Yuki Sudo³, Keiichi Kojima³, Masaki Nakama³ (¹*Grad. Sch. Adv. Health. Sci., Saga Univ.*, ²*Fac. Sci. Eng., Saga Univ.*, ³*Grad. Sch. of Med. Dent. & Pharm. Sci. Okayama Univ.*)

Microbial rhodopsins are the photoreceptors of micro-organisms using the retinal Schiff base chromophore. Many microbial rhodopsins are known to function as the oligomeric forms, and the oligomerization is thought to facilitate the functions of microbial rhodopsins as it improves thermal stability, ion transport activity, and so on. Although it has been thus suggested that the conformational change of the active site is induced by the oligomerization, the conformational change occurring in the oligomers has been largely unclear. In this study, we analyzed the conformation of the retinal Schiff base chromophore in monomeric and trimeric forms of thermophilic rhodopsin using Raman optical activity spectroscopy.

[2-12-1748*](#) 近赤外光を吸収する新規酵素ロドプシン(RhGC)の反応特性
Reaction characteristics of near-infrared light absorbing enzyme rhodopsin (RhGC)

Kazuki Ishikawa¹, Shoko Hososhima¹, Masahiro Sugiura¹, Leonid S Brown², Satoshi Tsunoda², Hideki Kandori¹ (¹*Graduate School of Engineering, Nagoya Institute of Technology.*, ²*the Department of Physics, University of Guelph.*)

RhGC, rhodopsin guanylyl cyclase, is a transmembrane protein consisting of a rhodopsin domain with all-*trans* retinal as a chromophore, and an enzyme domain functioning as a GC. All previously known RhGCs absorb visible light. However, novel RhGCs absorbing near-infrared light have been discovered very recently. Striking differences are found in the amino acid sequences between visible- and near-infrared-RhGCs. Several acidic amino acid residues surrounding the chromophore are crucial for near-infrared absorption. It is assumed that the visible- and near-infrared-RhGCs form functional heterodimers. Here, we report on spectroscopic properties of near-infrared-RhGCs and investigate their light-induced GC activity to address the molecular mechanisms of their function.

2-12-1800* ロドプシグアニル酸シクラーゼ (Rh-GC) の光反応ダイナミクス
Photoreaction Dynamics of Rhodopsin Guanylate Cyclase (Rh-GC)

Masahiro Sugiura¹, Satoshi Tsunoda¹, Haon Futamata², Wataru Shihoya², Osamu Nureki², Hideki Kandori¹, Yuji Furutani¹ (¹*Nagoya Inst. Tech.*, ²*Grad. Sch. Sci., Tokyo Univ.*)

Rhodopsin guanylate cyclase (Rh-GC) is a photoactivatable membrane protein composed of a rhodopsin domain and a guanylate cyclase (GC) domain at cytoplasmic side. The GC domain is activated through conformational change induced at rhodopsin domain by light. This is one of the interesting aspects of Rh-GC which is different from conventional rhodopsins. Since its discovery in 2014, no study has been reported on photoreaction dynamics of Rh-GC. Therefore, we applied time-resolved FTIR spectroscopy at room temperature to reveal its light-induced molecular dynamics. As a result, we succeeded in capturing signals of Rh-GC including the enzyme domain accompanied with the rhodopsin domain. Finally, we propose a photocycle model of Rh-GC.

2-12-1812* ヘリオロドプシン特有の波長制御メカニズムの構造基盤
Structural basis for unique color tuning mechanism in heliorhodopsin

Tatsuki Tanaka¹, Manish Singh², Wataru Shihoya¹, Keitaro Yamashita¹, Hideki Kandori², Osamu Nureki¹ (¹*Grad. Sch. of Sci., Univ. of Tokyo*, ²*Grad. Sch. of Eng., Nagoya Inst. of Tech.*)

In microbial rhodopsins, a retinal is covalently bonded to a lysine residue through the retinal Schiff base (RSB) and stabilized by a negatively charged counterion. The interaction between the RSB and a counterion is closely related to the light absorption. However, in heliorhodopsin (HeR), E to D mutation of the counterion exhibits an identical absorption spectrum to the wild-type. The crystal structure of the HeR counterion mutant revealed that interaction between the RSB and the counterion becomes weaker and the serine cluster form a distinct interaction network around the RSB. The absorption spectra of the double mutants suggested that the serine influences the spectral shift by compensating for the weaker counterion interaction.

2-12-1824* アニオンチャネルロドプシンのプロトンを経たアニオン透過機構の解明
Proton-mediated gating mechanism of anion channelrhodopsin-1

Masaki Tsujimura¹, Keiichi Kojima², Shiho Kawanishi², Yuki Sudo², Hiroshi Ishikita^{1,3} (¹*Grad. Sch. Eng., Univ. Tokyo*, ²*Grad. Sch. Med. Dent. Pharm., Okayama Univ.*, ³*RCAST, Univ. Tokyo*)

Anion channelrhodopsin from *Guillardia theta* (*GtACR1*) has Asp234 and Glu68 near the protonated Schiff base. Here we investigate mutant *GtACR1*s expressed in HEK293 cells. The influence of the acidic residues on the absorption wavelengths are analyzed, using a quantum mechanical/molecular mechanical approach. The calculated protonation pattern indicates that Asp234, which was proposed to be protonated, is deprotonated in the crystal structures. The measured and calculated absorption wavelengths of D234E and E68Q/D234N *GtACR1*s confirm that Asp234 is deprotonated. Molecular dynamics simulations show that a proton transfer pathway from the Schiff base toward Glu68 via deprotonated Asp234 forms upon the Glu68 reorientation, which is likely a basis of the gating mechanism.

2-13-1315 ペプチド核酸の Taq ポリメラーゼに対する鑄型活性を利用したタンパク質から DNA への転写活性の検出
Detection of transcription activity of amino acids into DNA using Peptide Nucleic Acid (PNA) as a template for *Taq* DNA polymerase

Hidekazu Kuwayama (*University of Tsukuba, Faculty of Life and Environmental Sciences*)

Here, I demonstrate that a thermostable DNA polymerase, *Thermus aquaticus* (*Taq*) polymerase, exhibits transcriptase activity when a peptide nucleic acid (PNA) oligomer is used as a template and that genetic information of the oligomer can be amplified by polymerase chain reaction (PCR) using DNA primers. Furthermore, the insertion of a glutamine peptide stretch in the middle part of the PNA template did not interfere with the transcription; it was transcribed into a guanosine or adenosine stretch. Intriguingly, this amino acid-to-DNA transcription did not occur when glycine residues were inserted. A synthetic PNA oligomer can, therefore, function as a template for a DNA polymerase, and polyglutamine peptides can be transcribed into guanosine or adenosine.

[2-13-1327](#) 飢餓状態における解糖系の振動現象
Role of Glycolytic Oscillation in Starvation

Seiji Hatano¹, Noboru Nagata¹, Yutetsu Kuruma², Toshihiro Kawakatsu¹, Masayuki Imai¹ (¹*Grad. Sch. Sci., Tohoku Univ.*, ²*Japan Agency for Marine-Earth Science and Technology*)

The life is the system that reproduces itself using nutrients taken from the environment, which is maintained by very complex chemical reaction networks, so-called metabolism. In the origin of life, how to sustain the metabolism under starvation is critical. We consider that the key to survival under the starvation lies in the glycolytic oscillation. It is well known that the production of NADH in the glycolysis of yeasts starts to oscillate when the supply of glucose is reduced. We have examined the relationship between the glycolytic oscillation and glucose supply from experimental and theoretical points of view and discussed the role of chemical oscillation in the starvation. Especially we monitored concentration of glucose in a cell using micro-Raman spectroscopy.

[2-13-1339](#) 人工 RNA 複製システムのダーウィン進化による複雑化
Evolutionary complexification of an artificial RNA replication system

Ryo Mizuuchi^{1,2}, Taro Furubayashi³, Norikazu Ichihashi^{1,4,5} (¹*Komaba Inst. Sci., Univ. Tokyo*, ²*JST, PRESTO*, ³*Appl. Chem., Univ. Tokyo*, ⁴*Life Sci., Univ. Tokyo*, ⁵*Univ. Biol. Inst., Univ. Tokyo*)

In prebiotic evolution, how could simple RNA replicators have complexified by expanding their information and functions? Theoretically, this process could occur through the successive appearance of novel replicators that interact with one another to form replication networks. Here, we performed long-term replication experiments (1,200 h, 600 generations) using an artificial RNA replication system and found that a single ancestral RNA replicator evolved into a multiple replicator network. The network consisted of five types of RNAs that show diverse interactions, including cooperation that unites all replicators in the network. Our results support the capability of RNA replicators to spontaneously develop complexity through Darwinian evolution.

[2-13-1351](#) Mechanism of chiral-selective aminoacylation of an RNA minihelix studied by quantum mechanics/molecular mechanics free energy simulations

Tadashi Ando^{1,2}, Takato Masui¹ (¹*Adv. Eng., Tokyo Univ. Sci.*, ²*Res. Ins. Sci. Tech., Tokyo Univ. 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 (QM/MM) molecular dynamics (MD) simulations combined with an umbrella sampling method, we examined free energy profiles along a reaction coordinate for the aminoacylation of L- and D-amino acids in the RNA minihelix. QM/MM MD simulations started from the structures adopting a geometry required for the chemical reaction sampled in classical MD simulations. We will discuss the simulation results in the meeting.

[2-13-1403](#) 単純なペプチドから RNA ポリメラーゼコアドメインへの進化過程の実験的再現
Reconstructing the evolutionary pathway of the core domain in RNA polymerases from simple peptide

Sota Yagi, Shunsuke Tagami (*Center for Biosystems Dynamics Research, RIKEN*)

The modern proteins are thought to have evolved from ancient short and simple ancestors with prototype folds. The double-psi beta-barrel (DPBB) is one of the ancient prototype folds and conserved in the core domain of RNA polymerase. Here, we reconstructed its evolutionary pathway started by interdigitating homo-dimer of a half-size peptide (~43aa), followed by gene duplication and fusion. Furthermore, by restriction of the amino acid repertoire in the peptide, we reconstructed the DPBB with only 7 amino acid types (Ala, Asp, Glu, Gly, Lys, Arg, and Val), which can be coded by only GNN and ARR codons in the modern genetic code. Thus, the DPBB fold could have been emerged at the early evolutionary stage of the genetic code when only ~7 amino acid types were available.

[2-13-1415](#) 細菌の群集がしめす適応的な表現型構造
Adaptive phenotypic structures of bacterial communities

Takao Suzuki¹, Motomu Matsui¹, Wataru Iwasaki² (¹*Grad. Sch. Sci., UTokyo*, ²*Grad. Sch. Front. Sci., UTokyo*)

How bacterial community structures are assembled is one of fundamental questions in population biology. Recent progress on sequence technologies, “metagenomics”, provides us to identify species from natural environments. Here we use a large-set data of 1,525 bacterial communities from three environmental conditions (soil, marine, human gut), and revealed adaptive phenotypic structures of them. We found that trait compositions in communities are significantly similar within a single environmental condition. Nevertheless, bacterial communities showed quite different in species compositions among communities. These results may suggest that the phenotypic compositions of communities are strongly attracted to the stable point, regardless of the constituent species.

[2-13-1427*](#) (1S10-3) アミノ酸配列と連携した原始生体膜の成長
(1S10-3) Growth of Primitive Cell Membrane Coupled with Amino Acid Sequence

Akiko Baba¹, Ulf Olsson², Masayuki Imai¹ (¹*Grad. Sch. Sci., Univ. Tohoku*, ²*Grad. Sch. Sci., Univ. Lund*)

Evolution is change shifted toward greater fitness over time. The fitness is a measure of replication rate and is determined by genetic information: sequence of nucleotide or amino acid in nucleic acid or protein. Therefore, to elucidate relationship between the fitness and the genetic information is essential to understand the evolution. We believe that the simplest relationship has emerged in the prebiotic era, when fatty acid vesicles coexist with numerous primitive molecules such as nucleotides, amino acids, and peptides. Here, we demonstrate amino acids and peptides encourage the growth of fatty acid vesicles. Especially, the growth rate strongly depends on the type of amino acids and amino acid sequence in peptides, which might be the origin of evolution.

[2-13-1439*](#) 鋳型重合と連携したベシクルの自己生産サイクル：自律的なプロトセルの構築を目指して
Reproduction cycles of vesicle coupled with template polymerization: toward autonomous synthetic protocell

Minoru Kurisu¹, Ryosuke Katayama¹, Yuka Sakuma¹, Peter Walde², Masayuki Imai¹ (¹*Grad. Sch. Sci., Tohoku Univ.*, ²*Dept. Materials Sci., ETH Zurich*)

The life is the system that reproduces itself, which is maintained by very complex chemical networks. To elucidate the physical basis for the origin of life, one of the promising approaches is to construct simple autonomous vesicle reproduction systems. Recently we developed reproduction cycles of AOT vesicles coupled with template polymerization of aniline. The system has chemical network composed of three essential domains: (i) the production of energy currencies, (ii) the processing of information polymer, and (iii) the membrane growth. Thus, this is a “semi” autonomous vesicle reproduction system. We derive a kinetic model that describe the reproduction of vesicles supported by the chemical network, which will reveal the stability of our synthetic protocell.

[2-13-1451*](#) (1S10-7) 多相液滴のコアを用いた人工細胞内転写反応場の構築
(1S10-7) Development of a transcription field in the artificial cell by the core of multiphase droplets

Kanji Tomohara, Yoshihiro Minagawa, Hiroyuki Noji (*Dept. Appl. Chem., Grad. Sch. Eng., Univ. Tokyo*)

In this work, we developed core-shell structured droplets as compartments for artificial cells and found out if the core of the droplets could serve as a field of enzymatic reactions and rectify the reaction pathway. First, we demonstrate that the mixture of three polymers, intrinsically disordered protein, dextran, and PEG, generates core-shell structured droplets by liquid-liquid phase separation. Next, we have engineered this system so that the core of the droplet, the IDP-rich phase, can incorporate proteins, including enzymes. Finally, NTP and DNA, both substrates for transcription, were observed to be naturally recruited into the IDP-rich phase. Based on these results, we are now trying to conduct transcription inside the core of this artificial cell compartment.

[2-13-1503*](#) 多段階酵素反応による DNA 液滴ベース人工細胞の分裂制御

Controlled division of DNA-droplet-based artificial cells coupled with enzymatic reaction cascade

Tomoya Maruyama¹, Akihiro Yamamoto², 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*)

Artificial cells can be used as new biomaterials or bio-inspired systems. To utilize artificial cells for such systems, artificial cells are expected to realize several dynamics such as growth or division. The DNA droplet is a liquid-like self-assembled microstructure of DNA nanostructures and DNA-droplet-based artificial cell division was previously realized by the one-step enzymatic reaction. However, it cannot control the size or numbers of the divided droplets. In this study, we succeeded in the controlled division of homogeneously mixed DNA droplets into two different DNA droplets by an enzymatic reaction cascade. We believe that this technology contributes to the construction of new biomaterials such as drug delivery or the understanding of primitive cells.

[2-13-1515*](#) 無細胞翻訳系を用いた DNA の自己複製による相分離液滴の形成

Formation of phase-separated droplets by DNA self-replication using cell-free protein synthesis system

Moe Yabuta, Yoshihiro Minagawa, Hiroyuki Noji (*Dept. App. Chem., Grad. Sch. Eng., Univ. Tokyo*)

Recently, we found that phase separation of Dextran (Dex) and Poly Ethyleneglycol (PEG) is stabilized by enriched DNA (950 ng/ μ l), and DNA amplification induced the phase separation from one phase state. We focused on the phase-separated Dex droplets for our artificial cell compartment, which would grow by DNA replication. We aim to create an artificial cell with evolvability in which DNA replication by enzymes encoded on self-DNA (DNA self-replication) and Dex compartment growth is coupled. To achieve our aims, we prepared the plasmid encoding phi29 DNA polymerase and performed DNA self-replication using a cell-free protein synthesis system. After several optimizations of the reaction conditions, we succeeded in inducing Dex droplets from one phase state.

[2-13-1527*](#) 共通要素は解糖系とタンパク質合成系の共役再構成系の動態を制御する

Common elements regulate the dynamics of the conjugated system of glycolysis and protein-synthesis reconstituted *in vitro*

Gaku Sato, Saki Kinoshita, Takahiro Yamada, Akira Funahashi, Nobuhide Doi, Kei Fujiwara (*Grad. Sch. Sci. Technol. Univ. Keio*)

With the progress of biochemistry, various biochemical systems were reconstituted *in vitro* and their behavior was analyzed. However, how life emerges from the cooperation of these systems has not been understood. Here, we reconstituted the conjugated system of glycolysis and protein-synthesis, and found that the dynamics of the conjugated system is regulated by the common elements of them. In addition, by adding ATP-degrading enzyme to the conjugated system, we revealed that “third party” systems, such as ATP-degrading enzyme, facilitate the coupling of the system. These results indicate that the dynamics of the conjugated system changes significantly depending on the interaction between the constituent systems.

[2-13-1600*](#) 胚発生期に海馬の細胞運命を決定する動的な分子制御ネットワークの構築

A Dynamic Molecular Regulatory Network to Determine Hippocampal Cell Fate during Embryogenesis

Zi Wang, Mariko Okada (*Lab. of Cell Sys., IPR, Osaka Univ.*)

The full picture of molecular interactions and regulatory networks relevant to hippocampal development remains elusive. This study aims to establish a method to integrate time-series scRNA-seq data into interpretable gene regulatory networks (GRNs), revealing intermolecular regulatory mechanisms during embryonic hippocampal cell differentiation. We performed unsupervised clustering of time-series scRNA-seq data from developing hippocampus, and made 12 GRNs from gene expression patterns in pre- and post-temporal causal states. By comparing the GRNs constructed for each cell lineage, we propose specific gene regulatory patterns may dominate points of divergence that determine differentiation between neuronal and glial cells.

[2-13-1612*](#) DNA1 分子からの無細胞遺伝子発現ノイズ解析
Noise analysis of cell-free gene expression from single-molecule DNA

Seiya Noro, Yoshihiro Minagawa, Hiroyuki Noji (*Dept. App. Chem., Grad. Sch. Eng., Univ. Tokyo*)

Gene expression noise (GEN) causes heterogeneity of protein synthesis yield among genetically identical cells. Although GEN is thought to have biologically fundamental roles, it hampers rational designing of gene circuits in cells or artificial cell systems. Whereas GEN has been analyzed in bacterial cells or cultured cells, it has not been well characterized in artificial cell systems. In this work, we aimed to analyze GEN using a uniform cell-sized microreactor array and cell-free gene expression system. We observed gene expression from a set of single-molecule DNAs encoding different fluorescent proteins and measured extrinsic and intrinsic noises. These values provide the noise from components involved in gene expression and stochasticity of reactions, respectively.

[2-13-1624*](#) 発現量ノイズの伝搬を利用した隠れた相互作用の検出
Capturing hidden regulation by utilizing expression noise propagation

Thoma Itoh^{1,2}, Takashi Makino³ (¹*Department of Basic Biology, School of Life Science, The Graduate University for Advanced Studies, SOKENDAI*, ²*Department of Biology, Faculty of Science, Tohoku University*, ³*Graduate School of Life Sciences, Tohoku University*)

Recent progress in single cell RNA-seq has activated the development of network inferring methods. Most network estimations assume that perturbations produce downstream effects. However, the effects of gene perturbations are sometimes compensated by a gene with redundant functionality (functional compensation). We hypothesized that functional compensation may emerge as a noise change without mean change (noise-only change) due to varying physical properties and strong compensation effects. We investigated this hypothesis on STP1 and STP2, which have strong functional compensation, and found that noise-only change genes are enriched in their redundantly regulated genes. We suggest the noise difference comparison could be a new strategy for network estimation.

[2-13-1636](#) 左右軸決定における、マウスノード不動繊毛への機械刺激依存的な *Cer12* mRNA 分解の活性化
Mechanical stimuli to a mouse nodal immotile cilium activate *Cer12* mRNA decay for left-right symmetry breaking

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Immotile cilia at the node of mouse embryo sense a flow-dependent signal for L-R patterning of the embryo. The cation channel *Pkd2* is required for sensing the flow and triggers *Cer12* mRNA decay, however, it is unknown how cilia sense the flow. Here, we show that the immotile cilium at the node functions as a mechanosensor. Upon applying mechanical stimuli to the immotile cilium by the optical tweezers, the decay of *Cer12* mRNA was monitored. The mRNA decay was induced by mechanical stimuli ($65\pm 21\%$; $n=28$), while it was not detected with *Pkd2*^{-/-} embryos ($105\pm 11\%$; $n=7$). Furthermore, 3-D imaging revealed the nodal flow imposes passive ventral-bending in cilia on the L-side. This bending likely activates cilia on the L-side cilium and triggers the L-R symmetry breaking.

[2-13-1648](#) G146V 変異アクチンのサプレッサー変異はクレフト周辺に位置する
Intragenic suppressor mutations of G146V mutant actin are located around the nucleotide binding cleft

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G146V mutant actin is dominantly lethal to *S. cerevisiae*, and in vitro, dominantly inhibits cofilin binding to WT actin protomer in copolymers. This suggests that G146V significantly affects cooperative conformational changes of actin filaments. To further gain insight into the effects of G146V, we previously found V152A mutation by intragenic suppressor screening of G146V mutant actin. Here, we performed improved suppressor screening and found seven suppressor mutants. These mutations were well distributed around the cleft between the large and small domains. These results suggested that G146V and its suppressor mutations affect ATP hydrolysis and/or conformational changes between the two domains, such as flattening during polymerization and cofilin-induced tilting.

[2-13-1700](#) 転写因子の動的な集合体形成はエンハンサーの長距離間相互作用を媒介する
Dynamic clustering of transcription factors mediates long-range regulatory communication in *Drosophila* embryos

Koji Kawasaki, Takashi Fukaya (*Inst. for Quantitative Biosciences, Research Center for Biological Visualization, Univ. of Tokyo.*)

Temporal dynamics of gene transcription is highly regulated by transcription factors (TF) recruited to enhancers. Importantly, recent imaging studies have revealed that TF forms ~300-nm size dense clusters within a nucleus. However, functional significance of such cluster formation in gene expression remains largely unclear. Here, we developed super-resolution live-imaging system that permits simultaneous visualization of enhancer activity and TF dynamics in living *Drosophila* embryos. Quantitative 3D image analysis revealed the co-occurrence of TF clustering and transcriptional bursting. Our data suggest that multivalent interaction of TF helps to increase the efficiency of burst induction especially when only weak TF binding sites are present at distal enhancers.

[2-13-1712](#) 中立的な競争とニッチを伴う幹細胞のクローン増殖に関する生物物理学的モデル
Biophysical model for clonal expansion of stem cells with neutral competition and niches

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Tissue stem cells maintain stem cell numbers and constantly supply differentiated cells. Although this stem cell homeostasis is critical in the maintenance of tissues and reproduction, the mechanism is still controversial. So far, the hierarchical model and the neutral competition model (NC model) have been proposed. In this study, we developed a new mathematical model, which seamlessly links the two existing models, and focused on the intermediate situation called the hierarchical neutral competition model (hNC model). Using mathematical analysis and numerical simulation, we showed that the size of each clone repeatedly showed transient bursts in the hNC model, which was not observed in two existing models. This research provides new insight to stem cell homeostasis.

[2-13-1724](#) 自己組織化過程における細胞の挙動解析
A dynamic self-organization of single cells

Ryuta Watanabe, Riichi Horikawa, Ryu Kidokoro, Shota Nozaki, Yuuta Moriyama, Toshiyuki Mitsui (*Dept. Phys., Aoyama Gakuin Univ.*)

During the process of embryonic development, cells organize themselves in a higher order of structures while undergoing cell division and cell fate specification. Such spatio-temporal organization of embryonic cells also occurs after dissociation and culture in vitro. However, the dynamics of cell reengagement have not thoroughly examined. We analyzed the trajectories of individual cells in multi-layers for zebrafish self-organizing cells over 2 hour using confocal microscopy. The mean square displacements of these cells are plotted and the scaling exponent is estimated. As a result, we found anomalous scaling exponent changes at 120 min where $\Delta r \sim 30 \mu\text{m}$, which is close to the cell diameter. We will also discuss the aging of cell behavior by evaluating ergodicity.

[2-13-1736](#) ヒト胚発生を模倣するための単純化された反応拡散 in vitro モデル実験系
Simplified reaction-diffusion in vitro model to mimic human embryonic development

Kiyoshi Ohnuma (*Bioeng., Nagaoka Univ Tech*)

Reaction-diffusion is well known as a model of embryonic development. However, animal experiments include many uncontrollable and hidden parameters, limiting the understanding of the mechanisms. Here we fabricated a unidirectional perfusion microchamber for human iPS cells to make a simplified but fully controllable embryo model. The cells can be maintained as 2D dispersed culture in a chemically defined medium, enabling to control signal input via medium and physical contact. Adding an activator, BMP4, differentiates cells, which is inhibited by a cell-secreted inhibitor, Noggin. As a result, although the upstream cells were differentiated, downstream cells were not, suggesting success in simplifying the reaction-diffusion to mimic organizer function in the embryo.

2-13-1748 分子動力学法による MED26 の天然変性蛋白質認識メカニズムの検討

Molecular dynamics study on multiple binding modes of MED26 to recognize intrinsically disordered proteins

Satoshi Goto¹, Kota Kasahara², Hidehisa Takahashi³, Junichi Higo⁴, Takuya Takahashi² (¹*Grad. Sci. Life Sci., Ritsumeikan Univ.*, ²*Coll. Life. Sci., Ritsumeikan Univ.*, ³*Grad. Sch. Med., Yokohama City Univ.*, ⁴*Res. Org. Sci. Tech., Ritsumeikan Univ.*)

The N-terminal domain of MED26 (MED26NTD), a subunit of the mediator complex, is known to play an important role by interacting with intrinsically disordered proteins including AFF4, EAF1, and TAF7. In this study, we applied the multicanonical MD simulation to investigate recognizing mechanism via identifying the complex structures for the three ligands. As a result, all the three ligands, EAF1, AFF4, and TAF7, formed multiple and unstable bound structures. Only TAF7 formed a helical structure in the bound form. EAF1 and AFF4 bound an alternative binding site on the MED26NTD surface, implying that these two ligands are recognized competitively.

2-14-1315* ヒト iPSC 細胞由来ニューロンの神経突起伸長過程における駆動力のゆらぎ解析

Fluctuation analysis of driving forces for development processes of neurites of human iPSC-derived neurons

Narumi Maeda¹, Yusuke Shibasaki¹, Yuka Shirakawa², Minoru Saito^{1,2} (¹*Grad. Sch. of Integ. Bas. Sci., Nihon Univ.*, ²*Nat. Inst., Nihon Univ.*)

We analyzed the two-dimensional morphologies of neurites of *in vitro*-cultured human iPSC-derived neurons. For driving forces calculated by a mathematical method (Loewner equation) for development processes of the neurites, detrended fluctuation analysis (DFA) was performed, and the morphological characteristics of the neurites were quantified using scaling exponents. The day *in vitro* (DIV)-dependent behaviors of the scaling exponents showed that differences between healthy and Alzheimer's disease (AD) neurites can be observed from the early stage (DIV3) of their development. Additionally, immunofluorescence-staining results showed that these differences precede significant expressions of β -amyloid and phosphorylated tau known as biological factors causing AD.

2-14-1327* 画像データから上皮細胞の力学パラメータを推定する手法の開発

Image-based parameter estimation for epithelial mechanics

Goshi Ogita^{1,2}, Takefumi Kondo¹, Keisuke Ikawa^{2,3}, Tadashi Uemura¹, Shuji Ishihara^{4,5}, Kaoru Sugimura^{2,3,5} (¹*Grad. Sch. Bio., Kyoto Univ.*, ²*Grad. Sch. Sci., Univ. Tokyo*, ³*iCeMS, Kyoto Univ.*, ⁴*Grad. Sch. Arts and Sci., Univ. Tokyo*, ⁵*UBI, Univ. Tokyo*)

Measuring mechanical parameters in tissues, such as the elastic modulus of cells, is essential to decipher the mechanical control of morphogenesis. However, their measurement *in vivo* is technically challenging. Here, we developed an image-based statistical method to estimate the mechanical parameters of epithelial cells. A test using synthetic data confirmed the accuracy of parameter estimation. By applying this method to *Drosophila* epithelial tissues, we found that a negative spring constant of cell junction increased with cell rearrangement. This method also clarified how alterations in tissue polarity and stretching affect the anisotropy in tension parameters. Thus, our method provides a novel approach to uncover the mechanisms governing epithelial morphogenesis.

2-14-1339* 細胞区画内のセルフリー遺伝子発現における液液相分離現象とぬれ効果

Liquid-liquid phase separation and wetting in compartmentalized cell-free expression reactions

Shuzo Kato¹, David Garenne², Vincent Noireaux², Yusuke Maeda¹ (¹*Dept. Phys., Kyushu Univ.*, ²*Sch. Phys. Astro., Univ. of Minnesota*)

Liquid droplets of proteins are formed via liquid-liquid phase separation (LLPS) in cells. However, the detailed mechanism of the interplay of droplet formation and intracellular reactions remains unknown. We study LLPS of cell-free reactions (TXTL), which is from *E. coli* cytoplasm and capable of gene expression. The reactions exhibit droplets when concentrated at 2.8 times volume fractions. This droplet formation is induced when they are encapsulated in a water-in-oil emulsion and dehydrated through evaporation. Droplets coalesce, wet the membrane, and coarsens into two distinct liquid domains with crowding agents which sequester synthesized proteins. Thus, cell-free systems can pave the way to understand membrane-less compartments having gene expression capacity.

[2-14-1351*](#) プロトセル空間における反応拡散波の示す時空間パターンの頑健性と可塑性
Robustness and plasticity of spatiotemporal patterning by a reaction-diffusion wave entrapped in protocells

Sakura Takada¹, Natsuhiko Yoshinaga^{2,3}, Nobuhide Doi¹, Kei Fujiwara¹ (¹*Dept. Biosci. Info., Keio Univ.*, ²*AIMR, Hokue Univ.*, ³*MathAM-OIL, AIST*)

Reaction-diffusion coupling (RDC) is a mechanism that regulates spatiotemporal patterning in cells. However, due to its parameter sensitivity, it is not clear whether spatiotemporal patterning by RDC could exist in primitive organisms. Here, we reconstituted Min wave, which is RDC as a regulator of cell division plane, in a protocell, and analyzed its parameter dependency. We found that spatiotemporal patterning of Min wave is robust against parameter fluctuation in the protocell, and it also showed plasticity against temperature and components concentration and transits between two patterns: traveling wave (found in amoeba) and standing wave (found in bacteria). These findings suggest that RDC has an important role in emergence of spatiotemporal pattern in protocells.

[2-14-1403*](#) ミトコンドリア呼吸鎖の活性と熱発生メカニズム解析
Mechanistic analysis of mitochondrial respiratory activity and heat generation

Ikuo Kujiraoka¹, Taku Mukoshiba¹, Nuning Namari¹, Kotaro Takeyasu^{2,3}, Junji Nakamura^{2,3} (¹*Graduate school of science and technology, Univ. Tsukuba*, ²*Faculty of pure and applied sciences, Univ. Tsukuba*, ³*Tsukuba research center for energy materials science, Univ. Tsukuba*)

Mitochondria effectively convert ADP to ATP using electrochemical energies. On the other hand, a part of the energy should drive the electrochemical reactions before the dissipation as heat. We aim to understand the energetic mechanisms in the electrochemical system under non-equilibrium condition in mitochondria using both of the experiments and model calculations. We have evaluated the respiration activity of yeast cells dispersed in water from the concentration of oxygen in a closed system. The respiration activity showed a maximum at the oxygen concentration of ~20% and then decreased as the oxygen concentration decreased. The respiration activity is to be compared with the local temperature in cells.

[2-14-1415](#) インシュリンシグナルは線虫のスケールフリー行動を制御する
Scale-free behaviors of *C. elegans* is shaped by insulin signaling

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Behaviors of animals including human are commonly characterized by a power law distribution. Here, we videorecorded *C. elegans* cultured in a new microfluidic device for 3 days and analyzed their behaviors. The power law distribution shown in *C. elegans* had a common feature with those of human and mice, i.e., actively-moving state and inactive state had a critical time scale or not, respectively. We found that the critical time scale disappeared in starved *C. elegans*, and it was restored by the addition of 1 g/L glucose. It was also disappeared in insulin signaling mutants, *daf-2* and *daf-16*. Insulin signaling regulates *C. elegans* scale-free behavior, and behavioral disorder in diabetes patients may be a defect in scale-free organization of human behaviors.

[2-14-1427](#) 2種細胞群間の境界パターン形成の動態モデル構築と定量解析
Physical model construction and quantitative analysis of boundary pattern formation between binary cell groups

Kosuke Mori, Yuhei Yasui, Akinori Awazu, Masashi Fuji (*Department of Mathematical and Life Sciences, Graduate School of Integrated Sciences for Life, Hiroshima University*)

The myotendinous junction (MTJ), which is the junction between skeletal muscle and tendon, are formed by the cell-cell and cell-extracellular matrix bindings. Particularly in the MTJ, a wave-like boundary pattern formation called the finger-like process has been observed. However, it is unclear how the boundary pattern is formed by mechanical actions during development process. Moreover, the relationships among the properties of the cell groups, the boundary pattern and the mechanical strength of the MTJ remain unclear. In this study, in order to simulate the process of MTJ formation process, we constructed a framework for a coarse-grained model of multicellular systems and examined the quantitative analyses for the boundary patterns.

2-14-1439 特異点をもつ2次元領域における細胞配向とトポロジカル欠陥**Cell Alignment and Topological Defects in Two-Dimensional Geometries with Corner Singularities****Hiroki Miyazako**¹, Hiroyuki Sato², Takaaki Nara^{1,2} (¹*Grad. Sch. IST, Univ. Tokyo*, ²*Sch. Eng., Univ. Tokyo*)

In recent studies, it has been revealed that the cell alignment induces singular points called topological defects, at which the cell alignment angle cannot be defined. Although many studies have focused on biophysical properties of the alignment and defects by patterning cells in two-dimensional geometries, there remains little understanding of how the singularities of the geometries (e.g., corner points) affect the cell alignment and defects. This study proposes a numerical calculation method for the cell alignment and defects in the geometries with corner points using complex analysis theories. We compare the numerical calculation with the experimental results by patterning mouse myoblast cells on PDMS structures.

2-14-1451 Representation and inference of cell growth and division by neural-network-aided point processes**Atsushi Kamimura**, Tetsuya J. Kobayashi (*Institute of Industrial Science, The University of Tokyo*)

The regulations of cell growth and division are long-standing problems in cell physiology. Recent single-cell measurements using microfluidic devices have provided quantitative time-series data on physiological parameters of cells. To clarify the regulatory laws and associated relevant parameters, developing a novel method will be helpful, which can handle noisy multidimensional data more exhaustively than conventional ones. By using size control as an example, we apply a neural network method, originally developed for history-dependent temporal point processes. It can effectively segregate history-dependent deterministic factors and unexplainable noise from given data by flexibly representing the functional forms of the deterministic relation and noise distribution.

2-14-1503 波打つ場が誘起する上皮細胞の集団運動と秩序形成**Collective motion of active epithelial cells induced by wave-like hydrogel folds****Yusuke Maeda**¹, Kazuyuki Shigeta¹, Tatsuya Fukuyama¹, Riku Takahashi², Aya Tanaka² (¹*Kyushu Univ., Dept. Phys.*, ²*NTT, BRL/BMC*)

The active matter such as migrating cells is known to show collective motions from turbulent state to vortex formation due to their orientation interaction. Epithelial cells have been extensively studied to understand the mechanism of collective dynamics, however, the dynamics of epithelial cells on three-dimensional (3D) structures reflecting actual folds and wrinkles in biological tissues has not been clarified. In this study, we developed an experimental system to study the collective motion of MDCK cells under a 3D wavy crinkle-like hydrogel. Our analysis revealed that the collective motion has a spatial correlation along the hydrogel pattern and its geometric dependence indicates that the 3D spatial constraint can induce ordered dynamics in epithelial monolayer.

2-14-1600 遺伝子発現制御ネットワークモデルのダイナミクス定量解析**Quantitative analysis of gene regulatory network dynamics****Masayo Inoue**¹, Kunihiko Kaneko² (¹*IMS, Meiji Univ.*, ²*Univ. of Tokyo*)

Living organisms respond appropriately according to environmental changes. To address the question of how cells can make accurate and robust responses, we have investigated gene regulatory networks that mutually activate or inhibit, and have demonstrated that complex entangled networks can provide appropriate input-output relationships. Since such a complex network is composed of a large number of closely interacting elements, it is difficult to quantitatively analyze its dynamics (information transmission process). In order to realize quantitative analysis, we applied "dynamic mode decomposition", which is a big data analysis method, to perform dimensional compression of dynamics.

[2-14-1612](#) Boolean modeling and state analysis of gene regulatory networks

Yoshiaki Horiike, Shin Fujishiro, Masaki Sasai (*Dept. Appl. Phys., Nagoya Univ.*)

Emergent behaviors of gene regulatory networks (GRNs) are crucial for cell fate decisions. Boolean modeling is an efficient method for analyzing large-scale GRNs, but the state transition dynamics of the Boolean network becomes obscured when the asynchronous updating rule is used. To overcome this problem, we developed a framework using a Gillespie's algorithm like method, which qualitatively reproduces small networks' continuous variable dynamics. We analyzed the state transition dynamics of the larger network with this method by introducing a new index representing the similarity between states as the similarity between dynamical regulatory relationships. Mean-field approximation can reproduce the distribution of this new index obtained from real biological networks.

[2-14-1624](#) Effects of epigenetic modifications on the intermediate states of epithelial-mesenchymal transitions

Kenichi Hagiwara, Masaki Sasai (*Dept of Appl. Phys., Nagoya. Univ*)

The epithelial-mesenchymal transitions (EMT) play a critical role in cancer metastasis, where the EMT goes through intermediate states between epithelial and mesenchymal states. Various theoretical models have been proposed to describe these intermediate states, but their features are not well defined yet. We hypothesized that the slower epigenetic regulation than the transcription factor binding, including histone modifications, is responsible for the intermediate state. We extended a gene network model of Jolly et al. (*Phys Biol* 2019) by introducing slowly varying variables that represent histone states of genes in the network to examine their effects on the intermediate states of EMT.

[2-14-1636](#) 出芽酵母の DNA 二本鎖切断時における染色体動態の数理モデル Mathematical model of chromosomal dynamics in budding yeast during DNA double strand break

Shinjiro Nakahata, Masashi Fujii, Akinori Awazu (*Graduate School of Integrated Sciences for Life, Hiroshima University*)

Genome DNA playing the central roles of intracellular activities is frequently damaged by various stresses. Most serious DNA damage is double-strand-break (DSB) often induced by the radiations. Since the damaged DNA involves the potentials to promote the cancer or improper gene expressions, living organisms developed various mechanisms to recognize and repair such damages. Recent studies reported various intranuclear dynamics during damaged DNA repair, for example the strong diffusion and localization at nuclear periphery of DSB sites were observed in budding yeast. However, the mechanisms of them are still unclear. To reveal the mechanism of such dynamics, we constructed and simulated the model of nucleus of yeast with normal genome and that with damaged genome.

[2-14-1648](#) ES 細胞のクロマチンドメイン変化による染色体動態制御のモデル A model for regulation of chromosome dynamics in mouse ES cells by chromatin domain changes

Tetsushi Komoto, Masashi Fujii, Akinori Awazu (*Grad. Sch. Integrated Sciences for Life, Univ. Hiroshima*)

The genomic activities of mammalian X chromosomes (X chrs) are mutually suppressed to make only one X chr is active in each cell. Such X chromosome inactivation (XCI) enables X chr number compensation of gene expression level. In mouse embryo, one of two X chrs is inactivated in inner clump of cells on blastocyst stage. The experiment of mouse ES cell suggested that mutual spatial approach of X chrs and localization of X chrs at the nuclear envelope occur after induction of differentiation. On the other hand, the mechanism how X chrs could search their homologous pair in mouse nucleus containing 40 chromosomes is still unclear. In this study, we developed the coarse-grained models of chromosome in mouse ES cell and simulated to unveil this mechanism.

[2-14-1700](#) Lifetime analysis of nucleotides bound to KaiC

Damien Stephane Simon^{1,2}, Atsushi Mukaiyama^{1,2}, Yoshihiko Furuike^{1,2}, Shuuji Akiyama^{1,2} (*¹Institute for Molecular Science, ²SOKENDAI*)

The circadian clock system of cyanobacteria, composed by clock proteins KaiA, KaiB and KaiC, can be reconstituted in vitro in the presence of ATP. Previous reports have shown that the ATPase activity of KaiC is one of the crucial factors defining the frequency of the system, but the details of the ATPase reaction remain unknown. In this study, we aim to determine which elementary reaction step of the ATPase cycle of KaiC determines the system's rate. For that mean, we have established a method to track the temporal changes of nucleotides bound to KaiC. We applied this method to a variety of mutants and observed how the rate constants were affected by the period length of the system. In this presentation, we would like to discuss about the significance of these results.

[2-14-1712](#) 代謝漏出による微生物の共存共栄戦略

The advantage of leakage of essential metabolites and resultant symbiosis of diverse microbes

Junpei Yamagishi¹, Nen Saito^{2,3}, Kunihiro Kaneko^{1,3} (*¹Grad. Sch. of Arts and Sci., Univ. Tokyo, ²ExCELLS, NINS, ³UBI, Univ. Tokyo*)

Microbial communities display extreme diversity. Besides the fittest strain or species under isolation conditions, many others coexist. Population dynamics with appropriate cell-to-cell interaction would provide such diversity, but how this interaction is achieved remains elusive. Secretion of beneficial metabolites from the fittest strain could feed others and enable the coexistence; however, why do cells leak out such essential components? We numerically and analytically demonstrate that appropriate leakage of essential metabolites is, counterintuitively, beneficial to the leaking cells. A symbiotic relationship among diverse cells is then established: each cell cross-feeds others by secreting out essential metabolites that are usefully consumed by others.

[2-14-1724](#) がん進行にともなう代謝変化のネットワーク構造に基づく解析

Network structure-based analysis of metabolic changes associated with cancer progression

Atsuki Hishida^{1,2}, Ayuna Hattori¹, Takahiro Ito¹, Atsushi Mochizuki¹ (*¹Institute for Frontier Life and Medical Sciences, Kyoto University, ²Graduate School of Science, Kyoto University*)

Carcinogenesis is known to induce the reprogramming of cellular metabolism. An amino acid metabolic enzyme BCAT1 was shown to be upregulated during progression of chronic myelogenous leukemia (CML). However, the observed metabolite changes and the flux analysis were considered to be inconsistent with the expectations from BCAT1 mediated reactions on the metabolic network. We studied effects of progression of CML on the metabolic system by "structural sensitivity analysis", by which qualitative responses of chemical concentrations to enzymatic changes are determined from topology of a reaction network alone. We found that observed changes in concentrations are rather reasonable from the network, and that amino acid production rates possibly increase in CML progression.

[2-14-1736](#) ステージ特異的な細胞周期調節機構の、ネットワーク構造に基づく解明

Independent regulation of the G₁-S and G₂-M transition realized by topology of the cell cycle network

Yuhei Yamauchi, Atsushi Mochizuki (*Department of Mathematical Biology, Kyoto University*)

In the yeast cell cycle, the G₁-S and G₂-M transition are regulated by the Cdc2-Cdc13 and Cig2-Cdc2 complex, respectively. The activity of each complex should rise specifically at different stages. The reactions that control the activity of these two complexes share common molecules, forming a complex network. We study how "independent regulation" of these two complexes is realized using "structural sensitivity analysis" previously established by our group. We found that activities of two complexes are regulated by separate sets of reaction parameters in the system. Our result can be understood in terms of "buffering structures", which determine the extent to which a change in the reaction rate influences and are defined in the light of network topology.

[2-15-1315*](#) 全神経活動リアルタイム計測のための全自動全神経細胞捕捉システムの開発
Development of a whole neural network tracking system for real-time high-resolution light-field imaging in freely behaving *C. elegans*

Haruka Maeoka, Kazuki Shigyou, Takuma Sugi (*Univ. Hiroshima*)

How does the spatiotemporal pattern of brain networks decline in the aging process? Understanding such patterns requires a method for quantifying neural activities noninvasively and repeatedly throughout life-course. Here, we are developing a system to quantify a whole-brain activity in freely behaving nematode *C. elegans*. We developed the software extracts fluorescence of a calcium indicator G-CaMP expressed in all neurons of worms. Then, this software controls the motorized stage to keep all neurons of a worm under the field of view of the microscope. Combining this tracking system with our developed high-resolution light-field microscopy for real-time, scan-less imaging will allow for examining the neural networks at single-cell resolution in the future.

[2-15-1327*](#) 繊毛虫 *Tetrahymena* における螺旋遊泳行動の三次元観察
Direct three-dimensional observation of helical swimming behavior of the ciliate *Tetrahymena*.

Akisato Marumo, Masahiko Yamagishi, Junichiro Yajima (*Grad. Arts & Sci., Univ. Tokyo*)

Ciliates are ciliated protists that swim in the water along helical paths by beating the thousands of cilia coating the cell body. Their swimming motions have been described through 2D observations; however, ciliates are three-dimensional entities, and their helical swimming pathway are not limited to only one focal plane. In this study, we conducted three-dimensional tracking of fluorescent beads within a cell to directly visualise the helical swimming of ciliates and showed that ciliate *Tetrahymena* swims along a right-handed helical path with right-handed rolling; influx of Ca^{2+} into cilia caused different patterns of 3D-trajectories of *Tetrahymena* swimming, indicating the orientation of torque generated by cilia as the determining factor in its swimming behavior.

[2-15-1339*](#) Structure-based analysis and evolution of a monomerized red-color chromoprotein from jellyfish *Olindias formosa* for bioimaging

Le Zhai (*Graduate School of Frontier Bioscience, Osaka University*)

GFP-like chromoproteins that generally do not fluoresce can be applied for bioimaging tools such as FRET-based indicators and photoacoustic probes. Here we report a novel chromoproteins cloned from *Olindias formosa*. The crystal structure of the protein with 2.1 Å resolution revealed the nonplanar *trans*-chromophore. To expand the absorption spectrum hue, we developed yellow, orange, and magenta variants by rationally-designed mutagenesis. Since Phe140 is considered as a key factor in the non-fluorescent property, we replaced it and its adjacent residue with other amino acids, making the chromoproteins fluoresce. In addition, we found that pKa of this mutant was 9.2, so that this could be applied to the imaging in alkaline ecological systems or alkaliphiles in future.

[2-15-1351*](#) 酸化ストレス下の単一細胞における液-液相分離のラマンイメージング測定
Raman imaging of liquid-liquid phase separation in a living single cell under oxidative stress

Ren Shibuya¹, Shinji Kajimoto^{1,2}, Takakazu Nakabayashi¹ (¹*Fac. Pharm. Sci., Univ. Tohoku*, ²*JST PRESTO*.)

Recently, liquid-liquid phase separation (LLPS) has attracted a great attention in cell biology. LLPS is a phenomenon in which a specific protein separates into concentrated and dilute phases and is involved in various biological reactions. In this study, we performed Raman imaging of stress granules formed via LLPS in a living cell. We measured Raman images of cells subjected to oxidative stress by the addition of sodium arsenite and analyzed the change in spectral shape. We found that the intensities of the Raman bands assignable to the main components of stress granules increased in some regions of cytoplasm after the oxidative treatment. In addition, using hierarchical cluster analysis, we succeeded in visualizing the distribution of stress granules on Raman images.

2-15-1403* ラマンおよび自家蛍光顕微鏡による生細胞内の薬剤ナノ粒子の代謝過程の観測
Observation of metabolism of drug nanoparticles in living cells using Raman and autofluorescence microscopy

Masato Machida¹, Toshiki Sugimura², Taemaitree Farsai³, Yoshitaka Koseki³, Hitoshi Kasai³, Shinji Kajimoto^{1,2,4}, Takakazu Nakabayashi^{1,2} (¹*Faculty of Pharmaceutical Sciences, Tohoku University*, ²*Graduate School of Pharmaceutical Sciences, Tohoku University*, ³*Institute of Multidisciplinary Research for Advanced Materials, Tohoku University*, ⁴*JST PRESTO*)

Nanoparticles as large as 100 nm accumulate in tumor tissues with high efficiency which is called EPR effect. Anti-cancer drug delivery systems using nanoparticles have extensively been investigated based on the concept of EPR effect. However, it is still not understood how nanoparticles are taken up into cells and metabolized in cells. In this study, we introduced nanoparticles of cholesterol-linked anti-cancer drug SN-38 (CLS NPs) into cells and followed their dynamics in a label-free manner using a combination of Raman and auto-fluorescence spectroscopies. Raman images show that CLS NPs were effectively introduced into the cytoplasm of cells. The shift to longer wavelength of auto-fluorescence suggests that CLS NPs were metabolized into SN-38 in cells.

2-15-1415* ラマンイメージングと Deep Learning の融合によるラベルフリー細胞内解析手法の開発
Development of label-free intracellular analysis methods by integrating Raman imaging and deep learning

Hiroaki Takahashi¹, Shinji Kajimoto^{1,2}, Takakazu Nakabayashi¹ (¹*Grad. Sch. Pharm. Sci., Tohoku Univ.*, ²*JST PRESTO*)

Raman imaging, which enables direct observation of molecules with high spatial resolution, has attracted much attention as a label-free method for analyzing living cells; however, it has the disadvantage of weak signals. To extract various information from noisy Raman image, we developed a new method to automatically analyze Raman images using deep learning. We show the artificial intelligence (AI) that can detect nuclear and cytoplasmic regions from Raman images of cells, and the AI that can visualize intracellular temperature from the spectra of water molecules. With the developed AI, we can classify cell images with an accuracy of about 85% per pixel, and able to predict the intracellular temperature with mean absolute error of 2.6°C per pixel.

2-15-1427* 構造化照明超解像ラマン顕微鏡の構築と生細胞への応用
Construction of a structured illumination super-resolution Raman microscope and application to a living cell

Akira Abe¹, Shinji Kajimoto^{1,2}, Takakazu Nakabayashi¹ (¹*Grad. Sch. Pharm. Sci., Univ. Tohoku*, ²*JST PRESTO*)

Structured illumination microscopy (SIM) is a highly applicable super-resolution microscopic technique that allows us to obtain super-resolution only by using the structured illumination light. In this study, we have developed a super-resolution Raman imaging system that enables high-speed Raman imaging by combining SIM with a wide-field Raman microscope. Only Raman scattered light in a certain wavenumber region was extracted using a dichroic mirror and a band pass filter, and Raman images were acquired using a CCD without a spectrometer. We report the improved spatial resolution of Raman images of a living HeLa cell in the C–H stretching band region with an acquisition time of 90 seconds.

2-15-1439* 情報理論を取り入れた手法によるラマン分光イメージ中での化学的空間不均一性の解析
Analysis of chemical heterogeneity in Raman spectral image with information theory

Ryoya Kondo¹, James N. Taylor², Jean-Emmanuel Clement², Yuta Mizuno^{1,2,3}, Katsumasa Fujita⁴, Yoshinori Harada⁵, Tamiki Komatsuzaki^{1,2,3} (¹*Grad. Sch. Sci. & Tec., Hokkaido Univ.*, ²*Res. Inst. electron Sci., Hokkaido Univ.*, ³*WPI-ICReDD, Hokkaido Univ.*, ⁴*Grad. Sch. Tec., Osaka Univ.*, ⁵*Kyoto Pre. Univ. Med.*)

Nonalcoholic fatty liver disease is a condition in which the liver accumulates lipids without drinking history and is regarded as a major liver disease. Raman spectral imaging of liver tissues obtained from a rat disease model was analyzed to identify pathology of the tissue and observe relationships among pathology and spatial heterogeneity. We analyzed the spatial heterogeneity in the images using information theory to gain new insights into pathology. We classified spectral heterogeneity around pixels using the information bottleneck method that enables us to classify the data in a functional space, which may be widely applied to various fields. We will identify an optimal number of clusters and hyperparameter value with consideration of photon-counting fluctuations.

[2-15-1451](#) A sample preparation method using the resin-embedding for digital holographic microscopy

Yuki Ide¹, Yuji Matsukawa¹, Shigeki Mayama², Kazuo Umemura¹ (¹Tokyo Univ. Sci., ²Tokyo Gakugei Univ.)

Digital holographic microscope (DHM) techniques are becoming one of the standard microscopic techniques to study micron size samples. In this work, we embedded diatomite which is fossils of diatoms in was SYLGARD 184 (refractive index (RI) 1.410), mount media (RI 1.520), and 1.5% agar (RI 1.355) to improve resolution of DHM images. Firstly, individual diatomite was stably observed with all the resins. When similar diatomite was observed in water, DHM observation was a little unstable due to perturbation of water. Secondly, detailed structures of diatomite could be observed only with SYLGARD 184. The RI of SYLGARD 184 was rather close to RI of diatomite (around 1.5). Our results revealed that the embedding was effective to stabilize and improve DHM observations.

[2-15-1503](#) 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内ケラチンタンパク質の選択的観察

Selective IR super-resolution imaging of keratin proteins in biological samples by micro-spectroscopy based on non-linear optical process

Hirona Takahashi, Tetsuya Ida, Kohei Katayama, Makoto Sakai (*Grad. Sch. Sci., Okayama Univ. of Sci.*)

Keratin is one of the most important structural proteins. We have already succeeded in IR super-resolution imaging of keratins inside the feather or animal hairs and revealed the distribution and orientation 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. In this study, we developed a new IR super-resolution micro-spectroscopy based on the 4-wave mixing, which is the third-order non-linear optical process, and try to detect keratin proteins in the bulk area. The comparison of the selective IR super-resolution imaging by two micro-spectroscopies is also discussed in the presentation.

[2-15-1515](#) 相関顕微鏡法 (CLEM) による同一試料観察に向けた相関・位置合わせ精度の改善
Improvement of correlation and alignment accuracy toward the same sample observation by CLEM

Yuki Gomibuchi¹, Risa Ezoe², Hiroko Takazaki^{1,3}, Yasuhisa Honda¹, Yaoki Yamamoto¹, Yusuke V. Morimoto¹, Takuo Yasunaga¹ (¹Dept. of Phys. Info. Tech., Kyushu Inst. Tech., ²Dept. of Biosci. Bioinfo., Kyushu Inst. Tech., ³IPR. Osaka Univ.)

A variety of samples including biomolecules are valuably observed by utilizing the merits of both LM and EM. Correlative Light and Electron Microscopy (CLEM) is effective for observing the region of interest in the same field. Thus, we used fluorescent beads as markers and performed coordinate calculation and stage movement by SerialEM to evaluate the errors and its procedures. As a result, the accuracy was improved when 20-25 markers were placed around the target, and the error was within 5 μm. It is possible to guarantee that the observed object is the same sample if it is within 10 μm. For the automation of CLEM, we are developing suitable protocols to automatically detect marker beads from images and a new program to align two images.

[2-15-1527](#) 診療録からの症状半自動抽出システムの開発
Development of semi-automatic phenotype extraction system from medical records

Yoshino Jibiki¹, Eisuke Dohi², Kota Ninomiya^{3,4}, Toyofumi Fujiwara⁵, Takanori Sasaki¹ (¹Fac. Adv. Math. Sci., Meiji Univ., ²Dept. Neuroscience Disease, Brain Research Inst., Niigata Univ., ³Natl. Inst. Public Health., ⁴Grad. Sch. Pharm. Sci., The Univ. of Tokyo, ⁵DBCLS)

For identification of about 6,000 types of rare/hereditary diseases by clinicians, automatic extraction of medical conditions from medical reports is considered to be useful. In this study, we developed a system, Phenotype Ontology Extractor from Text (POET) which extracts phenotype information from medical records with a variety of expressions for medical conditions. In fact, we created the extended version of the Japanese translation of the Human Phenotype Ontology (HPO) by utilizing the medical dictionary Manbyo-Jisyo, and extracted the texts for medical conditions from 32 case reports. As a result, the extraction accuracy by POET was better than that by regular HPO. In this presentation, we will report the details of the automatic extraction accuracy of POET.

2-15-1600 グラフェン電界効果トランジスタ表面におけるノイラミニダーゼ反応の電気的バイオセンシング
Electrical Biosensing for Neuraminidase Reaction at the Surface of Graphene Field-Effect Transistors

Takao Ono^{1,2}, Kaho Kamada¹, Ryota Hayashi¹, Alba Rosa Piacenti³, Calum Gabbutt³, Naruto Miyakawa⁴, Kaori Yamamoto¹, Nongluk Sriwilajaroen⁵, Hiroaki Hiramatsu⁶, Yasushi Kanai¹, Tomohiro Koyama^{1,7}, Koichi Inoue¹, Shota Ushiba⁴, Ayumi Shinagawa⁴, Masahiko Kimura⁴, Shin-ich Nakakita⁸, Toshio Kawahara⁶, Yutaka Ie¹, Yohei Watanabe⁹, Yasuo Suzuki⁶, Daichi Chiba^{1,7}, Sonia Contera³, Kazuhiko Matsumoto¹ (¹SANKEN, Osaka Univ., ²JST-PRESTO, ³Dept. Phys., Univ. Oxford, ⁴Murata Mfg., ⁵Fac. Med., Thammasat Univ., ⁶Col. LHS, Chubu Univ., ⁷CSRN, Osaka Univ., ⁸LSRC, Kagawa Univ., ⁹Grad. Sch. Med. Sci., KPUM)

Reactions at the surface are difficult to be measured, due to a small amount of their products. Graphene, a surface-sensitive two-dimensional material, has a potential for the measurement. Here we show an electrical biosensing for neuraminidase (NA) reaction to sialoglycan(SG)-modified graphene surface [1]. Influenza virus uses NA for the propagation, which cleaves sialic acid terminus of SG at the cell surface. NA inhibitors are a major class of anti-influenza drugs. NA reactions were monitored in real time as a dissociation of negatively-charged sialic acid from the surface. NA inhibition by Relenza® was also measured. Moreover, liquid-AFM imaging revealed hierarchical structures of reaction molecules on the surface. [1] T. Ono, *et al.*, *bioRxiv* 2020.03.18.996884.

2-15-1612 Diffusion of LLPS Droplets Consisting of Poly(PR) Dipeptide Repeats and RNA on Chemically Modified Glass Surface

Chen Chen¹, Kohsuke Kanekura², Yuhei Hayamizu³ (¹Tokyo Tech, Earth-Life Science Institute, ²Tokyo Medical University, Department of Molecular Pathology, ³Tokyo Tech, School of Materials and Chemical Technology)

The liquid-liquid phase separation (LLPS) of proteins and RNA has recently emerged as a crucial role in various cellular functions and some fatal neurodegenerative disease like ALS. Normally, LLPS droplets are characterized by optical microscopy with transparent substrates. With the liquid and wetting properties on a glass surface, LLPS droplets have been immobilized on the surface by some technical protocols. However, the interactions between LLPS droplets and glass surface still remain unclear. Here, we used single-particle tracking method to observe the surface dynamics of LLPS droplets on the untreated glass surface and chemically-modified glass surface with positive charges. This research could provide a novel insight to understand the LLPS formation.

2-15-1624 多次元 *in vitro* 酵素スクリーニング法の開発
Development of multidimensional *in vitro* enzyme screening system

Shingo Honda¹, Yoshihiro Minagawa², Hiroyuki Noji^{1,2}, Kazuhito Tabata² (¹Dept. Bioeng., Grad. Sch. Eng., Univ. Tokyo, ²Dept. Appl. Chem., Grad. Sch. Eng., Univ. Tokyo)

In vitro enzyme screening is a powerful method to select enzymes with desired properties, in which genes of enzyme mutants are individually encapsulated in myriads of small compartments and selected. Each mutant is expressed in the compartment and evaluated and sorted by the activity. However, the condition for evaluation is often non-optimal since, after expression, the solution cannot be exchanged keeping the genes and enzymes inside. Also, selection based on multiconditional assay is difficult. In this study, we develop an *in vitro* enzyme screening with solution exchanges by immobilizing individual genes and enzymes in arrayed micro-chambers, enabling screenings under desired condition(s). We have succeeded in immobilizing tagged genes and enzymes in each chamber.

2-15-1636 リコンビナント LOX-1 受容体に結合する LDL の特性
Physical properties of low-density lipoproteins recognized by recombinant LOX-1 receptor

Seiji Takeda¹, Kanajo Ushirogata², Ao Hamamuki¹, Agus Subagyo³, Taichi Takasuka² (¹Dept. Pharm., Hokkaido Univ. of Sci., ²Grad. Sch. GFR., Hokkaido University, ³Grad. Sch. Info. Sci. Tech., Hokkaido University)

Oxidation changes low-density lipoprotein (LDL) properties and it alters affinity to modified LDL receptors that are related to development of various diseases. Although Young's modulus of LDLs were decreased by the oxidation, Young's modulus of the LDL recognized by the receptors are not well investigated. In this study, a recombinant LOX-1, one of the modified LDL receptors, were used. The LOX-1 properties were analyzed by BLI method. The LOX-1 was immobilized on a mica substrate. Topographies and Young's modulus of LDLs recognized by the LOX-1 were analyzed using AFM. With increasing oxidation of LDL, Young's modulus of the LDL decreased and number of observed LDLs particles increased. We will discuss the physical properties of LDL recognized by the LOX-1.

[2-15-1648](#) インターカレーターは生きた細胞内のクロマチンの動きを抑制する
Intercalator suppresses chromatin motion in living human cells

Yuji Itoh, Aoi Otsuka, Kazuhiro Maeshima (*NIG*)

Some of the intercalators such as daunomycin (Daun) and doxorubicin (Doxo) are used as anticancer drugs. Intercalators are inserted into adjacent DNA base pairs and inhibit topoisomerase II, resulting in DNA double-strand breaks. However, the effect of intercalators on chromatin behavior remains unclear. To approach this issue, we investigated genome-wide chromatin behavior in living human cells using single-nucleosome imaging. We found that intercalators drastically suppress chromatin motion. The suppressed chromatin motion recovered after Daun/Doxo was washed out, suggesting that the motion suppression effects are reversible. These results indicate that intercalators alter chromatin motion and structure in living cells, which may contribute to the anticancer effects.

[2-15-1700](#) Localized in vivo Mechanical Characterisation of Normal and Abnormal Cell Nuclei by Atomic Force Microscopy

Sivashanmugan Kundan¹, Takehiko Ichikawa¹, Eishu Hirata^{1,2}, Mohammad Shahidul Alam¹, Mohammad Mubarak Hosain¹, Tetsuya Shirokawa¹, Keisuke Miyazawa^{1,3}, Kazuki Miyata^{1,3}, Takeshi Fukuma^{1,3} (¹*WPI Nano Life Science Institute (WPI-NanoLSI), Kanazawa University, Kakuma-Machi, Kanazawa, 920-1192, Japan*, ²*Division of Tumor Cell Biology and Bioimaging, Cancer Research Institute of Kanazawa University, Kakuma-Machi, Kanazawa, 920-1192, Japan*, ³*Division of Electrical Engineering and Computer Science, Kanazawa University, Kakuma-Machi, Kanazawa, 920-1192, Japan*)

Intracellular organelles, such as those in the nuclei of cancer cells, are key to revealing the normality of nucleus function during cancer cell metastasis. Atomic force microscopy (AFM) measurements have consistently shown that cancer cells are softer than normal cells. The variations in cellular mechanical properties can be correlated with their metastatic potential. The mechanical mapping can indirectly detect intracellular mechanics, there is no direct measurement of the cell interior. Recent work using an AFM nanoprobe has investigated the in vivo mechanical properties of normal and abnormal cell nuclei with suspected metastatic activity and additional biochemical studies can provide new and important insight into the metastasis process.

[2-15-1712](#) Development of a method for quantitative profiling of microRNAs in single exosomes

Cinya Chung¹, Ryo Iizuka², Takashi Funatsu¹ (¹*Grad. Sch. Pharm. Sci., Univ. Tokyo*, ²*Dept. Biol. Sci., Grad. Sch. Sci., Univ. Tokyo*)

Exosomes are nano-sized membrane vesicles secreted by various types of cells. Recent studies have shown that cancer cells secrete higher levels of exosomes compared to normal cells, and that these exosomes contain specific microRNAs (miRNAs). Therefore, exosomal miRNAs are considered as potential biomarkers for cancer diagnosis. However, there is still no efficient method to analyze miRNAs in individual exosomes. To enable earlier and more accurate cancer diagnosis, we devised a microfluidic-based method for profiling of miRNAs from single exosomes. We demonstrated the feasibility of our method using synthetic miRNAs with high reproducibility.

[2-15-1724](#) 1分子超解像イメージングを用いたRNAポリメラーゼIIとクロマチンのナノスケール相互作用解析
Single-molecule super-resolution analysis for nano-scale interaction between RNA polymerase II and chromatin

Yuma Ito, Makio Tokunaga (*Sch. Life Sci. Tech., Tokyo Tech*)

In the transcriptional regulation of eukaryotic cells, RNA polymerase II (Pol II) physically interacts with the highly organized structure of chromatin. However, the precise structure of Pol II-bound chromatin and how it functions in transcription are still elusive. Here, we simultaneously visualized the dynamics of individual Pol II molecules and the nanometer-scale structure of adjacent chromatin in living cells. The local angular distribution analysis revealed that the spatially polarized distribution of histone molecules and its distance to the Pol II localization were sensitive to the change of histone acetylation state by TSA treatment. These results suggest that epigenetic states control the accessibility of Pol II to adjacent chromatin nanostructures.

[2-15-1736](#) (3S6-2) 微小電気穿孔法を用いた細胞膜の機械特性と遺伝子発現の統合解析
(3S6-2) A combined analysis of membrane-mechanical phenotyping and transcriptomics using nanoelectroporation

Akifumi Shiomi, Taikopaul Kaneko, Kaori Nishikawa, Hirofumi Shintaku (*Hakubi, CPR, RIKEN*)

Mechanical properties of the cellular membrane are phenotypic expression that are involved in various biological contexts, especially aging. However, these detailed molecular cascade remains to be uncovered due to the complex physiological processes and the unexplained initiation factors. Here, we report an approach that enables a combination analysis on membrane-mechanical phenotype and gene expression in each of thousands of single cells leveraging nanoelectroporation, dubbed ELASTomics (electroporation-based lipid-bilayer assay for stiffness and transcriptomics). Applying ELASTomics to human TIG-1 fibroblasts, we dissect the link between the membrane-mechanical phenotype and gene expression along with the cellular senescence at single-cell resolution.

[2-15-1748](#) 1分子超解像イメージングによる細胞周期がもたらすヘテロクロマチンの構造変化
Structural changes in heterochromatin involved in cell cycle using single-molecule and super-resolution imaging

Masanori Nakano, Yuma Ito, Makio Tokunaga (*Sch. Life Sci. Tech., Tokyo Inst. Tech.*)

Heterochromatin is a key structure for regulating gene expression by repressing the access of transcription factors to DNA. However, the dynamics of its structure during the cell cycle are still largely unknown. Here, we observed the localization of histone H3 variants H3.1 and H3.3 using single-molecule super-resolution imaging. Localization analysis of histone variants throughout the cell cycle in synchronized 3T3 cells revealed that H3.1 was distributed including heterochromatin regions and changed the clustering strength during the S phase. In contrast, H3.3 in transcriptionally active regions was distributed uniformly throughout the S phase. We discuss the quantitative characteristics of heterochromatin-specific structural dynamics.

[2-15-1800](#) Genetically encodable tool for live-imaging and manipulation of endogenous RNAs in living cells

Akira Takai¹, Yasushi Okada^{1,2} (¹*BDR, RIKEN*, ²*Dept. Phys., Grad. Sch. Sci., Univ. Tokyo*)

In this study, we show 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.

[2-15-1812](#) 異なる翻訳後修飾を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 with different epigenetic modifications

Masanori Hirose, Yuma Ito, Makio Tokunaga (*Sch. Life Sci. Tech., Tokyo Tech*)

Chromatin status, such as post-translational modifications, controls the gene expression dynamically. However, the relationship between a particular chromatin state and its physical mobility is not well understood. Using U2OS cells that co-express Halo-tagged histone H4 and mCherry-HP1 α , we quantitatively analyzed the dynamics of individual histone molecules in heterochromatin. The mean square displacement obtained from histone H4 trajectories revealed that the diffusion coefficient and the anomalous exponent were decreased in heterochromatin, suggesting a confined environment of heterochromatin. We discuss the state-specific dynamics of chromatin using various indicators that visualize distinct features of single-molecule mobility.

[2-15-1824](#) 核小体タンパク質の生細胞 1 分子イメージングを用いた RNA に依存した相分離動態の定量解析
Single-molecule imaging analysis of RNA-dependent dynamics of phase-separated nucleolar
proteins in living cells

Yuma Ito, Supanut Sirisukhodom, **Makio Tokunaga** (*Sch. Life Sci. Tech., Tokyo Tech*)

The nucleolus is composed of three different subcompartments, including FC, DFC, and GC. Although liquid-liquid phase separation through protein-RNA interaction has essential roles in maintaining its structure, the effect of RNA on the dynamics of nucleolar proteins is still unclear. Using single-molecule imaging in living cells, we quantified the mobility of NPM1, FBL, and RPA194 in GC, DFC, and FC, respectively. The inhibition of RNA synthesis using Actinomycin D increased the mobility of FBL and RPA194 and decreased that of NPM1. The RNA accumulation by knockdown of small subunit processome components decreased FBL mobility, suggesting distinct contributions of RNA on the dynamics of nucleolar subcompartments.

[2-16-1315*](#) Development of a genetically encoded fluorescent indicator for molecular crowding with large
dynamic range and high sensitivity

Shinya Sakai (*Graduate School of Frontier Bioscience, Osaka University*)

Molecular crowding affects the mobility, folding and association of the biomolecules. Despite of the important parameter for biological functions, only few analytical tools are available. Here, we report a genetically encoded indicator for molecular crowding, which has a big dynamic range (975 %) in vitro. With this indicator, we successfully and easily detected spatio-temporal changes in molecular crowding associated with sorbitol-induced upshifts in intracellular osmotic pressure. This indicator would contribute to understanding of how molecular crowding is involved in cellular functions.

[2-16-1327*](#) ヨーロッパモノアラガイの咀嚼調節ニューロンのカルシウムイメージングー味覚嫌悪学習前後
のカルシウムシグナルの比較ー
Fluorescence calcium imaging for the feeding modulatory neuron of the pond snail

Ayaka Itoh¹, Yoshimasa Komatsuzaki², Monoru Saito¹ (¹*Grad. Sch. of Integ. Bas. Sci., Nihon Univ.*, ²*Coll. Sci. Tech., Nihon Univ.*)

Associative learning in the pond snail *Lymnaea stagnalis* has been used for investigating the mechanism of learning and memory. It includes taste aversive conditioning that is a form of classical conditioning using feeding behavior. In this study, we examined calcium signal in the cerebral giant cell (CGC) that modulates feeding rhythm in *Lymnaea*, and compared it before and after taste aversive conditioning. Here, we used fluorescence calcium imaging for calcium signal measurement. A calcium-sensitive dye, Cal-520, was injected into the CGC by a microelectrode. The preparation was illuminated by an Ar Laser (488 nm), and the 520 nm fluorescence images were acquired through a Nipkow confocal unit and an EM-CCD camera.

[2-16-1339*](#) 細胞内温度イメージングを用いた神経分化機構の解明
Elucidation of Neural Differentiation Using Intracellular Temperature Imaging

Shunsuke Chuma^{1,2}, 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 intra- and extra-cellular factors. Although recent studies have shown that thermal stimulation influences neural differentiation, the involvement of intracellular temperature remains elusive. Here, we investigated the contribution of intracellular temperature change to neural differentiation in PC12 cells. Using a fluorescence polymeric thermometer, we found that the intracellular temperature increased during neural differentiation in a transcription and translation dependent manner. Additionally, local heating of the nucleus by infrared laser promoted neurite outgrowth. Therefore, we propose that intracellular thermogenesis during differentiation contributes to neurite outgrowth.

[2-16-1351*](#) 高速 AFM によるヒストン H2A-DNA 相互作用およびその凝集性のリアルタイムダイナミクスの解明

Investigation of real-time dynamic histone H2A-DNA interaction and H2A-DNA condensation/de-condensation using high-speed AFM

Goro Nishide¹, Keesiang Lim², Akiko Kobayashi^{2,3}, Masaharu Hazawa^{2,3}, Takahiro Nakayama², Noriyuki Kodera², Toshio Ando², Richard Wong^{2,3}
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Nucleus is the storage and regulator of genetic information that shapes the blueprint of life. Octameric histone complex and DNA form the structural/functional unit of chromatin known as nucleosome. Dynamic histones-DNA interaction is essential for gene regulation, in which tight histone-DNA interaction restricts gene expression or vice versa. Today, real-time observation of histones-DNA interaction, including factors that affect the interaction, remain elusive. Weak tapping force and high spatiotemporal resolution make HS-AFM feasible for real-time imaging of biomolecule interactions. Therefore, we aim to reveal the real-time dynamic histone H2A-DNA interaction by using HS-AFM. We will discuss the details during the presentation.

[2-16-1403*](#) Development of the nanoendoscopy AFM technique for visualizing inter-cellular structures in living cells

Mohammad Shahidul Alam¹, Marcos Penedo^{2,5}, Tetsuya Shirokawa³, Mohammad Mubarak Hosain¹, Takahiko Ichikawa², Keisuke Miyazawa^{2,3}, Kazuki Miyata^{1,2,3}, Chikashi Nakamura⁴, Takeshi Fukuma^{1,2,3} (¹Graduate school of frontier science initiative, Division of Nano Life Science, Kanazawa University, ²Nano Life Science Institute (WPI-NanoLSI), Kanazawa University, ³Graduate school of natural science and technology, Division of Electrical Engineering and Computer Science, Kanazawa University, ⁴National Institute of Advanced Industrial Science and Technology (AIST), ⁵Laboratory for Bio- and Nano-Instrumentation, Swiss Federal Institute of Technology Lausanne (EPFL), Lausanne, Switzerland.)

The knowledge of the molecular-scale dynamics of intracellular components is necessary to explain cell functions and the key mechanisms of disease. To understand those processes, we have developed a unique AFM-based nanoendoscopy technique that permits label-free imaging of nanoscale biomolecular dynamics inside living cells, without breaking them apart. A long ultrathin nanoprobe is inserted into living cells to perform 2D and 3D AFM imaging. We can image and reconstruct from the whole cell structure to unsupported actin fibers, proving that such an imaging method based on ultrathin nanoprobes does not dramatically affect cell's viability. The nanoendoscopy AFM technique will aid in the understanding of intra-cellular biological processes.

[2-16-1415*](#) レーザー照射による固液界面でのリポソームの捕捉と破壊
Capture and rupture of liposomes at the solid-liquid interface by laser irradiation

Takumi Uchida (*Grad. Sch. Sci., The Univ. of Tokyo*)

Lipid vesicles are important for biological transport processes, and the vesicle manipulation is a key aspect to develop new synthetic biological applications. Currently, optical tweezers are commonly used to manipulate micro/nanoparticle, but its optical requirement hinders to handle biological vesicle due to small differences in refractive index. Therefore, we use thermophoresis on silicon-based substrate to manipulate liposome. In this talk, we talk the investigation of liposome manipulation under our silicon-based thermophoresis system. We observed that the trapping behavior of liposome depends on the ionic concentration of the solvent and the laser intensity, which means that our system can be used as a fundamental tool for the vesicle-based applications.

[2-16-1427*](#) パッチクランプ機能付き高速 AFM の開発
Development of Patch-Clamp High-speed Atomic Force Microscopy

Takeru Matsubara¹, Shinji Watanabe², Kenichi Umeda², Ayumi Sumino², Toshio Ando², Noriyuki Kodera² (¹Grad. Sch. NanoLS., Kanazawa Univ., ²WPI-NanoLSI, Kanazawa Univ.)

The structure and function of ion channels have been studied separately by either electrophysiological or structural biological methods (e.g., X-ray crystallography and cryo-electron microscopy). We have been developing a high-speed AFM (HS-AFM) system that can simultaneously observe the function of an ion channel and the accompanying structural changes by performing patch-clamp analysis during HS-AFM imaging. Last year, we reported that the basic experimental system including mechanical and electrical parts were established, so that we can observe the nano-pipette end with an aperture size of ~100 nm by HS-AFM while doing ion current measurement. Now, we are doing an application study using a pore-forming toxin. In the presentation, we will report the progress.

[2-16-1439*](#) CALHM2 をナノポアとして用いた多様なサイズの分子検出法の開発
Development of a variety size of molecule detection method using CALHM2 as a nanopore

Sotaro Nakamura, Hirohito Yamazaki, Wataru Shihoya, Osamu Nureki, Sotaro Uemura (*Department of Biological Sciences, The University of Tokyo*)

Biological nanopore become the attractive single molecule sensing method due to its ability to analyze building blocks of DNA, RNA, and peptides with high resolution. In our study, we use Calcium homeostasis modulator protein 2 (CALHM2) nanopores, which has potential to tune pore size from 2.5 nm to 6 nm, as new type of biological nanopore sensor to target much wide range of molecule size. Using physiological measurement, we saw CALHM2 nanopores have variety conductance from 1 nS to 24 nS, implying that CALHM2 nanopores have multiple nanopore conformations. Also, when we added RNA at 30 mV, we observed blockade current which have never been seen without RNA, which indicates molecular sensing ability of this pore.

[2-16-1451](#) 曲率の大きいエッジを持つナノポアと DNA の相互作用
Pathways for DNA into sharp-edged nanopores

Shin Takano, Takumi Yoshikawa, Sho Matsuki, Shimba Ichino, Yuuta Moriyama, Toshiyuki Mitsui (*Dept. of Phys. Aoyama Gakuin Univ.*)

Solid state nanopores are expected to become a DNA sequencing as well as commercial sequencing made of biological nanopores. One of issues would be the DNA dynamics when a DNA molecule enters into a nanopore affected by the nanoscale pore geometry. Therefore, we intentionally made pores with the shape containing high curvature edges and observed DNA dynamics into these pores. The “sharp-edged” pores provided anisotropic entry paths for DNA translocations. Furthermore, the pores dramatically reduced the probability of DNA clogging. The numerical simulation by a finite element method suggests that the force by osmosis exceeds the electrophoresis near the sharp-edge. Finally, we will discuss the nanopore shapes to control the entry routes of DNA for its sensing.

[2-16-1503](#) カラストレス印加下におけるタンパク質の動態イメージングのための高速 AFM 用基板伸縮システムの開発
Development of Substrate Stretching System for High-Speed AFM for Dynamic Imaging of Proteins under Mechanical Stress

Fengyueh Chan, Ryo Kurosaki, Takayuki Uchihashi (*Grad. Sch. Sci., Nagoya Univ.*)

Cell adapts to mechanical stimuli by regulating its cytoskeleton and other related proteins. High-speed atomic force microscopy (HS-AFM) is one of the promising techniques to examine the detailed dynamics down to the resolution of a single molecule at a high frame rate. Thus, by using a tip-scan atomic force microscope (TS-HS-AFM), we can apply versatile stimuli to the proteins located on the capacious sample stage. Here we present a TS-HS-AFM incorporating a substrate stretching mechanism to stimulate and observe the protein dynamics on the surface-modified polydimethylsiloxane (PDMS). Our demonstration with filament actin and microtubule indicates that the TS-HS-AFM-based substrate manipulator provides a new study method for studying the sophisticated design of life.

[2-16-1515](#) Photothermally enhanced single molecule nanopore sensing

Hirohito Yamazaki, Sotaro Uemura (*Department of Biological Sciences*)

In this presentation, we present methods that laser irradiation to solid-state nanopore can enhance sensing modalities. First, we found that photoexcitation of a silicon nitride nanopore using a visible laser results in a localized thermal gradient that produces both ion and DNA thermophoresis. We utilize this ion thermophoresis effect to probe thermal melting in biomolecules that are heated at the nanopore. Additionally, we found that a side-effect of the observed heating was that the material degradation under high power illumination. Combining this laser etching with dielectric breakdown, nanopores of arbitrary dimensions as small as 1–2 nm in diameter and thickness can easily be fabricated without using an electron beam, which allows detecting single-strand DNA.

[2-16-1527](#) Hidden Markov Modeling of Biomolecular Conformational Dynamics from Atomic Force Microscopy Time-Series Images

Tomonori Ogane, Yasuhiro Matsunaga (*Grad. Sch. of Eng. Sci., Saitama Univ.*)

High-speed atomic force microscopy (HS-AFM) is a powerful technique for measuring the structural dynamics of biomolecules. However, the structural information contained in HS-AFM images is limited to the surface shape of the molecule. Inferring latent three-dimensional structures from HS-AFM images is thus important for getting more insights into the dynamics of the molecule. Here, in order to make accurate estimations of molecular orientations and structures from HS-AFM time-series images, we have developed a method based on hidden Markov models. Using simulated HS-AFM image data as a test case, we show that our time-series analysis method makes more accurate estimations of molecular orientations and structures than the estimations from individual images.

[2-16-1600](#) 自動化1分子イメージングシステムによる受容体動態の大規模解析
Large-scale analysis of receptor behaviors with automated single-molecule imaging system

Michio Hiroshima^{1,2}, Daisuke Watanabe³, Masahiro Ueda³ (¹*RIKEN BDR*, ²*RIKEN CPR*, ³*FBS Osaka Univ.*)

We have achieved fully automated single-molecule imaging with employing AI and robotics. Inefficiencies arose from manual operations and expertise in the conventional microscopy were eliminated, applicable to a large-scale analysis. Single-molecule mobility and clustering of receptor proteins were shown to be sensitive to its activation level. This quantitative property can be effectively utilized when combining with the large-scale analysis. We are starting 1) cellular heterogeneity analysis regarding the activation of epidermal growth factor receptor (EGFR) and 2) single-molecule drug screening on EGFR kinase inhibitors. Comparison with the conventional methods, more informative screening considering molecular behaviors and cellular heterogeneity will be available.

[2-16-1612](#) 超解像顕微鏡の分解能を向上する事後処理の計算補償光学顕微鏡法
Post-processing, computational adaptive optics for 3D super-resolution microscopy

Atsushi Matsuda (*Advanced ICT Research Institute, National Institute of Information and Communications Technology*)

Recent development of adaptive optics (AO) microscopy has revealed its significant potential to improve resolution and signal to noise ratio in advanced microscopy by correcting sample-induced optical aberration. While AO has been successful, it is not yet used widely in biology due to its complex optics, expensive devices, and demanding operations. Here we report post-processing, computational AO of the 3D fluorescence images and 3D structured illumination microscopy (3D-SIM) images already acquired. We show that our method can separate two points that are previously recognized as a single point object, and the resulting FWHM of a fluorescent bead is close to the diffraction limit. Our approach has number of advantages over hardware-based AO.

[2-16-1624](#) 細菌が形成する動くバイオフィルムのASEMとcryo-TEMによる観察
Mobile biofilm formed by bacteria was observed using ASEM and cryo-TEM

Chikara Sato¹, Masami Naya¹, Naoki Kasahata¹, Mari Sato¹, Keiko Sato² (¹*Health Medical Res. Inst., AIST*, ²*Graduate School Biomedical Sciences, Univ. Nagasaki*)

Biofilm formed by bacteria is deleterious because the bacteria inside biofilm tend to be resistant against immune system and antibiotics. *Flavobacterium johnsoniae* forms spreading colony. It was analyzed for biofilm formation by ASEM[1] and cryo-TEM in hydrophilic conditions, decreasing the risk of changes of the water-rich biofilm. Filamentous network around mobile bacterial colonies were revealed by PTA and MCMIR stained ASEM, suggesting the formation of biofilms. Surface of the biofilm critical for the resistance was expected to be examined using newly developed grid-stamp negative stain method[1] and immuno-labeling[2-3]. [1] Sato et al. Sci. Rep. 11,967, 1-16(2021). [2] Sakai et al. Sci. Rep.11, 5722, 1-17(2021). [3] Sugimoto et al. Sci. Rep. 6, 25889, 1-13 (2016).

2-16-1636 蛍光イメージング法によるケラチノサイト細胞内 Mg^{2+} 動態の可視化
Visualization of intracellular Mg^{2+} dynamics in keratinocytes by fluorescent imaging

Keigo Fujita¹, Yutaka Shindo¹, Yuji Katsuta², Makiko Goto², Kohji Hotta¹, Kotaro Oka¹ (¹*Grad. Sch. Sci and Tech. Keio Univ.*, ²*Shiseido Global Innovation Center*)

Mg^{2+} is the richest divalent cation in living cells. However, the role of intracellular Mg^{2+} is unclear in keratinocytes, the major cell type in epidermis. Spatio-temporal dynamics of Mg^{2+} in keratinocytes in response to various stimuli were visualized with Mg^{2+} selective indicator, KMG-104. As a result, we found addition of H_2O_2 , one of the reactive oxygen species (ROS), caused intracellular Mg^{2+} concentration ($[Mg^{2+}]_i$) increase in keratinocytes. We further examined the H_2O_2 -induced $[Mg^{2+}]_i$ increase under several conditions and found that the Mg^{2+} was not mobilized from major Mg^{2+} sources: extracellular Mg^{2+} entry, release from mitochondria, and ATP-Mg hydrolysis. Our results suggest that keratinocytes have other unknown intracellular Mg^{2+} source.

2-16-1648 細胞内温度分布の追跡が単一細胞内の遅いエネルギー散逸を明らかにする
Tracking Intracellular Temperature Mapping Reveals Slow Energy Dissipation in Single Cells

Masaharu Takarada¹, Kohki Okabe^{1,2}, Takashi Funatsu¹ (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 distributions. Furthermore, this method revealed that the temperature relaxation rate of cells was 7.2×10^3 times slower than that calculated based on the heat transfer model, suggesting the existence of slow intracellular energy dissipation.

2-16-1700 High temporal observation of CheY-binding and dissociation during rotational switching of a single flagellar motor

Taro Yuri, Yumiko Uchida, Yong-Suk Che, Akihiko Ishijima, Hajime Fukuoka (*Grad. Sch. Frontier Bio Sci. Osaka Univ*)

Recently, we have showed the binding/dissociation of CheY-P directly switch CW/CCW rotation of a motor by single cell imaging of CheY-GFP. However, the temporal resolution was insufficient to elucidate the detailed process of switching by binding of CheY. Here, we developed mNeonGreen(mNG)-fusion of CheY, which is brighter than EGFP, for high temporal observation. We succeeded in measuring the binding of CheY-mNG at 5-ms resolution, which is 4-fold faster than that of our previous study. We are measuring the time difference between the binding of CheY and the switching of the motor, and binding/dissociation process of CheY during rotational switching. These are important to understand the process of switching by CheY, so we will discuss the detail results at the meeting.

2-16-1712 細胞内の温度変動に対する微小管の寄与
The contribution of microtubules on intracellular temperature variations

Takeshi Ueda¹, Takashi Yanagi¹, Koki Okabe^{1,2}, Takashi Funatsu¹ (¹*Grad. Sch. Pharm., Univ. Tokyo*, ²*JST PRESTO*)

Temperature is one of the most fundamental physical quantities and contributes greatly to life activities. Recently, it was found that intracellular temperature is an important factor in cell biology. For example, a cell uses localized heat to trigger cellular functions. However, it is still unclear how microtubules, which are widely distributed in cells, are involved in intracellular temperature changes. Therefore, we investigated the relationship between microtubules and intracellular temperature. By comparing microtubule-disrupted cells with normal cells, we found that the temperature increases in a cell upon either endogenous and exogenous heat production was dependent on microtubules, revealing that microtubules contribute to the temperature increase of the cells.

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- [2-16-1724](#) 大腸菌走化性応答適応過程 (CW バイアス) を簡単かつリアルタイムに数値化するポータブル顕微鏡システムの構築
Construction of a portable microscope system that easily and in real time digitizes E. coli chemotaxis adaptation process (CW bias)

Hiroto Tanaka, Yasuaki Kazuta, Amina Yano, Hiroaki Kojima (*Adv ICT Res Inst, NICT*)

We have developed a solution evaluator using E. coli chemotaxis response (10-minute CW bias measurement using tethered assay). We report on the development of a portable, inverted microscope system to realize the on-site use of this solution evaluator. The features of this portable microscope system are that it adopts an inverted type and has a work space above the sample that enables solution exchange, the weight of the microscope system (main body, camera, light source) is about 2.3 kg, and realizing real-time analysis of CW bias using a notebook computer. The image analysis program is self-made and can be customized. At the annual meeting, we would like to introduce actual usage situations and discuss the possibility of usage development.

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- [2-16-1736](#) 細胞内の温度変化に対する高分子の影響の解明
Elucidation of the effect of macromolecules on temperature changes in cells

Shunsaku Nagai¹, Koki Okabe^{1,2}, Takashi Funatsu¹ (¹*Grad. Sch. of Pharm. Sci., The Univ of Tokyo*, ²*JST, PRESTO*)

Previous studies showed a unique phenomenon in which local temperature inside the cell fluctuates spatiotemporally, and this local temperature change contributes to cellular functions. In this study, to elucidate the effect of macromolecules on temperature changes in cells, we measured the temperature change upon heating when the amount and state of molecules were manipulated in live cells. In these experiments, we found that the temperature rise and relaxation process of the cells depended on the macromolecules. This result suggests that the structure and concentration of the macromolecules expressed in the cells may govern the temperature fluctuations and non-uniform temperature distribution in cells.

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- [2-16-1748](#) Influence of Intra-Cellular Nanoendoscopy-AFM Measurements on Cell Viability and Functions

Mohammad Mubarak Hosain¹, Mohammad Shahidul Alam¹, Ichikawa Takechiko¹, Marcos Penedo^{1,2}, Tetsuya Shirokawa³, Sivashanmugan Kundan¹, Keisuke Miyazawa^{1,3}, Kazuki Miyata^{1,3}, Fukuma Takeshi^{1,3} (¹*Division of Nano Life Science Institute (WPI-NanoLSI) and Nano Life Science Institute, Kanazawa University*, ²*Laboratory for Bio- and Nano-Instrumentation, Swiss Federal Institute of Technology Lausanne (EPFL), Lausanne, Switzerland*, ³*Division of Electrical Engineering and Computer Science, Kanazawa University*)

Nanoendoscopy AFM is a method for investigating the morphology, dynamics, and characteristics of intra-cellular structures. Three-dimensional and two-dimensional mapping inside living cells help compile information about the internal structures' morphology. This investigation was performed by inserting a long, ultrathin nanoprobe fabricated with focused ion beam (FIB) milling, into the cell. However, there is a possibility of internal damage to living cells after penetration, such as changes in their morphology, functionality and viability. The results indicate that cells enter division after 3-D whole-cell nanoprobe endoscopy, which confirmed cell viability. This study suggests great potential for future development of the intra-cellular live-cell measurements.

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- [2-16-1800](#) Fluorometric digital ATPase assay with single-enzyme detection sensitivity

Hiroshi Ueno, Mio Sano, Mayu Hara, Hiroyuki Noji (*Grad. Sch. Eng., Univ. Tokyo*)

Digital enzyme assays using fL reactors are an emerging bioanalytical tool for highly sensitive, quantitative analysis of biomolecules, with single-molecule detection sensitivity. However, current digital enzyme assays require a fluorescent substrate for detection, limiting the applicability of this method. Here, we developed the three enzyme-coupled fluorometric digital enzyme assay system for ATPase that has no fluorogenic substrates. This system achieved the detection of the ATP hydrolysis activity of single F₁-ATPase. Furthermore, we succeeded in distinguishing the single ATPase activity of F₁s with different activities. Since this system detects ADP, it is expected to be applied to the measurement of single molecule activity of various enzymes that produce ADP.

[2-16-1812](#) 補償光学系を用いた 1 分子輝点 3 次元位置精度の改善のシミュレーション研究
A simulation study to evaluate improvement of three-dimensional localization precision of single molecule images using adaptive optics

Xiang Zhou, Yuma Ito, Makio Tokunaga (*Sch. Life Sci. Tech., Tokyo Tech*)

Single-molecule tracing (SPT) allows us to investigate molecular dynamics and interactions in living cells. To overcome the limitation of tracking ability in optical-axis direction, three-dimensional SPT methods are beginning to be developed. However, poor signal-to-noise ratios of out-focus images largely inhibit to improve three-dimensional localization precision. Here, we implement a simulation framework to evaluate a method of point spread function (PSF) engineering with adaptive optics for improving the localization precision. We measured the localization precision of engineered PSFs in three dimensional, especially in the optical-axis direction. It was shown that adaptive-optics-based microscopy is useful for three-dimensional single-molecule tracking.

[2-16-1824](#) Plunus Lanessiana から抽出した色素の pH 依存蛍光特性と水素化アモルファスシリコン上での薄膜
A pH depend fluorescent properties of pigment extracted from Plunus Lanessiana and the thin film on hydrogenated amorphous silicon film

Yutaka Tsujiuchi¹, Koyu Akiyama¹, Mao Izumi¹, Satomi Kimura¹, Kazunori Takada¹, Hiroshi Masumoto² (¹*Grad. Mat. Sci. Univ. Akita*, ²*Fris. Univ. Tohoku*)

Fluorescent property of pigment extracted from Plunus Lanessiana was characterized for investigating a highly ultraviolet absorption and visible light emission molecule. And the thin film contains the pigments on hydrogenated amorphous silicon (a-Si:H) was fabricated and analyzed the fluorescent spectrums depend on electric field for study the interaction of pigment and hydrogen rich subsurface of a-Si:H. The result was that the pigment emits turquoise color in high pH environment and revealed isosbestic points.

[3-01-1330](#) Towards understanding eukaryotic and prokaryotic protein interactions in loop regions

Lin Zhang¹, Hafumi Nishi^{1,2,3} (¹*Graduate School of Information Sciences, Tohoku University*, ²*Faculty of Core Research, Ochanomizu University*, ³*Tohoku Medical Megabank Organization, Tohoku University*)

Loops are much more than mere connection elements between other secondary structural elements. They often play a crucial functional role. Here we investigated loop interactions on a large-scale. In this study, 452,170, 76,190, and 20,753 loops were detected from three protein datasets, which are Entire PDB, human, and *E. coli*. We found that more than 70% of them were identified at least one binding site. Moreover, loops from *E. coli* tend to bind to more partners compare to human proteins. But human and *E. coli* proteins may not show significant bias on amino acid usage in binding to other molecules. Additionally, we found that binding site residues prefer arginine and tyrosine, whereas non-binding site residues prefer glycine.

[3-01-1342](#) 超音波照射を利用した夾雑物存在下における $\beta 2$ ミクログロブリンのアミロイド線維形成反応の研究
Study on amyloid fibril formation of $\beta 2$ -microglobulin in presence of concomitants by ultrasonication assay

Kichitaro Nakajima¹, Keichi Yamaguchi¹, Suguru Yamamoto², Hirotsugu Ogi³, Yuji Goto³ (¹*Global Center for Med. Eng. Info., Osaka Univ.*, ²*Med. Sch., Niigata Univ.*, ³*Grad. Sch. Eng., Osaka Univ.*)

$\beta 2$ -microglobulin ($\beta 2m$) forms amyloid fibrils in the body of long-term dialysis patients, causing dialysis-related amyloidosis that is a serious complication of dialysis treatment. Although the fibril formation of $\beta 2m$ has been widely investigated using pure $\beta 2m$ solutions, the effects of the concomitants on the $\beta 2m$ fibril formation are not fully understood. In this study, we investigated the fibril formation of $\beta 2m$ in the presence of concomitants, such as serum albumin, using an originally developed ultrasonication instrument. The concomitants showed an inhibition effect on the fibril-formation reaction. Furthermore, the experimental result using the human serum revealed that the extent of the inhibition effect depended on the status of blood donors.

[3-01-1354](#) CRAF は 14-3-3 結合サイトへの変異で N-/C-端ドメインを含む分子内複合体の状態が変わる
Mutations in 14-3-3 binding sites affect the intramolecular complex formation of CRAF involving its N- and C-terminus domains

Kenji Okamoto, Yasushi Sako (*CPR, RIKEN*)

The activity of CRAF, a kinase protein in the RAS-MAPK pathway, is thought to be regulated by the interactions of its three domains (RBD, CRD, and kinase) connected with linkers. But, details of CRAF conformation in live cells are not clearly understood. We have developed an ALEX system for single-molecule FRET measurement of diffusing proteins in the cytosol of live cells and successfully measured the conformation distribution of wt-CRAF. Here, we newly measured CRAF molecules with mutations at the 14-3-3 binding motifs or in the CRD domain and suggest structural models of the intramolecular complex including N-/C-terminus domains based on a 14-3-3 dimer as a scaffold. Two types of closed autoinhibitory conformation may be differently responsive to cell stimulation.

[3-01-1406](#) Dynamic Residue Interaction Network Analysis of Primary Mutations in Protease that Confer Drug Resistance in HIV-1

Ryoga Miyawaki, Mohini Yadav, Norihumi Yamamoto (*Chiba Tech*)

The human immunodeficiency virus (HIV) is the pathogen of the Acquired Immune Deficiency Syndrome (AIDS). AIDS has become a disease that can be controlled in the long term by anti-HIV drugs. However, due to prolonged treatment, 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 protease are known to directly and substantially reduce drug efficacy against anti-HIV drugs. These mutations are referred to as "primary mutations". In this study, we investigated the dynamic correlation between the drug binding site and its primary mutation site in HIV-1 protease using dynamic residue interaction network (dRIN) analysis based on molecular dynamics simulations.

[3-01-1418](#) β シート内における隣接ストランド間の $C\alpha$ 間距離の解析
Analysis of $C\alpha$ distances between adjacent strands in β -sheets

Hiromi Suzuki (*Sch. Agri., Meiji Univ.*)

We selected 21,312 protein chains from PDB and analyzed $C\alpha$ distances located on the adjacent strands in β -sheets. Average $C\alpha$ distances of anti-parallel strands were 5.25Å and 4.50Å for hydrogen bond (HB) and non-hydrogen bond (nHB) pairs, respectively, and 4.82Å for parallel strands. Among nHB pairs, Gly-pairs and Leu-pairs showed the shortest and longest $C\alpha$ distances, respectively, while Leu-pairs showed the shortest $C\alpha$ distances among HB pairs. The standard deviation (SD) values of Gly-pairs among HB pairs were explicitly larger than any other pairs, while among nHB pairs, values of Gly-pairs were slightly larger than those of Cys- and Asp-pairs. For parallel pairs, Gly-pairs showed the largest SD values, but there was not precise tendency for $C\alpha$ distances.

[3-01-1430](#) 生物分子モーターベースの群れは、貨物をロード・デリバリー・アンロードする分子トランスポーターとしての役割を果たす
Construction of biomolecular motor-based swarm as a molecular transporter to load-deliver-unload cargo

Mousumi Akter¹, Jakia Jannat Keya¹, Arif Md. Rashedul Kabir¹, Daisuke Inoue², Henry Hess³, Kazuki Sada¹, Akinori Kuzuya⁴, Hiroyuki Asanuma⁵ (¹*Fac. Sci., Univ. Hokkaido*, ²*Fac. Des., Univ. Kyushu*, ³*Dep. Biomed. Eng., Univ. Columbia*, ⁴*Grad. Sch. Chem. Mat. Eng., Univ. Kansai*, ⁵*Grad. Sch. Eng., Univ. Nagoya*)

Living beings often adopt swarming as a strategy to accomplish cooperative tasks i.e., load-deliver-unload cargoes. Swarms of animals not only ensure delivery of cargoes to a destination but also facilitate transportation of large-sized or number of cargoes. Transportation of cargoes by swarms has been implemented in artificial systems using mechanical robots which emerges as a new discipline, swarm robotics. Implementation of such swarm-based cargo transportation in the microscopic world has not been reported yet. Here we demonstrate cooperative cargo transportation by the swarms of the self-propelled cytoskeletal filament microtubules, driven by kinesins. This work shows the advantages of the swarm system in molecular transportation over single transporters.

[3-01-1442](#) Relationship between the acceptor specificity and the loop structure of catalytic domain in bacterial glucansucrases

Takafumi Inoue, Ko-hei Yano, Hideyuki Komatsu (*Dept. of Bioscience and Bioinformatics, Kyushu Inst.Tech.*)

Leuconostoc or *Lactobacillus* glucansucrase catalyzes glucose-transfer from sucrose to not only physiological substrate glucan but also a wide range of artificial acceptors. Here, we have compared the acceptor-specificities between *Lactobacillus* glucansucrase (GTFA) and other type of *Streptococcus* glucansucrase (GTFI). GTFA exhibited the broad specificity, but GTFI transferred glucose to fewer acceptors than GTFA. Comparing between GTFA structure and GTFI homology model, a loop structure was found near the sucrose-binding site in only GTFI but not GTFA catalytic domain. Phylogenetic analysis also shows that this loop region is specific for *Streptococcus*. Therefore, the acceptor specificity is probably due to the loop structure.

[3-01-1454](#) ヒト S100A3 の変異体を用いた四量体構造解析に向けた研究
Research for tetramer structure analysis using mutants of human S100A3

Hiroyuki Iida¹, Kenzi Ite^{1,2}, Masaki Unno^{1,2} (¹*Grad. Sci. Eng., Ibaraki Univ.*, ²*iFRC, Ibaraki Univ.*)

S100A3 protein (S100A3) is a calcium-binding protein that is abundantly expressed in hair cuticular cells. If its arginine residues are converted to citrulline by peptidylarginine deiminase, a Ca²⁺-dependent enzyme, S100A3 increases affinity for calcium and zinc ions, and assembles to tetramers from dimers depending on these metal ions. To date, the R51Q mutant has been used as a model for the citrullinated S100A3, but the structure of this tetramer has not been characterized in detail. In this study, we used R51Q+R77Q mutant and compared its oligomerization states with R51Q mutants, and confirmed that R51Q+R77Q mutant has a higher tetramer existence ratio. The results obtained here will be useful for the tetramer structure analysis of Ca²⁺/Zn²⁺-bound S100A3.

[3-01-1506](#) アミロイド β(16-22)ペプチドのアミロイド線維形成メカニズムの解明
Elucidation of the mechanism of amyloid fibril formation of amyloid-β(16-22) peptide

Moe Yamazaki (*Faculty of Pharmaceutical Sciences, University of Toyama*)

Identifying factors that influence the formation of neurotoxic amyloid fibrils can provide insights into the treatment of neurological diseases. Here, we investigated aggregation kinetics of amyloid-β fragment peptide, Aβ₁₆₋₂₂ (KLVFFAE), which plays an important role in amyloid fibril formation. Transmission electron microscopy revealed that Aβ₁₆₋₂₂ formed short, thin fibrils in a few seconds at neutral pH and 25°C, and that longer, thicker fibrils were formed over several minutes, through elongation and lateral association of the thin fibrils. The results with addition of salts or alcohols to the peptides suggested that electrostatic interactions inhibited the fibril elongation and hydrophobic interactions inhibited the lateral association of the fibrils.

[3-01-1518](#) 抗体製剤の凝集体形成に及ぼす物理化学的製剤特性の影響
Effect of Physicochemical Formulation Properties on the Formation of aggregate in Antibody Preparations

Maki Mitani, Hiroyuki Suetomo, Chihiro Wayu, Toshihito Hosokawa (*Bio Process Research and Development Laboratories, Kyowa Kirin Co., Ltd.*)

Due to the nature of proteins, biopharmaceutical products have a risk of aggregates formation under a variety of stresses. A lot of time and the amount of active ingredient are required to establish an optimal formulation. However, they are limited especially at early stage of pharmaceutical development. In order to overcome those limitations, high throughput screening system which can evaluate the lots of kind of formulations at small amount of active ingredient has developed and applied to formulation development for a monoclonal antibody formulation study. In future, we plan to optimize a formulation for each protein by not only physicochemical data, but also in silico approaches such as a predicted 3D structure modeling.

3-02-1330 Structural intermediates in rotary V/A-ATPase from initial to steady state visualized by time-resolved cryo-electron microscopy

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Rotary ATPases catalyze the interconversion process between ATP and ADP-phosphate through a rotary mechanism that is coupled to ion flow across the membrane. It is believed that ATP binding triggers the sequential structural change, but how rotary ATPases initiate the sequential process has not been investigated. Here we use time-resolved cryo-electron microscopy (cryo-EM) to capture short-lived states of *Thermus thermophilus* V/A-ATPase (*Tth* V/A-ATPase) from initial ATP binding to steady state. We found that sulphate delayed initial ATP binding to *Tth* V/A-ATPase, resulting in snapshots of *Tth* V/A-ATPase just after initial ATP binding, that unveil structures from initial to steady state through sequential ATP binding to its three catalytic sites.

3-02-1342 ポンプ型チャネルロドプシン ChRmine のイオン透過機構の構造基盤
Structural basis for channel conduction in the pump-like channelrhodopsin ChRmine

Keiichiro Kishi¹, Yoon Kim², Masahiro Fukuda¹, Tsukasa Kusakizako³, Elina Thadhan^{2,4}, Eamon Byrne², Joseph Paggi⁴, Charu Ramakrishnan⁵, Toshiki Matsui¹, Keitaro Yamashita⁶, Takashi Nagata^{7,8}, Masae Konno^{7,8}, Peter Wang², Masatoshi Inoue², Tyler Benster², Tomoko Uemura⁹, Kehong Liu⁹, Mikihiko Shibata¹⁰, Norimichi Nomura⁹, So Iwata^{9,11}, Osamu Nureki³, Ron Dror^{4,12}, Keiichi Inoue⁷, Karl Deisseroth^{2,5,13,14}, Hideaki Kato^{1,3,15} (¹*Komaba Institute for Science, The University of Tokyo*, ²*Department of Bioengineering, Stanford University*, ³*Department of Biological Sciences, Graduate School of Science, The University of Tokyo*, ⁴*Department of Computer Science, Stanford University*, ⁵*CNC Program, Stanford University*, ⁶*MRC Laboratory of Molecular Biology, Cambridge Biomedical Campus*, ⁷*The Institute for Solid State Physics, The University of Tokyo*, ⁸*PRESTO, Japan Science and Technology Agency*, ⁹*Department of Cell Biology, Graduate School of Medicine, Kyoto University*, ¹⁰*High-speed AFM for Biological Application Unit, Institute for Frontier Science Initiative, Kanazawa University*, ¹¹*RIKEN Spring-8 Center*, ¹²*Institute for Computational and Mathematical Engineering, Stanford University*, ¹³*Howard Hughes Medical Institute, Stanford University*, ¹⁴*Department of Psychiatry and Behavioral Sciences, Stanford University*, ¹⁵*FOREST, Japan Science and Technology Agency*)

ChRmine, a recently discovered bacteriorhodopsin-like cation channelrhodopsin exhibits puzzling properties (large photocurrents, red-shifted spectrum, and high light-sensitivity) that have opened up new opportunities in optogenetics. Here we present the cryo-electron microscopy structure of ChRmine at 2.0 Å resolution. The structure reveals unusual architectural features including the trimeric assembly, short transmembrane helix 3 unwound in the membrane, twisting extracellular loop 1, the large intra- and extracellular cavities, and a hydrophilic pore through the center of the trimer. Together with the electrophysiological, spectroscopic, and computational analyses, our findings provide insight into the channel gating and passive ion conduction of ChRmine.

3-02-1354 Structural analysis of amyloid disaggregation reaction by the novel FT-IR technique

Takashi Nomura¹, Yoshiko Nakagawa^{1,2}, Yusuke Komi¹, Shingo Tamai^{1,3}, Motomasa Tanaka¹ (¹*CBS, Riken*, ²*Dept. of Life Sci. & Tech., Tokyo Tech.*, ³*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 disaggregated are poorly understood. Here we developed a novel FT-IR spectrophotometer coupled with a microfluidic device to observe the disaggregation reaction under the physiological conditions. We investigated possible structural changes of Sup35 Sc4 amyloid induced by Ssa1/Sis1 binding (the first step of the disaggregation reaction in yeast cells) and found that the amide I signal derived from β -sheet of Sc4 amyloid showed an upshift upon Ssa1/Sis1 binding. This result will provide insights into how amyloid fibrils elicit neurodegenerative disorders by cell-to-cell propagation.

3-02-1406 X線結晶構造解析による2機能的ミモシン合成酵素の反応機構解明に向けて
Structural Insights into Catalytic Reaction Mechanism for bifunctional enzyme, Mimosine Synthase, from *Leucaena leucocephala*

Masaki Horitani^{1,2}, Risa Maeda¹, Shigeki Oogai², Masakazu Fukuta^{2,3}, Hirosuke Oku^{2,4}, Hiroshi Sugimoto⁵ (¹*Fac. of Agri., Saga Univ.*, ²*United Grad. Agri. Sci., Kagoshima Univ.*, ³*Grad. Sch. Agri., Univ. Ryukyuu*, ⁴*Trop. Bios. Res. Cent., Univ. Ryukyuu*, ⁵*Harima Inst., Riken*)

Mimosine is a toxic non-protein amino acid and is found in the legumes, *Leucaena leucocephala* and *Mimosa pudica*. Recently, cloning and expression of mimosine synthase from *Leucaena leucocephala* have been reported and the homology analysis revealed that mimosine synthase has 73 % similarity with plant cysteine synthase. Interestingly, mimosine synthase can catalyze both reactions of mimosine and cysteine biosynthesis. To elucidate how mimosine synthase can catalyze dual reaction, we have performed X-ray crystallographic studies for wild-type and mutant mimosine synthase in the presence and absence of substrates. Our results showed only one mutation in the active site resulted in the ability to produce the mimosine with no loss of production ability for cysteine.

[3-02-1418](#) 酸化型及び還元型の cryptdin 4 の抗菌活性発現に関与する構造の解析
Structural analysis to clarify antimicrobial mechanisms of oxidized and reduced cryptdin-4

Weiming Geng, Yi Wang, Yuchi Song, Shaonan Yan, Wendian Yang, Tomoyasu Aizawa (*Grad. Sch. of Life Sci, Hokkaido Univ*)

Cryptdin-4 (Crp4) is a mouse Paneth cell α -defensin which has the most potent bactericidal activity *in vitro* among its isoforms (Crp1 – Crp6). There are two types of structures *in vivo*, oxidized Crp4 (Crp4_{Oxi}) with β -sheet structure maintained by three disulfide bonds and reduced Crp4 (Crp4_{Red}) with linear structure without disulfide bonds. Previous research indicated Crp4_{Oxi} and Crp4_{Red} have selective antibacterial activity against commensal bacteria depending on its disulfide bonds. Thus, the secondary structures of Crp4_{Oxi} and Crp4_{Red} were investigated in membrane mimetic conditions using Circular Dichroism (CD), showing that Crp4_{Oxi} maintained stable β -sheet structure, whereas flexible Crp4_{Red} transformed to an α -helical structure in high TFE concentration.

[3-02-1430](#) Crystal Structure of Soluble Family II Inorganic Pyrophosphatase Revealed the Mechanism of Catalysis and Structure Dynamics

Kantaro Sakamoto¹, Hiroshi Sugimoto², Masaki Horitsni¹ (¹*Grad. Sch. Agric., Univ. Saga*, ²*Harima Inst., Riken*)

Inorganic pyrophosphatase from *Shewanella* sp. AS-11 (Sh-PPase) catalyzes hydrolysis reaction of inorganic pyrophosphate to phosphate (Pi). Previously we have reported that Sh-PPase has two transition metal ions in active site, the optimized temperature of enzyme activity showed characteristic metal ion dependencies and overall structure was changed from open to close conformation by bound of substrate. The mechanism of catalysis and dynamics is, however, unclear. Therefore, in this study, we have performed X-ray crystallographic studies. The intermediate structures of Co activated Sh-PPase complexed with 2Pi were successfully determined, and results revealed the mechanism for the catalysis and structure dynamics of Sh-PPase.

[3-02-1442](#) 単粒子解析における投影パラメータ分布推定と初期モデル生成
Estimation of projection parameter distribution and initial model generation in single particle analysis

Nobuya Mamizu^{1,2}, Takuo Yasunaga¹ (¹*Grad. Sch. Comp. Sci., Kyushu Inst. Tech.*, ²*System in frontier Inc.*)

In this study, we propose the projection parameter estimation and initial model generation method in single particle analysis. The model formula for 3D reconstruction follows RELION [1], and for the prior distribution probability calculation for parameter search, the next probability model is generated from the multiplication of the elements extracted from the distribution in the previous step. This algorithm can be used in the initial model generation as well. We evaluate this method using simulation projection data generated from PDB and experimental images, in the restoration of 3D structure, the possibility of initial model generation, and the calculation time. [1] Sjors H.W. Scheres, JSB Vol. 180, Issue 3, page 519-530. (2012).

[3-02-1454](#) クモ糸フィブロインからなるナノファイバー構造の解明
Nanofiber Structure Composed of Spider Silk Fibroin

Haruya Kajimoto¹, Yusuke Okamoto¹, Kento Yonezawa², Takehiro Sato³, Yoichi Yamazaki¹, Sachiko Toma¹, Hironari Kamikubo^{1,2,4} (¹*NAIST, MS*, ²*NAIST, CDG*, ³*Spiber Inc.*, ⁴*KEK, IMSS*)

Fibroin is a protein that forms the hierarchical structure of spider silk. We have revealed a precursor composed of fibroin molecules responsible for nanofibers (NFs) formation. Based on the reaction kinetics of the NF formation, we assumed that the precursor is a kind of building block of the NFs. However, it is still unclear how the precursors are aligned in the NFs. In this study, to clarify the alignment of the precursor in NFs, gold nanoparticles (AuNPs) were adsorbed onto NFs prepared from N-terminally His-tagged fibroins and observed by AFM. When AuNPs were added to NFs, AuNPs were observed to bind to the NFs highly organized. The present study suggests that the precursor has a repeating structure.

[3-03-1330](#) The conformational stability analysis of dengue virus envelope domain III(ED3) wild type and its mutants by molecular dynamics simulation

Jingwen Xian¹, Hiromichi Tsurui², Atsushi Kurotani³, Yutaka Kuroda¹ (¹*Tokyo University of Agriculture and Technology*, ²*Department of Immunological Diagnosis, Juntendo University School of Medicine*, ³*Center for Sustainable Resource Science, RIKEN Institute*)

Dengue fever is major disease in tropical and subtropical area. ED3 of dengue virus is a 103 residues domain that can fold independently and contains both the epitope regions and the receptor binding regions, and it contains a large number of mutations throughout the four serotypes. In this work, we used molecular dynamics simulations to assess the stability of ED3 wild type (3VTT) and its two mutants (3VTT_V310M, 3VTT_V310M_I318T), by calculating the root mean square deviation and the root mean square fluctuation, pairwise the root mean square deviation and Principal Component Analysis. We compared the results of the molecular dynamics simulation to experimental data to determine how well the conformational stability of ED3 can be assessed using these parameters.

[3-03-1342](#) Analysis of amino acid sequence variation in the RBD of SARS-CoV-2

Cheng ZhiRui¹, Yutaka Kuroda¹, Atsushi Kurotani² (¹*Tokyo University of Agriculture and Technology*, ²*Center for Sustainable Resource Science, RIKEN Institute*)

Since the outbreak of the novel coronavirus in Wuhan, China, in late 2019 causing a worldwide pandemic. The cause of lasting pandemic is the massive mutations resulting in high transmission variants. In preparation for our study, we retrieved the RBD (Receptor Binding Domain) of the spike protein of SARS-COV2 variant sequences from the GISAID database. Our research objectives are to determine hotspot sites (high mutation residues) and to analyze: (1) the structural characteristics of hotspot sites, (2) the correlation between hotspot variant appearance and regional and time series, and (3) the codon usages in hotspot variant. In addition, we plan to use these information to predict novel hotspot variants.

[3-03-1354](#) SEC-SAXS/紫外可視分光で測定した行列データの自動解析ソフトウェア開発
Development of software for automatic processing of matrix data measured with SEC-SAXS/UV-Vis. spectroscopy

Kento Yonezawa^{1,2}, Masatsuyo Takahashi¹, Keishi Oyama¹, Keiko Yatabe¹, Yasuko Nagatani¹, **Nobutaka Shimizu**¹ (¹*PF, IMSS, KEK*, ²*CDG, NAIST*)

SEC-SAXS, small-angle X-ray scattering combined with size-exclusion chromatography, is a recent standard method in SAXS for solution samples of biological macromolecules (BioSAXS). In SEC-SAXS, hundreds to thousands of scattering curves are continuously collected while the solution is eluted from the gel filtration column. In order to acquire the scattering curve of target molecule from such a large amount of data, we have developed the automatic processing software, MOLASS, which considers this data as matrix and uses matrix optimization techniques. MOLASS can lead to more accurate results by combining SAXS with UV-Vis. spectroscopy. In this presentation, we will introduce the analytical problems of SEC-SAXS and the detailed specifications of MOLASS to solve them.

[3-03-1406](#) 質問学習を活用した HLA class II 結合性ペプチドの予測
Prediction of HLA class II-binding peptides by training with query learning

Keiko Udaka¹, Morito Chabata¹, Kousuke Onoue², Yoshiko Yamashita², Yuki Tanaka² (¹*Department of Immunology, School of Medicine, Kochi University*, ²*AI Drug Development Division, NEC*)

The prediction of MHC class II-binding peptides remains as a technical hurdle to develop peptide vaccines for tumors and infectious agents where T-cell recruitment is crucial. Unlike MHC class I molecules MHC class II molecules are open-ended and longer peptides can bind. Thus, the core peptides which have direct contact with MHC class II molecules need to be identified within the sequences deposited in the databases. We developed a flow cytometry-based peptide binding assay using end-protected random 11-mer peptides bearing peptidase resistant amino acids. We then developed a SK-SVM-based platform to predict HLA-DRB1*04:05 and DRB1*08:03-binding peptides. The performance of the platform was evaluated in comparison with the leading *in silico* platforms.

3-03-1418 抗原-抗体界面の塩橋の安定性とその役割に関する理論的研究

A theoretical study on the salt bridge stability in the antigen-antibody interface and its effect

Takefumi Yamashita (*RCAST, Univ. Tokyo*)

Since antibodies recognize their antigens specifically, they are widely used as drugs. To develop a high-affinity antibody, it is important to understand how the antigen-antibody interaction is strengthened. In this study, we study the antigen-antibody interface by using MD simulations. In the case of an anti-ROBO1 antibody (B5209B), we found that the salt bridge played important role to control the binding enthalpy. To understand the origin of salt bridges in the antigen-antibody interface, we followed the constructivist approach and developed a series of reduced salt bridge models. The analysis showed the importance of environment. Even the hydrophobic residues significantly affect the salt bridge stability.

3-03-1430 シアニデオシゾン由来 Branching Enzyme の MD シミュレーションによる構造解析
Molecular Dynamics Simulation of Starch Branching Enzyme Derived from *Cyanidioschyzon merolae***Kosuke Nariyama**¹, Yoh Noguchi^{1,3}, Motokuni Nakajima¹, Hironao Yamada^{2,3}, Ryota Morikawa¹, Masako Takasu¹, Shoko Fujiwara¹ (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*)

Branching enzymes (BE) are enzymes that catalyze the formation of starch branching structures. The optimal temperature for BE is lower than the temperature at which starch shows high reactivity, and improvements in the heat resistance of BE are being considered. Based on the report that the heat resistance of BE derived from *Cyanidioschyzon merolae* (CmeBE) was improved by introducing an ancestral sequence, we analyzed the structure of wild-type (WT) and ancestral-sequenced mutant (MT) of CmeBE using MD simulations. We analyzed the distances between the ancestral sequences and the C- and N-terminal residues forming the random coil, and found differences between WT and MT.

3-03-1442 サポニン B と脂質分子の分子動力学シミュレーション
Molecular dynamics simulations of Saposin B with a bound lipid**Matsuyuki Shirota** (*Grad. Sch. Med., Tohoku Univ.*)

Saposin B is a lysosomal protein that activates the metabolism of lipid molecules by solubilizing them out of lipid bilayer. To study the molecular mechanism of its interaction with lipid molecules, we analyzed the dynamics of a Saposin B homo-dimer bound to a distearoyl- β -phosphoethanolamine (DSPE) in lysosomal condition by using molecular dynamics simulations. Compared to the starting X-ray structure of the complex of Saposin B and DSPE, two carbohydrate tails of DSPE get more deeply buried in the hydrophobic cavity of Saposin B dimer. Polar atoms in glycerol and phosphoethanolamine groups were hydrogen-bonded by arginine and tyrosin side chains of Saposin B. These results suggest the binding mode of Saposin B and lipid in physiological conditions.

3-03-1454 Capturing drastic state transitions of biological macromolecules by molecular dynamics simulation and nonlinear dimensionality reduction**Mao Oide**¹, Yuji Sugita^{1,2,3} (¹*CPR, RIKEN*, ²*BDR, RIKEN*, ³*R-CCS, RIKEN*)

Molecular dynamics (MD) simulation is a great help for us to understand structural mechanisms behind functionality process of biological macromolecules, and dimensionality reduction for conformational distribution of the target molecule is crucial in order to understand the dynamics intuitively. The most common dimensionality reduction methods are linear mode decomposition methods e.g., principal component analysis. However, complicated dynamics involving drastic state transitions is generally difficult to capture with linear methods and should be analyzed by nonlinear methods instead. Here, we will report investigation results of an applicability of UMAP, a novel nonlinear method developed in 2018, to analyses of MD simulation data with drastic state transitions.

3-03-1506 分子動力学シミュレーションによって明らかになった SLC26A9 塩化物イオントランスポーターのゲート運動機構
Mechanism of the gating motion of SLC26A9 chloride ion transporter revealed by the molecular dynamics simulations

Satoshi Omori¹, Yuya Hanazono², Hafumi Nishi^{1,3}, Kengo Kinoshita^{1,4,5} (¹*GSIS, Tohoku Univ.*, ²*Med. Res. Inst., Tokyo Medical and Dental Univ.*, ³*Faculty of Core Res., Ochanomizu Univ.*, ⁴*ToMMo, Tohoku Univ.*, ⁵*Inst. of Dev. Aging and Cancer, Tohoku Univ.*)

Solute Carrier family 26 member A9 (SLC26A9) is a membrane-transport protein that exhibits chloride transporter activity and plays essential roles in physiological processes. The cryo-EM structures of homo-dimeric SLC26A9 suggest that the cytoplasmic (STAS) domain mediates the interactions between the subunits. However, the detailed mechanism is still unknown. In this study, we performed the MD simulations of SLC26A9 with the full-length, the C-terminus removal (ΔC), and the STAS removal models. The gating motions and the stable bindings of the chloride ions were observed only in ΔC model. These results suggest that the removal of the C-terminus triggers the gating motion and the motion of the STAS domain promotes the formation of the stable ion binding mode.

3-03-1518 微小管つぎ目領域におけるチューブリン構造集団の全原子分子動力学シミュレーションによる解析
Tubulin conformational ensemble in seam region of microtubule investigated by all-atom molecular dynamics simulation

Koji Umezawa^{1,2}, Naoyuki Furuta¹, Takuma Todoroki¹ (¹*Grad. Sch. of Sci. & Tech., Shinshu Univ.*, ²*IBS, Shinshu Univ.*)

Microtubules (MTs) play an essential role as a cellular component, which is related to their structural stability. The structure of MT is built by assembling $\alpha\beta$ -tubulin heterodimers (TUBs) like a hollow cylindrical tube. There is a seam region in the MT structure, where interaction between the neighboring TUBs is different from the other region. It is a key factor for the whole stability of MT. Then, we investigated the details by conformational ensembles of the seam region. We prepared 9 TUBs including tubulin C-terminal tails (CTTs) as MT-seam model. All-atom molecular dynamics simulations were performed for the MT-seam models binding GTP or GDP. The results show that the bending patterns are different. Nucleotide dependency and CTT distribution will be discussed.

3-04-1330 Recombinant production and antibacterial activity assay of reduced and oxidized cryptdin-6

Shaonan Yan, Yuchi Song, Yi Wang, Weiming Geng, Wendian Yang, Tomoyasu Aizawa (*Graduate School of Life Sciences, Hokkaido University*)

Cryptdin (Crps) is an α -defensin family from mouse containing Crp1-6 which has strong antimicrobial activity. Now, there are few published studies about other isoforms except Crp4 and the efficient system of recombinant production is unclear. In this study, by recombinant expression using co-expression system in *E. coli* Origami2 strain, the expression level of Crp6 as inclusion body form had the strongest improvement among Crp family. After large scale expression, purification and refolding, both recombinant Crp6red and Crp6oxi were successfully obtained and the system of peptide production was established. From bactericidal activity assay, both Crp6red and Crp6oxi were effective in killing *E. coli*, and the bactericidal activity of Crp6red was stronger than Crp6oxi.

3-04-1342 gREST 法による Nanobody CDR H3 ループ構造のサンプリング
Enhanced Conformational Sampling of Nanobody CDR H3 Loops by Generalized Replica-Exchange with Solute Tempering

Ren Higashida, Yasuhiro Matsunaga (*Grad. Sch. Sci. Eng., Saitama Univ.*)

Single domain antibodies, known as nanobodies, are potential substitutes for conventional antibodies. Here, we apply an enhanced sampling method, generalized replica-exchange with solute tempering (gREST) developed by Kamiya and Sugita (*JCP*, 2018), to sample nanobody CDR H3 loop structures. In the conventional replica-exchange methods, temperatures of only a whole system are exchanged to boost sampling. In gREST, we define the CDR H3 loop as a temperature-exchange region and investigate which potential energy term should be scaled for efficient sampling of the loop structures. The results of several nanobody simulations suggest that scaling the dihedral-angle terms is the best for efficient sampling although there are exceptions depending on nanobody structures.

[3-04-1354](#) 一分子蛍光法による RNA 結合と液滴形成に伴う LAF-1 RGG 構造変化の解明
Single molecule fluorescence investigations on the structure transitions of LAF-1 RGG upon the RNA binding and the droplet formation

Kanna Fujita^{1,2}, Michiko Kimura^{1,2}, Hiroto Takahashi^{1,2}, Satoshi Takahashi^{1,2}, Hiroyuki Oikawa^{1,2} (¹*IMRAM, Tohoku Univ.*, ²*Grand. Sch. Life Sci., Tohoku Univ.*)

Despite the considerable attention on liquid-liquid phase separation (LLPS), the structural properties of disordered proteins inside and outside of assembled droplets are largely unknown. We explored the structures of the RGG domain of LAF-1 (LAF-1 RGG), essential for LLPS, which is RNA helicase causing the assembly of P-granules in *C. elegans*. For the Fluorescence Resonance Energy Transfer (FRET) measurements of LAF1 RGG, we labeled it with Alexa488 at the N-terminus and Alexa647 at the C-terminus. Using home-made confocal laser scanning microscopy, we discovered that the FRET efficiency inside the droplets formed upon the mixing of the sample with poly-rA is higher than that in the solvent, demonstrating significant structural change upon the droplet formation.

[3-04-1406](#) 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 mechanisms of cold-adapted glucokinase

Akane Yato¹, Rio Asaka², Hiroshi Sugimoto³, Keiichi Watanabe², Masaki Horitani² (¹*Grad. Sch. Adv. Hea. Sci., Saga Univ.*, ²*Agr., Saga Univ.*, ³*RIKEN, SPring-8 center*)

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.

[3-04-1418](#) Studies on Cry j 7, a Novel Allergen from Japanese cedar

Jignkang Zheng, Tomona Iizuka, 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 (*Cryptomeria japonica*) as the pollen allergen to make cross-reactivity with food allergens cause pollen-food allergy syndrome (PFAS). In our study, the amino acid sequence of Cry j 7 was searched in FroestGen database and the N-terminal was predicted by homologs alignment from Cup s 7 (European cypress). After the recombinant Cry j 7 was successfully overexpressed by *Pichia pastoris*, stable proteins were produced for characterization analysis. The results clearly indicated that recombinant Cry j 7 formed a correct folding structure and exhibited a strong antigenicity cross-related with fruit GRP allergens.

[3-04-1430](#) Amyloid accumulation dynamics in physiological condition

Masahiro Kuragano, Shinya Yamanaka, Kiyotaka Tokuraku (*Grad. Sch. Eng., Muroran Inst. of Tech.*)

Abnormal aggregation and accumulation of misfolded proteins are involved in the development of various amyloidosis. Here, we analyzed the process of aggregation and accumulation of amyloid β ($A\beta$), which causes the development of Alzheimer's disease (AD), by real-time 3D imaging under physiological conditions using the quantum-dot nanoprobe. We found that the amount and size of aggregates were dramatically decreased in 40% glycerol solution mimicking the human blood viscosity. Furthermore, the numerical calculation reveals that several decades are required to fully develop the settling velocity and diameter of $A\beta$ aggregates in physiological conditions. This time span is consistent with the actual syptom progression of AD.

[3-04-1442](#) ラッサウィルスの表面タンパク質を覆う糖鎖の構造ダイナミクス
Structure and dynamics of glycans on Lassa virus envelop protein

Suyong Re¹, Kenji Mizuguchi^{1,2} (¹ArCHER, NIBIOHN, ²IPR, Osaka Univ.)

The protein glycosylation affects a protein-antibody interaction, but a little is known about the effect because of the diverse structures and interactions of glycans. Here, we built an atomistic model of a fully glycosylated envelope protein complex of the Lassa virus. Using molecular dynamics simulations, we show that the glycosylation non-uniformly shields the protein surface to give rise to the formation of distinct clusters. We integrated the simulation results with existing sequence- and structure-based epitope prediction methods and successfully recovered known protein epitopes. This work provides a molecular basis for integrating otherwise elusive structural properties of glycans into vaccine and neutralizing antibody developments.

[3-04-1454](#) PSD95-PDZ3 の一残基置換による高温での可逆的なオリゴマー (RO) 形成の阻害およびアミロイド線維の抑制
Blocking PSD95-PDZ3's amyloidogenesis through point mutations that inhibit high-temperature reversible oligomerization (RO)

Tomonori Saotome^{1,2,3}, Sawaros Onchaiya¹, Taichi Mezaki³, Jose Martinez⁴, Shun-ichi Kidokoro³, Yutaka Kuroda^{1,2} (¹Dept. of Biotech. and Life Sci., Tokyo Univ. of Agric. and Tech., ²Insti. of Glob. Innov. Res., Tokyo Univ. of Agric. and Tech., ³Dept. of Bio., Nagaoka Univ. of Tech., ⁴Dept. of Phys. Chem. and Insti. of Biotech., Univ. of Granada.)

The wild type third PDZ domain of postsynaptic density protein 95 (PSD95-PDZ3) is a natively folded small globular protein, but it exhibits a peculiar three-state thermal denaturation by forming a reversible oligomerization (RO) at high temperatures. In addition, PSD95-PDZ3 has a propensity to form amyloid fibrils at high temperatures. Here, we examined RO's role in PDZ3's amyloidogenesis at high temperature by performing an alanine scanning experiment by individually replacing seven surface-exposed hydrophobic residues to alanine. As a result, two single mutations (F340A and L342A) that inhibited the high-temperature-RO and yielded variants that denatured according to a two-state model completely suppressed amyloidogenesis as assessed by Thioflavin T fluorescence.

[3-05-1330](#) Free Energy Landscape of RNA Binding Dynamics in Start Codon Recognition by Eukaryotic Ribosomal Pre-Initiation Complex

Takeru Kameda¹, Katsura Asano^{2,3,4}, Yuichi Togashi^{1,5} (¹College of Life Sciences, Ritsumeikan University, ²Molecular Cellular and Developmental Biology Program, Division of Biology, Kansas State University, ³Hiroshima Research Center for Healthy Aging (HiHA), ⁴Graduate School of Integrated Sciences for Life, Hiroshima University, ⁵RIKEN Center for Biosystems Dynamics Research (BDR).)

Specific interaction between the start codon and the anticodon ensures accurate initiation of translation. Recent studies show that several near-cognate start codons (e.g. GUG) can play a role in initiating translation in eukaryotes. However, the mechanism allowing initiation through mismatched base-pairs at the ribosomal decoding site is still unclear at an atomic level. In this work, we propose an extended simulation-based method to evaluate free energy profiles. Our method provides not only the free energy penalty for mismatched start codons relative to the AUG start codon, but also the preferred pathways of transitions between bound and unbound states, which has not been described by previous studies.

[3-05-1342](#) 構造レベルでの RRF と tRNA によるリボソームリサイクリングの解明
Structural basis for ribosome recycling by RRF and tRNA

Takehito Tanzawa^{1,2}, Dejian Zhou³, Jinzhong Lin³, Gagnon Matthieu G.^{2,4} (¹Inst., for Protein Res., Osaka Univ., ²Dept. of Microbiol. & Immunol., Univ. of Texas Med. Branch, ³Schl. of Life Sci., Zhongshan Hospital, Fudan Univ., ⁴Sealy Center for Struct. & Biophys., Univ. of Texas Med. Branch)

The bacterial ribosome is recycled into subunits by two conserved proteins, elongation factor G (EF-G) and the ribosome recycling factor (RRF). The molecular basis for ribosome recycling by RRF and EF-G remains unclear. Here, we report the crystal structure of a posttermination *Thermus thermophilus* 70S ribosome complexed with EF-G, RRF and two tRNAs at a resolution of 3.5 Å. The deacylated tRNA in the P site moves into a previously unsuspected state of binding (peptidyl/recycling, p/R) that is analogous to that seen during initiation. The terminal end of the p/R-tRNA forms nonfavorable contacts with the 50S subunit while RRF wedges next to central inter-subunit bridges, illuminating the active roles of tRNA and RRF in dissociation of ribosomal subunits.

[3-05-1354](#) DNA複製一分子観察にむけた酵母レプリソームのDNA結合の評価
Evaluation of DNA binding of yeast replisome toward single-molecule observation of DNA replication

S. Mayu Terakawa, Tsuyoshi Terakawa (*Grad. Sci. Kyoto Univ.*)

Eukaryotic DNA replication initiation is a highly complex process in which at least 18 proteins are involved. Thus, the molecular mechanism of DNA replication initiation has remained elusive. The replication initiation can be divided into three steps: 1) Two Mcm2-7 molecules are loaded onto the ARS DNA sequence, 2) Cdc45 and GINS are loaded onto the Mcm2-7 molecules to assemble a pre-replicative complex, and 3) the firing factors make the pre-replicative complex capable of replicating DNA. In this study, we purified all the proteins required to reconstitute the DNA replication. By magnetic beads pull-down assays, we confirmed that the purified proteins are properly loaded onto the ARS and tried to verify whether the pre-replicative complex formed in our system.

[3-05-1406](#) 薬剤耐性機構の解明に向けた、クライオ電子顕微鏡解析によるNTMリボソームへのマクロライド結合様式の解明
Elucidation of the binding mode of a macrolide antibiotic to NTM ribosome for understanding drug resistance mechanism by using cryo-EM

Tsubasa Hashimoto¹, Nozomi Takada¹, Takuma Chiashi¹, Hanako Fukano², Kentaro Yamamoto², Masato Suzuki³, Yoshihiko Hoshino², Takeshi Yokoyama¹, Yoshikazu Tanaka¹ (¹*Grad. Sch. Life Sci., Tohoku Univ.*, ²*Leprosy Res. Center, Nat. Ins. of Infectious Diseases*, ³*AMR Center, Nat. Ins. of Infectious Diseases*)

The incidence of non-tuberculous mycobacterial (NTM) infections has increased rapidly recent years and it raises concerns in healthcare. Many NTMs often acquire resistance to multiple antimicrobial agents such as macrolides that target bacterial ribosomes, making their treatment difficult. As the structural details of NTM ribosome is unknown, it is important to obtain structural information of the ribosome for the development of effective drug to suppress NTM infections. In this study, we report the structure of NTM ribosome in complex with macrolide at a resolution of 2.65 Å using single particle cryo-EM. Based on this structure, the mechanism of action of macrolides on NTM ribosomes and the drug-resistance acquired by ribosomal RNA modification are discussed.

[3-05-1418](#) In-cell NMR法によるヒト生細胞内環境下の核酸の塩基対ダイナミクスの解析
In-cell NMR study on the base pair dynamics of nucleic acid in the living human cells

Yudai Yamaoki^{1,2}, Takashi Nagata^{1,2}, Keiko Kondo¹, Tomoki Sakamoto², Shohei Takami², Masato Katahira^{1,2} (¹*Inst. Adv. Energy, Kyoto Univ.*, ²*Grad. Sch. Energy Sci., Kyoto Univ.*)

It is expected that the structural dynamics of nucleic acids in living cells are affected by endogenous molecules and different from those under *in vitro* conditions. The in-cell NMR technique is a powerful tool to investigate the base pair dynamics of nucleic acids in the living cells. In this study, we measured the exchange rates of imino protons contained in base pairs in living human cells by using in-cell NMR technique. The exchange rates of imino protons under *in vitro* conditions were also obtained and evaluated the base pair lifetimes. The comparison of the exchange rates of imino protons under *in vitro* and in-cell conditions indicated that the base pair lifetimes in living human cells are different from those under *in vitro* conditions.

[3-05-1430](#) c-MYC遺伝子のグアニン四重鎖の圧力変性に関するFTIR研究
FTIR study of pressure-induced denaturation of the guanine quadruplex of the c-MYC gene

Kohei Miyauchi¹, Yudai Yamaoki², Hiroshi Imamura¹, Minoru Kato¹ (¹*Grad. Sch. Life Sci., Univ. Ritsumei*, ²*Advanced Energy Inst., Univ. Kyoto*)

The c-MYC gene has a quadruplex structure, which is present in the promoter region of cancer-related genes and is a target of anticancer drugs. In this study, we have investigated the effect of pressure on the structural stability of the guanine quadruplex of the c-MYC gene using by FTIR up to 1500 MPa. As marker bands for monitoring the secondary structure of the c-MYC gene, we used the C=O stretch vibrational band of guanine observed at 1670 cm⁻¹. Increasing pressure induced a decrease in the peak intensity of the band, which is similar to the change in the spectrum due to the heat denaturation of the guanine quadruplex. From the pressure dependence of the intensity, we obtained the volume change accompanying the pressure denaturation.

[3-05-1442](#) Simultaneous monitoring of DNA, RNA, and DNA:RNA hybrid G-quadruplexes, and their interaction with arginine-glycine-rich peptide by NMR

Chihiro Nakayama^{1,2}, Yudai Yamaoki^{1,2}, Keiko Kondo¹, Takashi Nagata^{1,2}, Masato Katahira^{1,2} (¹*Inst. Adv. Energy, Kyoto Univ.*, ²*Grad. Sch. Energy Sci., Kyoto Univ.*)

Guanine-rich sequences of DNA and RNA are known to form G-quadruplex structures (GQs). GQs can comprise not only DNA (DGQ) or RNA (RGQ), but also both of them, which is known as DNA:RNA hybrid GQ (HGQ). These GQs are thought to be involved in different biological events. Tracking the activities of these GQs individually in the biological context is challenging. We have recently identified the NMR signals of DGQ, RGQ, and HGQ that are isolated from each other using a sample containing all of them. We demonstrated that these NMR signals can be used to probe the binding between individual GQs with arginine-glycine-rich peptide. Our results strongly suggest that our system can be applied to search for and develop the molecules that specifically recognize DGQ, RGQ, or HGQ.

[3-06-1330](#) 生体運動メカニズムの統一的理解
Unified Understanding of Active Motions Driven by Proteins

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Active motions driven by motor proteins are classified as translational, rotational, and expanding (polymerizing) motions. Recently, Sasaki-Kaya-Higuchi (SKH) model has been proposed [*Biophys. J.* 2018] to reproduce motions of translational motors (kinesin-1, dynein-1 and myosin-V). However, whether SKH model explains motions of other motors and what the model means physically are unknown. To answer these questions, we explain that the SKH model holds not only for translational motions but also for rotational ones of DNA polymerase, RNA polymerase and F1-motor. We also introduce a chemical reaction model that reproduces the features of the SKH model to discuss the physical meaning of SKH model.

[3-06-1342](#) Molecular dynamics simulations of the yeast condensin holo complex towards elucidation of the mechanism of DNA loop extrusion

Hiroki Koide, Shoji Takada, Tsuyoshi Terakawa (*Kyoto Univ. Dep. of Science Takada Lab.*)

Chromatin higher-order structural formation in metaphase is important for sister chromatid segregation. Previous studies have shown that condensin, one of the structural maintenance of chromosomes proteins, extrudes DNA loops with its molecular motor activity to accomplish the chromatin structural formation. However, the detailed molecular mechanism of DNA loop extrusion has remained elusive. In this study, we performed coarse-grained molecular dynamics simulations to observe the conformational transitions of the yeast condensin holo complex in the ATP cycle. This study paves the way for the future simulation works in which we can directly observe DNA loop extrusion by condensin.

[3-06-1354](#) ショウジョウバエの左右非対称性を制御する Myosin1C と Myosin1D の解析
Molecular analysis of Myosin1C and Myosin1D, determinants of left-right asymmetry in *Drosophila*

Kohei Yoshimura¹, Takeshi Haraguchi¹, Takuma Imi¹, Asuka Yamaguchi², Chinami Maeda², Kenji Matsuno², Kohji Ito¹ (¹*Grad. Sch. Sci., Univ. Chiba*, ²*Grad. Sch. Sci., Univ. Osaka*)

Left-right (LR) asymmetry is essential for organisms' early development. In *Drosophila*, Myosin1C (Myo1C) and Myosin1D (Myo1D) have been identified as determinants of LR asymmetry; however, the molecular mechanism by which these myosins disrupt symmetry remains poorly understood. To better understand this mechanism, we performed a detailed analyses of motor activities of Myo1C and Myo1D, such as velocities, ATPase activities, and curvature of actin tracks. Our results showed that Myo1D has faster motility and higher ATPase activity compared to Myo1C. Surprisingly, not only Myo1D but also Myo1C induces clockwise circular movements of actin filaments. Based on our results, we propose a model of LR asymmetry formation by Myo1D and Myo1C.

3-06-1406 病原性大腸菌 EPEC が有する III 型分泌装置の ATPase 複合体の機能解析
Functional analysis of ATPase complex in Type Three Secretion System of Enteropathogenic *Escherichia coli*

Aya Suzuki¹, Yuki Tajimi², Ryo Kurosaki², Hiroshi Ueno¹, Takayuki Uchihashi², Hiroyuki Noji¹ (¹*Dept. Appl. Chem., Grad. Sch. Eng., Univ. Tokyo*, ²*Dept. Matl. Sci., Grad. Sch. Sci., Nagoya Univ.*)

Enteropathogenic *E. coli* (EPEC) utilizes type III secretion system (T3SS) that is essential for the injection of virulence effector proteins into host cells. Among the components of T3SS, ATPase complex is proposed to play a significant role in energizing secretion events and substrate recognition. As ATPase subcomplex, the hexameric EscN forms the stator ring, where the central shaft EscO is inserted into the central cavity. Here, to demonstrate the estimated rotational catalytic mechanism of the EPEC T3SS ATPase subcomplex, EscN hexamer rings were formed by incubating with nucleotides, and the enzymatic property was characterized by ATPase activity assay. The stability and the conformational change of the EscN rings were investigated by using High-speed AFM imaging.

3-06-1418 高速原子間力顕微鏡と電子顕微鏡によるダイナクチンサイドアームのダイナミクスの可視化
Visualization of conformational dynamics of dynactin sidearm by high-speed AFM and negative stain EM

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Dynactin is a huge protein complex, which interacts with various microtubule-binding and vesicle-binding proteins, and it regulates the motility of dynein. Although previous cryo EM studies revealed its averaged structure, our knowledge on the structure of sidearm in dynactin complex is still limited because of its flexibility. Here, we report conformational change of dynactin sidearm observed by AFM and EM. We found that 1) the dynein-binding domain in p150 subunit (CC1) underwent a conformational change between the folded and extended forms, and 2) the mobility of microtubule-binding domain in p150 was regulated by the conformation of the nearby intrinsically disordered region. Our results reveal dynamic aspects of the domains crucial for dynactin function.

3-06-1430 高度好塩菌アーキアの回転モーターにおける化学走性
Chemotaxis of the archaeal motor in *Haloferax volcanii*

Yoshiaki Kinoshita, Rikiya Watanabe (*CPR, RIKEN*)

Motile archaea form the ATP-driven rotary motor called an archaeal flagellum. Although it has no similarity with the bacterial flagellum, the switching from CCW to CW rotation is mediated by the same chemotaxis system. Here, to elucidate how this switching occurs, we conducted the mutagenesis and bead assay, allowing direct observation of the motor's rotational direction. CheF is believed to be necessary for CW switching, but the lacking strain exhibited 50 % CW rotation with the frequent switching. Now, we purify this protein and characterize the function *in vitro*. The combination of permeabilized-ghost model and purified-CheY proteins could control the motor switching manually. We will discuss the difference and similarities in switching between bacteria and archaea.

3-07-1330 無細胞タンパク質発現系による生体分子モーターの試験管内合成とデザイン
In vitro synthesis and design of biomolecular motors by cell-free protein expression system

Daisuke Inoue¹, Keisuke Ohashi^{2,3}, Taichi Takasuka^{2,3}, Akira Kakugo⁴ (¹*Faculty of Design, Kyushu University*, ²*Graduate School of Global Food Resources, Hokkaido University*, ³*Research Faculty of Agriculture, Hokkaido University*, ⁴*Faculty of Science*)

The biomolecular motor system (microtubule-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 using bacteria is time-consuming to produce and design kinesins. Here, we demonstrated *in vitro* synthesis of kinesins using a cell-free protein expression system that expresses proteins from DNA templates in coupled transcription and translation systems. Synthesized kinesins propelled microtubules on a kinesin-coated substrate. We also successfully introduced a specific tag into kinesins by using PCR fragments with the tag sequence. Our method will accelerate the study of biomolecular motor systems.

[3-07-1342](#) (1S1-3) Engineering of hybrid kinesin-1 dimer with synthetic linker by tuning the neck linker length

Jakia Jannat Keya¹, Akasit Visootsat¹, Akihiro Otomo¹, Sanghun Han², Kazushi Kinbara², Ryota Iino¹ (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 dimer by conjugating with a synthetic linker through the neck-linker regions. Single-molecule fluorescence imaging of a hybrid revealed unidirectional processive motion with the velocity of 202 nm/s and run length of 1084 nm at 1 mM ATP, although lower than those of the wild-type (690 nm/s and 2740 nm). By removing 9 additional glycine linkers and 1 amino acid residue of the neck linker from the original hybrid, velocity and run length increased to 362 nm/s and 1930 nm respectively, indicating the critical role of neck linker length for fast and long processive motion. By tuning the neck linker and synthetic linker lengths, we are trying to further improve the velocity and run length of the hybrid kinesin-1 to outperform the wild-type.

[3-07-1354](#) 微小管群ロボット操作のための人工 DNA フェロモンの開発
Designed DNA pheromone for automatic controlling of microtubules swarming

Daiki Matsumoto¹, Kohei Nishiyama², Ibuki Kawamata^{1,4}, Satoshi Murata¹, Akira Kakugo^{2,3}, Shin-ichiro M. Nomura¹ (¹*Department of Robotics, Graduate School of Engineering, Tohoku University*, ²*Graduate School of Chemical Sciences and Engineering, Hokkaido University*, ³*Department of Chemistry, Faculty of Science, Hokkaido University*, ⁴*Natural Science Division, Faculty of Core Reserch, Ochanomizu University*)

Biomolecular motors such as microtubules (MTs) and kinesins are promising candidate of actuators for molecular swarm robots. It has been demonstrated that the swarming can be controlled by functionalizing MTs with DNA through precise control of their local interactions. On the other hand, swarming in nature, ants find a shortest path between preys and a nest, laying down the pheromone trails. Here, if swarming of MTs controlled by the local interaction like pheromone trails, molecular swarming that solves shortest path problems extensively in distributed manner will be viable. In this study, we designed DNA based artificial pheromone which will guide the behavior of the DNA functionalized MTs. Here, we will discuss about the visualization of the DNA pheromone trails.

[3-07-1406](#) ポリエチレングリコールを用いたアクトミオシン運動の輸送能力試験
Test on in vitro transport capacity of actomyosin using polyethylene glycols

Yuma Sunada, Kuniyuki Hatori (*Grad. Sch. Sci. Eng., Yamagata Univ.*)

Myosin motors generate mechanical work from ATP hydrolysis and move along actin filaments. Extensive research on cargo transport in motor proteins has been performed; however, it is not yet well understood how large cargo the actomyosin sliding can transport. We investigated the transport capacity by way of binding of four different sizes of polyethylene glycols (PEGs) to actin. PEG-bound actin filaments were prepared with various mixing ratios of PEG-actin to intact actin. In an in vitro motility assay with ATP, the sliding velocity of the actin filaments on heavy meromyosin slightly decreased with the increase in PEG-actin ratio under 2k in size. Meanwhile, the percentage of moving filament obviously decreased as PEG size increased up to 10k.

[3-07-1418](#) In vitro でのアクチンフィラメントへの lifeact-GFP の不均一かつ安定的な結合の観察
Uneven and stable binding of lifeact-GFP to actin filaments observed in vitro

Yuuya Aoki, Yousuke Yamazaki, Taro Q.P. Uyeda (*Dept. Physics, Waseda Univ.*)

Structural polymorphism of actin filaments (AF) has been implicated in the regulation of certain actin binding proteins. Lifeact-GFP is generally believed to rapidly bind to and dissociate from all AF in cells. The dwell time of lifeact on AF in lamellipodia showed a single exponential decay with a half-life of 23 ms (kiuchi *et al.*, 2015). Here, we imaged Lifeact-monomeric eGFP along AF in vitro. Surprisingly, lifeact-GFP formed clusters along AF, and remained bound for extended periods of time after washing out lifeact-GFP in solution. We thus speculate that the affinity of Lifeact-GFP to AF varies depending on the local conformational variation of the filaments. We are now investigating factors that affect actin binding kinetics of lifeact-GFP.

[3-07-1430](#) Photocontrol of small GTPase Ras using its regulatory factor GEF modified with photochromic azobenzene derivative

Yuichi Imamura, Nobuyuki Nishibe, Yuichi Imamura (*Grad.Sch.Eng., Univ. Soka*)

Ras is a central regulator of cellular signal transduction processes. There are two kinds of regulatory factor for Ras, GEF and GAP. GEF exchange GDP to GTP. In this study, functional sites of SOS which is one of GEF were directly modified with photochromic molecule in order to control GDP-GTP exchange of Ras photo-reversibly. We have designed the sites in Ras to be modified by azobenzene and expressed the Ras mutants by E. coli expression system. The mutants S732C, S881C, H905C and H911C were prepared. Azobenzene derivative N-(4-phenylazophenyl) maleimide (PAM) was incorporated into the cysteine of each mutant. Photocontrol of Ras GTPase activity in the presence of GAP and PAM modified SOS mutants was examined under UV and visible light irradiations.

[3-08-1330](#) 細胞内物質輸送を理解する新しい接近方：機械学習とイメージプロセッシング技術の応用について
Understanding of vesicle transport using machine learning and image processing technology

Seohyun Lee¹, Hyuno Kim¹, Masatoshi Ishikawa¹, Hideo Higuchi² (¹*Data Science Reserach Division, Information Technology Center, The University of Tokyo*, ²*Department of Physics, Graduate School of Science, The University of Tokyo*)

Vesicle transport refers to the overall internal process of information delivery occurring in living cells, which is an essential biological procedure for living organisms. Although vast amounts of researches have revealed the mechanism of vesicle movement at the molecular level, the studies about the actual movement of vesicles interacting with cytoskeletons in a living cell are often limited due to the complexity of both imaging and the vesicle movement itself. Here, we present a machine learning approach and a computer image processing method to better understand the behavior of vesicle in a living cell, particularly in terms of the interaction between cytoskeletons.

[3-08-1342](#) 原子間力顕微鏡による上皮ドームの力学解析
Mechanical analysis of epithelial dome using atomic force microscopy

Kenta Shigemura, Kaori Kuribayashi-Shigetomi, Agus Subagyo, Kazuhisa Sueoka, Takaharu Okajima (*Grad. Sch. Inform. Sci., Univ. Hokkaido*)

Epithelial domes that enclose a pressurized lumen is a fundamental biological process existing in tissues. Recent studies reported that epithelial cells retain their dome structure under high tension [Latorre et al., *Nature* 563, 203 (2018)]. However, the mechanical property of single cells forming dome is still unclear. In this study, we investigated the mechanical behavior of Madin-Darby canine kidney cell monolayers and domes by atomic force microscopy. We observed that domes exhibited a mechanical behavior that does not follow the Hertzian contact theory modeling the deformation of homogeneous bulk sample, indicating that AFM has an ability to quantify the effect of both tension and elastic modulus in domes. We thank Dr. Yasuyuki Fujita for providing cell samples.

[3-08-1354](#) Observations of structural change in epithelial dome under constant electric field

Mataka Nagano, Miyu Ogawa, Yuki Fujii, Takaharu Okajima (*Grad. Sch. Inform. Sci. and Tech., Univ. Hokkaido*)

The electric field response of epithelial cells has been widely investigated in single cells and monolayers in terms of cell migration, called electrotaxis or galvanotaxis. However, little is known about how three-dimensional epithelial samples change their structure in response to electric field. In this study, we investigated the electric field response of Madin-Darby canine kidney (MDCK) cells forming dome-shaped structures (Latorre et al. *Nature* 2018) in vitro. We found that the MDCK dome underwent a transition to monolayer sheet in response to an electric field, and the structural change in MDCK dome occurred over a threshold and also depended on the formed dome size. We thank Dr. Yasuyuki Fujita for providing cell samples.

[3-08-1406](#) 極性形成に関わる膜タンパク質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

Rinshi Kasai¹, Yuri Nemoto² (¹*GCORE, Gifu Univ.*, ²*OIST*)

Planar cell polarity (PCP) is orchestrated by various proteins. Adhesion GPCR (G-protein coupled receptor) forms a homophilic complex at the cell-cell interface. Based on this, other proteins like Frizzled are cooperatively and exclusively organized. However, the mechanism how these proteins are regulated remains unclear. By observing them at the single molecule level at the cell-cell interface, we found that Frizzled and other proteins are specifically accumulated and immobilized, whereas some of them are diffusing (around 3 times slower than typical membrane proteins). These findings suggest that PCP-related proteins are mostly anchored to structural proteins like actin, but some of them are dynamically exchanging, which could be important for plasticity of polarity.

[3-08-1418](#) 酵母 G1 期核内での染色体分布とそのフラクタル次元に関する X 線回折イメージング
X-ray diffraction imaging study on the distribution and fractal dimensions of chromosomes in yeast nuclei in G1 phase

So Uezu^{1,2} (¹*Dept. Phys., Keio Univ.*, ²*RSC, RIKEN*)

We studied structures of the nuclei of budding yeast in the G1 phase by X-ray diffraction imaging (XDI) using X-ray free electron laser. XDI enables us to illustrate the structures of non-crystalline particles without chemical labeling and sectioning. From the projection electron density maps retrieved from high quality diffraction patterns, the distribution of chromosomes was visualized in the nuclei with ellipsoidal shapes. In addition, the generalized scattering function applied to the sum of circularly averaged 60 diffraction patterns yielded the mass and surface fractal dimensions of chromatin assemblies composing chromosomes. Together the projection maps and fractal characteristics of chromatins, we will discuss models on the distribution of chromosomes.

[3-08-1430](#) 蛍光顕微鏡複合型高速 AFM による細胞のナノ粒子取り込み過程の計測
The cellular uptake observation of nanoparticles by high-speed AFM combined with fluorescent microscopy

Akito Matsui¹, Hayato Yamashita¹, Akihiro Tsuji¹, Asuka Yamaguchi², Madoka Suzuki³, Masayuki Abe¹ (¹*Grad. Sch. Eng. Sci., Osaka Univ.*, ²*Grad. Sch. Sci., Osaka Univ.*, ³*IPR Osaka Univ.*)

Fluorescent nanodiamonds (FNDs) are nanoparticles that are widely used for drug delivery system or intracellular imaging and sensing. It has been reported that the efficiency of the cellular uptake depends on morphological features (size or shape) of FNDs [1]. However, the relationship between FND morphologies and cell membrane structural characteristics remains unclear. In order to reveal the mechanism of cellular uptake, it is necessary to visualize the dynamics of cell membrane interacting with FNDs. In this study, we introduced a wide range scanner and fluorescence detection system in high-speed AFM to observe such cellular processes. We successfully visualized the morphology of FNDs attached on the cellular surface. [1] B. Zhang, et al. *Sci. Rep.* 7, 46462 (2017)

[3-08-1442](#) 細胞外小胞のサブタイプと取り込み経路の解明：超解像顕微鏡法と 1 粒子追跡法による研究
Subtypes of small extracellular vesicles and their uptake routes as revealed by super-resolution microscopy and single-particle tracking

Koichiro M. Hirose¹, Yasunari Yokota², Kenichi G.N. Suzuki^{1,3} (¹*GCORE, Gifu Univ.*, ²*Dept. Eng., Gifu Univ.*, ³*CREST, JST*)

Small Extracellular Vesicles (sEV) have received an extensive attention as intercellular messengers. Recent studies suggested that sEV play a critical role in tumor metastasis. However, heterogeneity of the sEVs and their uptake routes into target cells are totally unknown. Here, we investigated whether sEV have subtypes and how sEV are taken up by the cells. Single-particle analysis showed that marker proteins are not necessarily colocalized with each other in the same sEV, suggesting that sEV can be classified into several subtypes. Furthermore, we simultaneously performed single-particle tracking of sEVs and super-resolution imaging of membrane structures in living cell, revealing that the uptake route of sEVs into target cells differed among their subtypes.

[3-08-1454](#) Measuring the conformational changes in clathrin light chain at single sites of endocytosis with FLIM-FRET-CLEM

Kazuki Obashi, Kem Sochacki, Marie-Paule Strub, Justin Taraska (*National Heart, Lung, and Blood Institute, National Institutes of Health*)

The dynamic nanoscale localizations, interactions, and conformations of endocytic proteins are crucial regulators of clathrin-mediated endocytosis. However, information about these nanoscale changes are largely unknown due to the lack of available measurement tools. To span this gap, we developed a correlative FLIM-FRET and EM imaging method. Here, FRET-based atomic distances can be mapped to EM-visible nanoscale cellular structures at the plasma membrane. Using this method, we discovered that clathrin light chain undergoes a conformational switch as clathrin lattices gain curvature. We hypothesize that these dynamics promote the transition from flat to curved vesicles. These new correlative light and EM data will help develop a complete atomic model of endocytosis.

[3-08-1506](#) Application of photothermal agarose microfabrication technology for spatiotemporal analysis of collective cell migration

Mitsuru Sentoku, Hiromichi Hashimoto, Kenji Yasuda (*Dept. Pure & Appl. Phys., Grad. Sch. Adv. Sci. & Eng., Waseda Univ.*)

Unlike conventional microfabrication technologies, which require complicated pre-designing, our agarose microfabrication allows flexible real-time fabrication even during cell cultivation. We adopted this technique to probe collective cell behavior in confined geometry, ranging from 10 to 211- μm width straight channels. Tracking the cell sheet indicated a velocity peak around 30- μm channel. Single-cell tracking revealed (1) the decrease of velocity in the narrower width was caused by an increased aspect ratio, and (2) the reduction in the broader channels was caused by the increase of the random walk-like behavior of cells. Hence, we confirmed that our technology provides a more facilitated preparation of topological confinements for probing collective cell behavior.

[3-08-1518](#) 原子間力顕微鏡の往復フォースカーブを用いた初期発生胚のレオロジーマッピング
Mapping rheological parameters of embryonic cells during early developmental stages using atomic force microscopy force curves

Tomohiro Matsuo, Yosuke Tsuboyama, Megumi Yokobori, Yuki Fujii, Takaharu Okajima (*Grad. Info. Sci. & Tech., Univ. Hokkaido*)

Atomic force microscopy (AFM) allows us to measure the stiffness of embryonic cells in the developmental process [1]. In this study, using AFM we investigated the rheological properties of cells in ascidian embryo during the early developmental stages. We first determined that the relaxation modulus followed single-power law rheology involving static modulus. Using approach and retract AFM force curves, we mapped the rheological parameters of embryonic cells during early developmental stages, showing that the modulus increased, while the exponent decreased toward the cell division. Furthermore, a universal correlation between the modulus and the exponent of cells was observed during the gastrulation. [1] Y. Fujii, et al., *Commun. Biol.* 2021.

[3-09-1330](#) tau-RNA 液滴形成の熱量解析
Calorimetric study of RNA-induced formation of tau droplet

Kan Matsuda, Junta Kashima, Hideyuki Komatsu (*Dept. of Bioscience and Bioinformatics, Kyushu Inst. Tech.*)

Microtubule-associated protein tau aggregate is a major component of Alzheimer neurofibrillary tangle. Liquid-liquid phase separation (LLPS) of tau has been considered to be an important process of the tau aggregation. Thus, RNA-tau interaction is thought to undergo LLPS into tau-concentrated droplet. Here, we have studied thermodynamics of RNA-induced tau droplet formation by using isothermal titration calorimetry (ITC). In preliminary ITC, endothermic heat was observed at the condition where the tRNA-tau droplet formed, implying an entropic driven process. Tau droplet formation by single-strand RNA will also be analyzed. In addition, the curve-fitting based on detergent micellization thermodynamics will be employed (*Anal. Chem.* 2020, **92**, 1154).

[3-09-1342](#) 心毒性検査法の効率化を目指したハイスループット薬剤応答解析
High-throughput cardiotoxicity detection system for simultaneously analysis of 64 samples

Kentaro Kito, Naoki Tadokoro, Masahito Hayashi, Tomoyuki Kaneko (*LaRC, FB, Hosei Univ*)

To save the cost and time for cardiotoxicity tests, we have developed an *in vitro* electrocardiogram that can simultaneously measure the extracellular potentials of 64 cardiomyocyte colonies. In this report, we analyzed the Field Potential Durations (FPDs) and Inter-Spike Intervals (ISIs) responding to known cardiotoxic agents. FPD elongation was detected as the response to hERG channel blockers, E-4031 and quinidine, while FPD shortening was detected as that to Ca²⁺ channel blocker, verapamil. Short-term variability of FPD and ISI was increased for all the agents. These results suggest that our system is useful for the cardiotoxicity tests of drug candidates.

[3-09-1354](#) リアルタイムフィードバック機構を内蔵した心臓細胞への機械的刺激システム
Development of a mechanical device for stimulus on cardiac cells with feedback control system

Ayu Sasaki, Kazuki Mammoto, Ryu Kidokoro, Shota Nozaki, Yuuta Moriyama, Toshiyuki Mitsui (*Dept. Phys., Aoyama Gakuin Univ.*)

The heart is known to sensitive to stress in order to effectively circulate blood through an entire body as the heartbeat. Because the beats occur periodically, it is interesting to investigate the response of stress as stimuli synchronized with the beat period. We have developed a mechanical device to generate deformation on a cardiac cell cluster as stimulus *in vitro* with a real-time feedback control in response to cluster's beats. In this presentation, we will describe the device build moderately reasonable using a USB camera with LabVIEW based platform. Although the response, as a time constant, is still 0.1 sec corresponding to three framing time of 30Hz imaging, phase controlled mechanical stimuli can be applied to a cardiac cell cluster.

[3-09-1406](#) リアルタイムフィードバック制御による力学的刺激に影響を受けた心筋細胞の拍動変化
Change in phase stability of cardiac cell clusters affected by to mechanical stimulus with feedback control

Shota Nozaki, Ryu Kidokoro, Kaito Kojima, Ayu Sasaki, Yuuta Moriyama, Toshiyuki Mitsui (*Dept. Phys., Aoyama Gakuin Univ.*)

Synchronization of the heart from single cells is one of enigmatic phenomena observed in biology. To understand its mechanism, it requires realization of electronic properties of single cells and their interactions. Furthermore, recent studies indicate the direct influence of mechanical deformations on the synchronization. We have developed a system to apply periodic deformations on a cardiac cell cluster *in vitro*. In our preliminary experiments, no significant deviations on cluster's beats were observed except the beating phases. Therefore, we added a real-time feedback control of phases to the system in response to cluster's beats. We will be shown that in-phase stimulus stabilized the beating of cardiac cell clusters, out of phase stimulus showed unstable motions.

[3-09-1418](#) 機械学習を用いた細胞の集団運動ダイナミクスの次元圧縮とメカノバイオロジ的な効果
Dimension compression and mechanobiological effects of collective cell movement dynamics using machine learning

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Multicellular motions *in vivo* are extremely complex and diverse, and collective motions such as migration and aggregation cause medically important phenomena such as wound healing, angiogenesis, and metastasis of cancer cells. However, it is practically impossible to understand them from the molecular level due to the enormous degree of freedom of cells, and here we consider a data-driven approach using experimental data. The video data of vascular endothelial cells is binarized using the position of the center of each cell, and the multidimensional time series data is dimensionally reduced using manifold learning techniques and a time-delay autoencoder to investigate the mechanobiological effects, such as when pressure is applied to the cells.

[3-09-1430](#) 初期ニワトリ胚における中胚葉細胞の動的網目構造の自己組織化
Dynamical network structure formation of mesoderm cells in early chick embryo

Mitsusuke Tarama, Yukiko Nakaya, Tatsuo Shibata (*RIKEN BDR*)

How individual cells self-organize into complex multi-cellular morphological structures of tissue is one of the fundamental questions in developmental biology. In our experiment, we found that the mesoderm cells that appear at the primitive streak form a dynamical three-dimensional network structure between the epiblast and the endoderm while migrating away from the primitive streak. Using agent-based theoretical model, we investigate the mechanism of the self-organization of such network structure. We identified that the cell elongation, the cell-cell adhesion, and the cell density play important roles for the network structure formation, and the additional cell migration makes the structure dynamic.

[3-09-1442](#) 細胞性粘菌の細胞型特異的な運動形状ダイナミクスの定量的解析
Quantitative analysis of cell-type specific morphology dynamics in *Dictyostelium discoideum*

Natsuki Murayama¹, Satoshi Kuwana², Masahito Uwamichi², Hidenori Hashimura², Satoshi Sawai² (¹*Grad. Sch. Sci., Univ. Tokyo*, ²*Grad. Sch. Arts & Sci., Univ. Tokyo*)

Crawling migration take several distinct modes (e.g. protrusive- and blebbing/contractile -based) depending on how motility and directionality are governed. Much of the physical basis and their migratory strategies remain to be elucidated. Here we studied repertoires of migratory modes exhibited by differentiated *Dictyostelium* cells by quantifying the morphology dynamics by confocal and light-sheet microscopy. We show that the main cell-types isolated from the stage of slug to culmination exhibit cell-type dependent morphodynamics characterized by distinct pseudopodial forms, blebbing and extent of cell polarization. We will discuss their implications to the general concepts of migratory modes based on the spherical harmonics and a deep-learning based feature space.

[3-09-1454](#) 納豆菌が生産する水溶性メナキノン-7の構造研究
Structural study of water-soluble complex of menaquinone-7 produced by *Bacillus subtilis natto*

Toshiyuki Chatake¹, Yasuhide Yanagisawa², Risa Murakami², Tadanori Ohsugi³, Hiroyuki Sumi³, Aya Okuda¹, Ken Morishima¹, Rintaro Inoue¹, Masaaki Sugiyama¹ (¹*KURNS, Kyoto Univ.*, ²*Fac. Pharm., Chiba Inst. Sci.*, ³*Dep. Life Sci., Kurashiki Univ. Sci. Arts*)

Japanese traditional food *natto* abundantly contains menaquinone-7 (MK-7). MK-7 belongs to the vitamin K₂ family and is involved in osteogenesis. While MK-7 is a fat-soluble compound, *Bacillus subtilis natto* produces water-soluble complex of MK-7 (*natto*-MK-7). This solubility in water has nutritional and medical applications, including pharmaceutical preparation. The major component of *natto*-MK-7 is peptides, which was called K-binding-factor (KBF). In the present study, *natto*-MK-7 containing only KBF and menaquinone-7 can be obtained and its particle structure is confirmed by dynamic light scattering technique. Mass spectrometry of KBF shows the multiple peaks around $m/z = 1050$, suggesting that KBF might have ~1k basic units with different amino acid sequences.

[3-10-1330](#) 脂質二分子膜への有毒物質の吸着
Adsorption of toxic molecules into lipid bilayer membranes

Kazunari Yoshida, Naofumi Fujiwara (*Grad. Sch. Sci Eng., Yamagata University*)

Toxic acetonitrile incorporation into a 1,2-dioleoyl-*sn*-glycero-3-phosphocholine (DOPC) vesicle is numerically estimated using shape data obtained from previous direct observations. A bilayer-couple (BC) model is used to determine the quantitative disparity in acetonitrile incorporation between outer and inner leaflets. These disparities suggest that the difference in acetonitrile molecule incorporation between the outer and inner leaflets of bilayers is $\Delta N = 1.4 \times 10^3$. The value indicates that the amount of incorporated acetonitrile molecules in outer leaflet is quite larger than that of transferred molecules to inner leaflet due to the polarity of acetonitrile.

[3-10-1342](#) 膜曲率依存的な KcsA チャネル構造変化を蛍光ラベルで検出する

Fluorescence detection of membrane curvature-induced structural changes in the KcsA potassium channel

Misuzu Ueki, **Masayuki Iwamoto** (*Dept. Mol. Neurosci., Facul. Med. Sci., Univ. Fukui*)

Highly curved structures in biomembrane, such as caveolae and transport vesicles, are essential for signal transduction and membrane trafficking. The curvature of the lipid bilayer physically stresses membrane proteins in these regions, but the effect of this stress on protein structure and function remains unclear. This study established an experimental procedure to evaluate membrane curvature-induced structural changes in the prototypical potassium channel, KcsA. The effect of a large membrane curvature was estimated using fluorescently labeled KcsA by incorporating it into liposomes with a small diameter (< 30 nm). We found that a large membrane curvature significantly affects the activation gate conformation of the KcsA channel.

[3-10-1354](#) 金プローブを用いた自動チャネル電流測定装置の開発

Development of an automated system for measuring channel currents using a gold probe

Minako Hirano¹, Masahisa Tomita², Chikako Takahashi¹, Nobuyuki Kawashima³, Toru Ide⁴ (¹*GPI*, ²*Tom's factory*, ³*SYSTEC Corporation*, ⁴*Grad. Sch. Interdiscip. Sci. Engr. Health Syst., Okayama Univ.*)

We have developed an automated channel current measurement system using a hydrophilically modified gold probe. In the system, a lipid bilayer membrane containing ion channels is promptly made on the probes' hydrophilic area by automatically plunging the probe into a recording solution through a lipid solution. We optimized the shape of the probe and chemical modification of the probe surface, and found that use of probes with rounded tips and introducing a hydrophobic area on the probe surface, beside the hydrophilic one, increased measurement efficiency. Using the optimized probes, we were able to automatically measure channel currents and analyze the effects of a blocker on channel activity.

[3-10-1406](#) アガロースゲルビーズを用いた新規チャネル電流測定法の開発

Development of a novel channel current measurement method using agarose gel beads

Mami Asakura¹, Daiki Yamamoto¹, Minako Hirano², Toru Ide¹ (¹*Grad. Sch. Health Sys., Okayama Univ.*, ²*Photo-Bio. GPI*)

We have developed novel channel current measurement techniques using artificial lipid bilayers. The formation of rapid and stable lipid bilayers is key to improve the efficiency and accuracy for channel current recordings. By using agarose gel bead as a support of lipid bilayers, we were able to simplify the lipid bilayer formation technique and dramatically shorten the time needed for the current measurement. Here, we show additional results of channel current measurement using several kinds of agarose gel beads. We expect that our method using agarose gel beads makes it possible to reduce the size of the channel current measurement device.

[3-10-1418](#) チャネル電流測定のためのゲルビーズ上の人工膜の形成

Artificial bilayers on a hydrogel bead for channel current recordings

Daiki Yamamoto¹, Mami Asakura¹, Minako Hirano², Toru Ide¹ (¹*Grad. Sch. Health Sys., Okayama Univ.*, ²*Photo-Bio. GPI*)

We have developed a method of single channel recordings using agarose gel beads. We previously reported on forming artificial lipid bilayers on surface of gel beads, into which we incorporated channel proteins and recorded single ion channel current. Here, we will introduce the new method of single channel recordings using gel beads which improve the technique for immobilization of gel beads and formation of lipid bilayers. These methods enable us to record ion channel current more quickly and more easily. There is some possibility of an automated multi-channel measurement system by using these methods.

[3-10-1430](#) Analysis of water permeability of human Aquaporin6 using moving membrane method

Takahisa Maki¹, Shigetoshi Oiki², Masayuki Iwamoto¹ (¹*Dept. Mol. Neurosci., Facal. Med. Sci., Univ. Fukui*, ²*Biomed. Imaging. Res. Ctr., Univ. Fukui*)

Aquaporins (AQPs) are responsible for the selective permeation of water across the cell membrane, but the intramolecular machinery to control the water permeability remains undiscovered. To elucidate its mechanism, we aimed to quantify the AQP's activity under the regulated lipid bilayer environment by applying the recently developed moving membrane (MM) method (Yano et al., *J. Memb. Sci.*, 2021). First, we constructed an expression system of human AQP6 (hAQP6) using the budding yeast *S.cerevisiae* and confirmed hAQP6 localization to the cell membrane. Then, we verified the water permeability of purified hAQP6 by the conventional stopped-flow method and the MM method. We would like to discuss the function of reconstituted hAQP6 and the applicability of our new method.

[3-10-1442](#) Thermo-responsive deformable liposomes, towards micron scale bio-hybrid robotics

Richard James Archer, Shinichiro Nomura, Satoshi Murata (*Tohoku University Graduate School of Engineering Department of Robotics*)

Biomimetic materials replicate naturally occurring functionalities using synthetic materials, however, to date most reports on have been structural and static in nature. One important aspect of biological matter is the ability to move or respond dynamically to environmental stimuli. Here we report attempts at producing environmentally triggered, dynamic and reversible physical responses in multicellular liposomes through use of synthetic thermo-responsive ionic copolymers, able to effect changes in osmotic pressure and thereby controlling water flow across the lipid membrane. The ability to produce triggered dynamic changes in biomaterials is an important step towards smart responsive and programmable materials which are also compatible with physiological conditions.

[3-10-1454](#) Adhesion of giant liposomes with cells using lipid-conjugated DNA towards DNA-mediated fusion

Sho Takamori, Hisatoshi Mimura, Toshihisa Osaki, Shoji Takeuchi (*Kanagawa Institute of Industrial Science and Technology*)

A benefit of DNA-based nanodevices is the predictability of intermolecular interactions. In this study, we use lipid-conjugated small DNA structures to achieve the adhesion of giant liposomes to cultured cells. The liposome-cell interactions programmed by our DNA is specific and can selectively attach giant liposomes to cells. Our DNA has been designed based on the structure of previously reported SNARE-inspired DNA constructs and may be able to fuse attached giant liposomes and cells. To this end, we first demonstrate the DNA-mediated adhesion of giant liposomes to cultured cells. Then, we investigate the feasibility of DNA-mediated fusion. We believe the optimisation of experimental conditions may ultimately enable the fusion of the attached giant liposomes and cells.

[3-11-1330](#) Intermolecular interaction dynamics between PYPs and downstream PYP-binding proteins

Suhyang Kim¹, Yusuke Nakasone¹, Akira Takakado², Yoichi Yamazaki³, Hironari Kamikubo³, Masahide Terazima¹ (¹*Grad. Sch. Sci., Univ. Kyoto*, ²*Grad. Sch. Sci., Univ. Gakushuin*, ³*Div. Mat. Sci., NAIST*)

PYP is a bacterial light sensor protein found in more than 100 species and its photoreaction has been studied extensively. Recently, we have found PYP's downstream protein PBP (PYP-binding protein) from two different species, *Rhodobacter capsulatus* (Rc) and *Leptospira biflexa* (Lb). We previously reported that Rc-PYP forms a complex with Rc-PBP upon UV light illumination, and the complex dissociates upon blue light illumination. In this study, we investigated the interaction dynamics between Lb-PYP and Lb-PBP and found that they form large complexes with molecular weights of hundreds of kDa in the dark state. This complex dissociates upon blue light excitation. These findings represent the diverse signaling mechanisms of PYP-PBP systems.

[3-11-1342](#) RcPYP の複合体形成反応に対する塩濃度効果
Effect of salt concentration on the complex formation reaction of RcPYP

Yoko Narahara¹, Yoichi Yamazaki¹, Kento Yonezawa², Sachiko Toma¹, Hironari Kamikubo^{1,2,3} (¹NAIST, MS, ²NAIST, CDG, ³KEK, IMSS)

Rhodobacter capsulatus Photoactive Yellow Protein (RcPYP), binds to the PYP Binding Protein (PBP) in a light-dependent manner, but the interaction mechanism is still unclear. In order to investigate the effect of electrostatic interaction on the complex formation, we measured the photoreaction and the interaction under various salt concentration conditions. Depending on the salt concentration, while the absorption maxima of inactivated RcPYP were changed, there was no change in the activated RcPYP and the RcPYP complexed with PBP. The interaction with PBPs was weakened at higher salt concentrations. The mutant analysis of RcPYP revealed that K72 was involved in the presumed interaction sites. We assumed that the positive charge on K72 is responsible for the interaction.

[3-11-1354](#) 発色団水素結合を欠損した桂皮酸導入 RcPYP の光反応・相互作用
Photoreaction and interaction of cinnamic acid-incorporated RcPYP lacking chromophore hydrogen bond

Kai Okubo¹, Yoichi Yamazaki¹, Kento Yonezawa², Sachiko Toma¹, Hironari Kamikubo^{1,2,3} (¹NAIST, MS, ²NAIST, CDG, ³KEK, IMSS)

Rhodobacter capsulatus PYP (RcPYP) is a photoreceptor protein with p-coumaric acid (pCA) as a chromophore. pCA's phenolic oxygen forms hydrogen bonds with E45 and Y41 and plays a central role in absorption spectra and photoreactions. In this study, to investigate the contribution of hydrogen bonds to the light-dependent binding of PYP-binding protein (PBP), we prepared PYP-CA with cinnamic acid, which has no phenolic oxygen moiety. The absorption peak of RcPYP-CA was at 310 nm, photoreaction was confirmed, but unlike pCA, the photoreaction cycle was lost. In addition, the light-dependent complex formation with PBP was confirmed by SEC analysis. The absence of phenolic oxygen significantly altered the absorption wavelength, but the binding ability was maintained.

[3-11-1406](#) 赤色光照射による植物光受容蛋白質フィトクロム A の構造変化
Red-light induced structural changes in plant photoreceptor protein phytochrome A

Mao Oide^{1,2}, Masayoshi Nakasako^{1,2} (¹Dept. Phys., Keio Univ., ²RSC, RIKEN)

Phytochrome A (phyA) is a photoreceptor protein of plants regulating the red/far-red light photomorphogenic responses. PhyA displays photoreversible interconversion between inactive red light-absorbing (Pr) and active far-red light-absorbing (Pfr) forms to act as a light-driven phosphorylation enzyme. To understand the molecular mechanism, we studied the molecular structures of phyA from *Pisum sativum* by small-angle X-ray scattering combined with multivariate analyses applied to molecular models predicted from the scattering profiles. Pr dimer had a four-leaf shape with the subunit approximated as a bent rod of 175 × 50 Å, and Pfr dimer exhibited a butterfly shape composed of subunits with a straight rod, indicating conformational changes in the interconversion.

[3-11-1418](#) 部位特異的変異導入によるビリリン結合光センサー RcaE の光変換機構の解析
Analysis of the proton transfer mechanism of the bilin-based photosensor RcaE by site-directed mutagenesis

Yuu Hirose, Takanari Kamo, Toshihiko Eki (*Toyohashi Univ. of Tech. Appl. Chem. & Life Sci.*)

RcaE is green- and red-light sensing photosensor protein of the phytochrome superfamily that binds a linear tetrapyrrole (bilin) as a chromophore. RcaE regulates the photosynthetic activity of cyanobacteria and is also applied as a light-regulated photoswitch in synthetic biology. The green/red photoconversion of RcaE involved C15-Z/C15-E photoisomerization and subsequent protonation/deprotonation of the bilin chromophore. We recently revealed the molecular structure of RcaE in its red-absorbing state and discovered the unique bilin conformation and its interacting amino acid residues. Here, we performed site-directed mutagenesis in the highly conserved residues in RcaE and elucidated the detailed role of each residue in the green/red photoconversion.

[3-11-1430](#) 高速 AFM によるグラナ膜に内在する PSII 側方運動の可視化
Visualizing the lateral mobility of photosystem II in grana membrane by HS-AFM

Misato Ide¹, Daisuke Yamamoto² (¹Grad. Sch. Sci., Fukuoka Univ., ²Fac. Sci., Fukuoka Univ.)

Thylakoid membranes in chloroplasts consists of photosynthetic protein complexes that convert light energy into chemical energy. The dissipation of excess excitation energy is assumed to be associated with dynamic rearrangement of photosystem II (PSII) and its associated antenna proteins. Thus, the photosynthetic protein complexes are presumably mobile in the membranes. However, the dynamic nature of the proteins in the membranes remains to be elucidated. Here, we applied high-speed atomic force microscopy (HS-AFM) to directly observe the lateral movement of the photosynthetic proteins in the grana membrane from spinach. The PSII complexes fluctuating in the membrane were evident in HS-AFM images. We will discuss the detail of the mobility of PSII observed by HS-AFM.

[3-11-1442](#) パターン化人工膜におけるチラコイド膜再構築技術の開発
Reconstitution of thylakoid membrane in a patterned model membrane

Yuka Kusunoki¹, Daisuke Takagi², Seiji Akimoto³, Syouhei Maekawa³, Kenichi Morigaki^{1,4} (¹Grad. Sch. Agr., Univ. Kobe, ²Agr. Univ. Setsunan, ³Grad. Sch. Sci., Univ. Kobe, ⁴Bio signal Research Center, Univ. Kobe)

The photosynthetic functions are regulated by the distribution of proteins and lipids in thylakoid membrane. However, the functional roles of the dynamic organization are difficult to study *in vivo*. In order to mimic the 2D organization of thylakoid membrane in a controlled geometry, we developed a hybrid thylakoid membrane of native thylakoid membrane and synthetic phospholipids (*e.g.* DOPC) in a patterned model membrane. The type and state of reconstituted light harvesting proteins were evaluated with the chlorophyll fluorescence, and the electron transfer activity of PSII was assessed by adding DMBQ and hydroxylamine. We discuss the possibilities to apply the hybrid thylakoid membrane in the photosynthesis research.

[3-11-1454](#) ストリークカメラを検出器とした細胞内局所での時間分解顕微蛍光分光
Microscopic Time-Resolved Fluorescence Spectroscopy within a Single Chloroplast based on the Streak Camera

Yuki Fujita, XianJun Zhang, Naoya Kaneda, Yutaka Shibata (*Grad. Sch. Sci., Univ. Tohoku*)

Time-resolved fluorescence (FL) spectroscopy by the streak camera is a strong tool to evaluate the energy transfer kinetics within a photosynthetic complex. However, with *in vivo* studies, overlap of the FL spectra from different components makes accurate quantification difficult. Here, we propose a method to resolve the overlapped FL components by spatial decomposition based on the microscope. To achieve this, we developed Streak-Cryo-Microscope system so that one can acquire a time-wavelength 2-D FL image (streak image) of local areas in a microscope image. We succeeded in obtaining the streak images from the subregions enriched in photosystems I and II within a chloroplast at 80 K. This method enables detailed analysis of local energy transfer in the photosystems.

[3-11-1506](#) 二光子顕微鏡法での AMPK イメージングと ATP イメージングで見たマウス桿体視細胞の代謝回復
Two-Photon AMPK and ATP Imaging Reveals Metabolic Recovery in Mouse Rod Photoreceptor Cells

Shinya Sato^{1,2}, Jiazhou He¹, Masamichi Yamamoto², Kenta Sumiyama³, Yumi Konagaya⁴, Kenta Terai⁵, Michiyuki Matsuda^{1,5,6} (¹Grad. Sch. Biostudies, Kyoto Univ., ²National Cerebral and Cardiovascular Center Research Institute, ³Osaka Inst., Riken, ⁴Weill Cornell Med., ⁵Grad. Sch. Med., Kyoto Univ., ⁶iCeMS, Kyoto Univ.)

Rod and cone photoreceptor cells consume ATP very rapidly. To understand the metabolism of rods and cones, we visualized cellular AMP-activated protein kinase (AMPK) activity and ATP levels by two-photon microscopy. Transgenic mice expressing a hyBRET-AMPK biosensor and GO-ATeam2 biosensor were used for measuring the AMPK activity and ATP level, respectively. Metabolic responses were detected in the live retinal explants upon drug perfusion. A glycolysis inhibitor, 2-deoxy-D-glucose (2-DG), activated AMPK and reduced ATP. These effects were clearly stronger in rods than in cones. Notably, rod AMPK and ATP started to recover at 30 min from the onset of 2-DG perfusion. We propose that rods become less dependent on glycolysis within 60 min upon the glycolysis inhibition.

[3-11-1518](#) **マイクロビーム用いた細胞質損傷を起因とした防衛的な細胞応答の解析**
Microbeam irradiation and analysis on cytoplasm damage induced defensive cellular response

Teruaki Konishi¹, Alisa Kobayashi^{1,2}, Daisuke Ohsawa¹, Masakazu Oikawa^{1,2}, Jun Wang³ (¹Single Cell Radiation Biology Group, National Institutes for Quantum and Radiological Science and Technology, ²Electrostatic Accelerator Operation Section, National Institutes for Quantum and Radiological Science and Technology, ³Key Laboratory of High Magnetic Field and Ion Beam Physical Biology, Chinese Academy of Sciences)

Primary target of radiation is the cellular DNA, but consequence of cytoplasmic damage is yet to be understood. Taking advantage of SPICE-QST microbeam, we performed a cytoplasm targeted irradiation (Cyto-IR) of the WI-38 cells to investigate the cytoplasmic damage response. We focused on the activation of nuclear factor (erythroid-derived 2)-like 2 (NRF2) and its antioxidative signaling pathway. As a result, Cyto-IR induced mitochondria fragmentation, which accelerated the mitochondrial superoxide (MitoSOX) production. MitoSOX triggered the NRF2 nucleus translocation and upregulated the expression of its target genes, such as heme oxygenase 1. Overall, NRF2 antioxidative response is suggested to play a key role against DNA damage under cytoplasmic irradiation.

[3-12-1330](#) **細胞内シグナリング経路を表したタンパク質間相互作用の有向グラフ**
Directed Protein-Protein Interaction Network Representing Intracellular Signaling Pathways

Wenruo Cao, Ryotaro Koike, Motonori Ota (*Grad. Sch. Info., Univ. Nagoya*)

By the modern technology of proteomic analysis, a large number of data for protein-protein interactions (PPI) have been revealed. However, they do not indicate the directions of information processing. Here, we describe the directed PPI network for intracellular signaling pathways. From the SwissProt database, receptor proteins in cell membrane and DNA-binding proteins in nucleus were selected as starting and ending nodes. Using PPI data in HPRD, two proteins in two node groups were connected by solving the shortest path problem. We examined directed PPI network obtained in terms of path length, and feature and population of intermediate nodes, etc. The results in detail will be reported in the presentation.

[3-12-1342](#) **ジペプチドのエネルギー準位統計と分子進化**
Energy level statistics of dipeptides and molecular evolution

Masanori Yamanaka (*CST, Nihon Univ.*)

The energy level of the dipeptides was calculated by quantum chemistry calculation. The obtained energy levels were analyzed according to the procedure of energy level statistics. To generate statistical data, we performed a multipoint calculation on molecular structures produced via the molecular dynamics simulation. We try to determine the universality class in the random matrix theory for the valence orbitals and the unoccupied orbitals. These dipeptides are considered to be in a type of critical state, which is relevant for proteogenesis, the molecular evolution of protein.

[3-12-1354](#) **グラフニューラルネットワークを使ったタンパク質-補酵素結合予測**
Protein-cofactor binding prediction with graph neural networks

Masafumi Shionyu, Atsushi Hijikata (*Fac. Biosci., Nagahama Inst. Bio-Sci. Tech.*)

Several computational approaches for predicting protein functions were so far developed. However, many amino acid sequences are not functionally annotated yet. Thanks to state-of-the-art methods for predicting protein 3D structures, such as AlphaFold, we can use 3D structure information for many function-unknown proteins to predict their ligands or cofactors. We developed a graph neural network model named ProLMS-GNN, which learns simple features of cofactor binding residues, such as binding propensity and surface geometry, to predict cofactor-binding residues and cofactor binding. ProLMS-GNN showed high prediction performance compared with other methods and could detect cofactor binding without learning features from homologous proteins.

3-12-1406 単一インフルエンザウイルス集団中のヘマグルチニンゲノム配列の分布測定
Heterogeneity of Hemagglutinin Gene within Single-Plaque Population of Influenza Virus
Revealed by Single-Molecule Sequencing Method

Kenji Tamao¹, Masayuki Suetsugu², Hiroyuki Noji¹, Kazuhito Tabata¹ (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 developed a sequencing protocol of single-molecule influenza virus genome to investigate sequence heterogeneity of hemagglutinin (HA) gene. As a result of single-molecule sequencing of HA gene of influenza A/PR/8/34, various mutations were found in single-plaque population. It should include mutations due to viral replication and errors due to sequencing reactions. Thus, this study showed that single plaque population has significant heterogeneity in HA gene, and for more quantitative analysis, the effect of sequence error needs to be studied.

3-12-1418 疾患—タンパク質—ドラッグのネットワークグラフを用いた新しい創薬ターゲット予測法
A new method to predict potential drug targets using a disease-protein-drug network graph

Atsushi Hijikata, Masafumi Shionyu, Tsuyoshi Shirai (*Nagahama Inst. Bio-Sci. Tech.*)

One of the major bottlenecks in drug development studies is identifying potential drug targets. At the last annual meeting, we have reported Drug Target eXcavator (DTX), an integrative database for exploring new potential drug targets in the molecular network. We extensively analyzed the shortest molecular paths between the disease-drug pairs in the DTX database, and used the path information for machine learning. We found that a GBDT approach with molecular features of nodes in the paths could accurately discriminate between the paths from diseases to the therapeutic and non-effective drugs. This result indicated that evaluating the shortest paths from a given disease to a protein by DTX makes it possible to predict a new potential drug target.

3-12-1430 Revisiting structural and functional features of phosphorylation sites

Hafumi Nishi^{1,2,3} (¹*Grad. Sch. Info. Sci., Tohoku Univ.*, ²*Fac. Core Res., Ochanomizu Univ.*, ³*ToMMo, Tohoku Univ.*)

Phosphorylation is one of the most common post-translational modifications in various species. It is reported that phosphorylation sites have unique structural characteristics, which are strongly related to their molecular and cellular function. However, most phosphosites are in disorder regions, and the lack of complete structural information prevents a full understanding of their structural features. Here I performed a comprehensive analysis of human phosphorylation sites with the AlphaFoldDB models. A significant fraction of phosphosites were located on high pLDDT score regions, namely predicted structured regions or short loops. Additionally, around 10% of phosphosites were identified as buried, which can be potential sites causing structural changes.

3-12-1442 回転並進同変なニューラルネットワークを用いた蛋白質間相互作用部位予測の検討
Towards protein interface prediction using roto-translation equivariant neural network

Tsukasa Nakamura (*JSPS-PD/Grad. Sch. Info. Sci., Tohoku Univ.*)

Predicting protein interfaces from protein monomer structures is important for large-scale structure prediction of protein complexes. SE(3)-Transformer is one of the neural network models that take as input a connected graph in which each node has coordinate information, such as a graph constructed from a 3D point cloud. In this model, equivariance is guaranteed for 3D rotational and translational transformations of input, and stable feature computation is possible. In this study, I applied this model to structure data of protein-protein interfaces. A structure data is a 3D point cloud of atoms, and in this sense, it is expected that using this model will have an advantage in prediction performance.

3-13-1330 Whole-mount cryo-TEM 観察による *Mycobacterium avium* 株間の菌体基礎形態情報の比較検討
Comparison of fundamental cell morphology between strains of *Mycobacterium avium*
examined with whole-mount cryo-TEM

Hiroyuki Yamada¹, Kinuyo Chikamatsu¹, Akio Aono¹, Kazuyoshi Murata², Naoyuki Miyazaki^{2,3}, Youko Kayama⁴, Satoshi Mitarai^{1,5} (¹Dept. *Mycobacterium Ref. Res., RIT, JATA.*, ²NIPS, ³Ohtsuka Pharm., ⁴Terabase Inc., ⁵Nagasaki Univ.)

Mycobacterium avium (MAV) is one of the pathogenic bacterial species belonging to the genus *Mycobacterium*, which contains *M. tuberculosis* and *M. leprae*. MAV represents varied individual cell morphology between and within strains. In this study, a total of more than 1000 fundamental cell morphologies of the eleven strains of MAV were analyzed through a whole-mount cryo-TEM examination. Cell diameter, length, perimeter, circularity, and aspect ratio were measured with Fiji/ImageJ. Among all comparisons, only 20% of comparisons were non-significant, the other comparisons between strains showed significant differences. In addition, it is revealed that the ratio of the longest vs. the shortest cell length (L/S ratio) differentiate two groups with the cut-off value of 3.3.

3-13-1342 液中 AFM による肺がん細胞の薬剤耐性獲得に伴うナノスケール表面構造変化の解明
Changes in Nanoscale Surface Structures of Lung Cancer Cells Associated with Acquisition of
Drug Resistance Investigated by In-Liquid AFM

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Molecular-targeted drugs bind specifically to cancer cells with relatively few side effects. However, cancer cells often acquire drug resistance after long-term administration. Lung cancer cells A925L and H1975 are respectively resistant to crizotinib and osimertinib associated with epithelial-mesenchymal transition (EMT). However, it is difficult to recognize this transition in morphological diagnosis. In this study, we performed atomic force microscopy measurements for detecting the differences between the lung cancer cells (A925L, H1975) with and without the drug resistance. Interestingly, both A925L and H1975 showed a significant decrease in cell surface microvilli and changes in elastic modulus after the acquisition of drug resistances.

3-13-1354 生体高分子の 3D-AFM 像の走査速度依存性の理論予測
A theoretical prediction of dependency of three-dimensional atomic force microscopy images
of biopolymers on scanning velocity

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Three-dimensional atomic force microscopy (3D-AFM) has resolved three-dimensional distribution of solvent molecules at solid-liquid interfaces and is being expected to resolve 3D structures of biopolymers such as chromosomes when it is applied to them. So far, we developed a method to compute 3D-AFM images of biopolymers using polymer simulation. Here, we simulated 3D-AFM images of biopolymers with changing vertical scanning velocity. It was found that insufficient force acts between probe and sample when scanning velocity is slower than the intrinsic speed of the sample. When scanning velocity is too fast, fiber structure was not resolved. Thus, the optimal velocity was found to exist in the range of several to ten-times faster than the intrinsic speed of the sample.

3-13-1406 NMR メタボロームを用いた昆虫食に関する研究
Research of Entomophagy by NMR-based Metabolomics

Li Gan, Zihao Song, Yuki Ohnishi, Hiroyuki Kumeta, Yasuhiro Kumaki, Tomoyasu Aizawa (*Grad. Sch. Life Sci., Univ. Hokkaido*)

Eri silkworm (*Samia cynthia ricini*) is a traditional source of food in northeast India. Although the nutrient composition of eri silkworm pupa has been studied, there are few studies on its taste and metabolite changes during pupal periods. Therefore, the study was undertaken to research the changes of taste-related components of eri silkworm pupa (day 1, day 2, and day 3) by using NMR-based metabolomics. The metabolome consisted of 28 metabolites, including amino acids, sugars, organic acids, and other organic components. Quantitative analysis showed that the amount of taste-related metabolites composition of eri silkworm pupa on different pupal periods was significantly different. Some taste-related components decreased with pupal growth.

[3-13-1418](#) Application of low field, benchtop NMR for discriminating metabolic signature of DSS-induced colitis model mice from the healthy

Zihao Song¹, Yuki Ohnishi¹, Seiji Osada², Li Gan¹, Hiroyuki Kumeta¹, Yasuhiro Kumaki¹, Kiminori Nakamura¹, Tokiyoshi Ayabe¹, Kazuo Yamauchi³, Tomoyasu Aizawa¹ (¹*Grad. Sch. Life Sci., Univ. Hokkaido*, ²*Nakayama Co., Ltd.*, ³*Instrumental Analysis Section, OIST*)

Metabolomics has shown its potential of recognizing a range of diseases. Indeed, high-field nuclear magnetic resonance (NMR) spectroscopy represents one of the routinely used approaches for metabolomics study while further application for the point-of-care diagnosis suffers from large size, high cost and transportation limitation. In this study, we applied low field NMR (60 MHz) and high field NMR (800 MHz) to characterize and compare 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 healthy control. In addition, the concentration of acetate can be quantified with high accuracy based on 60 MHz NMR spectra.

[3-13-1430](#) Manganese-enhanced MRI enables early detection of neuroinflammation in the rat brain

Sosuke Yoshinaga¹, Satoshi Fujiwara¹, Shigeto Iwamoto¹, Sayaka Shibata², Aiko Sekita², Nobuhiro Nitta², Tsuneo Saga², Ichio Aoki², Hiroaki Terasawa¹ (¹*Fac. Life Sci., Kumamoto Univ.*, ²*NIRS, QST*)

Neuroinflammation is initiated by many types of neural disorder as a defensive response of the innate immune system in the central nervous system. Neuroinflammation is typically accompanied by the disruption of Calcium ion (Ca²⁺) homeostasis. Manganese ion (Mn²⁺) is a useful positive MRI contrast agent that behaves like Ca²⁺ *in vivo*, and is utilized in Manganese-Enhanced MRI (MEMRI) for functional neuroimaging. We sought to determine whether MEMRI could be used to assess the cellular alterations caused by acute neuroinflammation *in vivo*, by focusing on Mn²⁺ accumulation in the brain. In the hippocampus of the neuroinflammation model rat, MEMRI signal-enhanced areas corresponded to the areas with activated microglia, revealed by immunohistochemical analyses.

[3-14-1330](#) 透過型電子顕微鏡の最大感度をもたらす φ ヒルベルト位相板
φ-Hilbert Phase Plates That Assure the Highest Sensitivity of Transmission Electron Microscopy

Kuniaki Nagayama (*N-EM Laboratories*)

In transmission electron microscopy (TEM), two classes of phase plates (PPs) are known, one is the Zernike PP, which retards the electron wave phase by $\pi/2$ and the other the Hilbert PP, which does by π . Images obtained with the two kind of PPs are connected through the Hilbert transform and hence they are equivalent in sensitivity. Recently, we have found the third class that can exceed the two classes in sensitivity, namely ϕ -Hilbert PPs where ϕ is the PP phase close to $3\pi/4$. The comprehensive theory of 4-dimensional (4D) EM tells that ϕ -Hilbert PPs are not only best among the three classes of PPs but also better in sensitivity than any other EM methods that has been proposed so far. Its theoretical foundation together with TEM simulations will be shown.

[3-14-1342](#) ナノスケール量子計測を用いたラベルフリー脂質二重層相転移計測
Label-free phase change detection of lipid bilayers using nanoscale diamond magnetometry

Hitoshi Ishiwata^{1,2}, Hiroshi C. Watanabe^{1,3}, Shinya Hanashima⁴, Takayuki Iwasaki², Mutsuko Hatano² (¹*PRESTO JST*, ²*School of Engineering, Tokyo Institute of Technology*, ³*Quantum Computing Center, Keio University*, ⁴*Department of Chemistry, Graduate School of Science, Osaka University*)

The cell membrane (lipid bilayer) is a nanoscale (~5nm thick) 2D fluid crystalline assembly with sub-compartment phases that determines cellular functions. In this manuscript, diffusion constant of a lipid bilayer, a biological parameter that determines the dynamics of the lipid bilayer, was determined by making use of extremely small detection volume offered by nanoscale NMR using NV center in diamond. Observation of diffusion constant reveals different phases of lipid bilayer which identifies sub-compartment domains that are critical for cellular functions. The result builds foundation for label-free imaging of cell membranes for observation of phase composition and pristine dynamics that determines cellular functions.

[3-14-1354](#) 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を用いたガスセンサシステム

Gas sensor system using composite molecular film of fatty acid and coumarin enhanced by hydrogenated amorphous silicon

Hikaru Hatakeyama¹, Kairi Shimazaki¹, Shu Mugita¹, Takuro Sato¹, Kenta Shirasu¹, Hiroshi Masumoto², Yutaka Tsujiuchi¹
(¹Grad. Mat. Sci. UNiv. Akita, ²Fris. Univ. Tohoku)

For the purpose of designing a high precision bio sensor, ionic state of composite molecular film of fatty acid and coumarin and fluorescent properties was 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 fluorescent intensity of 7-hydroxy-4-methylcoumarin (7C) and 4-hydroxymethylcoumarin (4C) depend on the concentration of a volatile organic compound, ammonia was measured. 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.

[3-14-1406](#) 電子顕微鏡を利用した繊維状蛋白質の解離定数の新規測定法の開発

Development of a new method to measure dissociation constant of filamentous protein complexes by electron microscopy

Masato Watanabe¹, Hiroshi Imai¹, Tomoko Miyata³, Fumiaki Makino^{3,4}, Etsuko Muto⁵, Christoph Gerle², Kaoru Mitsuoka⁶, Genji Kurisu², Keiichi Namba³, Takahide Kon¹ (¹Grad. Sch. Sci., Osaka Univ., ²IPR, Osaka Univ., ³Grad. Sch. Frontier Biosci., Osaka Univ., ⁴JEOL, ⁵Chuo Univ., ⁶Res. Ctr. UHVEM, Osaka Univ.)

Assembly and disassembly of filamentous protein complexes play important roles in eukaryotic and procaryotic cells. However, there is no method to simultaneously measure the protein structure and association/dissociation parameters. Here we have developed a new method to measure dissociation constant by negative stain electron microscopy. As a test sample, we have used glutamate dehydrogenase (GDH) hexamers. We observed EM images of GDH hexamers under a wide range of protein concentration (0.002-5 mg/ml) and successfully determined dissociation constant of GDH hexamer by counting the particle number of GDH oligomers in the EM images. This new method would be applicable for determination of dissociation constant of varieties of filamentous protein complexes.

[3-14-1418](#) Visualizing individual dengue virus maturation states using high-speed atomic force microscopy

Steven John McArthur, Noriyuki Kodera (*WPI-Nano Life Sciences Inst., Kanazawa Univ.*)

One of the key steps in the lifecycle of dengue viruses (DENV) is the proteolytic maturation of the membrane precursor (prM) glycoprotein. Maturation is required for infectivity, and involves significant conformational changes of the viral protein coat. Immature virions at neutral pH exhibit trimeric spikes of prM-envelope (E) protein complexes; in mature particles these spikes have dissociated and re-formed in a dimeric smooth herringbone-like pattern. While these phenomena have been observed in vitrified samples by cryoEM, the maturation of individual particles in a liquid buffer at ambient temperature has never been observed. Here, we apply high-speed atomic force microscopy to directly observe the spiky and smooth conformations of individual DENV-2 particles.

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Horiike, Yoshiaki (堀池 由朗)	2-14-1612			Iida, Akane (飯田 茜)	2-09-1624
Horikawa, Kazuki (堀川 一樹)	1S13-6			Iida, Hiroyuki (飯田 泰由)	3-01-1454
Horikawa, Riichi (堀川 凜一)	2-13-1724			Iida, Takahiro (飯田 高広)	2S2-7
Horikawa, Sayuri (堀川 小百合)	1-13-1342			Iida, Takahito (飯田 隆仁)	2-04-1503
Horikoshi, Naoki (堀越 直樹)	2-02-1327			Iida, Tatsuya (飯田 龍也)	1-07-1430
Horitani, Masaki (堀谷 正樹)	1-02-1418			Iijima, Mikuru (飯島 美来)	2-03-1415
	3-02-1406			Iino, Ryota (Iino Ryota)	1S1-3
	3-04-1406				3-07-1342
Horitsni, Masaki (堀谷 正樹)	3-02-1430			Iino, Ryota (飯野 亮太)	1-07-1430
Horonushi, Dan (襲主 暖)	1-08-1342			Iizuka, Ryo (飯塚 怜)	1-16-1406
	1-09-1342				1-16-1518
Hosain, Mohammad Mubarak (ホサイン モハマッドム バロケ)	2-16-1748				2-15-1712
Hosain, Mohammad Mubarak (ホサイン モハマッドム バラク)	2-16-1403			Iizuka, Tomona (飯塚 友菜)	2-02-1427
Hoshino, Yoshihiko (星野 仁彦)	3-05-1406				3-04-1418
Hosokawa, Chic (細川 千絵)	2-09-1600			Ikawa, Keisuke (井川 敬介)	2-14-1327
Hosokawa, Naoki (細川 直輝)	2-01-1636			Ikeda, Atsushi (池田 篤志)	2-08-1624
Hosokawa, Toshihito (細川 俊仁)	2-01-1700			Ikeda, Keisuke (池田 恵介)	1-10-1454
				Ikeda, Kota (池田 幸太)	1-14-1430
				Ikeda, Mari (池田 真理)	2-09-1327

Ito, Hiroshi (伊藤 浩史)	1S7-7	Izri, Ziane (イズリ ジャン)	2-08-1415
Ito, Honami (伊藤 帆奈美)	2-11-1612	Izumi, Mao (和泉 真生)	2-16-1824
Ito, Keisuke (伊藤 敬佑)	1-16-1406	Izumi, Yoshihiro (和泉 自泰)	3S6-5
Ito, Kenta (伊藤 健太)	2-07-1515	Jha, Siddharth (Jha Siddharth)	1S7-5
Ito, Kohji (伊藤 光二)	2-07-1427	Jia, Tony Z (Jia Tony Z)	1S10-1
	3-06-1354	Jibiki, Yoshino (地引 芳乃)	2-15-1527
Ito, Kota (伊藤 滉太)	1-04-1454	Jin, Jianshi (Jin Jianshi)	3S6-6
Ito, Mei (伊藤 芽)	1-16-1518	Joshua, Stanfield (Joshua Stanfield)	2-06-1439
Ito, Minako (伊藤 美菜子)	1S13-5	Jung, Jaewoon (Jung Jaewoon)	1S3-4
Ito, Nana (伊藤 那奈)	2-09-1648		2S6-1
Ito, Natsuki (伊藤 夏希)	1-10-1330		2-01-1712
Ito, Takahiro (伊藤 貴浩)	2-14-1724	Jung, Jaewoon (鄭 載運)	1-03-1330
Ito, Yuma (伊藤 由馬)	2-15-1724	Jurica, Peter (ユリツァ ペテル)	2-14-1415
	2-15-1748	Justin, Chan (ジャスティン チャン)	2-11-1800
	2-15-1812	Kabir, Arif Md. Rashedul (Kabir Arif Md. Rashedul)	2-07-1812
	2-15-1824		3-01-1430
	2-16-1812	Kabir, M. Golam (Kabir M. Golam)	1-04-1506
Ito-Miwa, Kumiko (三輪 久美子)	2S5-5	Kadokura, Hiroshi (門倉 広)	2S2-6
Ito-Miwa, Kumiko (三輪 (伊藤) 久美子)	2S5-1		1-02-1506
Itoh, Ayaka (伊藤 綾香)	2-09-1612	Kadono, Ai (楞野 亜衣)	2-11-1736
	2-16-1327	Kagawa, Yuki (加川 裕貴)	2-07-1315
Itoh, Kaho (伊藤 夏穂)	2-09-1700		2-07-1824
Itoh, Satoru (伊藤 暁)	2-05-1724	Kage, Azusa (鹿毛 あずさ)	2-07-1451
Itoh, Shigeru (伊藤 繁)	2-11-1700		2-09-1748
Itoh, Thoma (伊藤 冬馬)	2-13-1624	Kaida, Shingo (海田 新悟)	2-01-1439
Itoh, Yuji (伊藤 優志)	2-15-1648	Kaizuka, Yoshihisa (貝塚 芳久)	1-08-1454
Iwadate, Yoshiaki (岩楯 好昭)	2-08-1339	Kaji, Mizuki (榎 瑞基)	2-10-1636
	2-08-1600	Kajimoto, Haruya (梶本 遥也)	3-02-1454
Iwai, Shigenori (岩井 成憲)	2-11-1712	Kajimoto, Shinji (梶本 真司)	2-04-1600
	2-11-1724		2-04-1624
Iwaki, Mitsuhiro (岩城 光宏)	1-15-1518		2-04-1636
	2-07-1636		2-15-1351
Iwaki, Nanako (岩城 奈那子)	1-04-1518		2-15-1415
Iwamoto, Hiroyuki (岩本 裕之)	1-04-1342		2-15-1427
	2-08-1724	Kajimoto, Shinji (梶本 真司)	2-15-1403
Iwamoto, Koji (岩本 浩司)	2-08-1327	Kajimura, Naoko (梶村 直子)	2-07-1403
Iwamoto, Masayuki (岩本 真幸)	3-10-1342	Kajino, Hiroki (梶野 洗樹)	1-10-1418
	3-10-1430	Kajiwara, Riichi (梶原 利一)	2-09-1451
Iwamoto, Shigeto (岩本 成人)	3-13-1430	Kakizuka, Taishi (垣塚 太志)	1S13-6
Iwanaga, Misaki (岩永 美咲)	2-08-1339	Kakugo, Akira (Kakugo Akira)	2-07-1812
Iwasaki, Kenji (岩崎 憲治)	2S1-3	Kakugo, Akira (角五 彰)	1-16-1354
	2-02-1327		3-07-1330
Iwasaki, Shintaro (岩崎 信太郎)	3S2-1		3-07-1354
Iwasaki, Takayuki (岩崎 孝之)	3-14-1342	Kamada, Kaho (鎌田 果歩)	2-15-1600
Iwasaki, Wataru (岩崎 渉)	2-13-1415	Kamagata, Kiyoto (鎌形 清人)	1S4-4
Iwase, Hiroki (岩瀬 裕希)	2-04-1736		1-04-1518
Iwashita, Tomoya (岩下 智哉)	2S6-2	Kamarulzaman, Latiefa (Kamarulzaman Latiefa)	1S5-5
	2-03-1327	Kameda, Takeru (亀田 健)	3-05-1330
Iwata, Seiya (岩田 聖矢)	2-06-1403	Kameda, Tomoshi (亀田 倫史)	2-05-1600
Iwata, So (岩田 想)	2-06-1403	Kamei, Kenichiro F. (亀井 健一郎)	1-15-1418
	3-02-1342	Kameo, Yoshitaka (亀尾 佳貴)	1-14-1506
Iwata, Tatsuya (岩田 達也)	2-11-1527	Kamikubo, Hironari (上久保 裕生)	2S5-3
Iwaya, Katsuhisa (岩屋 克尚)	2-04-1439		

	1-01-1442	Kasahara, Kota (笠原 浩太)	1-03-1506
	1-04-1442		1-12-1442
	2-04-1800		1-13-1418
	3-02-1454		2-03-1527
	3-11-1330		2-03-1736
	3-11-1342		2-03-1812
	3-11-1354		2-13-1748
Kamimura, Atsushi (上村 淳)	2-14-1451	Kasahara, Kouta (笠原 浩太)	2-02-1712
Kamimura, Shinji (上村 慎治)	1-04-1342	Kasahata, Naoki (笠畑 尚喜)	2-16-1624
	2-07-1403	Kasai, Chic (笠井 千枝)	2-06-1439
Kamiya, Koki (神谷 厚輝)	2-04-1339	Kasai, Hitoshi (笠井 均)	2-15-1403
	2-10-1315	Kasai, Rinshi (笠井 倫志)	1-10-1342
Kamo, Takanari (加茂 尊也)	3-11-1418		3-08-1406
Kanai, Yasushi (金井 康)	2-15-1600	Kasai, Rinshi S (笠井 倫志)	1-09-1354
Kanakubo, Yuki (金久保 有希)	2-10-1712	Kasai, Rinshi S. (笠井 倫志)	1-15-1342
Kanamamaru, Shuji (金丸 周司)	1-04-1354	Kasai, Takuma (葛西 卓磨)	2-05-1712
	1-16-1506	Kashihara, Kenichiro (榎原 賢一朗)	2-06-1427
Kanamamaru, Tomoko (金丸 朋子)	1-16-1506	Kashima, Junta (鹿嶋 純太)	1-09-1454
Kanamura, Setsuko (金村 節子)	1S14-6		3-09-1330
Kanbayashi, Saori (上林 さおり)	1-04-1518	Kashino, Yasuhiro (菓子野 康浩)	2-11-1700
Kanda, Tomoki (神田 知樹)	2-11-1403	Kashiwagi, Hiroko (柏木 広子)	1-08-1518
Kandori, Hideki (神取 秀樹)	1-11-1418	Katahira, Masato (片平 正人)	3-05-1418
	1-11-1454		3-05-1442
	2-02-1339	Katayama, Kohei (片山 康平)	2-15-1503
	2-04-1700	Katayama, Kota (片山 耕太)	1S6-7
	2-06-1403		2-04-1700
	2-11-1527		2-06-1403
	2-12-1439		2-12-1700
	2-12-1636		2-12-1712
	2-12-1648	Katayama, Ryosuke (片山 涼介)	2-13-1439
	2-12-1700	Katayama, Yoshiki (片山 佳樹)	1-08-1354
	2-12-1712		1-08-1406
	2-12-1748		2-10-1339
	2-12-1800	Kato, Hideaki (加藤 英明)	2-01-1515
	2-12-1812		3-02-1342
Kaneda, Naoya (金田 直也)	2-11-1351	Kato, Koichi (加藤 晃一)	2-04-1724
	3-11-1454	Kato, Koji (加藤 公兎)	2-12-1503
Kaneko, Jun (金子 淳)	1S3-5	Kato, Kosuke (加藤 広介)	2-02-1327
Kaneko, Kunihiko (金子 邦彦)	1S14-1	Kato, Minoru (加藤 稔)	3-05-1430
	2-14-1600	Kato, Shuzo (加藤 修三)	2-14-1339
	2-14-1712	Kato, Soichiro (加藤 壮一郎)	2-02-1339
Kaneko, Ryusei (金子 竜晟)	1S13-5	Kato, Takasumi (加藤 貴純)	1-02-1430
Kaneko, Taikopaul (金子 泰洗ボール)	3S6-2	Kato, Takayuki (加藤 貴之)	1-02-1442
	2-15-1736		2-01-1800
Kaneko, Tomoyuki (金子 智行)	2-10-1403		2-07-1403
	2-10-1748		2-07-1439
	3-09-1342	Kato, Yuki (加藤 佑樹)	2-11-1612
Kaneko, Toshiyuki (金子 智之)	2-07-1612	Katoh, Takanobu A (加藤 孝信)	2-13-1636
Kanekura, Kohsuke (金蔵 孝介)	2-15-1612	Katsurashima, Yuro (桂嶋 優呂)	1-14-1518
Kanemaki, Masato (鐘巻 将人)	1S7-2	Katsuta, Yuji (勝田 雄治)	2-16-1636
Kanematsu, Yusuke (兼松 佑典)	1S3-3	Kawabata, Takeshi (川端 猛)	2-03-1700
Kano, Kohei (加納 康平)	2-02-1403	Kawade, Raiji (河出 来時)	2-04-1315
Kasahara, Keisuke (笠原 慶亮)	2-04-1315	Kawagishi, Ikuro (川岸 郁朗)	1-01-1454

	1-07-1518		3-09-1354
	2-06-1427		3-09-1406
	2-09-1648		3-04-1454
Kawagoe, Soichiro (川越 聡一郎)	2-04-1812	Kidokoro, Shun-ichi (城所 俊一)	2-05-1712
Kawaguchi, Kazutomo (川口 一朋)	2-10-1503	Kigawa, Takanori (木川 隆則)	2-02-1503
	2-11-1648	Kihara, Daisuke (木原 大亮)	1-09-1506
Kawahara, Rui (川原 るい)	2-06-1351	Kijima, Saku (貴嶋 紗久)	2S1-1
Kawahara, Toshio (河原 敏男)	2-15-1600	Kikkawa, Masahide (吉川 雅英)	2S2-6
Kawai, Hisako (河合 寿子)	2S2-3		1-02-1506
Kawakami, Keisuke (川上 恵典)	1-02-1330		2-02-1415
	1-02-1342	Kikuchi, Hiroto (菊地 浩人)	2-11-1339
	2-11-1700	Kikuchi, Kenji (菊地 謙次)	2-09-1748
Kawakami, Kouki (川上 耕季)	2-01-1515	Kikuchi, Rio (菊地 莉緒)	2-06-1315
Kawakami, Tohru (川上 徹)	2-06-1700	Kikuchi, Takeshi (菊地 武司)	1-03-1442
Kawakatsu, Toshihiro (川勝 年洋)	2-13-1327		1-03-1454
Kawakubo, Wataru (川久保 渉)	1-16-1518	Kikuchi, Yousuke (菊池 洋輔)	2-01-1648
Kawama, Kosuke (河間 光祐)	2-02-1636	Kikukawa, Takashi (菊川 峰志)	1-02-1430
Kawamata, Ibuki (川又 生吹)	1-16-1354		1-06-1330
	2-05-1527		1-11-1430
	3-07-1354		1-11-1442
Kawamoto, Akihiro (川本 晃大)	2-01-1315		2-06-1327
Kawamura, Izuru (川村 出)	2-12-1403		2-06-1339
Kawamura, Masato (川村 勝人)	2-02-1724		2-06-1415
	2-02-1736		2-12-1503
Kawamura, Mina (河村 味奈)	2-06-1748		2-12-1724
Kawamura, Ryuzo (川村 隆三)	2-01-1748	Kim, Eunchul (金 恩哲)	2S2-3
Kawanishi, Shiho (川西 志歩)	2-12-1612	Kim, Hyuno (Kim Hyuno)	3-08-1330
	2-12-1824	Kim, Sooyeon (金 水縁)	1S5-5
Kawano, Ryuji (川野 竜司)	2S7-4	Kim, Suhyang (金 穗香)	3-11-1330
	2-04-1648	Kim, Yoon (Kim Yoon)	3-02-1342
	2-05-1327	Kimura, Akatsuki (木村 暁)	2-07-1712
	1S11-2		2-08-1403
Kawasaki, Hisashi (川崎 寿)	2-13-1700	Kimura, Akihiro (木村 明洋)	2-11-1700
Kawasaki, Koji (川崎 洸司)	1-02-1354	Kimura, Hiroshi (木村 啓志)	2-14-1415
Kawasaki, Masato (川崎 政人)	2-12-1327	Kimura, Masahiko (木村 雅彦)	2-15-1600
Kawasaki, Yuma (川崎 佑真)	3-10-1354	Kimura, Michiko (木村 美智子)	1-04-1518
Kawashima, Nobuyuki (川島 信幸)	1-04-1430		3-04-1354
Kawata, Yasushi (河田 康志)	2-09-1327	Kimura, Satomi (木村 聡見)	2-16-1824
Kawato, Suguru (川戸 佳)	3-13-1330	Kimura, Tetsunari (木村 哲就)	1S3-2
Kayama, Youko (香山 容子)	1S6-6		1-02-1454
Kazama, Kazuki (風間 一輝)	2-01-1451		1-02-1518
	2-16-1724		1-06-1406
Kazuta, Yasuaki (數田 恭章)	1-08-1406	Kimura, Yusuke (木村 優介)	1-10-1454
KC, Biplab (KC Biplab)	1-08-1354	Kinbara, Kazushi (Kinbara Kazushi)	1S1-3
KC, Biplab (ケーシー ビップラブ)	1S14-3		3-07-1342
Keegstra, Johannes M. (Keegstra Johannes M.)	1S1-3	Kinoshita, Kengo (木下 賢吾)	2S1-5
Keya, Jakia Jannat (Keya Jakia Jannat)	3-01-1430		1-12-1406
	3-07-1342		3-03-1506
Keya, Jakia Jannat (ケヤ ジャナット ジャキア)	1-16-1354	Kinoshita, Masahiro (木下 正弘)	2-02-1724
	2-07-1748	Kinoshita, Miki (木下 実紀)	2-07-1527
Khanh Huy, Bui (カーン フイ ブイ)	2-10-1636	Kinoshita, Saki (木下 紗季)	2-13-1527
Kibata, Hideto (木畑 秀仁)	2-13-1724	Kinoshita, Seisho (木下 清晶)	2-04-1748
Kidokoro, Ryu (城所 龍)		Kinosita, Yoshiaki (木下 佳昭)	3-06-1430

Kise, Yoshiaki (木瀬 孔明)	1-06-1442	2-16-1427
Kishi, Koichiro (岸 孝一郎)	3-02-1342	3-14-1418
Kishikawa, Jun-ichi (岸川 淳一)	1-02-1442	Koga, Nobuyasu (古賀 信康)
	3-02-1330	1S6-6
Kishimoto, Hiraku (岸本 拓)	2-11-1636	2-01-1439
Kishimura, Akihiro (岸村 顕広)	1-08-1354	2-01-1451
	1-08-1406	Koide, Hiroki (小出 洋輝)
	2-10-1339	3-06-1342
Kita, Tomoki (北 智輝)	2-07-1327	Koike, Ryotaro (小池 亮太郎)
Kitajima-Ihara, Tomomi (北島(井原) 智美)	2-11-1600	1-04-1454
Kitamura, Ryota (北村 嶺太)	1-09-1330	1-12-1330
Kitamura, Taiki (北村 太樹)	3-13-1342	1-12-1418
Kitamura, Yoshihiro (北村 美一郎)	2-09-1439	1-13-1330
Kitanishi, Takuma (北西 卓磨)	2S3-1	3-12-1330
Kitao, Akio (北尾 彰朗)	1S11-6	2-09-1636
	1-03-1430	1-12-1430
	1-06-1518	1-08-1442
	2-03-1515	Koizumi, Nobuo (小泉 信夫)
Kito, Kentaro (鬼頭 健太郎)	3-09-1342	2-09-1600
Kitoh, Hirotaka (鬼頭 宏任)	2-11-1700	Kojima, Hiroaki (小嶋 寛明)
Kiuchi, Ryunosuke (木内 龍之介)	1-03-1430	2-08-1724
Kiyonaka, Riku (清中 大陸)	1-09-1442	2-16-1724
	1-09-1454	1-11-1430
	1S6-5	Kojima, Kaito (小島 快斗)
Kiyono, Ken (清野 健)	2-14-1415	3-09-1406
Kiyooka, Ryota (清岡 亮太)	2-03-1824	Kojima, Keiichi (小島 慧一)
Kizuka, Yasuhiko (木塚 康彦)	2-08-1503	1-11-1330
Kobayakawa, Tomoya (小早川 友哉)	2-05-1700	2-12-1612
Kobayashi, Akiko (小林 亜紀子)	2-16-1351	2-12-1624
Kobayashi, Alisa (小林 亜利紗)	3-11-1518	2-12-1736
Kobayashi, Chigusa (Kobayashi Chigusa)	2S6-1	2-12-1824
	2-01-1712	Kojima, Rei (小島 嶺)
Kobayashi, Chigusa (小林 千草)	1-03-1330	2-02-1439
	1-03-1418	Kojima, Seiji (小嶋 誠司)
Kobayashi, J. Tetsuya (小林 徹也)	1S5-2	2-05-1700
Kobayashi, Kan (小林 幹)	2-01-1515	2-08-1612
Kobayashi, Kazuhiro (小林 和弘)	2-01-1515	Kojima, Yoshino (児島 よしの)
Kobayashi, Mika (小林 美加)	1-05-1354	2-02-1315
Kobayashi, Naoya (小林 直也)	2-01-1439	2-04-1415
Kobayashi, Naritaka (小林 成貴)	2-01-1748	1S7-5
Kobayashi, Ryohei (小林 稜平)	1S1-1	Kole, Swapnil (Kole Swapnil)
	1-07-1418	1S9-5
	1-07-1454	Komaki, Shohei (小巻 翔平)
Kobayashi, Takuya (小林 拓也)	2-06-1403	1-09-1442
Kobayashi, Takuya (小林 琢也)	2-07-1624-Canceled	1-09-1454
	3-06-1418	3-01-1442
Kobayashi, Tetsuya J. (小林 徹也)	2-14-1451	3-09-1330
Kobayashi, Chigusa (小林 千草)	1S3-4	Komatsuzaki, Tamiki (小松崎 民樹)
Kobori, Yasuhiro (小堀 康博)	1-02-1518	1S4-7
	2-11-1527	2-15-1439
Kodera, Noriyuki (古寺 哲幸)	1-04-1418	Komatsuzaki, Yoshimasa (小松崎 良将)
	2-02-1327	2-16-1327
	2-16-1351	Komatsuzaki, Yoshimasa (小松崎 良将)
		2-09-1612
		Komi, Yusuke (小見 悠介)
		3-02-1354
		Komiyama, Ken (小宮 健)
		1-16-1454
		Komoto, Tetsushi (小本 哲史)
		2-14-1648
		Kon, Takahide (昆 隆英)
		2-07-1403
		3-14-1406
		Konagaya, Yumi (小長谷 有美)
		3-11-1506
		Kondo, Hiroko X. (近藤 寛子)
		1S3-3
		Kondo, Kaori (近藤 香織)
		1-11-1430
		Kondo, Keiko (近藤 敬子)
		3-05-1418
		3-05-1442
		Kondo, Naoshi (近藤 直)
		1S8-3
		2-02-1600
		2-02-1624

Kuwana, Satoshi (桑名 悟史)	3-09-1442	Maru, Takamitsu (丸 喬光)	1-02-1354
Kuwano, Wako (桑野 わ子)	2-06-1439	Marumo, Akisato (丸茂 哲聖)	2-15-1327
Kuwashima, Yutaro (桑島 佑太郎)	2S2-4	Maruta, Shinsaku (Maruta Shinsaku)	2-05-1636
	1-15-1330	Maruta, Shinsaku (丸田 晋策)	2-07-1351
Kuwata, Takumi (桑田 巧)	2-04-1427	Maruyama, Atsushi (丸山 厚)	2S7-6
Kuwayama, Hidekazu (桑山 秀一)	2-13-1315	Maruyama, Tomoki (丸山 朋輝)	2-10-1339
Kuzuya, Akinori (Kuzuya Akinori)	3-01-1430	Maruyama, Tomoya (丸山 智也)	2-13-1503
Laage, Damien (Laage Damien)	1S8-6	Maruyama, Yutaka (丸山 豊)	2-02-1351
Lee, Seohyun (Lee Seohyun)	3-08-1330	Marin, María del Carmen (María del Carmen Marin)	2-12-1515
Lei, Yici (雷 宜慈)	2-07-1403		2-12-1451
Li, Hongjie (Li Hongjie)	1S11-1	Masae, Konno (Masae Konno)	2-09-1451
Li, Meng (Meng Li)	2-12-1339	Masatoshi, Nishikawa (西川 正俊)	2-09-1648
Li, Shujie (李 書潔)	1-06-1418	Masuda, Youichi (増田 容一)	1-16-1342
Li, Xinxuan (Li Xinxuan)	1-09-1406	Masui, Ayumi (益井 歩未)	1-04-1430
Lim, Keesiang (Lim Keesiang)	2-16-1351	Masui, Takato (増井 貴登)	2-13-1351
Lin, Jinzhong (Lin Jinzhong)	3-05-1342	Masukawa, Marcos (Masukawa Marcos)	2-05-1415
Liu, Chujie (劉 楚傑)	2-06-1612	Masukawa, Marcos (マスカワ マルコス)	1-16-1430
Liu, Kehong (Liu Kehong)	3-02-1342	Masumoto, Hiroshi (増本 博)	2-16-1824
Liu, Runjing (劉 潤晶)	2-03-1403		3-14-1354
Liu, Yang (Yang Liu)	2-12-1339	Matsubara, Hitomi (松原 暉)	1-15-1518
Loo, Daniel WK (Loo Daniel WK)	1S10-5	Matsubara, Ryosuke (松原 亮介)	1-02-1454
Lowe, Lauren (Lowe Lauren)	1S10-5	Matsubara, Takeru (松原 猛)	2-16-1427
Lucena-Agell, Daniel (Lucena-Agell Daniel)	1-04-1342	Matsubara, Takumi (松原 巧)	2-11-1600
Machida, Manabu (町田 学)	1S12-5	Matsuda, Aozora (松田 青創楽)	1-15-1430
Machida, Masato (町田 雅斗)	2-15-1403	Matsuda, Atsushi (松田 厚志)	2-16-1612
Maebayashi, Masahiro (前林 正弘)	2-04-1527	Matsuda, Kan (松田 貫)	3-09-1330
Maeda, Chinami (前田 知那美)	3-06-1354	Matsuda, Kyohei (松田 恭平)	2-07-1427
Maeda, Narumi (前田 成海)	2-14-1315	Matsuda, Michiyuki (松田 道行)	1S7-4
Maeda, Risa (前田 理沙)	3-02-1406		3-11-1506
Maeda, Yusuke (前多 裕介)	1S10-6	Matsuda, Teruhiko (松田 瑛彦)	2-04-1612
	2-08-1415	Matsui, Akito (松井 爽斗)	3-08-1430
	2-14-1339	Matsui, Motomu (松井 求)	2-13-1415
	2-14-1503	Matsui, Takashi (松井 崇)	1S3-5
Maekawa, Syouhei (前川 昌平)	3-11-1442	Matsui, Toshiki (松井 俊貴)	3-02-1342
Maenaka, Katsumi (前仲 勝実)	2S1-4	Matsui, Yukino (松井 ゆきの)	1-13-1354
Maeno, Tatsumi (前野 達海)	2-11-1748	Matsukawa, Yuji (松川 雄二)	2-15-1451
Maekawa, Haruka (前岡 遥花)	2-15-1315	Matsuki, Hitoshi (松木 均)	2-10-1327
Maeshima, Kazuhiro (前島 一博)	1S7-2	Matsuki, Sho (松木 翔)	2-16-1451
	2S4-3	Matsukura, Lisa (松倉 里紗)	2-03-1315
	2-15-1648		2-03-1824
Maki, Takahisa (真木 孝尚)	3-10-1430	Matsumori, Nobuaki (松森 信明)	2S7-5
Maki-Yonekura, Saori (真木 さおり)	1-02-1342	Matsumoto, Daiki (松本 大輝)	1-16-1354
Makino, Fumiaki (牧野 文信)	2-07-1439		3-07-1354
	2-08-1624	Matsumoto, Kazuhiko (松本 和彦)	2-15-1600
	3-14-1406	Matsumoto, Masaki (松本 雅記)	3S6-5
Makino, Takashi (牧野 能士)	2-13-1624	Matsumoto, Sairi (松本 彩里)	1-01-1330
Makino, Yoshiteru (横野 義輝)	2-12-1403		2-01-1327
Mamizu, Nobuya (馬水 信弥)	3-02-1442	Matsumura, Fumiki (松村 郁希)	1S8-3
Mammoto, Kazuki (万本 和輝)	3-09-1354		2-02-1624
Manabe, Shota (眞鍋 昇大)	2-09-1636	Matsumura, Kazuaki (松村 和明)	3S3-4
Marin Perez, Maria del Carmen (Marin Perez Maria del Carmen)	2-12-1451	Matsumura, Waka (松村 和香)	2-06-1736
	3-04-1454	Matsunaga, Kyoko (松永 恭子)	2-11-1315
Martinez, Jose (Martinez Jose)		Matsunaga, Yasuhiro (松永康佑)	1S3-4

	1S4-2	Mitani, Shohei (三谷 昌平)	2-09-1315
	1-03-1418	Mitarai, Satoshi (御手洗 聡)	3-13-1330
	2-16-1527	Mitra, Shrutarshi (MITRA Shrutarshi)	2-06-1451
	3-04-1342	Mitsui, Toshiyuki (三井 敏之)	2-13-1724
Matsuno, Kenji (松野 健治)	3-06-1354		2-16-1451
Matsuo, Keisuke (松尾 佳祐)	1-13-1442		3-09-1354
Matsuo, Koichi (松尾 光一)	2-10-1648		3-09-1406
Matsuo, Koishi (松尾 光一)	3S5-4	Mitsumoto, Masaya (三本 齊也)	1S6-6
	2-10-1351		2-01-1451
Matsuo, Tomohiro (松尾 智大)	2-08-1439	Mitsuoka, Kaoru (光岡 薫)	2-07-1403
	3-08-1518		3-02-1330
Matsuoka, Daisuke (松岳 大輔)	2-02-1503		3-14-1406
	2-03-1451	Mitsutake, Ayori (光武 亜代理)	1S6-4
Matsuoka, Hideki (松岡 英樹)	2-09-1612		2-02-1351
Matsuoka, Satomi (松岡 里実)	1S14-4		2-03-1339
	2-08-1327		2-06-1515
Matsuoka, Shigeru (松岡 茂)	2-01-1503	Miura, Haruko (三浦 晴子)	2-08-1427
Matsuura, Tomoaki (松浦 友亮)	1S3-5	Miura, Masato (三浦 正人)	1-08-1518
Matsuura, Uchu (松浦 宇宙)	2-04-1636	Miura, Toru (三浦 徹)	2-09-1315
Matsuzaki, Kohei (松崎 興平)	1-07-1342	Miura, Yuki (三浦 勇輝)	1-07-1518
Matsuzawa, Yuki (松沢 佑紀)	1-14-1406	Miyajima, Shogo (宮島 将吾)	2-04-1724
Matthieu G., Gagnon (Matthieu G. Gagnon)	3-05-1342	Miyakawa, Naruto (宮川 成人)	2-15-1600
Matubayasi, Nobuyuki (松林 伸幸)	2-02-1700	Miyake, Takahito (三宅 崇仁)	3S2-3
Mayama, Shigeki (真山 茂樹)	2-15-1451	Miyamoto, Shunsuke (宮本 隼輔)	2-02-1736
Mayanagi, Kouta (真柳 浩太)	2S1-6	Miyamoto, Syunsuke (宮本 俊輔)	2-02-1724
McArthur, Steven John (McArthur Steven John)	3-14-1418	Miyanoiri, Yohei (宮ノ入 洋平)	2-02-1327
			2-11-1636
Meshcheryakova, Irina (Meshcheryakova Irina)	2-08-1351	Miyashita, Naoyuki (宮下 尚之)	2-03-1315
	1-13-1342		2-03-1824
Metsugi, Shoichi (目次 正一)	3-04-1454		2-05-1800
Mezaki, Taichi (目崎 太一)	3-10-1454	Miyata, Kazuki (Miyata Kazuki)	2-15-1700
Mimura, Hisatoshi (三村 久敏)	1S10-2		2-16-1748
Mimura, Masahiro (三村 真大)	2-11-1351	Miyata, Kazuki (宮田 一輝)	1-08-1506
Minagawa, Jun (皆川 純)	1-05-1354	Miyata, Kazuki (宮田 一輝)	2-16-1403
Minagawa, Yoshihiro (皆川 慶嘉)	1-16-1418	Miyata, Makoto (宮田 真人)	2-06-1700
	2-13-1451		2-07-1415
	2-13-1515	Miyata, Tomoko (宮田 知子)	2-07-1439
	2-13-1612		2-08-1624
	2-15-1624		3-14-1406
Minakuchi, Yohei (水口 洋平)	2-09-1315	Miyauchi, Kohei (宮内 滉平)	3-05-1430
	2-09-1339	Miyawaki, Ryouga (宮脇 綾我)	3-01-1406
Minami, Chika (南 知香)	2-05-1800	Miyazaki, Makito (宮崎 牧人)	2-08-1415
Minami, Shintaro (南 慎太郎)	1-12-1330	Miyazaki, Masaya (宮崎 真也)	2-10-1451
Minamino, Tohru (南野 徹)	2-07-1439	Miyazaki, Midoka (宮崎 美登香)	1-10-1506
	2-07-1527	Miyazaki, Naoyuki (宮崎 直幸)	3-13-1330
	2-08-1800	Miyazako, Hiroki (宮廻 裕樹)	2-14-1439
Mino, Hiroyuki (三野 広幸)	2-11-1624	Miyazawa, Keisuke (Miyazawa Keisuke)	2-15-1700
Mishima, Senji (三島 銃侍)	1-01-1430		2-16-1748
Mishima, Yuichi (三島 優一)	2-06-1700	Miyazawa, Keisuke (宮澤 佳甫)	1-08-1506
Mitani, Maki (三谷 麻綺)	2-01-1700		2-16-1403
	3-01-1518	Mizuguchi, Kenji (水口 賢司)	3-13-1342
		Mizukami, Taku (水上 卓)	3-04-1442
			2-02-1748

Mizuno, Daisuke (水野 大介)	2-07-1800	Murakami, Risa (村上 理沙)	3-09-1454
Mizuno, Katsutoshi (水野 克俊)	2-13-1636	Murakami, Satoshi (村上 聡)	1S11-2
Mizuno, Yuta (水野 雄太)	2-15-1439	Muramoto, Kazumasa (村本 和優)	1-06-1430
Mizutani, Azuki (水谷 淳生)	2-03-1800	Murata, Hiroto (村田 裕斗)	1-01-1430
Mizuuchi, Ryo (水内 良)	2-13-1339		1-03-1518
Mochizuki, Atsushi (望月 敦史)	2-14-1724	Murata, Kazuyoshi (村田 和義)	3-13-1330
	2-14-1736	Murata, Michio (村田 道雄)	2-01-1503
Mori, Kosuke (森 功佑)	2-14-1427	Murata, Satoshi (村田 智)	2-05-1527
Mori, Takaharu (Mori Takaharu)	2S6-1		3-07-1354
	2-01-1712		3-10-1442
Mori, Takaharu (森 貴治)	2-02-1503	Murata, Takeshi (村田 武士)	1S6-6
Mori, Takeshi (森 健)	1-08-1354		2S1-3
	1-08-1406		1-02-1354
	2-10-1339		2-01-1451
Morigaki, Kenichi (森垣 憲一)	1-10-1342		2-12-1515
	1-10-1430	Murata, Takeshi (村田 武志)	1-07-1430
	3-11-1442	Murata, Yutaka (村田 隆)	1-05-1430
Morikawa, Ryota (森河 良太)	3-03-1430	Murayama, Keiji (村山 恵司)	1S2-5
Morimatsu, Masatoshi (森松 賢順)	1-09-1406	Murayama, Natsuki (村山 菜月)	3-09-1442
	2-07-1612	Murayama, Takashi (村山 尚)	2-07-1624-Canceled
Morimoto, Naoya (森本 直也)	2-12-1315		3-06-1418
Morimoto, Yusuke V. (森本 雄祐)	1S14-2	Murayama, Yoshihiro (村山 能宏)	2-09-1724
	2-02-1451		2-09-1736
	2-15-1515	Muta, Mikihisa (牟田 幹悠)	1-16-1518
Morishima, Ken (守島 健)	3S4-2	Muto, Etsuko (武藤 悦子)	3-14-1406
	2-04-1351	Mutoh, Risa (武藤 梨沙)	2S2-7
	3-09-1454		2-06-1700
Morita, Hiroyoshi (盛田 宏義)	2-11-1712		2-11-1636
Morita, Kohei (森田 康平)	1-06-1330	N.Taylor, James (N.Taylor James)	2-15-1439
Morita, Miho (森田 美穂)	2-02-1600	Nabika, Hideki (並河 英紀)	2-09-1624
Moritsugu, Kei (森次 圭)	2S6-4	Nagae, Fritz (長江 文立津)	2-05-1339
	2-03-1503	Nagai, Ken H. (永井 健)	1S7-7
Moriya, Toshio (守屋 俊夫)	1-02-1354	Nagai, Rurika (永井 るりか)	1-10-1342
Moriyama, Yuuta (守山 裕大)	2-13-1724	Nagai, Shunsaku (永井 駿作)	2-16-1736
	2-16-1451	Nagai, Takeharu (永井 健治)	1S13-6
	3-09-1354		1-15-1354
	3-09-1406		1-15-1406
Motomura, Haruka (本村 晴佳)	2-09-1800		2-01-1736
Mubarak Hosain, Mohammad (Mubarak Hosain)		Naganathan, Athi N. (Naganathan Athi N.)	2-06-1451
Mohammad)	2-15-1700	Nagano, Mataka (永野 真莞)	3-08-1354
Mugita, Shu (麦田 修)	3-14-1354	Nagano, Yuta (永野 優大)	2-11-1451
Muhammad Jauhari, Insyeeerah Binti (Insyeeerah Binti)			2-11-1503
Muhammad Jauhari)	2-12-1600		2-11-1515
Mukai, Daichi (向 大地)	2-06-1712	Nagao, Hidemi (長尾 秀実)	2-10-1503
Mukaiyama, Atsushi (向山 厚)	2S5-4		2-11-1648
	2S5-5	Nagao, Masaaki (長尾 正明)	2S6-2
	2-14-1700		2-03-1327
Mukoshiba, Taku (向柴 巧)	2-14-1403	Nagao, Ryo (長尾 遼)	2-11-1315
Mullah, Yuval (Mullah Yuval)	1S14-3		2-11-1600
Muneyuki, Eiro (宗行 英朗)	1-07-1442	Nagao, Satoshi (長尾 聡)	2-06-1439
Murai, Yuka (村井 裕佳)	1-06-1330	Nagao, Takemasa (長尾 壮将)	2-06-1736
Murakami, Hiroshi (村上 洋)	1S8-7	Nagasue, Tomoya (永末 智也)	2-09-1600
Murakami, Kazuki (村上 一輝)	2-04-1624	Nagata, Noboru (永田 昇)	2-13-1327

Nagata, Taisei (永田 大晴)	2-01-1812	Nakanishi, Mio (中西 未央)	1S13-3
Nagata, Takashi (永田 崇)	2S3-3	Nakanishi, Taito (中西 大斗)	2-09-1403
	2-12-1315	Nakaniwa, Tetsuko (仲庭 哲津子)	2-11-1327
	3-02-1342	Nakano, Masanori (中野 真徳)	2-15-1748
	3-05-1418	Nakano, Minoru (中野 実)	1-10-1454
	3-05-1442	Nakano, Ryosuke (中野 僚介)	1S6-6
Nagatani, Yasuko (永谷 康子)	3-03-1354		2-01-1451
Nagatoishi, Satoru (長門石 暁)	2-04-1315	Nakano, Takuto (中野 卓斗)	2-10-1636
Nagayama, Kuniaki (永山 國昭)	3-14-1330	Nakano, Yuta (中野 雄太)	1-12-1442
Nagino, Kimiko (名木野 貴美子)	2-07-1315		1-13-1418
Nair, Asha V. (Nair Asha V.)	1S11-2		2-03-1527
Naito, Akira (内藤 晶)	2-12-1403	Nakano, Yuuta (中野 雄太)	2-03-1736
Naito, Kazuma (内藤 一馬)	1-09-1354	Nakao, Hiroyuki (中尾 裕之)	1-10-1454
Naka, Ayaka (仲 絢香)	1-02-1518	Nakao, Shin (中尾 新)	1-11-1330
Nakabayashi, Seiichiro (中林 誠一郎)	2-01-1748	Nakao, Toshiki (中尾 俊樹)	2-10-1327
Nakabayashi, Takakazu (中林 孝和)	2-04-1600	Nakaoka, Ikuya (中岡 育也)	2-04-1812
	2-04-1624	Nakasako, Masayoshi (中迫 雅由)	2-01-1800
	2-04-1636		2-02-1612
	2-15-1351		3-11-1406
	2-15-1403	Nakasone, Yusuke (中曾根 祐介)	2-04-1812
	2-15-1415		3-11-1330
	2-15-1427	Nakatani, Kohta (中谷 航太)	3S6-5
Nakafukasako, Miho (中深迫 美穂)	2-02-1451	Nakaue, Tatsuya (中植 達也)	2-08-1636
Nakagawa, Hiroshi (中川 洋)	3S3-3	Nakaya, Yukiko (仲矢 由紀子)	3-09-1430
	2-04-1736	Nakayama, Chihiro (中山 千尋)	3-05-1442
Nakagawa, Yoshiko (中川 幸姫)	3-02-1354	Nakayama, Takahiro (中山 隆宏)	2-16-1351
Nakahara, Toshiaki (中原 敏彰)	2-09-1439	Nakayama, Yohei (中山 洋平)	1-07-1442
Nakahata, Shinjiro (中畑 伸児郎)	2-14-1636	Nakazawa, Yuki (中澤 友紀)	2-08-1527
Nakajima, Hiroto (中島 碩士)	2-11-1451	Namari, Nuning (Namari Nuning)	2-14-1403
Nakajima, Kichitaro (中島 吉太郎)	2-05-1612	Namba, Keiichi (難波 啓一)	2S1-2
	3-01-1342		2-07-1439
Nakajima, Motokuni (中島 基邦)	3-03-1430		2-07-1527
Nakajima, Yoshiki (中島 芳樹)	1S11-1		2-08-1624
	1-02-1330		3-14-1406
Nakakido, Makoto (中木戸 誠)	2-04-1748	Namba, Tatsuki (難波 樹)	2-03-1415
Nakakita, Shin-ich (中北 慎一)	2-15-1600	Namba, Toshinori (難波 利典)	1-15-1430
Nakama, Masaki (仲間 政樹)	2-12-1736	Namiki, Hazuki (並木 葉月)	2-01-1503
Nakamura, Aya (Nakamura Aya)	2-08-1351	Naoi, Takuma (直井 拓磨)	2-07-1315
Nakamura, Chikashi (史 中村)	2-16-1403	Nara, Takaaki (奈良 高明)	2-14-1439
Nakamura, Haruki (中村 春木)	2S1-99	Narahara, Yoko (橘原 陽子)	3-11-1342
	2-03-1700	Narai, Shun (奈良 井 峻)	1-02-1418
Nakamura, Junji (中村 潤児)	2-14-1403	Narikawa, Rei (成川 礼)	2S3-6
Nakamura, Kiminori (中村 公則)	3-13-1418	Narita, Yoshinori (成田 義規)	1-13-1342
Nakamura, Mai (中村 麻愛)	2-11-1712	Nariyama, Kosuke (成山 幸助)	3-03-1430
	2-11-1724	Naruse, Keiji (成瀬 恵治)	1-09-1406
	1-08-1442		2-07-1612
Nakamura, Shuichi (中村 修一)	2-16-1439	Nasada, Kaho (名定 加峰)	2-06-1748
Nakamura, Sotaro (中村 宗太郎)	3-12-1442	Nasrin, Syeda Rubaiya (Nasrin Syeda Rubaiya)	2-07-1812
Nakamura, Tsukasa (中村 司)	2-02-1712		2-16-1624
Nakamura, Yui (中村 優似)	2-13-1712	Naya, Masami (納谷 昌実)	1-03-1342
Nakamuta, Asahi (中牟田 旭)	2-07-1451	Negami, Tatsuki (根上 樹)	2-08-1351
Nakane, Daisuke (中根 大介)	3-02-1330	Nemoto, Yuri (Nemoto Yuri)	3-08-1406
Nakanishi, Atsuko (中西 温子)	3S3-1	Nemoto, Yuri (根本 悠宇里)	
Nakanishi, Masahiro (中西 真大)			

Nemoto, Yuri L (根本 悠宇里)	1-09-1354	Noireaux, Vincent (Noireaux Vincent)	2-14-1339
Niina, Toru (新稲 亮)	1-05-1430	Noji, Hiroyuki (野地 博行)	1S1-1
	2-06-1648		1S10-7
Niino, Motoki (新野 素生)	1-07-1342		1-05-1354
Ninomiya, Kota (仁宮 洸太)	2-15-1527		1-07-1418
Nishi, Hafumi (西 羽美)	1-12-1406		1-07-1454
	3-01-1330		1-16-1418
	3-03-1506		2-04-1503
	3-12-1430		2-07-1503
Nishibe, Nobuyuki (西部 伸幸)	3-07-1430		2-13-1451
Nishida, Mizuho (西田 水穂)	1-01-1406		2-13-1515
Nishida, Yuya (西田 優也)	2-06-1736		2-13-1612
Nishide, Goro (西出 梧朗)	2-16-1351		2-15-1624
Nishiguchi, Tomoki (西口 知輝)	1-15-1342		2-16-1800
Nishikawa, Kaori (西川 香里)	3S6-2		3-06-1406
	2-15-1736		3-12-1406
Nishikawa, Kohei (西川 航平)	2-12-1736	Noma, Ryohei (野間 涼平)	2-01-1736
Nishikawa, Masatoshi (西川 正俊)	1-07-1518	Nomoto, Akira (野本 晃)	2-04-1712
	2-06-1427	Nomura, Mai (野村 舞)	2-01-1503
Nishikino, Tatsuro (錦野 達郎)	1-02-1442	Nomura, Norimichi (野村 紀通)	3-02-1342
Nishimura, Yoshifumi (西村 善文)	1-03-1342	Nomura, Shin-ichiro M. (野村 M. 慎一郎)	1-16-1354
Nishina, Takumi (仁科 拓海)	1-01-1518		3-07-1354
Nishinami, Suguru (西奈美 卓)	2-04-1712	Nomura, Shin-ichiro M. (野村 M. 慎一郎)	2-05-1439
Nishio, Takashi (西尾 天志)	2-05-1315	Nomura, Shinichiro (野村 慎一郎)	3-10-1442
Nishiyama, Kohei (西山 晃平)	1-16-1354	Nomura, Takashi (野村 高志)	3-02-1354
	3-07-1354	Norioka, Naoko (乗岡 尚子)	2-11-1327
Nishiyama, Masayoshi (西山 雅祥)	1-09-1406	Noro, Seiya (野呂 聖弥)	2-13-1612
	2-07-1612	Nozaki, Shota (野崎 庄太)	2-13-1724
Nishiyama, So-ichiro (西山 宗一郎)	1-01-1454		3-09-1354
	2-09-1636		3-09-1406
Nishiyama, Tomoko (西山 朋子)	2S4-1	Nozaki, Takuro (野崎 拓郎)	2-04-1351
Nishizaka, Takayuki (西坂 崇之)	2-07-1451	Nreki, Osamu (濡木 理)	1-02-1406
	2-09-1748	Nureki, Osamu (濡木 理)	1-06-1442
Nishizawa, Tomohiro (西澤 知宏)	1-02-1406		2-01-1515
	2-01-1515		2-04-1403
	2-04-1403		2-12-1800
	3-02-1330		2-12-1812
Nitta, Nobuhiro (新田 展大)	3-13-1430		2-16-1439
Nitta, Takahiro (新田 高洋)	1-16-1330		3-02-1342
Niwa, Shinsuke (丹羽 伸介)	2-07-1315	Obashi, Kazuki (小橋 一喜)	3-08-1454
Niwa, Shinsuke (丹羽 伸介)	1S1-6	Oda, Kazumasa (小田 和正)	2-04-1403
	2-07-1327	Oda, Takashi (小田 隆)	3S4-4
	2-07-1824	Oda, Yoshinori (織田 祥徳)	1-10-1518
Niwa, Tatsuya (丹羽 達也)	1-12-1330	Odagiri, Kenta (小田切 健太)	1-14-1430
	1-13-1354		3-09-1418
Nobunaga, Shingo (延永 慎吾)	2-02-1712	Ogane, Tomonori (大金 智則)	2-16-1527
	2-03-1812	Ogasawara, Satoshi (小笠原 諭)	1-02-1354
Noga, Akira (苗加 彰)	2-08-1648	Ogata, Kazuhiro (緒方 一博)	1-06-1506
Noguchi, Daiki (野口 大輝)	2-03-1339		2-03-1527
Noguchi, Hiroshi (野口 博司)	1-14-1418	Ogawa, Miyu (小川 美優)	3-08-1354
Noguchi, Takumi (野口 巧)	2-11-1600	Ogawa, Rei (小川 令)	1S12-2
	2-11-1612		3-09-1418
Noguchi, Yoh (野口 瑤)	3-03-1430	Ogawa, Tomohisa (小川 智久)	1S3-5

Ogawa, Yuichi (小川 雄一)	1S8-3 2-02-1600 2-02-1624	Okada, Yasushi (岡田 康志)	1-15-1442 2-15-1800
Ogi, Hirotsugu (荻 博次)	2-05-1612 3-01-1342	Okada, Yuki (岡田 由紀)	2S4-5
Ogita, Goshi (荻田 豪士)	2-14-1327	Okahata, Misaki (岡畑 美咲)	2-09-1315 2-09-1339
Ogoshi, Susumu (大越 奨)	2-09-1636	Okajima, Takaharu (岡嶋 孝治)	2-08-1439 3-08-1342 3-08-1354 3-08-1518
Oh-oka, Hirozo (大岡 宏造)	2-11-1636	Okamoto, Kenji (岡本 憲二)	3-01-1354
Ohashi, Keisuke (大橋 慧介)	3-07-1330	Okamoto, Yuko (岡本 祐幸)	2S6-7
Ohki, Yuya (大木 優也)	2-12-1724	Okamoto, Yusuke (岡本 悠介)	3-02-1454
Ohmachi, Masashi (大町 優史)	2-07-1636	Okazaki, Kei-ichi (岡崎 圭一)	1S4-3
Ohnishi, Yuki (大西 裕季)	3-13-1418	Oki, Hideyuki (沖 英幸)	1-02-1354
Ohno, Hirohisa (大野 博久)	2-05-1439	Okimura, Chika (沖村 千夏)	2-08-1339 2-08-1600
Ohnuki, Jun (大貫 隼)	2-03-1415 2-07-1339 2-12-1427	Okitsu, Takashi (沖津 貴志)	2-12-1403
Ohnuma, Kiyoshi (大沼 清)	2-13-1736	Oku, Hirosuke (屋 宏典)	3-02-1406
Ohsawa, Daisuke (大澤 大輔)	3-11-1518	Okubo, Kai (大久保 海)	3-11-1354
Ohsugi, Tadanori (大杉 忠則)	3-09-1454	Okubo, Rihito (大窪 理仁)	1-01-1506
Ohta, Akane (太田 茜)	2-09-1315 2-09-1339 2-09-1800	Okuda, Aya (奥田 綾)	3S4-2 2-04-1351 3-09-1454
Ohta, Masateru (大田 雅照)	2-02-1636	Okumura, Hisashi (奥村 久士)	3S5-6 2-05-1724
Ohta, Yoshihiro (太田 善浩)	1-08-1430 1-08-1518 1-11-1430	Okura, Kaoru (大蔵 かおる)	1-09-1518
Ohtake, Ryohei (大竹 峻平)	1-11-1430	Okura, Reiko (大倉 玲子)	1-15-1418
Ohtake, Ryouhei (大竹 峻平)	2-12-1724	Okuyama, Akari (奥山 あかり)	2-12-1648
Ohue, Masahito (大上 雅史)	2-03-1712	Olivucci, Massimo (Olivucci Massimo)	2-12-1451
Oide, Mao (大出 真央)	2-01-1800 2-02-1612 3-03-1454 3-11-1406 1-08-1430	Olsson, Ulf (オルソン ウルフ)	1S10-3 2-13-1427
Oie, Yoshiki (尾家 佳樹)	1-08-1430	Omori, Satoshi (大森 聡)	3-03-1506
Oikawa, Hiroyuki (Oikawa Hiroyuki)	2-06-1451	Omori, Toshihiro (大森 俊宏)	2-09-1748 2-13-1636
Oikawa, Hiroyuki (小井川 浩之)	1-04-1518 2-06-1624 3-04-1354	Onai, Kiyoshi (小内 清)	2S2-7
Oikawa, Masakazu (及川 将一)	3-11-1518	Onchaiya, Sawaros (Onchaiya Sawaros)	3-04-1454
Oiki, Shigetoshi (老木 成稔)	3-10-1430	Ong, Gabrielle (オン ガブリエル)	1-08-1354
Oiwa, Kazuhiro (大岩 和弘)	2-07-1700 2-08-1724 1-03-1406	Onishi, Satoru (大西 悟)	2-04-1800
Ojima, Ayaka (尾島 彩夏)	2-16-1636	Ono, Ryohei (小野 稜平)	2-04-1403
Oka, Kotaro (岡 浩太郎)	2-11-1327	Ono, Shinji (小野 慎司)	2-05-1403
Oka, Naohiro (岡 直宏)	2-01-1351	Ono, Takao (小野 堯生)	2-15-1600
Oka, Yoshiki (岡 芳樹)	3S2-5	Onoue, Kousuke (尾上 広祐)	3-03-1406
Okabe, Kohki (岡部 弘基)	2-16-1339 2-16-1648 2-16-1712 2-16-1736	Oogai, Shigeki (大貝 茂希)	3-02-1406
Okabe, Koki (岡部 弘基)	2-09-1700 2-13-1600	Ooka, Koji (大岡 紘治)	2-03-1351 2-03-1403
Okada, Mariko (岡田 真里子)		Ookubo, Shigeki (大久保 成貴)	1-08-1418
		Or Rashid, Md. Mamun (オアラシッド エム ディ マムン)	2-10-1600
		Ori, Ryota (折井 良太)	1-14-1454
		Oroguchi, Tomotaka (荳口 友隆)	2-02-1800
		Osada, Seiji (長田 誠司)	3-13-1418
		Osaki, Toshihisa (大崎 寿久)	2-10-1736 3-10-1454

Oshima, Atsunori (大嶋 篤典)	1S11-3 1-10-1518	Sada, Kazuki (Sada Kazuki)	2-07-1812 3-01-1430
Oshima, Hiraku (尾嶋 拓)	1-04-1406	Saga, Tsuneco (佐賀 恒夫)	3-13-1430
Oshima, Masanobu (大島 正伸)	1-08-1506	Sagawa, Wataru (佐川 航)	2-03-1600
Ota, Hideaki (太田 英暁)	2-08-1315	Saha, Samiron Kumar (サハ サミロン クマール)	2-10-1600
Ota, Honoka (太田 帆香)	2-04-1812	Saio, Tomohide (齋尾 智英)	3S4-3 2-04-1812
Ota, Motonori (太田 元規)	1-04-1454 1-12-1330 1-12-1418 1-13-1330 3-12-1330	Saito, Claire (齋藤 くれあ)	1S9-5
Ota, Sadao (太田 禎生)	1S5-3	Saito, Hirohide (齋藤 博英)	1-05-1454 2-05-1439
Otani, Risako (大谷 理紗子)	1-06-1342	Saito, Kai (齋藤 開)	1-16-1518
Otomo, Akihiro (Otomo Akihiro)	1S1-3 3-07-1342	Saito, Kei (齋藤 慧)	3-06-1418
Otomo, Akihiro (大友 章裕)	1-07-1430	Saito, Keisuke (齋藤 圭亮)	2-11-1403 2-11-1415
Otosu, Takuhiro (乙須 拓洋)	2-10-1439	Saito, Minoru (齋藤 稔)	2-09-1327 2-09-1612 2-14-1315
Otsubo, Shiho (大坪 史歩)	1-01-1406 1-01-1418	Saito, Monoru (齋藤 稔)	2-16-1327
Otsuka, Aoi (大塚 碧)	2-15-1648	Saito, Nen (齋藤 稔)	2-14-1712
Otsuka, Yumeto (大塚 夢斗)	2-02-1315	Saito, Shigeru (齋藤 茂)	1S9-5
Ottawa, Masaki (大多和 克紀)	2-03-1824	Saitoh, Takahiro (齋藤 崇啓)	1-15-1518
Ouyang, Dongyan (歐陽 東彦)	2S5-5	Sakaguchi, Miyuki (坂口 美幸)	2-10-1439
Oyama, Keishi (小山 恵史)	3-03-1354	Sakaguchi, Reiko (坂口 怜子)	1S9-1
Oyama, Kotaro (大山 廣太郎)	2-06-1612	Sakai, Kazumi (酒井 佳寿美)	1-11-1342 1-11-1354
Ozawa, Takeaki (小澤 岳昌)	1-15-1342	Sakai, Makoto (酒井 誠)	2-15-1503
Paggi, Joseph (Paggi Joseph)	3-02-1342	Sakai, Shinya (酒井 伸弥)	2-16-1315
Parkinson, John S. (Parkinson John S.)	1S14-3	Sakai, Yuji (境 祐二)	1S7-2
Patricia, Mc Gahan (パトリシア ミキャン)	1-14-1406	Sakai, Yusuke (酒井 佑介)	1-12-1442 1-13-1418 2-03-1527
Pedraza-Gonzalez, Laura (Pedraza-Gonzalez Laura)	2-12-1451 2-16-1748	Sakakibara, Hitoshi (榎原 斉)	2-07-1700 2-08-1724
Penedo, Marcos (Penedo Marcos)	2-16-1748	Sakamoto, Kantaro (坂本 貫太郎)	3-02-1430
Penedo, Marcos (ペネド マルコス)	2-16-1403	Sakamoto, Kazufumi (坂本 一史)	1-14-1342 1-14-1354
Piacenti, Alba Rosa (Piacenti Alba Rosa)	2-15-1600	Sakamoto, Kei (坂本 溪)	2-02-1712
Pigolotti, Simone (ピゴロッティ シモーネ)	2-05-1403	Sakamoto, Masayuki (坂本 雅行)	2-12-1612
Prabhu, Apoorva (Apoorva Prabhu)	2-12-1339	Sakamoto, Naoaki (坂本 尚昭)	1-08-1330
Prioux, Magali (Prioux Magali)	1-09-1430 1S2-1	Sakamoto, Ryota (坂本 遼太)	2-08-1415
Qian, Lulu (Qian Lulu)	1-04-1506	Sakamoto, Tomoki (坂本 知樹)	3-05-1418
Rahman, Nafsoon (Rahman Nafsoon)	1-04-1506	Sakamoto, Yuta (坂本 悠太)	2-09-1712
Rajan, Robin (Rajan Robin)	3S3-4	Sakaue, Takahiro (坂上 貴洋)	1-05-1330 2-08-1403
Rajendran, Divya (Rajendran Divya)	2-06-1451	Sakiyama, Tomoko (崎山 朋子)	2-09-1712
Ramakrishnan, Charu (Ramakrishnan Charu)	3-02-1342	Sako, Yasushi (佐甲 靖志)	2S2-4 1-15-1330 2-14-1415 3-01-1354
Ramaswamy, Sriram (Ramaswamy Sriram)	1S7-5	Sakuma, Daisuke (佐久間 大輔)	2-07-1451
Rapenne, Gwenael (ラッペネル ゲナエル)	2-10-1636	Sakuma, Shinya (佐久間 臣耶)	3S6-4
Raturi, Sagar (Raturi Sagar)	1S11-2		
Re, Suyong (Re Suyong)	2S6-1 2-01-1712		
Re, Suyong (李 秀榮)	3-04-1442		
Rikhy, Richa (Rikhy Richa)	1S7-3		
Rinke, Christian (Christian Rinke)	2-12-1339		
Rioual, Elisa (Rioual Elisa)	2-05-1712		
Rozenberg, Andrey (Andrey Rozenberg)	2-12-1515		
Rufiat, Nahar (Rufiat Nahar)	2-05-1636		

Sakuma, Yuka (佐久間 由香)	2-10-1415 2-13-1439	Sato, Yusei (佐藤 優成)	2-07-1427
Sakuraba, Shun (桜庭 俊)	1-06-1506 2-03-1427	Sato, Yusuke (佐藤 佑介)	2-05-1415 2-05-1427 2-07-1515
Sakuraba, Shun (桜庭 俊)	2-11-1800	Satou, Takechiro (佐藤 健大)	2-04-1800
Sakurai, Mika (櫻井 実香)	1-13-1342	Sawai, Satoshi (澤井 哲)	3-09-1442
Sakurai, Minoru (櫻井 実)	2-03-1748	Schiessel, Helmut (Schiessel Helmut)	1-05-1330
Sakurai, Takeshi (櫻井 武)	2S3-2	Seki, Hayto (関 隼斗)	2-12-1403
Sakurai, Tatsunari (櫻井 建成)	2-08-1339 2-08-1600	Sekiguchi, Tetsushi (関口 習一)	1-16-1518
Sano, Mio (佐野 美桜)	2-01-1427 2-16-1800	Sekita, Aiko (関田 愛子)	3-13-1430
Sano, Yoshiaki (佐野 仁亮)	2-05-1515	Senda, Miki (千田 美紀)	2-02-1327
Saotome, Tomonori (早乙女 友規)	3-04-1454	Senda, Toshiya (千田 俊哉)	2S1-3 1-02-1354
Sasada, Ko (笹田 航)	1-02-1454	Sengoku, Toru (仙石 徹)	1-03-1342 1-06-1506 2-03-1527
Sasai, Masaki (笹井 理生)	2S5-2 1-05-1418 2-01-1812 2-05-1736 2-14-1612 2-14-1624	Sentoku, Mitsuru (千徳 光)	2-08-1515
Sasaki, Ayu (佐々木 亜優)	3-09-1354 3-09-1406	Sentoku, Mitsuru (千徳 光)	3-08-1506
Sasaki, Kaito (佐々木 海渡)	1S8-4	Shah, Syed Hashim (Shah Syed Hashim)	1-05-1406
Sasaki, Kazuo (佐々木 一夫)	3-06-1330	Shahidul Alam, Mohammad (Shahidul Alam Mohammad)	2-15-1700
Sasaki, Ryo (佐々木 暲)	2-07-1824	Shen, Jian-Ren (沈 建仁)	1S11-1 1-02-1330 2-11-1315
Sasaki, Takanori (佐々木 貴規)	1-12-1430 1-13-1430 2-15-1527	Shibagaki, Mitsuki (柴垣 光希)	2-02-1403
Sato, Chikara (佐藤 主税)	2-16-1624	Shibahara, Keita (芝原 慶太)	1-03-1442
Sato, Daisuke (佐藤 大輔)	2-04-1427	Shibasaki, Koji (柴崎 貢志)	1S9-6
Sato, Gaku (佐藤 岳)	2-13-1527	Shibasaki, Yusuke (柴崎 雄介)	2-14-1315
Sato, Hiroyuki (佐藤 弘之)	2-14-1439	Shibata, Daiki (柴田 大貴)	2-10-1503
Sato, Kazunobu (佐藤 和信)	2-06-1700	Shibata, Daiki (柴田 大輝)	2-04-1600 2-04-1624
Sato, Keiichiro (佐藤 圭一朗)	1-03-1506	Shibata, Keisei (柴田 桂成)	2-04-1403
Sato, Keiko (佐藤 啓子)	2-16-1624	Shibata, Keitaro (柴田 桂太郎)	2-01-1636
Sato, Ko (佐藤 光)	1-06-1506	Shibata, Mikihiko (柴田 幹大)	2-06-1712 3-02-1342
Sato, Kochi (佐藤 航地)	2-02-1612	Shibata, Satoshi (柴田 敏史)	2-02-1439
Sato, Mari (佐藤 真理)	2-16-1624	Shibata, Sayaka (柴田 さやか)	3-13-1430
Sato, Masaki (佐藤 昌樹)	2-10-1439	Shibata, Tatsuo (柴田 達夫)	2S7-1 1-10-1442 3-09-1430
Sato, Moritoshi (佐藤 守徳)	2-01-1403	Shibata, Yutaka (柴田 穰)	2-11-1351 3-11-1454 2-12-1612
Sato, Nao (佐藤 那音)	2-01-1339 2-01-1351	Shibukawa, Atsushi (渋川 敦史)	2-15-1351
Sato, Natsumi (佐藤 夏美)	1-07-1442	Shibuya, Ren (澁谷 蓮)	1-11-1342
Sato, Nobuhiro (佐藤 信浩)	3S4-2	Shichida, Yoshinori (七田 芳則)	2-11-1427
Sato, Renta (佐藤 連太)	1-03-1354	Shiga, Daisuke (志賀 大将)	2-14-1415
Sato, Shin-ichi (佐藤 慎一)	2-05-1315	Shiga, Itsuki (志賀 樹)	1-11-1354
Sato, Shinya (佐藤 慎哉)	3-11-1506	Shiga, Yasuhiro (志賀 靖弘)	3-08-1342
Sato, Takechiro (佐藤 健大)	1-01-1442 3-02-1454	Shigemura, Kenta (茂村 研太)	1-11-1454
Sato, Takuro (佐藤 匠朗)	3-14-1354	Shigemura, Shunta (重村 竣太)	2-12-1403
Sato, Yukino (佐藤 千乃)	2-12-1503 2-12-1724	Shigeta, Arisu (重田 安里寿)	2-14-1503
		Shigeta, Kazuyuki (繁田 和幸)	2-04-1824
		Shigeta, Yasuteru (重田 育照)	

Shigete, Yasuteru (重田 育照)	2-04-1515	Shionyu, Clara (塩生 くらら)	1-04-1454
Shigyō, Kazuki (執行 航希)	2-15-1315	Shionyu, Masafumi (塩生 真史)	3-12-1354
Shihoya, Wataru (志甫谷 渉)	2-01-1515		3-12-1418
	2-12-1800	Shiraga, Keiichiro (白神 慧一郎)	1S8-3
	2-12-1812		2-02-1600
	2-16-1439		2-02-1624
Shikakura, Takafumi (鹿倉 啓史)	2-12-1415	Shirai, Tsuyoshi (白井 剛)	3-12-1418
Shikata, Hiromasa (四方 明格)	2S3-4	Shirakawa, Yuka (白川 由佳)	2-14-1315
Shikata, Toshiyuki (四方 俊幸)	1S8-3	Shiraki, Kentaro (白木 賢太郎)	2-04-1712
	2-02-1600	Shirasaki, Yoshitaka (白崎 善隆)	3S6-3
	2-02-1624	Shirasu, Kenta (白須 健大)	3-14-1354
Shimabukuro, Katsuya (島袋 勝弥)	2-08-1451	Shiro, Yoshitsugu (基成 宜嗣)	1-02-1518
Shimada, Atsuhiko (島田 敦広)	1-06-1430	Shiroguchi, Katsuyuki (城口 克之)	3S6-6
Shimada, Ichio (嶋田 一夫)	3S4-5	Shirokawa, Tetsuya (Shirokawa Tetsuya)	2-15-1700
Shimada, Satoru (島田 悟)	1-06-1430		2-16-1748
Shimada, Yuichiro (嶋田 友一郎)	2-11-1600	Shirokawa, Tetsuya (城川 哲也)	2-16-1403
Shimamori, Keiya (島森 圭弥)	2-04-1451	Shirota, Matsuyuki (城田 松之)	3-03-1442
Shimamoto, Kanako (嶋本 佳那子)	2-06-1351	Shirouzu, Mikako (白水 美香子)	1S3-5
Shimamoto, Yuta (島本 勇太)	2-08-1415	Sho, Ayano (正 彩乃)	2-08-1503
Shimamura, Hirotaro (島村 博太郎)	2-01-1415	Shoji, Kyohei (庄司 響平)	2-07-1339
Shimazaki, Kairi (島崎 海理)	3-14-1354	Shoji, Mikio (庄司 幹郎)	2-02-1439
Shimizu, Hirofumi (清水 啓史)	1S9-2	Shoji, Osami (庄司 長三)	2-06-1439
	2-06-1724	Shoji, Shuichi (庄司 周一)	1-16-1518
Shimizu, Masahiro (清水 将裕)	3S4-2	Shuma, Madhabl Lata (シューマ マドビラタ)	
Shimizu, Nobutaka (清水 伸隆)	1-03-1342		2-10-1612
	1-04-1442	Simoda, Kenji (下田 賢司)	2-09-1351
	1-06-1442	Simon, Damien Stephane (Simon Damien Stephane)	
	2-04-1736		2-14-1700
	3-03-1354	Sims, Peter (Sims Peter)	3S6-1
Shimizu, Thomas (Shimizu Thomas)	1S14-3	Singh, Himansha (Singh Himansha)	1S11-2
Shimo, Rieko (下 理恵子)	2-07-1403	Singh, Manish (Singh Manish)	2-12-1812
Shimoda, Kenji (下田 賢司)	2-09-1415	Sirisukhodom, Supanut (Sirisukhodom Supanut)	
Shimoshige, Rino (下茂 梨乃)	2-01-1648		2-15-1824
Shimoyachi, Hiroto (下谷内 宏統)	2-11-1812	Sochacki, Kem (Sochacki Kem)	3-08-1454
Shimoyama, Hiromitsu (下山 紘充)	2-04-1824	Soma, Mika (相馬 ミカ)	2-09-1327
Shimura, Mari (志村 まり)	1S3-6	Song, Yuchi (宋 雨迟)	2-05-1824
Shinagawa, Ayumi (品川 歩)	2-15-1600		3-02-1418
Shindo, Yutaka (新藤 豊)	2-16-1636	Song, Yuchi (宋 雨遲)	2-05-1812
Shinkai, Yoichi (新海 陽一)	1S10-2		3-04-1330
Shino, Genki (篠 元輝)	2-05-1351	Song, Zihao (宋 子豪)	3-13-1406
Shinobu, Ai (信夫 愛)	1-03-1418		3-13-1418
Shinoda, Keiko (篠田 恵子)	1S11-2	Sonoyama, Masashi (園山 正史)	1-06-1330
Shinoda, Wataru (篠田 渉)	1-10-1354		1-06-1342
Shinohara, Yuka (篠原 由佳)	2-06-1327		2-01-1503
Shintaku, Hirofumi (新宅 博文)	3S6-2		2-06-1315
	2-15-1736		2-06-1327
Shintani, Seine (新谷 正嶺)	2-07-1600		2-06-1339
Shintani, Yasunori (新谷 泰範)	2-06-1736		2-06-1351
Shinzawa-Itoh, Kyoko (伊藤 (新澤) 恭子)	1-06-1430		2-06-1415
	2-06-1736		2-10-1451
Shiomi, Akifumi (塩見 晃史)	3S6-2	Sotoma, Shingo (外間 進悟)	3S2-4
	2-15-1736	Sowa, Yoshiyuki (曾和 義幸)	1-07-1518
Shiomi, Shunsuke (汐見 駿佑)	2-10-1403		2-06-1427

	2-09-1484		2-03-1451
Sriwilaijaroen, Nongluk (Sriwilaijaroen Nongluk)			3-03-1454
	2-15-1600	Sugita, Yukihiko (杉田 征彦)	3S1-3
Strub, Marie-Paule (Strub Marie-Paule)	3-08-1454	Sugiura, Kazunori (杉浦 一徳)	1-15-1406
Su'etsugu, Masayuki (末次 正幸)	1-16-1418		2-01-1736
Subagyo, Agus (スバキョ アグス)	2-15-1636	Sugiura, Masahiro (杉浦 雅大)	2-12-1748
Subagyo, Agus (スバキョ アグス)	3-08-1342		2-12-1800
Sudo, Yuki (須藤 雄気)	2S2-5	Sugiyama, Hironori (杉山 博紀)	2-10-1736
	1-11-1330	Sugiyama, Jun-ichi (杉山 順一)	1S8-1
	2-12-1403	Sugiyama, Masaaki (杉山 正明)	3S4-2
	2-12-1612		2-04-1351
	2-12-1624		3-09-1454
	2-12-1736	Sugiyama, Satoshi (杉山 聡)	2-03-1712
	2-12-1824	Sugiyama, Shigeru (杉山 成)	2-01-1503
Suematsu, J. Nobuhiko (末松 J. 信彦)	1-14-1430		2-02-1315
Suenaga, Shoma (末永 翔磨)	3S5-4	Sugo, Yu (菅生 優)	2-11-1415
	2-10-1351	Suito, Hiroshi (水藤 寛)	1S12-3
Sueoka, Kazuhisa (末岡 和久)	3-08-1342	Sumi, Hiroyuki (須見 洋行)	3-09-1454
Suetaka, Shunji (季高 駿士)	2-01-1339	Sumikama, Takashi (炭竈 享司)	3-13-1354
	2-01-1351	Sumikawa, Mizuki (澄川 瑞季)	2-12-1636
Suetake, Isao (末武 勲)	2-06-1700	Sumino, Ayumi (角野 歩)	2-06-1712
Suetani, Hiromichi (末谷 大道)	3-09-1418		2-16-1427
Suetomo, Hiroyuki (末友 裕行)	2-01-1700	Sumiyama, Kenta (隅山 健太)	3-11-1506
	3-01-1518	Sunada, Yuma (砂田 悠真)	3-07-1406
Suetsugu, Masayuki (末次 正幸)	3-12-1406	Sunami, Tomoko (角南 智子)	1-06-1454
Suga, Michi (菅 倫寛)	1S11-1	Suno, Chiyo (寿野 千代)	2-06-1403
Suganuma, Yoshiki (菅沼 芳樹)	1-08-1518	Suno, Ryoji (寿野 良二)	1S6-1
Sugawa, Mitsuhiro (須河 光弘)	2-07-1427		2-06-1403
Sugawara, Takeshi (菅原 武志)	1S14-1	Suziki, Kohei (鮎 洗平)	2-06-1403
Sugaya, Kanna (菅谷 幹奈)	1S6-6	Suzuki, Aya (鈴木 綾)	3-06-1406
	2-01-1451	Suzuki, Hiromi (鈴木 博実)	3-01-1418
Sugi, Takuma (杉 拓磨)	1S7-7	Suzuki, Kano (鈴木 花野)	1-02-1354
	2-15-1315		2-12-1515
Sugihara, Kaori (杉原 加織)	2-10-1700	Suzuki, Kenichi (鈴木 健一)	1-10-1342
Sugimachi, Ayane (杉町 純音)	1-10-1342	Suzuki, Kenichi G. N. (鈴木 健一)	2-08-1503
Sugimoto, Hiroshi (杉本 宏)	1-02-1518	Suzuki, Kenichi G.N. (鈴木 健一)	3-08-1442
	2-06-1439	Suzuki, Leo (鈴木 令和)	2-06-1624
	3-02-1406	Suzuki, Madoka (鈴木 団)	2-06-1612
	3-02-1430		3-08-1430
	3-04-1406	Suzuki, Makoto (鈴木 誠)	1S8-2
Sugimoto, Teppei (杉本 哲平)	2-12-1700	Suzuki, Masato (鈴木 仁人)	2-05-1451
Sugimoto, Yasunobu (杉本 泰伸)	1-04-1454		3-05-1406
Sugimura, Kaoru (杉村 薫)	2-14-1327	Suzuki, Masato (鈴木 允人)	2-10-1315
Sugimura, Toshiki (杉村 俊紀)	2-15-1403	Suzuki, Sota (鈴木 爽太)	1-08-1342
Sugita, Masatake (杉田 昌岳)	2-03-1712	Suzuki, Souta (鈴木 爽太)	1-09-1342
Sugita, Yuji (Sugita Yuji)	2S6-1	Suzuki, Takao (鈴木 誉保)	2-13-1415
	2-01-1712	Suzuki, Takehiro (鈴木 健裕)	2-11-1600
Sugita, Yuji (杉田 有治)	1S3-4	Suzuki, Tetsuhito (鈴木 哲仁)	1S8-3
	2S6-5		2-02-1600
	1-03-1330		2-02-1624
	1-03-1418	Suzuki, Tomohiko (鈴木 知彦)	2-02-1315
	1-04-1406	Suzuki, Yasuo (鈴木 康夫)	2-15-1600
	2-02-1503	Swenson, Jan (Swenson Jan)	1S8-5

Tabata, Kazuhito (田端 和仁)	2-15-1624	Takahashi, Riku (高橋 陸)	2-14-1503
	3-12-1406	Takahashi, Satoshi (Takahashi Satoshi)	2-06-1451
Tadokoro, Naoki (田所 直樹)	3-09-1342	Takahashi, Satoshi (高橋 聡)	1-04-1518
Tagami, Shunsuke (田上 俊輔)	2-13-1403		2-06-1624
Taguchi, Hideki (田口 英樹)	1-12-1330		3-04-1354
	1-13-1354	Takahashi, Takuya (高橋 卓也)	1-03-1506
Taguchi, Mai (田口 真衣)	2-07-1503		1-12-1442
Taguchi, Masahiko (田口 真彦)	2-11-1800		1-13-1418
Taguchi, Yuta (田口 裕大)	2-07-1339		2-02-1712
Tahara, Shinya (田原 進也)	2-04-1636		2-03-1527
Tajjima, Hiroataka (田島 寛隆)	2-09-1648		2-03-1736
Tajjima, Hiroataka (田島 寛隆)	1-01-1454		2-03-1812
	1-07-1518		2-13-1748
	2-06-1427	Takahashi, Tohru (高橋 徹)	2S3-2
Tajjima, Seiya (但馬 聖也)	2-12-1403	Takahashi, Yohei (高橋 洋平)	1-01-1454
Tajimi, Yuki (多治見 祐希)	3-06-1406	Takai, Akira (高井 啓)	2-15-1800
Takada, Hiroya (高田 弘弥)	3-09-1418	Takakado, Akira (高門 輝)	3-11-1330
Takada, Kazunori (高田 一範)	2-16-1824	Takakuwa, Kazuya (高桑 和也)	1-13-1342
Takada, Nozomi (高田 希美)	3-05-1406	Takami, Shohei (高見 昇平)	3-05-1418
Takada, Sakura (高田 咲良)	2-14-1351	Takamori, Sho (高森 翔)	3-10-1454
Takada, Shoji (高田 彰二)	1S4-2	Takano, Fumiaki (高野 史明)	2-11-1527
	2S4-2	Takano, Mitsunori (高野 光則)	2-03-1415
	1-05-1342		2-07-1339
	1-05-1406		2-12-1427
	1-05-1430	Takano, Shin (高野 辰)	2-16-1451
	1-12-1354	Takano, Yu (鷹野 優)	1S3-3
	2-03-1624	Takarada, Masaharu (寶田 雅治)	2-16-1648
	2-03-1800	Takashima, Hajime (高島 一)	2-01-1351
	2-05-1339	Takasu, Masako (高須 昌子)	3-03-1430
	2-05-1351	Takasuka, Taichi (高須賀 太一)	2-15-1636
	2-06-1636		3-07-1330
	2-06-1648	Takazaki, Hiroko (高崎 寛子)	2-06-1724
	3-06-1342		2-15-1515
Takagi, Daisuke (高木 大輔)	3-11-1442	Takeda, Kazuki (竹田 一旗)	2-03-1439
Takagi, Hiroaki (高木 拓明)	2-07-1636	Takeda, Seiji (武田 晴治)	2-15-1636
Takagi, Toshiyuki (高木 俊之)	1-06-1330	Takehara, Dai (竹原 大)	2-01-1351
	2-06-1351	Takehiko, Ichikawa (Takehiko Ichikawa)	2-16-1748
	2-10-1451	Takekawa, Norihiro (竹川 宜宏)	1-01-1406
Takahashi, Chikako (高橋 稚佳子)	3-10-1354		1-01-1418
Takahashi, Daichi (高橋 大地)	2-07-1415		1-01-1454
Takahashi, Hidehisa (高橋 秀尚)	2-13-1748		1-02-1442
Takahashi, Hideo (高橋 栄夫)	3S4-5		2-02-1439
Takahashi, Hikaru (高橋 輝)	2-09-1439		2-08-1612
Takahashi, Hiroaki (高橋 大智)	2-15-1415		2-08-1624
Takahashi, Hirona (高橋 広奈)	2-15-1503		2-08-1700
Takahashi, Hiroshi (高橋 浩)	1-06-1330		2-08-1800
	2-06-1351	Takemura, Kazuhiro (竹村 和浩)	1-03-1430
	2-10-1427		1-04-1354
	2-10-1451		2-03-1515
Takahashi, Hiroto (高橋 泰人)	3-04-1354	Takenaka, Satoshi (竹中 聡)	2-02-1327
Takahashi, Kanami (高橋 花南)	2-02-1327	Takeshi, Fukuma (Takeshi Fukuma)	2-16-1748
Takahashi, Leona (高橋 玲央奈)	1-14-1518	Takeuchi, Chihiro (竹内 千尋)	1-09-1418
Takahashi, Masatsuyo (高橋 正剛)	3-03-1354	Takeuchi, Koh (竹内 恒)	3S4-5

	3S5-5	Tashiro, Rintaro (田代 凛太郎)	1-11-1418
	2-02-1351	Tateishi, Keito (立石 圭人)	2-07-1800
Takeuchi, Shoji (竹内 昌治)	2-10-1736	Tatsumi, Hitoshi (辰巳 仁史)	1-08-1418
	3-10-1454		1-09-1518
Takeyasu, Kotaro (武安 光太郎)	2-14-1403	Tawa, Keiko (田和 圭子)	2-09-1600
Takiguchi, Sotaro (滝口 創太郎)	2-05-1327	Terada, Tohru (寺田 透)	1-03-1342
Takinoue, Masahiro (瀧ノ上 正浩)	2S4-4	Terada, Tomoki P. (寺田 智樹)	2-01-1812
	1-05-1442		2-05-1736
	1-05-1454		2-05-1736
	1-16-1430	Terai, Kenta (寺井 健太)	3-11-1506
	1-16-1442	Terakawa, S. Mayu (寺川 まゆ)	3-05-1354
	2-05-1415	Terakawa, Tsuyoshi (寺川 剛)	2-03-1624
	2-05-1427		2-05-1339
	2-05-1503		2-06-1636
	2-13-1503		3-05-1354
	2-06-1700		3-06-1342
Takui, Takeji (工位 武治)	2-06-1700	Teranishi, Mizuki (寺西 美月)	2-01-1427
Tama, Florence (Tama Florence)	1S11-4	Terasawa, Hiroaki (寺沢 宏明)	3-13-1430
Tamai, Nobutake (玉井 伸岳)	2-10-1327	Terashi, Genki (寺師 玄記)	2-02-1503
Tamai, Shingo (玉井 真悟)	3-02-1354	Terashima, Hiroyuki (寺島 浩行)	1-10-1418
Tamao, Kenji (玉尾 研二)	3-12-1406	Terashima, Mia (寺島 美亜)	1-11-1430
Tamemoto, Naoki (爲本 尚樹)	1-14-1418	Terazima, Masahide (寺嶋 正秀)	2S6-2
Tamura, Atsuo (田村 厚夫)	2-01-1315		2-03-1327
Tan, Cheng (譚 丞)	1-03-1330		2-04-1812
Tanabe, Aki (田部 亜季)	2-04-1315		3-11-1330
Tanaka, Akemi (田中 明美)	1-07-1354	Teshima, Tomohiro (手嶋 友寛)	1-07-1506
Tanaka, Aya (田中 あや)	2-14-1503	Thadhani, Elina (Thadhani Elina)	3-02-1342
Tanaka, Hideaki (田中 秀明)	2-11-1327	Thutupalli, Shashi (Thutupalli Shashi)	1S7-6
	2-11-1636		1-09-1430
	2-16-1724	Théry, Manuel (Théry Manuel)	2-05-1612
Tanaka, Hiroto (田中 裕人)	1S8-1	Toda, Hajime (戸田 元)	2-05-1612
Tanaka, Masahito (田中 真人)	3-02-1354	Todoroki, Takuma (轟 拓磨)	2-03-1612
Tanaka, Motomasa (田中 元雅)	3-02-1354		3-03-1518
Tanaka, Motomu (田中 求)	1S12-1	Togashi, Yuichi (富樫 祐一)	3-05-1330
Tanaka, Tatsuki (田中 達基)	2-12-1812	Toko, Kazuma (床 和真)	1-01-1342
Tanaka, Yoshikazu (田中 良和)	1S3-5	Tokudome, Shun (徳留 俊)	2-01-1503
	1-02-1418	Tokunaga, Makio (徳永 万喜洋)	2-15-1724
	2-05-1451		2-15-1748
	2-12-1503		2-15-1812
	3-05-1406		2-15-1824
	2-12-1503		2-16-1812
Tanaka, Yoshiki (田中 良樹)	2-09-1351	Tokunaga, Yuji (徳永 裕二)	1S8-1
Tanaka, Yuhei (田中 悠平)	3-03-1406		3S4-5
Tanaka, Yuki (田中 雄希)	2-02-1339	Tokuraku, Kiyotaka (徳樂 清孝)	1-09-1330
Tang, Jingyi (唐 靜一)	2-12-1600		2-01-1636
	1-13-1430		2-04-1451
Tani, Aoi (谷 葵衣)	1-13-1430		3-04-1430
Taniguchi, Kenji (谷口 健治)	1-13-1342		2S3-00
Taniguchi, Yuichi (谷口 雄一)	1S5-5	Tokutomi, Satoru (徳富 哲)	2-11-1351
Tanimoto, Haruka (谷本 悠)	1-12-1418	Tokutsu, Ryutarou (得津 隆太郎)	2-04-1800
Tanimoto, Hirokazu (谷本 博一)	1-14-1454	Toma, Sachiko (藤間 祥子)	3-02-1454
Tanimoto, Shoichi (谷本 勝一)	2-05-1724		3-11-1342
Tanzawa, Takchito (丹澤 豪人)	3-05-1342		3-11-1354
Taoka, Azuma (田岡 東)	2-01-1648		1-01-1442
Tarama, Mitsusuke (多羅間 充輔)	3-09-1430	Toma-Fukai, Sachiko (藤間 祥子)	2-12-1439
Taraska, Justin (Taraska Justin)	3-08-1454	Tomida, Sahoko (富田 紗穂子)	

Tomii, Kentaro (富井 健太郎)	2-04-1515	Tsunabuchi, Ryosuke (綱淵 稔介)	2-01-1636
Tominaga, Makoto (富永 真琴)	1S9-5	Tsuneishi, Taichi (恒石 泰地)	2-12-1624
Tominaga, Takashi (富永 貴志)	2-09-1451	Tsunoda, Satoshi (角田 聡)	1-11-1418
Tominaga, Yoko (富永 洋子)	2-09-1451		1-11-1454
Tomishige, Michio (富重 道雄)	1-07-1342		2-12-1648
	2-07-1800		2-12-1748
Tomita, Atsuhiko (富田 篤弘)	1-02-1406		2-12-1800
	2-01-1515	Tsunoyama, Taka A (角山 貴昭)	1-09-1354
Tomita, Masahisa (富田 正久)	3-10-1354	Tsunoyama, Taka A. (Tsunoyama Taka A.)	2-08-1351
Tomita, Shunsuke (富田 峻介)	1S10-2	Tsurui, Hiromichi (鶴井 博理)	1-14-1406
Tomo, Tatsuya (鞆 達也)	2-11-1315		3-03-1330
Tomohara, Kanji (友原 貫志)	1S10-7	Tsuruyama, Tatsuaki (鶴山 竜昭)	1S12-4
	2-13-1451	Tsutsumi, Akihisa (包 明久)	2S2-6
Tomono, Junta (伴野 詢太)	2-05-1451		1-02-1506
Tomoshige, Michio (富重 道雄)	1-07-1354		2-02-1415
Torisawa, Takayuki (鳥澤 嵩征)	2-07-1712	Tsutsumi, Kento (堤 建人)	2-04-1800
Tosaka, Toshiyuki (登坂 俊行)	2-04-1339	Tsuzuki, Yuka (都築 侑果)	1-01-1454
Tosha, Takehiko (當舎 武彦)	2-06-1439	Uchida, Kunitoshi (内田 邦敏)	1S9-4
Toshino, Kenta (歳納 健太)	2-05-1748	Uchida, Takumi (内田 匠)	2-16-1415
Toyabe, Sho (鳥谷部 祥一)	2-07-1515	Uchida, Yumiko (内田 由美子)	1-07-1506
Toyabe, Shoichi (鳥谷部 祥一)	1-07-1442	Uchida, Yumiko (内田 裕美子)	2-08-1736
	2-05-1403		2-08-1748
Toyoda, Atsushi (豊田 敦)	2-09-1315		2-16-1700
	2-09-1339	Uchihashi, Takayuki (Uchihashi Takayuki)	2-07-1812
Toyota, Taro (豊田 太郎)	2-10-1736	Uchihashi, Takayuki (内橋 貴之)	1S4-1
Tran, Duy (Tran Duy)	1-06-1518		2-04-1724
Tsubaki, Motonari (鏗木 基成)	1-02-1518		2-12-1636
	1-06-1406		2-16-1503
Tsubouchi, Masaki (坪内 聖樹)	2-09-1736		3-06-1406
Tsuboyama, Yosuke (坪山 洋介)	2-08-1439		3-06-1418
	3-08-1518	Uchikawa, Ryo (内川 亮)	1-13-1342
Tsuchida, Naoyuki (土田 直之)	2-06-1351	Uchikubo-Kamo, Tomomi (内窪 友美)	1S3-5
Tsuda, Koji (津田 宏治)	3S5-2	Uda, Koji (宇田 幸司)	2-02-1315
Tsuji, Akihiro (辻 明宏)	2-11-1439	Udaka, Keiko (宇高 恵子)	3-03-1406
	3-08-1430	Ueda, Masahiro (上田 昌宏)	1S14-4
Tsuji, Naruaki (辻 成瑛)	2-01-1748		2S2-4
Tsuji, Ryoga (辻 怜河)	2-10-1648		1-15-1330
Tsujimoto, Koichi (辻本 浩一)	2-06-1403		2-08-1327
Tsujimura, Masaki (辻村 真樹)	2-12-1824		2-16-1600
Tsujiuchi, Yutaka (辻内 裕)	2-16-1824		2-16-1600
	3-14-1354	Ueda, Takeshi (上田 健史)	2-16-1712
Tsukamoto, Takashi (塚本 卓)	1-02-1430	Ueda, Waka (上田 和佳)	2-02-1403
	1-11-1430	Uehori, Maria (上堀 まりあ)	2-08-1800
	1-11-1442	Ueki, Misuzu (植木 美鈴)	3-10-1342
	2-12-1503	Uemura, Eri (上村 英里)	1-12-1330
	2-12-1724	Uemura, Naoki (上村 直輝)	2-08-1451
	2-12-1503	Uemura, Sotaro (上村 想太郎)	1-16-1406
	2-12-1503		2-16-1439
Tsukazaki, Tomoya (塚崎 智也)	1-06-1430		2-16-1515
Tsukihara, Tomitake (月原 富武)	2S7-2	Uemura, Tadashi (上村 匡)	2-14-1327
Tsukiji, Shinya (築地 真也)	2-05-1415	Uemura, Tomoko (植村 智子)	3-02-1342
Tsumoto, Kanta (湊元 幹太)	2-04-1315	Ueno, Hiroshi (上野 博史)	1S1-1
Tsumoto, Kouhei (津本 浩平)	2-04-1748		1-07-1418
	2-05-1427		1-07-1430
Tsumura, Nozomi (津村 希望)			

	1-07-1454	Wang, Anna (Wang Anna)	1S10-5
	2-04-1503	Wang, Jun (王 军)	3-11-1518
	2-07-1503	Wang, Peter (Wang Peter)	3-02-1342
	2-16-1800	Wang, Yi (王 一)	2-05-1812
	3-06-1406		2-05-1824
Ueno, Mako (上野 真琴)	2-06-1415		3-02-1418
Uesaka, Kazuma (上坂 一馬)	1-13-1442	Wang, Zi (王 梓)	3-04-1330
Uezu, So (上江洲 奏)	3-08-1418	Washio, Takumi (鷺尾 巧)	2-13-1600
Umeda, Kenichi (梅田 健一)	2-16-1427	Watanabe, Chiho (渡邊 千穂)	2-07-1636
Umemura, Kazuo (梅村 和夫)	2-15-1451		1S10-4
Umezawa, Koji (梅澤 公二)	2-03-1612		2-10-1712
	3-03-1518		2-10-1724
Unno, Hideaki (海野 英昭)	2-01-1600	Watanabe, Daisuke (渡邊 大介)	2-16-1600
Unno, Masaki (海野 昌喜)	3-01-1454	Watanabe, Haruki (渡部 治樹)	2-09-1351
Unno, Masashi (海野 雅司)	2-12-1736		2-09-1415
Unno, Masasi (海野 雅司)	2-11-1427	Watanabe, Hiroshi C. (渡邊 宙志)	3-14-1342
Urade, Reiko (裏出 令子)	3S4-2	Watanabe, Jo (渡辺 穰)	2-12-1724
Urakami, Hiroshi (浦上 弘)	2-09-1636	Watanabe, Kaichi (渡辺 開智)	1-08-1330
Urano, Ryo (浦野 諒)	1-10-1354	Watanabe, Keiichi (渡邊 啓一)	3-04-1406
Usami, Masataka (宇佐美 将誉)	2-04-1648	Watanabe, Kohei (渡辺 航平)	2-12-1712
Ushiba, Shota (牛場 翔太)	2-15-1600	Watanabe, Masato (渡邊 真人)	3-14-1406
Ushida, Takashi (牛田 多加志)	2-04-1612	Watanabe, Rikiya (渡邊 力也)	3-06-1430
Ushirogata, Kanajo (後潟 夏菜子)	2-15-1636	Watanabe, Ryo (渡邊 亮)	1-07-1454
Uwamichi, Masahito (上道 雅仁)	3-09-1442	Watanabe, Ryuta (渡辺 隆太)	2-13-1724
Uyeda, Taro (上田 太郎)	2-04-1612	Watanabe, Satoshi (渡部 聡)	1-06-1442
Uyeda, Taro Q.P. (上田 太郎)	2-01-1636		2-02-1415
	2-05-1748	Watanabe, Satoshi (渡部 聡)	2S2-6
	2-13-1648		1-02-1506
	3-07-1418	Watanabe, Shinji (渡辺 信嗣)	2-16-1427
Uyeda, Taro QP (上田 太郎)	1-09-1506	Watanabe, Takuma (渡邊 拓真)	2-12-1724
Vaidehi, Nagarajan (Vaidehi Nagarajan)	1S6-3	Watanabe, Yohei (渡邊 洋平)	2-15-1600
Valente-Paterno, Melissa (Valente-Paterno Melissa)	2-07-1724	Wayu, Chihiro (和湯 千紘)	2-01-1700
	2-07-1724		3-01-1518
van Veen, Hendrik W. (van Veen Hendrik W.)	1S11-2	Wazawa, Tetsuichi (和沢 鉄一)	2-01-1736
Verhey, Kristen (Verhey Kristen)	1S1-5	Wei, Aguan D. (Wei Aguan D.)	2-09-1315
Vianay, Benoit (Vianay Benoit)	1-09-1430	Wong, Richard (Wong Richard)	2-16-1351
Viet Cuong, Nguyen (グエン ヴェト クーン)	2-02-1748	Xian, Jingwen (XIAN JINGWEN)	3-03-1330
Vilfan, Andrej (ビルファン アンドレ)	2-07-1700	Xie, Qilin (謝 祺琳)	1-12-1442
Visootsat, Akasit (Visootsat Akasit)	1S1-3		1-13-1418
	3-07-1342		2-03-1527
Vogel, Hans J. (Vogel Hans J.)	1-02-1430	Xu, Bu (Bu Xu)	2-03-1736
Wada, Akimori (和田 昭盛)	2-12-1403	Y. Toyoshima, Yoko (豊島 陽子)	2-12-1339
	2-12-1439	Yabunaka, Yuzuki (藪中 柚輝)	3-06-1418
Wada, Masamitsu (和田 正三)	1-09-1506	Yabuta, Moe (藪田 萌)	1-01-1454
Wada, Takumi (和田 卓巳)	1S5-4	Yadav, Mohini (Yadav Mohini)	2-13-1515
Wakabayashi, Ken-ichi (若林 憲一)	1S13-2		1-03-1406
Wakabayashi, Taiki (若林 大貴)	2-01-1800		3-01-1406
Wakamoto, Ryo (若本 稜生)	1-16-1342	Yadav, Mohini (ヤダフ モヒニ)	2-04-1327
Wakamoto, Yuichi (若本 祐一)	1-15-1418	Yagi, Hiromasa (八木 宏昌)	2-05-1712
Wakao, Shingo (若尾 真吾)	1-13-1406	Yagi, Sota (八木 創太)	2-13-1403
Walde, Peter (わるで ぴーたー)	1S2-3	Yagi, Toshiki (八木 俊樹)	1-04-1342
Walde, Peter (ワルデ ピーター)	2-13-1439		2-07-1403
			2-07-1736

Yagi-Utsumi, Maho (矢木 真穂)	3S5-7 2-04-1724	Yamane, Tsutomu (山根 努)	2-06-1503
Yajima, Junichiro (矢島 潤一郎)	1-07-1406 2-07-1427 2-15-1327	Yamano, Yumiko (山野 由美子)	2-11-1327
Yajima, Yoshiki (矢島 芳起)	2-10-1427	Yamano, Yuuhei (山野 雄平)	1S2-5
Yamada, Daichi (山田 大智)	2-11-1736 2-11-1748	Yamaoki, Yudai (山置 佑大)	3-05-1418 3-05-1430 3-05-1442
Yamada, Hironao (山田 寛尚)	3-03-1430	Yamashita, Eiki (山下 栄樹)	2S5-5 1-06-1430
Yamada, Hiroyuki (山田 博之)	3-13-1330	Yamashita, Hayato (山下 隼人)	2-11-1439 3-08-1430
Yamada, Takahiro (山田 貴大)	2-13-1527	Yamashita, Keitaro (山下 恵太郎)	2-01-1515 2-12-1812
Yamada, Yuma (山田 勇磨)	2-12-1624	Yamashita, Nagi (山下 和諒)	3-02-1342
Yamagishi, Jumpei (山岸 純平)	2-14-1712	Yamashita, Takahiro (山下 高廣)	1-16-1442 1-11-1342 1-11-1354
Yamagishi, Masahiko (山岸 雅彦)	1-07-1406 2-15-1327 2-07-1427	Yamashita, Takefumi (Yamashita Takefumi)	2-07-1812
Yamagishi, Msahiko (山岸 雅彦)	1-06-1406	Yamashita, Takefumi (山下 雄史)	3-03-1418
Yamaguchi, Aoi (山口 葵)	3-06-1354 3-08-1430	Yamashita, Yoshiko (山下 慶子)	3-03-1406
Yamaguchi, Asuka (山口 明日香)	2-08-1800 1-04-1430 2-05-1612 3-01-1342	Yamat, Takahisa (倭 剛久)	2-01-1624
Yamaguchi, Ayaka (山口 綾香)	2-10-1439	Yamauchi, Kazuo (山内 一夫)	3-13-1418
Yamaguchi, Keiichi (山口 圭一)	2-07-1427 1-06-1406	Yamauchi, Masataka (山内 仁喬)	1-05-1342
Yamaguchi, Shoichi (山口 祥一)	3-08-1430 2-08-1800 1-04-1430 2-05-1612 3-01-1342	Yamauchi, Yuhei (山内 悠平)	2-14-1736
Yamaguchi, Tomoko (山口 智子)	2-10-1439	Yamawaki, Yuta (山脇 佑太)	2-01-1600
Yamaguchi, Yohei (山口 陽平)	2-07-1439	Yamazaki, Hirohito (山崎 洋人)	2-16-1439
Yamamoto, Airi (山本 愛理)	2-07-1612	Yamazaki, Masahito (山崎 昌一)	2-16-1515
Yamamoto, Akihiro (山本 陽大)	2-06-1327 2-13-1503 3-10-1406 3-10-1418		3S5-3 2-10-1600 2-10-1612 2-10-1624
Yamamoto, Daiki (山本 大樹)	1-15-1454 3-11-1430	Yamazaki, Moe (山崎 萌)	3-01-1506
Yamamoto, Daisuke (山本 大輔)	2-11-1712 2-11-1724 2-11-1736 2-11-1748	Yamazaki, Yoichi (山崎 洋一)	1-01-1442 1-04-1442 2-04-1800 3-02-1454 3-11-1330 3-11-1342 3-11-1354
Yamamoto, Junpei (山元 淳平)	2-15-1600 2-08-1427	Yamazaki, Yoichi (山崎 洋一)	2S5-3
Yamamoto, Kaori (山本 佳織)	3-05-1406	Yamazaki, Yosuke (山崎 陽祐)	1-09-1506 2-05-1748
Yamamoto, Kei (山本 啓)	3-11-1506	Yamazaki, Yousuke (山崎 陽祐)	3-07-1418
Yamamoto, Kentaro (山本 健太郎)	2S1-5	Yamazawa, Toshiko (山澤 徳志子)	2-06-1612
Yamamoto, Masamichi (山本 正道)	3S3-2	Yan, Shaonan (YAN SHAONAN)	3-04-1330
Yamamoto, Masayuki (山本 雅之)	1-03-1406 2-04-1327	Yan, Shaonan (闫 少南)	2-05-1812
Yamamoto, Naoki (山本 直樹)	3-01-1406 2-07-1403	Yan, Shaonan (闫 少男)	3-02-1418
Yamamoto, Norifumi (山本 典史)	1-09-1430 3-01-1342	Yanagawa, Masataka (柳川 正隆)	2S2-4 1-15-1330
Yamamoto, Norihumi (山本 典史)	1-05-1330 2-15-1515	Yanagi, Takashi (柳 昂志)	2-16-1712
Yamamoto, Ryosuke (山本 遼介)	3S6-5	Yanagida, Toshio (柳田 敏雄)	2-07-1636
Yamamoto, Shohei (山本 昌平)	3-12-1342 3-04-1430	Yanagida, Yuki (柳田 侑樹)	2-04-1427 2-05-1624
Yamamoto, Suguru (山本 卓)		Yanagisawa, Keisuke (柳澤 溪甫)	2-03-1712
Yamamoto, Tetsuya (山本 哲也)			
Yamamoto, Yaoki (山本 八生起)			
Yamamura, Shohei (山村 昌平)			
Yamanaka, Masanori (山中 雅則)			
Yamanaka, Shinya (山中 真也)			

Yanagisawa, Miho (柳澤 実穂)	1S10-4 2-10-1712 2-10-1724	Yokoyama, Yasunori (横山 泰範)	1-06-1330 1S10-5
Yanagisawa, Sachiko (柳澤 幸子)	2-06-1736 2-06-1748	Yomo, Tetsuya (Yomo Tetsuya)	1-02-1330 1-02-1342 2-11-1700
Yanagisawa, Yasuhide (柳澤 泰任)	3-09-1454	Yonemori, Kazuko (米森 和子)	1-02-1354
Yang, Shun Kai (Yang Shun Kai)	2-07-1724	Yonezawa, Kento (米沢 健人)	2-04-1800
Yang, Wendian (杨 文典)	3-02-1418	Yonezawa, Kento (米澤 健人)	1-01-1442 1-03-1342 1-04-1442
Yang, Wendian (楊 文典)	2-05-1812 3-04-1330	Yoshida, Hiroshi (吉田 寛)	1-06-1442 3-02-1454 3-03-1354 3-11-1342 3-11-1354
Yano, Amina (矢野 亜美奈)	2-16-1724	Yoshida, Itsuki (吉田 樹生)	1-14-1330
Yano, Daichi (矢野 大地)	2-02-1315	Yoshida, Kazunari (吉田 一也)	2-05-1736 1-14-1518 3-10-1330
Yano, Ko-hei (矢野 耕平)	3-01-1442	Yoshida, Kiyomi (吉田 清美)	2-05-1624
Yano, Seiji (矢野 聖二)	3-13-1342	Yoshida, Natsumi (吉田 夏海)	2-06-1503
Yao, Min (姚 閃)	1-02-1418 2-12-1503	Yoshida, Yuki (吉田 祐貴)	1-15-1418
Yasuda, Kenji (安田 賢二)	1-08-1342 1-09-1342 1-14-1342 1-14-1354 1-15-1506 2-08-1515 2-09-1351 2-09-1415 3-08-1506	Yoshido, Kana (吉戸 香奈)	2-13-1712
Yasuda, Satoshi (安田 賢司)	1-02-1354	Yoshidome, Takashi (吉留 崇)	1-03-1354 1-07-1442 2-02-1636 2-02-1648
Yasuhara, Kazuma (安原 主馬)	2-10-1636	Yoshii, Tatsuyuki (吉井 達之)	3S1-5
Yasui, Yuhei (安井 優平)	1-08-1330 2-14-1427	Yoshikawa, Hiroshi (吉川 洋史)	2-01-1748
Yasunaga, Takuo (安永 卓生)	2-02-1451 2-06-1724 2-15-1515 3-02-1442	Yoshikawa, Kenichi (吉川 研一)	2-05-1315 2-05-1415
Yasuzawa, Mikito (安澤 幹人)	2-10-1327	Yoshikawa, Shinya (吉川 信也)	1-06-1430
Yatabe, Keiko (谷田部 景子)	3-03-1354	Yoshikawa, Takumi (吉川 匠)	2-16-1451
Yato, Akane (矢埜 紅音)	3-04-1406	Yoshikawa, Yasushi (吉川 寧)	2-03-1712
Ye, Shen (叶 深)	2-11-1351	Yoshikawa, Yuko (吉川 祐子)	2-05-1315
Yesbolatova, Aiya K. (Yesbolatova Aiya K.)	2-08-1403	Yoshimori, Akira (吉森 明)	2S6-2 2-03-1327
Yimeng, Zhao (Yimeng Zhao)	2-06-1712	Yoshimori, Atsushi (吉森 篤史)	2-01-1351
Yoda, Takao (依田 隆夫)	2-03-1636	Yoshimura, Hideaki (吉村 英哲)	1-15-1342
Yoko-o, Takechiko (横尾 岳彦)	2-13-1648	Yoshimura, Hideyuki (吉村 英恭)	1-16-1506
Yokobori, Megumi (横堀 惠美)	3-08-1518	Yoshimura, Kohei (吉村 孝平)	2-07-1427
Yokoi, Shun (横井 駿)	1S6-4 2-06-1515	Yoshimura, Kohei (吉村 考平)	3-06-1354
Yokosawa, Kohei (横澤 公平)	2-04-1600	Yoshimura, Masataka (吉村 匡隆)	2-01-1403 2-09-1315
Yokota, Hiroaki (横田 浩章)	2-06-1600	Yoshina, Sawako (吉名 佐和子)	2-14-1351
Yokota, Junpei (横田 淳平)	2-02-1315	Yoshinaga, Natsuhiko (義永 那津人)	3-13-1430
Yokota, Yasunari (横田 康成)	2-08-1503 3-08-1442	Yoshinaga, Sosuke (吉永 壮佐)	2-01-1636
Yokoyama, Ken (横山 謙)	3-02-1330	Yoshino, Atsuki (吉野 敦貴)	2-06-1339
Yokoyama, Takeshi (横山 武司)	1S3-5 2-05-1451 3-05-1406	Yoshizawa, Shingo (吉澤 慎吾)	2-04-1451 2-05-1415
		Yousif, Ragheed H. (Ragheed H. Yousif)	1-02-1330 2-03-1451
		Yu, Fujio (湯 不二夫)	1S1-5
		Yu, Huaxin (Yu Huaxin)	
		Yu, Isseki (優 乙石)	
		Yue, Yang (Yue Yang)	

Yumoto, Tenji (湯本 天嗣)	<u>2-13-1648</u>
Yunoki, Yasuhiro (柚木 康弘)	<u>3S4-2</u>
Yuri, Taro (由里 太郎)	<u>2-16-1700</u>
Yusuke, Sato (佐藤 佑介)	<u>2-05-1503</u>
Yuzu, Keisuke (柚 佳祐)	<u>1-04-1430</u>
	<u>2-04-1351</u>
	<u>2-04-1415</u>
Zanni, Martin (Zanni Martin)	<u>2S7-3</u>
Zhai, Le (Zhai Le)	<u>2-15-1339</u>
Zhang, Chuanlun (Chuanlun Zhang)	<u>2-12-1339</u>
Zhang, Lin (張 琳)	<u>3-01-1330</u>
Zhang, XianJun (張 先駿)	<u>2-11-1351</u>
	<u>3-11-1454</u>
Zhang, Yuxia (張 玉霞)	<u>2S2-6</u>
	<u>1-02-1506</u>
Zhao, Enming (趙 恩明)	<u>2-09-1427</u>
Zheng, Jigkang (鄭 靖康)	<u>3-04-1418</u>
Zheng, Jingkang (鄭 靖康)	<u>2-02-1427</u>
ZhiRui, Cheng (智 睿 程)	<u>3-03-1342</u>
Zhou, Dejian (Zhou Dejian)	<u>3-05-1342</u>
Zhou, Xiang (周 翔)	<u>2-16-1812</u>
Zimmermann, Noemi (ツィーマーマン ノエミ)	<u>2-08-1648</u>

PDB 50th Anniversary Symposium in Asia

50 years of the Protein Data Bank and the Frontier of Structural Biology in Asia

<Background>

In 1971, the structural biology community established the single global archive for 3D macromolecular structure data: the Protein Data Bank (PDB). In 2000, Protein Data Bank Japan (PDBj) started on-site data processing as a newly founded Asian hub. Since 2001, PDBj has provided our newly developed online Data-out services available freely and publicly through our own web site (<https://pdbj.org>), which we have enhanced through the years. With the establishment of the worldwide PDB in 2003, we have served as one of its regional data centers, collaborating on Data-in and Data-out activities on a global scale. In 2021, we are celebrating the 50th anniversary of our single global archive. Especially this time in Asia, and we want to discuss the frontier of the Structural Biology in Asia.

At e-poster session, students and postdoctoral fellows are eligible for the PDBj poster prize.

<Date>

Wednesday, 24 November 2021 (JST)

<Preliminary program>

AM Poster session

PM PDB 50th Anniversary Symposium

Genji Kurisu (Osaka U., Japan), Kyeong Kyu Kim (Sungkyunkwan U., R. O. Korea), Yuh-Ju Sun (NTHU, Taiwan), So Iwata (Kyoto U., Japan), Ichio Shimada (RIKEN, Japan), Keiichi Namba (Osaka U. & RIKEN, Japan), Wenqing Xu (NFPS & ShanghaiTech U., P.R.China), Sameer Velankar (EMBL-EBI, UK)

<Further information>

<https://pdbj.org/news/pdb50asiasympo>

<Secretariat>

c/o Protein Data Bank Japan

Institute for Protein Research

Osaka University, Japan

Email: db_sec@protein.osaka-u.ac.jp

第 59 回 日本生物物理学会年会 高校生・高専生向け 生物物理ワークショップ

日 時：11 月 23 日（火・祝）13:30～16:30

会 場：オンライン

主 催：日本生物物理学会

対象者：主に高校生および高専生。参加費無料。参加申し込み必要（11 月 12 日締め切り，年会 HP から）。

世話人：鳥谷部祥一（東北大），柴田 讓（東北大），羽鳥晋由（山形大），最上讓二（東北大），元池育子（東北大）

※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：次世代を担う高校生および高専生をメインターゲットにする会を企画した。高校生や高専生は生物物理学には馴染みが薄いと思われるが，生物物理学という分野を知っていただき，その魅力を伝え，将来の学会員の芽を育てることが目的である。講演だけでなく，グループディスカッション，発表会，交流会からなるインタラクティブなワークショップを予定している。

プログラム：

1. 講演 3 件

西口大貴（東京大学 理学系研究科 物理学専攻 助教）

微生物の泳ぎと群れの運動を物理学者と一緒に眺めてみよう！

柳澤実穂（東京大学 総合文化研究科 先進科学研究機構 准教授）

細胞の形とその力学：真似して造って理解する

白井 剛（長浜バイオ大学 フロンティアバイオサイエンス学科 教授）

「物理の力」で病気と闘う？

2. グループディスカッション（講演中に出される「お題」に関して，グループに分かれて議論。）

3. ディスカッションの内容をグループごとに発表。

4. 交流会（質問コーナー）



西口大貴氏
東京大学 理学系研究科
物理学専攻 助教



柳澤実穂氏
東京大学 総合文化研究科
先進科学研究機構 准教授



白井 剛氏
長浜バイオ大学 フロンティア
バイオサイエンス学科 教授

男女共同参画・若手支援委員会企画シンポジウム 働き方の多様性を考える～ After コロナ時代に向けて

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：2021年11月27日（土）12:00～13:30

会場：オンライン開催

形式：講演会

司会：田端和仁（東京大学）

シンポジスト：土屋理恵（Novozymes A/S）、石崎章仁（分子科学研究所）、伊藤奨太（日本学術振興会）

※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：新型コロナウイルス感染症がきっかけとなって、これまでの「働き方」は大きく変容しました。多くのイベントがオンライン上で完結するようになり、本年会のようなオンライン学会にも多くの方が滞りなく参加できていることは、before コロナ時代には思いもしなかったことだと思います。今後も「ちょっと Zoom で打ち合わせ」というように、オフラインとオンラインとをうまく併用しながらの生活になっていくでしょう。

日本生物物理学会では、男女共同参画と若手支援を目的とした企画シンポジウムを毎年の年会で開催してきました。多様なキャリアパス、多様な働き方・生き方、ワークライフバランスなどを取り上げることが多いですが、今年は特に After コロナ時代を見据えて、「働き方」が今後どうなるのか、どうしていきたいのか、どうありたいのか、ということを考えるきっかけになるようにと思い、このようなテーマのシンポジウムを企画しました。

ところで、コロナ禍の一番の弊害は、雑談が気軽にできなくなってしまったことだと思います。研究の話はオンライン学会で聞けても、オンライン学会ではなかなか「雑談」をすることができません。身近な人以外のキャリアの話やワークライフバランスの話がほとんど聞けなくなってしまったことに、強い危機感を持っています。本シンポジウムは、研究の話というよりは働き方に対する価値観や工夫、経験といった貴重な「雑談」に焦点を当てたいと思います。デンマークで長く働かれている Novozymes A/S の土屋理恵さん、分子科学研究所 教授であり育児休業制度の利用経験もある石崎章仁さん、研究業界から官公庁に入られた若手である伊藤奨太さんの3名の話を知りたいと思います。それぞれの講演者の雑談トークにより、皆さんが多様な働き方に触れ、来たる After コロナ時代に向けて働き方について考えるきっかけとなれば幸いです。

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：11月25日（木）12:00～13:00

形式：Zoom ミーティングでのライブ配信

※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！

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いたします。

【Part 1】 12:00～12:20 博士・PDの方の為の就活ガイダンス

徐々に企業の採用対象として存在感を増してきている博士人材ですが、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企業の採用活動の現在、②博士やPDの就職活動の実態、③博士人材が活躍できる企業の探し方を中心に紹介します。

【Part 2】 12:20～12:40 理系大学院生の就活ケーススタディ

周りを見れば大卒としてどのように就職活動しているか見えてくるかと思いますが、自身に最適な方法や目標を見つけるのは至難の業です。ここでは実際にアカリクで支援した方の情報をもとにして、状況に応じてどのような戦略や戦術が有効なのかを解説します。

【Part 3】 12:40～13:00 専門外就職へ向けて何をすべきか

専門性が高いほど技術や知識がそのまま活用できる仕事は少なくなりますが、その専門性を構成する要素を紐解くことで「専門外」の領域で幅広く活躍することが視野に入ります。専門外就職を目指す上で特に注意すべき「一貫性」を中心に書類の書き方や面接対策などのノウハウを解説します。

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。また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。お申込方法は年会ウェブサイトをご確認ください。

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：11月27日（土）12:00～13:00

会場：オンライン開催

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。

第59回生物物理学会バイオイジックスセミナー

switchSENSE® heliX® : measuring interactions from small molecules to cells

Thursday, November 25 at 12:00-12:50PM

Room : ch3

Alice Soldá, Irene Ponzó, Agnes Marsal, Daisy Paiva
Dynamic Biosensors GmbH



switchSENSE® is an automated, fluorescence-based biosensor chip technology that employs electrically actuated DNA nanolevers for the real-time measurement of binding kinetics (k_a , k_d) and affinities (with K_D values down to the fM range). The platform offers an automated ligand density control, which allows to conveniently discriminate between affinity and avidity in one single assay. Interactions between proteins, DNA/RNA, and small molecules can be detected with femto-molar sensitivity. At the same time, conformational changes and complex binding events can be measured using minimal amounts of sample.

Using heliX® instrument and the novel DNA Y-structure, we made it possible to characterize ternary complex formation of bifunctional small molecules like PROTACs (Proteolysis targeting chimeras). The E3 ligase as well as a target protein can be functionalized on each separate end of two FRET pair color-coded Y-arms. The Y-structure closes upon PROTAC binding and the subsequent ternary complex formation bringing together the green donor and the red acceptor dye into a closer, FRET sensitive, distance. The change in red fluorescence signal intensity directly correlates with ternary complex formation kinetics. We show that the Y-structure is an extremely versatile tool for studying any type of protein-protein complex formations with a

dissociation constant between 1nM to 10 μ M.

Moving from small molecules interactions to complex systems, we present a novel method to capture isolated cells and to measure the association and dissociation kinetics of fluorescently labeled antibodies to/from cell surface antigens in real-time. To this end, flow-permeable, mesh-like cell cages were designed to accommodate and physically retain single cells in the microfluidic channel of a commercially available biochip. Suspension or adherent cells can be loaded into the cages by an automated workflow using only a few microliters of sample and are subsequently exposed to binders under continuous flow. We validated the method by investigating a number of different antibody clones against various antigens (CD3, CD1d, CD7 and CD305) expressed on the surface of T-lymphocyte cancer cells. The engagement of antibodies to one or two antigens (affinity vs. avidity) on the cell surface and ultimately correlate avidity with the antigen expression level could be determined in a reproducible manner.

In this work we will highlight both recent advances that allows investigation of biomolecular interactions under conditions that are close to in-vivo situations in a highly automated workflow and thus useful for the screening and characterization of new drugs that intervene in the different cellular or biochemical processes..



お問い合わせ先

DKSHジャパン株式会社 テクノロジー事業部門 科学機器部

Tel : 03-5730-4510 Fax :03-5730-7605

e-mail: tp.labtyo@dksh.com

* This event will be presented in English language.

第 59 回日本生物物理学会年会 BP セミナー 2021 年 11 月 26 日 (金) ch2

PDB activities under ongoing Covid-19 situation, and up-to-date information on our quality improvement and data validation

By Genji Kurisu, Institute for Protein Research, Osaka University

PDBj (PDB Japan, <https://pdbj.org/>) is an Asian hub for the development of the single global archive for 3D macromolecular structure data as known as PDB, which is accessible freely online. In this session, we will talk how promptly we are trying to provide necessary information under the ongoing Covid-19 situation. We will also introduce our various quality improvement activities, and data validation system utilizing Cambridge Structural Database (CSD).

PDBj tools and services for analyzing and visualizing structural data.

By Gert-Jan Bekker, Institute for Protein Research, Osaka University

PDBj has developed multiple services for exploring, visualizing and retrieving data from the PDB. In this seminar, we will introduce some of the new functionality of the main PDBj website to search and explore PDB data. In addition, we will describe some of the new functionality of our WebGL based molecular viewer Molmil (<https://pdbj.org/molmil2/>) and show examples of how advanced visualization operations can be performed.

Services and databases for 3D electron microscopy data by PDBj and wwPDB

By Hirofumi Suzuki, Waseda University

The rate of increase in the number of electron microscopy (EM) data is still accelerating. EM raw images, 3D density maps, and atomic coordinates are stored in the databanks, EMPIAR, EMDB, and PDB, respectively. The seminar will cover recent trends in EM data in the databanks, new wwPDB activities such as validation reports for EM data, PDBj database activities, and services and tools for EM, such as EM Navigator and Omokage search.

Protein Data Bank Japan
<https://pdbj.org>

PDBj 事務局
565-0871 大阪府吹田市山田丘 3-2
大阪大学蛋白質研究所プロテインデータバンク研究室
TEL: 06-6879-4311 (事務局) 8634 (登録事務局)

* This event will be presented in English language.

第 59 回日本生物物理学会年会

サーモフィッシャーサイエンティフィック

バイオフィジックスセミナー

◆ 日時 : 2021 年 11 月 26 日 (金) 12:00-12:50

◆ 会場 : ch3

クライオトモグラフィーで実現する生体三次元構造解析の新時代:

生体分子構造から機能解析へ

甲斐 翼

サーモフィッシャーサイエンティフィック

The New Era of Advanced Structural and Functional Analysis of Biological Systems Driven by Cryo Tomography

Tsubasa Kai

Thermo Fisher Scientific

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。

細胞内やタンパク質複合体の微細構造は電子顕微鏡を用いることで観察することが可能である。現在、タンパク質の立体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を用いた単粒子解析法が大きな注目を集めているが、クライオ電子顕微鏡のアプリケーションはそれだけにとどまらない。そ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。つまり、クライオトモグラフィー法によって、各タンパク質やその複合体の独立した立体構造だけでなく、それらが相互作用し、機能している環境の様子までを詳細に三次元観察することで、これまでない視点から生体内の機能解析することが可能となる。本セミナーでは、クライオトモグラフィー法のワークフローを最新のアプリケーション事例とともに紹介する。

※このイベントは日本語で開催します。

* This event will be presented in Japanese language.

実際に手に取って見たコアユニット製品

～全反射蛍光観察および広視野多細胞観察について～

発表日：11月27日(土) 12:00 - 12:50 部屋番号：ch3

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(音声付ご紹介動画は <https://youtu.be/dLUpQW0lLfc> または



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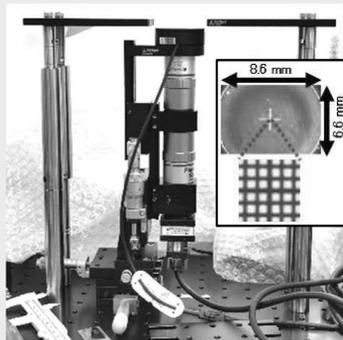
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「全反射顕微鏡を初構築して
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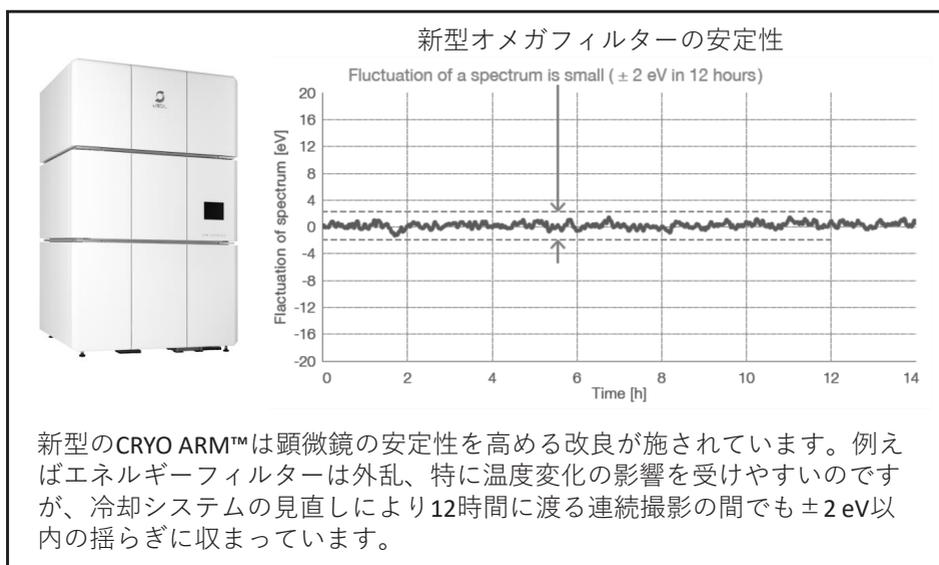
* This event will be presented in Japanese language.

“CRYO ARM™は新しい世代へ”

近年、クライオ電子顕微鏡による単粒子解析法の分解能は飛躍的に向上しており、タンパク質の構造解析に無くてはならない手法となりました。当社では長年培った極低温技術を盛り込んだクライオ電子顕微鏡に、より高い分解能を実現する冷陰極電子銃や多試料を装填可能なクライオステージを搭載したCRYO ARM™をリリースし、分解能レコードを塗り替えてきました。

しかし、これまでのクライオ電子顕微鏡を用いた単粒子解析法ワークフローは、スクリーニング用とデータ取得用の複数の電子顕微鏡で構成されており、使用者にとって運用コストが大きいという問題がありました。また、極低温の凍結試料を装置間で移動させる事への懸念があり、1台のクライオ電子顕微鏡でスクリーニングからデータ取得まですべてサポートすることが待ち望まれていました。さらに、より広くお客様に使用していただくためには、電子顕微鏡の扱いに慣れた特定の使用者だけではなく、これから電子顕微鏡を使い始めるユーザーにも使用できるようなユーザビリティの向上が必要とされていました。当社ではこうした要求に応えるべく、より短時間で、より簡単な操作で、より高品質のデータ取得を実現した次世代のCRYO ARM™ IIを開発しました。

本セミナーではCRYO ARM™ IIのテクノロジーを御紹介いたします。



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* This event will be presented in Japanese language.

微細構造の Live-Imaging を実現する超解像顕微鏡

Lattice SIM² & Airyscan2 Multiplex

市川 明彦

カールツァイス株式会社 リサーチマイクロスコピーソリューション, 102-0083 千代田区麹町 2-10-9

概要

顕微鏡の光学限界を超える分解能を得る手法として、超解像顕微鏡(SRM)法が確立されてから、多様な技術を用いた SRM が開発され、様々な研究分野に利用されている。そうした中、近年では固定化試料のみならず、1 細胞 1 分子を主対象とした動態研究としてライブイメージングへの需要が高まっている。

この需要に対して、従来の構造化照明顕微鏡(SIM)技術では、縞状照明の重複照射によるサンプルへのダメージやデータ取得に時間がかかるといったデメリットが存在する。これにより、褪色・光毒性で長時間の撮像が難しい、高速度の生命現象・反応を捉えられないなどの不都合が生じていた。

そこで、カールツァイス株式会社では独自の格子状の構造化照明(Lattice SIM)を採用することで、上記の問題点を解消し、取得速度を従来比で 2 倍の効率化を実現した。さらに、この度開発された Elyra7 with Lattice SIM² (図 1)では、演算方法を見直すことで、Lattice SIM のメリットはそのままに、最大 255fps (2D, Burst mode)の速度と 60nm(xy), 200nm(z)の分解能を得ることが可能となる(図 2)。

また SIM 技術に共通するメリットとして、専用色素やサンプリングに限定されることなく、一般的な蛍光色素を使用できるという点で汎用性に優れる。

本セミナーでは、この Lattice SIM²技術を搭載した超解像顕微鏡 ZEISS Elyra7 と共焦点顕微鏡ベースで使用可能な超解像検出器 Airyscan2 Multiplex について、その特徴であるライブイメージング技術を中心に最新の知見を交えて紹介する。

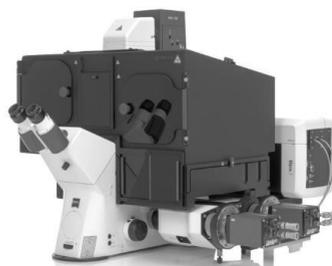


図 1 Elyra7 with Lattice SIM² システム

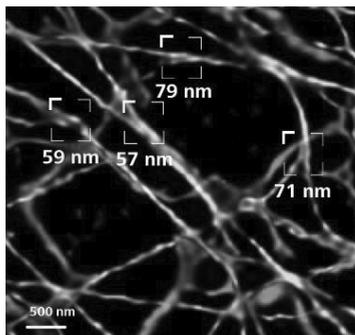


図 2 Lattice SIM² 参考画像

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キーワード

超解像顕微鏡、ライブイメージング、生細胞構造化照明(SIM)、分子動態、低毒性

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