

8th Japan-Korea Seminars on Biomolecular Science: Experiments and Simulation Program

Date: February 15 – 17, 2016

Venue: Okazaki Conference Center (<http://www.orion.ac.jp/occ-e/>)

February 15 (Mon)

【Chair: Takumi Yamaguchi】

- 10:00-10:25 **Steven P. Gross (UC Irvine, and KIAS)**
Single molecular motor heterogeneity and its implications for ensemble function
- 10:25-10:45 **Akihiko Nakamura (IMS)**
(short talk) Analysis of functional structure of cellulase by neutron crystallography
- 10:45-11:10 **Ryota Iino (IMS)**
Direct observation of intermediate states during the stepping motion of kinesin-1
- 11:10-11:35 **Sota Sato (Tohoku Univ. & JST)**
Biological functions implanted in artificial supramolecules
- 11:35-11:55 **Takayoshi Watanabe (Japan Adv. Inst. of Sci. & Tech.)**
(short talk) Novel method for site-specific protein pegylation using aromatic amine-containing non-natural amino acid
- 11:55-13:30 Lunch

【Chair: Ryota Iino】

- 13:30-13:55 **Keehyoung Joo (KIAS)**
Contact Assisted Protein Structure Modeling by Global Optimization in CASP11
- 13:55-14:20 **Nam Ki Lee (POSTECH)**
New single-molecule FRET method for observing fast dynamics and its application for dsDNA bending dynamics
- 14:20-14:45 **Masahide Terazima (Kyoto Univ.)**
Time-resolved study on conformation change and inter-domain change during protein reactions
- 14:45-15:10 **Kunihiro Kuwajima (Tokyo Univ.)**
The H/D-exchange kinetics of a fully unfolded protein studied by the DMSO-quenched and 2D NMR techniques
- 15:10-15:40 coffee break

【Chair: Julian Lee】

- 15:40-16:00 **Balachandran Manavalan (KIAS)**
(short talk) StrRate: Structure-based protein folding type classification and folding rate prediction
- 16:00-16:20 **Seung Hwan Hong (KIAS)**
(short talk) Template based modeling by dynamic fragment assembly: revisited
- 16:20-16:45 **Ji-Joon Song (KAIST)**
Understanding molecular Architecture of Huntington's disease protein
- 17:30- Banquet

February 16 (Tue)

【Chair: Changbong Hyeon】

- 10:00-10:25 **Fumio Hirata (Ritsumeikan Univ.)**
Multi-scale dynamics simulation of protein based on the generalized Langevin equation combined with 3D-RISM theory
- 10:25-10:45 (short talk) **InSuk Jung (KIAS)**
Efficient sampling of transition pathways using nudged elastic band and conformational space annealing
- 10:45-11:10 **Hisashi Okumura (IMS)**
Pressure induced structural change of proteins by molecular dynamics simulations
- 11:10-11:35 **Seokmin Shin (Seoul National Univ.)**
The two faces of self-assembly of peptides
- 11:35-12:00 **Jooyoung Lee (KIAS)**
Atomistic mechanism of conformational transition of adenylate kinase investigated by Lorentzian structure-based potential
- 12:00-13:30 Lunch

【Chair: Jooyoung Lee】

- 13:30-13:55 **Chaok Seok (Seoul National Univ.)**
Galaxy7TM: Modeling and docking of G-protein coupled receptors
- 13:55-14:15 (short talk) **Takumi Yamaguchi (Japan Adv. Inst. of Sci. & Tech.)**
Design and creation of Lewis X-expressing glycoclusters toward functional analyses of oligosaccharides in membrane systems
- 14:15-14:40 **Kazushi Kinbara (Tokyo Inst. of Tech.)**
Development of Stimuli-Responsive Multiblock Amphiphilic Molecules Mimicking Multipass Transmembrane Proteins
- 14:40-15:05 **Weontae Lee (Yonsei Univ.)**
NMR and X-ray crystallographic studies on syndecan, proteoglycan: Structure, function and diseases
- 15:05-15:35 coffee break

【Chair: Weontae Lee】

- 15:35-16:00 **Shinobu Itoh (Osaka Univ.)**
Activation mechanism of fungal tyrosinase
- 16:00-16:25 **Masafumi Odaka (Akita Univ.)**
Time-resolved crystallography of the reaction intermediate of nitrile hydratase: Revealing a role for the cysteinesulfenic acid ligand as a catalytic nucleophile
- 16:25-16:50 **Shuji Akiyama (IMS)**
Atomic-scale origins of slowness in the cyanobacterial circadian clock
- 16:50-17:15 **Dong Hae Shin (Ewha Womans Univ.)**
Structural properties of GmhA and GmhB from *Burkholderia thailandensis*
- 18:00- Free Discussion

February 17 (Wed)

【Chair: Koichi Kato】

- 10:00-10:25 **Takeshi Uchida (Hokkaido Univ.)**
Heme uptake proteins from *Vibrio cholerae*
- 10:25-10:50 **Hiroshi Sugimoto (RIKEN/SPring-8)**
Structural mechanism of the heme transporter complex from pathogenic bacteria
- 10:50-11:10
(short talk) **Norifumi Muraki (IMS)**
Crystal structures of HtaA and HmuT, heme uptake proteins from *Corynebacterium glutamicum*
- 11:10-11:35 **Jeong-Yong Suh (Seoul National Univ.)**
Structural basis for the preferential interaction of auxin-response transcriptional repressor with different transcription factors
- 11:35-11:55
(short talk) **Saeko Yanaka (IMS)**
Affinity improvement of antibody through mutational modification of the conformational dynamics
- 11:55-13:30 Lunch

【Chair: Shigetoshi Aono】

- 13:30-13:55 **Susumu Uchiyama (Osaka Univ.)**
Mass spectrometry of protein-ligand interactions
- 13:55-14:20 **Takafumi Ueno (Tokyo Inst. of Tech.)**
Protein Crystals for Designing Biohybrid Solid Materials
- 14:20-14:45 **Tadashi Satoh (Nagoya City Univ.)**
Structural insights into the working mechanisms of multi-domain enzymes involved in ER protein quality control
- 14:45-15:05
(short talk) **Jaeyoung Byeon (Soongsil Univ.)**
Protein contact prediction based on information theory
- 15:05-15:35 coffee break

【Chair: Kunihiro Kuwajima】

- 15:35-16:00 **Julian Lee (Soongsil Univ.)**
Prediction of protein rigid domains and hinge residues based on graph theory and elastic network model
- 16:00-16:25 **Takahiro Kosugi (IMS)**
De novo design of protein function
- 16:25-16:50 **Changbong Hyeon (KIAS)**
Mapping allosteric signaling of G protein-coupled receptors