

## Program

### February 15 (Mon)

10:00-10:25	<b>Steven P. Gross (UC Irvine, and KIAS)</b> Single molecular motor heterogeneity and its implications for ensemble function
10:25-10:45	<b>Akihiko Nakamura (IMS)</b> Analysis of functional structure of cellulase by neutron crystallography
10:45-11:10	<b>Ryota Iino (IMS)</b> Direct observation of intermediate states during the stepping motion of kinesin-1
11:10-11:35	<b>Sota Sato (Tohoku Univ. &amp; JST)</b> Biological functions implanted in artificial supramolecules
11:35-11:55	<b>Takayoshi Watanabe (Japan Adv. Inst. of Sci. &amp; Tech.)</b> Novel method for site-specific protein pegylation using aromatic amine-containing non-natural amino acid
11:55-13:30	Lunch
13:30-13:55	<b>Keehyoung Joo (KIAS)</b> Contact Assisted Protein Structure Modeling by Global Optimization in CASP11
13:55-14:20	<b>Nam Ki Lee (POSTECH)</b> New single-molecule FRET method for observing fast dynamics and its application for dsDNA bending dynamics
14:20-14:45	<b>Masahide Terazima (Kyoto Univ.)</b> Time-resolved study on conformation change and inter-domain change during protein reactions
14:45-15:10	<b>Kunihiro Kuwajima (Tokyo Univ.)</b> 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
15:40-16:00	<b>Balachandran Manavalan (KIAS)</b> StrRate: Structure-based protein folding type classification and folding rate prediction
16:00-16:20	<b>Seung Hwan Hong (KIAS)</b> Template based modeling by dynamic fragment assembly: revisited
16:20-16:45	<b>Ji-Joon Song (KAIST)</b> Understanding molecular Architecture of Huntington's disease protein
17:30-	Banquet (事前申込必要、会費 5,000 円)

## February 16 (Tue)

- 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 **InSuk Joung (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
- 13:30-13:55 **Chaok Seok (Seoul National Univ.)**  
Galaxy7TM: Modeling and docking of G-protein coupled receptors
- 13:55-14:15 **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
- 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)

- 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      **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      **Saeko Yanaka (IMS)**  
Affinity improvement of antibody through mutational modification of the conformational dynamics
- 11:55-13:30      Lunch
- 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      **Jaeyoung Byeon (Soongsil Univ.)**  
Protein contact prediction based on information theory
- 15:05-15:35      coffee break
- 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