Program for Joint Molecular Simulation Workshop between Institute of Science Tokyo and Keio University
(科学大・慶應大 合同分子シミュレーションワークショップ @東京科学大 大岡山キャンパス　プログラム)

July 14 (Mon)	Time	Name	Affiliation	Title	Chair
	14:30			Doors Open / 開場	
	15:00	Kenji Yasuoka(泰岡 顕治)	Dept. of Mechanical Engineeing, Keio University	Opening Remarks / 開会の挨拶	
PI 1	15:05	Akio Kitao (北尾 彰朗)	School of Life Science and Technology, Institute of Science Tokyo	Introduction to Kitao Laboratory / 北尾研究室 研究紹介	Kenji Yasuoka
Oral 1	15:15	Zhen Bai (白 臻)	School of Life Science and Technology (D3), Institute of Science Tokyo	Conformational Cycle of Sir2 in NAD⁺-Dependent Deacetylation of p53-ALY382	
Oral 2	15:35	Yusuke Takagi (髙木 悠丞)	Graduate School of Science and Technology (M2), Keio University	Introduction to Yamamoto Laboratory + Analysis of Heterogeneous Fields and Particle Behavior via Mesoscale Simulation 山本研究室 研究紹介 + メソスケールシミュレーションによる不均一場と粒子挙動の解析	Akio Kitao
Oral 3	15:52	Yuki Nakagaki (中垣 友希)	Graduate School of Science and Technology (M2), Keio University	Unveiling the Dynamics of Membrane-bound Protein AKT on Lipid Bilayers 脂質二重膜上における膜結合タンパク質AKTのダイナミクスの解明	
	16:05			(Break)	
PI 3	16:20	Noriyoshi Arai (荒井 規允)	Dept. of Mechanical Engineeing, Keio University	Introduction to Arai Laboratory / 荒井研究室 研究紹介	
Oral 4	16:30	Akihiro Yamaguchi (山口 晃寛)	Graduate School of Science and Technology (D3), Keio University	Study on Improving Adhesion at Phase-Separated Interfaces in Thermoplastic Starch/Biodegradable Polyester Composites 熱可塑性デンプン/生分解性ポリエステル複合材料における相分離界面の密着性向上に関する研究	Kenji Yasuoka
PI 4	16:50	Kenji Yasuoka (泰岡 顕治)	Dept. of Mechanical Engineeing, Keio University	Introduction to Yasuoka Laboratory / 泰岡研究室 研究紹介	
Oral 5	17:00	Sosuke Asano (浅野 綜介)	Graduate School of Science and Technology (M1), Keio University	An unsupervised deep learning method to identify characteristic amino acid residues from molecular dynamics simulation by comparing similar systems 類似系の分子動力学シミュレーション間の比較による特徴的なアミノ酸残基同定のための教師なし深層学習手法	Noriyoshi Arai
Poster	17:30			(Poster presentation)	
	19:30	Akio Kitao (北尾 彰朗)	School of Life Science and Technology, Institute of Science Tokyo	Closing Remarks / 閉会の挨拶	

Poster Presentation List / ポスター発表リスト

1	Meng Fan (孟 凡)	Graduate School of Science and Technology (D1), Keio University	Molecular Dynamics Simulation of Molecular Adsorption Behavior on FePt Metal Electrodes FePt金属電極への分子吸着挙動に関する分子動力学シミュレーション
2	Naoya Osato (大里 直也)	Graduate School of Science and Technology (M2), Keio University	Reverse Mapping from DPD Model to All-Atom MD Model of Star Polymer Self-Assembly Structures スターポリマー自己集合構造のDPDモデルから全原子MDモデルへのリバースマッピング
3	Toshiki Mori (森 俊貴)	Graduate School of Gifu University (D3, Visiting Student in Yamamoto Lab)	Regulation Mechanisms of K-Ras Signal Transduction by Lipid Domains as Revealed by High-Speed Super-Resolution Microscopy
4	Youtaro Takeda(武田 陽太郎)	Graduate School of Science and Technology (M2), Keio University	Vibrational and Diffusion Dynamics of Water Molecules in FUS Protein Condensates: Molecular Interpretation
5	Duy Phuoc Tran (陳 福 唯)	School of Life Science and Technology (Assisgtant Professor), Institute of Science Tokyo	G Protein Coupling Selectivity of the Adenosine A2A receptor
6	Soichiro Kijima (木島 壮一朗)	School of Life Science and Technology (D2), Institute of Science Tokyo	Nucleic acid-binding mechanisms in concert with intrinsically disordered region revealed by molecular dynamics simulations of FUS protein 分子動力学シミュレーションによる天然変性タンパク質FUSのジンクフィンガードメインと天然変性領域による協調的な核酸結合機構の解明
7	Lu Wenbo (陸 文博)	School of Life Science and Technology (D1), Institute of Science Tokyo	Investigating the Binding Characteristics between Glutathione S-Transferase and Anthocyanins
8	Vi Toan Lam	School of Life Science and Technology (M2), Institute of Science Tokyo	In silico study of transmembrane allosteric effect of CBD on CB1 receptor
9	Koki Yano (矢野晃紀)	Graduate School of Science and Technology (M2), Keio University	Investigating the Allosteric Inhibition Mechanism of PTP1B by Molecular Dynamics Simulation 分子動力学シミュレーションによるPTP1Bのアロステリック阻害メカニズム研究
10	Naonobu Kuribayashi(栗林直信)	Graduate School of Science and Technology (D2), Keio University	分子動力学法によるAQP4四量体ポア内を透過する水分子のゆらぎに関する研究 Investigation of Water Fluctuations through the AQP4 Tetramer Pore Using Molecular Dynamics Simulations