## \*15 minutes per talk

# Monday, March 1, 2021 (Day 1)

13:00-14:30 JST | 23:00 (Feb 28)-00:30 EST | 20:00-21:30 PST (Feb 28) | 5:00-6:30 CET

### Group A

- A-1 *In situ* genome sequencing Paul Reginato (Massachusetts Institute of Technology, USA)
- A-2 An integrative approach toward the Planarian Promoter Nucleosome Architecture Reza Bagherzadeh (Gakushuin University, Japan)
- A-3 Redefinition of Promoters and Super-enhancers Ranked by Histone H4 Hyperacetylation Identifies Transcription Factors Involved in Glioblastoma Stemness Nando Dulal Das (RIKEN Center for Biosystems Dynamics Research, Japan)
- A-4 DNA replication machinery contributes to development of eye in *Drosophila* Hidetsugu Kohzaki (Shumei University, Japan)
- A-5 Competition-based scaling of two pronuclei enables epigenetic maintenance in zygotes Hirohisa Kyogoku (Kobe University, Japan)
- A-6 Structure of RNA polymerase bound with transcription termination factor Rho Yuko Murayama (RIKEN Center for Biosystems Dynamics Research, Japan)

## Group B

- B-1 Role of the IgE variable heavy chain in FcεRIα and superantigen binding in allergy and immunotherapy
  Samuel Ken-En Gan (Experimental Drug Development Centre, A\*STAR, Singapore)
- **B-2** Deep neural network models to predict ion channel inhibitors with pre-learning of activity information of analogous proteins Tomohiro Sato (RIKEN Center for Biosystems Dynamics Research, Japan)
- **B-3** Development of FMODB and analysis of the inter- and intramolecular interaction data of biomolecules Daisuke Takaya (RIKEN Center for Biosystems Dynamics Research, Japan)
- B-4 Development of drug discovery support technology: inter- and intramolecular interaction analysis by fragment molecular orbital (FMO) calculation Chiduru Watanabe (RIKEN Center for Biosystems Dynamics Research, Japan)

- B-5 Activity cliff for 7-substituted pyrrolo-pyrimidine inhibitors of HCK explained in terms of predicted basicity of the amine nitrogen Hitomi Yuki (RIKEN Center for Biosystems Dynamics Research, Japan)
- B-6 Interaction-Induced and Motility-Induced Phase Separation in a Lattice Model Kyosuke Adachi (RIKEN Center for Biosystems Dynamics Research, Japan)

#### Group C

- C-1 In Vitro Reconstitution of the Wolffian Duct Using Human Pluripotent Stem Cells Junichi Taniguchi (RIKEN Center for Biosystems Dynamics Research, Japan)
- C-2 Tracking S-shape body formation towards understanding the mechanism of nephron maturation

Olena Trush (RIKEN Center for Biosystems Dynamics Research, Japan)

- C-3 Niche-Specific Regulation of MET Events within Kidney Organoids Rio Noto (RIKEN Center for Biosystems Dynamics Research, Japan)
- C-4 Recapitulating ventral hindgut development generates bladder organoids from human pluripotent stem cells Kazuhiro Ofuji (RIKEN Center for Biosystems Dynamics Research, Japan)
- C-5 FGF10 and testosterone are required for primary prostate induction in mouse embryo Wataru Uno (RIKEN Center for Biosystems Dynamics Research, Japan)

14:30-15:15 JST | 00:30-01:15 EST | 21:30-22:15 PST (Feb 28) | 6:30-7:15 CET Break

15:15-16:30 JST | 01:15-2:30 EST | 22:15-23:30 PST (Feb 28) | 7:15-8:30 CET

#### Group A

- A-7 A minimal model to understanding heterogeneous dynamics in live cell nucleosomes S.S Ashwin (Nagoya University, Japan)
- A-8 Multi-scale architecture of archaeal chromosomes Naomichi Takemata (Kyoto University, Japan)
- A-9 Role of nuclear membrane protein Bqt4 for the regulation of the nucleolus position and volume in fission yeast

Masaru Ueno (Hiroshima University, Japan)

- A-10 HiC1Dmetrics: Using 1D metrics to describe different structure from Hi-C data Jiankang Wang (Institute for Quantitative Biosciences, The University of Tokyo, Japan)
- Evolution of the core fold in RNA polymerase from ancient simple peptide A-11 Sota Yagi (RIKEN Center for Biosystems Dynamics Research, Japan)

#### **Group B**

B-7 Liquid Crystal Peptide/DNA Coacervates in the Context of Prebiotic Molecular **Evolution** 

Tony Z. Jia (Tokyo Institute of Technology, Japan)

- B-8 Lifespan and motility analysis of C.elegans expressing C-terminal fragments of ALScausative TDP-43 Yidan Lyu (Graduate School of Life Science, Hokkaido University, Japan)
- B-9 Liquid-liquid phase separation as organising principle in self-assembly of spider silk Ali D. Malay (RIKEN Center for Sustainable Resource Science, Japan)
- B-10 Role of ions on solubility and self-assembly of repetitive domain of spider dragline silk protein Nur Alia Oktaviani (RIKEN Center for Sustainable Resource Sciences, Japan)
- B-11 Liquid droplet enhances enzyme activity of L-lactate oxidase Tomoto Ura (RIKEN Center for Biosystems Dynamics Research, Japan)

#### Group C

- C-6 Understanding cell origin and the developmental signals during mammalian bladder development Filip Jos Wymeersch (RIKEN Center for Biosystems Dynamics Research, Japan)
- C-7 A Study of the Mechanism of the Glomerular Vascularization in vitro Kensuke Yabuuchi (RIKEN Center for Biosystems Dynamics Research, Japan)
- C-8 Non-monotonic fluidization generated by fluctuating edge tensions in confluent tissues Takaki Yamamoto (RIKEN Center for Biosystems Dynamics Research, Japan)
- C-9 A single-cell transcriptome approach to investigate the mechanism of mesoderm lineage-specification using human iPSCs

Wei Zhao (RIKEN Center for Biosystems Dynamics Research, Japan)

### Tuesday, March 2, 2021 (Day 2)

13:00-14:15 JST | 23:00 (March 1)-00:15 EST | 20:00-21:15 PST (March 1) | 5:00-6:15 CET

#### Group A

A-12 Structural basis for Rac activation by the ELMO1-DOCK5 bipartite guanine exchange factor

Mutsuko Kukimoto-Niino (RIKEN Center for Biosystems Dynamics Research, Japan)

- A-13 Regulation of Actin Dynamics by Phosphoinositides Yosuke Senju (Okayama University, Japan)
- A-14 A specific eIF4A paralog facilitates LARP1-mediated translation repression during mTORC1 inhibition

Yuichi Shichino (RIKEN Cluster for Pioneering Research, Japan)

A-15 Structural and biochemical analysis for translation regulatory protein from baculovirus Daijiro Takeshita (National Institute of Advanced Industrial Science and Technology

(AIST), Japan)

#### Group B

B-12 Molecular Dynamics of Dietary Poly Unsaturated Fatty Acids on Positive Allosteric Modulatory Domains of Vitamin D Receptor and its Consequential Effects on Skeletal Muscle Glucose Homeostasis Balaji Hari (JSS Academy of Higher Education and Research, JSS College of Pharmacy,

India)

B-13 Analysis of structural changes on E1/E2 transition of SR-Ca<sup>2+</sup>-ATPase using molecular dynamics simulations Chigusa Kobayashi (RIKEN Center for Computational Science, Japan)

**B-14 MDGRAPE-4A: a special purpose computer for molecular dynamics simulations** Gentaro Morimoto (RIKEN Center for Biosystems Dynamics Research, Japan)

- **B-15 DNA translocases reposition a nucleosome by the unwrap-shift-rewrap mechanism** Fritz Nagae (Kyoto University, Japan)
- B-16 Structural and functional characterization of *de novo* designed membrane coiled-coil peptide channels

Ai Niitsu (RIKEN Cluster for Pioneering Research, Japan)

Group C

- C-10 Cryo-EM structure of the photosynthetic RC-LH1-PufX supercomplex at 2.8 Å resolution Laura Bracun (RIKEN Center for Biosystems Dynamics Research, Japan)
- C-11 Engineering of pore-forming toxin: Grafting the transmembrane region of staphylococcal two-component hemolysin to one-component hemolysin Nouran Ghanem (RIKEN Center for Biosystems Dynamics Research, Japan)
- C-12 Crystal structure of ABC heme exporter Tamao Hisano (RIKEN Center for Biosystems Dynamics Research, Japan)
- **C-13** Structural changes in Cl- pump rhodopsin by time-resolved crystallography Toshiaki Hosaka (RIKEN Center for Biosystems Dynamics Research, Japan)
- C-14 Heme toxicity and its detoxification by an ABC-type efflux pump in Gram-positive pathogenic bacteria Hiro Nakamura (RIKEN Center for Biosystems Dynamics Research, Japan)

14:15-15:15 JST | 00:15-01:15 EST | 21:15-22:15 PST (March 1) | 6:15-7:15 CET Break

15:15-16:30 JST | 01:15-2:30 EST | 22:15-23:30 PST (March 1) | 7:15-8:30 CET

## Group A

- A-16 Mapping the Conformational Dynamics of Spike Protein in SARS-Cov-2 Hisham M. Dokainish (RIKEN Cluster for Pioneering Research, Japan)
   A-17 Molecular dynamics study of the dimeric SARS-CoV-2 main protease with 7 HIV inhibitors Teruhisa S. Komatsu (RIKEN Center for Biosystems Dynamics Research, Japan)
- A-18 Cryptic pockets in glycosylated SARS-CoV-2 spike proteins Lorena Zuzic (Agency for Science, Technology and Research Singapore, Singapore)
- A-19 Dynamics of a stochastic coronavirus (COVID-19) epidemic model with Markovian switching Mohamed El Khalifi (Ibn Tofail University, Morocco)

#### Group B

**B-17** Dimensionality reduction of macromolecular dynamics using UMAP Mao Oide (RIKEN Cluster for Pioneering Research, Japan)

- **B-18** Developments and Applications of Free-Energy Analysis for Protein-Ligand Binding Hiraku Oshima (RIKEN Center for Biosystems Dynamics Research, Japan)
- **B-19 Coarse-grained simulations of multiple intermediates along conformational transition pathways of multi-domain proteins** Ai Shinobu (RIKEN Center for Biosystems Dynamics Research, Japan)
- B-20 SSBD:database and SSBD:repository Online Open Resources for Bioimages and Quantitative Data for Biosystems Dynamics Hiroya Itoga (RIKEN Center for Biosystems Dynamics Research, Japan)
- **B-21** Self-assembling supramolecular nanostructure complexes constructed from protein nanobuilding blocks Ryoichi Arai (Shinshu University, Japan)

### Group C

- C-15 Investigation of the dynamics of GPCR microswitches related to functional selectivity Yutaro Ogaeri (RIKEN Center for Biosystems Dynamics Research, Japan)
- C-16 Cryo-EM structure of the MT<sub>1</sub>-G<sub>i</sub> signaling complex Hiroyuki Okamoto (Graduate school of science, The University of Tokyo, Japan)
- C-17 Phosphorylation-induced conformation of β2-adrenoceptor related to arrestin recruitment revealed by NMR Yutaro Shiraishi (RIKEN Center for Biosystems Dynamics Research, Japan)
- C-18 The bidirectional control of the intrinsic frequency of neurons by Na<sup>+</sup> and K<sup>+</sup> current around resting potential Tetsuya Yamada (The University of Tokyo, Japan)
- C-19 Structural insights into the selective interaciton between type IIa protein tyrosine phosphatase and the neuronal scaffolding protein, Liprin-alpha Atsushi Yamagata (RIKEN Center for Biosystems Dynamics Research, Japan)