

分子研研究会

日韓生体分子科学セミナー -実験とシミュレーション

6th Japan-Korea Seminars on Biomolecular Science:

Experiments and Simulation

Okazaki Conference Center

Institute for Molecular Science

Nov. 25 – 27, 2013

November 25 (Mon)

【Chair: Yuji Furutani (IMS)】

- 10:00-10:25 **Akihito Ishizaki (IMS)**
QUANTUM DYNAMIC ASPECTS IN PHOTOSYNTHETIC LIGHT HARVESTING – OLD ROOTS,
NEW SHOOTS
- 10:25-10:50 **Young Min Rhee (POSTECH)**
INTERPOLATED MECHANICS / MOLECULAR MECHANICS STUDIES ON THE DYNAMICS OF
FLUORESCENT PROTEINS

10:50-11:10 coffee break

【Chair: Shigetoshi Aono (IMS)】

- 11:10-11:35 **Yuji Furutani (IMS)**
STIMULUS-INDUCED DIFFERENCE FTIR SPECTROSCOPY ON ION-CHANNEL AND
ION-PUMP PROTEINS
- 11:35-12:00 **Osami Shoji (Nagoya Univ.)**
GASEOUS ALKANE HYDROXYLATION CATALYZED BY CYTOCHROME P450BM3 BY TRICKING
ITS SUBSTRATE RECOGNITION USING DECOY MOLECULES

12:00-13:30 lunch

【Chair: Young Min Rhee (POSTECH)】

- 13:30-13:55 **Jinwoo Lee (Kwangwoon Univ.)**
A NOVEL APPROACH TO NON-EQUILIBRIUM THERMODYNAMICS
- 13:55-14:20 **Nam Ki Lee (POSTECH)**
SINGLE-VESICLE FRET ASSAY FOR THE NEUROTOXICITY OF A-SYNUCLEIN OLIGOMERS
IN PARKINSON'S DISEASE: INHIBITING NEURONAL SNARE-MEDIATED VESICLE FUSION
- 14:20-14:45 **Naoyuki Inagaki (Nara Inst. of Sci. & Tech.)**
SIGNAL-FORCE TRANSDUCTION IN AXON OUTGROWTH AND GUIDANCE

14:45-15:05 coffee break

【Chair: Yuji Furutani (IMS)】

- 15:05-15:30 **Jaehoon Yu (Seoul National Univ.)**
A PEPTIDE MIMETIC OF APOLIPOPROTEIN A-I THAT CONTAINS 2-NAPHTHYLAMINE
RESIDUES ENHANCES CHOLESTEROL EFFLUX AND SEQUESTERS OXIDIZED LDL FROM
MACROPHAGE CELLS
- 15:30-15:55 **Changbong Hyeon (KIAS)**
UREA-INDUCED DENATURATION OF RNA
- 15:55-16:20 **Chaok Seok (Seoul National Univ.)**
GALAXY 2013 TESTED ON RECENT COMMUNITY-WIDE PREDICTION EXPERIMENTS

16:20-16:40 coffee break

【Chair: Hisashi Okumura (IMS)】

- 16:40-16:55 **Balachandran Manavalan (KIAS)**
RANDOM FOREST-BASED PROTEIN MODEL QUALITY ASSESSMENT (RFMQA) USING
STRUCTURAL FEATURES AND POTENTIAL ENERGY TERMS
- 16:55-17:10 **Takumi Yamaguchi (IMS)**
PARAMAGNETISM-ASSISTED NMR EVALUATION OF MOLECULAR DYNAMICS SIMULATIONS
FOR CONFORMATIONAL CHARACTERIZATION OF OLIGOSACCHARIDES
- 17:10-17:25 **Tadashi Satoh (Nagoya City Univ. & JST PRESTO)**
STRUCTURAL BASIS FOR PROTEASOME FORMATION MEDIATED BY ASSEMBLY CHAPERONE
NAS2
- 17:25-17:40 **Min-Kyu Kim (KIOST)**
CRYSTAL STRUCTURES OF COLD-ACTIVE β -MANNANASE AND ITS MANNOPENTAOSE
COMPLEXES FROM ANTARCTIC SPRINGTAIL, *Cryptopygus antarcticus*

18:00- Free Discussion/Mixer

November 26 (Tue)

【Chair: Jooyoung Lee (KIAS)】

- 9:30-9:55 **Julian Lee (Soongsil Univ.)**
EXACT PARTITION FUNCTION ZEROS OF THE WAKO-SAITÔ-MUÑOZ-EATON PROTEIN MODEL
- 9:55-10:20 **Fumio Hirata (Ritsumeikan Univ.)**
ROLE OF WATER TO CONVERT "NON-BIOLOGICAL" FLUCTUATION TO THE "BIOLOGICAL"
ONE
- 10:20-10:40 coffee break

【Chair: Seokmin Shin (Seoul National Univ.)】

- 10:40-11:05 **Jooyoung Lee (KIAS)**
HIGH-ACCURACY PROTEIN STRUCTURE MODELING AND ITS APPLICATION TO MOLECULAR
REPLACEMENT OF CRYSTAL PHASING
- 11:05-11:30 **Hisashi Okumura (IMS)**
REPLICA-PERMUTATION METHOD FOR PROTEIN SIMULATIONS AND PRESSURE-INDUCED
DENATURATION
- 11:30-11:55 **Sun Choi (Ewha Womans Univ.)**
COMPUTER-AIDED DRUG DESIGN AND MOLECULAR MODELING STUDIES FOR THE
DISCOVERY OF COVALENT INHIBITORS
- 11:55-13:30 lunch

【Chair: Sun Choi (Ewha Womans Univ.)】

- 13:30-13:55 **Seokmin Shin (Seoul National Univ.)**
UNDERSTANDING AMYLOID FORMATION
- 13:55-14:20 **Hirofumi Sato (Kyoto Univ.)**
MOLECULAR THEORIES OF SOLVATION, FLUCTUATION AND DIFFUSION IN AQUEOUS
SOLUTION
- 14:20-14:45 **Weontae Lee (Yonsei Univ.)**
STRUCTURE AND DYNAMICS OF C-TERMINAL REGULATORY DOMAIN OF *Vibrio vulnificus*
EXTRACELLULAR METALLOPROTEASE
- 14:45-15:05 coffee break

【Chair: Kunihiro Kuwajima (SOKENDAI)】

- 15:05-15:30 **Sung-il Yoon (Kangwon National Univ.)**
CONSERVED, BUT DISTINCT, ACTIVATION OF TOLL-LIKE RECEPTOR 5 BY FLAGELLIN
- 15:30-15:55 **Keehyoung Joo (KIAS)**
NMR STRUCTURE DETERMINATION BY CONFORMATIONAL SPACE ANNEALING
- 15:55-16:10 **Chihiro Kitatsuji (IMS)**
MOLECULAR MECHANISM FOR HEME-MEDIATED INHIBITION OF THE 5-AMINOLEVULINIC
ACID SYNTHASE 1
- 16:10-16:30 coffee break

【Chair: Koichi Kato (IMS)】

- 16:30-16:45 **Norifumi Muraki (IMS)**
STRUCTURAL BASIS FOR PROTOCHLOROPHYLLIDE REDUCTION IN THE CHLOROPHYLL
BIOSYNTHESIS
- 16:45-17:00 **In Suk Joung (KIAS)**
A SIMPLE STRUCTURE-BASED MODELING FOR EXPLORING MACRO-MOLECULAR
CONFORMATIONAL CHANGES
- 17:00-17:15 **Sim Jun (Soongsil Univ.)**
GRAPH-THEORY BASED COMPUTATION OF PROTEIN RIGID BLOCKS
- 18:00- Banquet

November 27 (Wed)

【Chair: Shingo Nagano (Tottori Univ.)】

9:30-9:55 **Hironari Kamikubo (Nara Inst. of Sci. & Tech.)**
FUNCTIONAL MODIFICATION OF A PROTEIN BY USING ELEMENT IMPLANTATION

9:55-10:20 **Shuji Akiyama (IMS)**
KaiC AS CIRCADIAN PACEMAKER OF CYANOBACTERIAL CIRCADIAN CLOCK

10:20-10:40 coffee break

【Chair: Soo Hyun Eom (GIST)】

10:40-11:05 **Genji Kurisu (Osaka Univ.)**
STRUCTURAL STUDIES OF THE CYTOPLASMIC DYNEIN MOTOR DOMAIN

11:05-11:30 **Koichi Kato (IMS)**
AN ARCHAEAL HOMOLOG OF PROTEASOME ASSEMBLY CHAPERONE FORMS A HOMOTETRAMER AND FUNCTIONS AS PROTEASOME ACTIVATOR

11:30-11:55 **Sun-Shin Cha (KIOST)**
ZINC-BINDING TO THE SURFACE OF PROTEINS AND ITS APPLICATION TO EXPERIMENTAL PHASING

11:55-13:30 lunch

【Chair: Fumio Hirata (Ritsumeikan Univ.)】

13:30-13:55 **Soo Hyun Eom (GIST)**
CRYSTAL STRUCTURE OF THE CORE DOMAIN OF HUMAN SWIPROSIN-1, CALCIUM DEPENDENT ACTIN BUNDLING PROTEIN

13:55-14:20 **Kunihiro Kuwajima (SOKENDAI)**
IRREVERSIBLE DENATURATION OF *Escherichia coli* MALTODEXTRIN GLUCOSIDASE

14:20-14:45 **Shun Hirota (Nara Inst. of Sci. & Tech.)**
OLIGOMERIZATION OF HEME PROTEINS BY DOMAIN SWAPPING

14:45-15:05 coffee break

【Chair: Shun Hirota (Nara Inst. of Sci. & Tech.)】

15:05-15:30 **Toshitaka Matsui (Tohoku Univ.)**
UNIQUE REACTION MECHANISMS OF IcdG-TYPE HEME DEGRADING ENZYMES FROM PATHOGENIC BACTERIA

15:30-15:55 **Shingo Nagano (Tottori Univ.)**
STRUCTURE AND HEME ACQUISITION MECHANISM OF A HEMOPHORE HasA HAVING UNUSUAL 5-COORDINATED HEME

15:55-16:20 **Shigetoshi Aono (IMS)**
STRUCTURAL BASIS FOR THE TRANSCRIPTIONAL REGULATION OF HEME HOMEOSTASIS IN LACTOCOCCUS LACTIS