

# Sihyun Ham Protein Symposium 2022

## Program (Korean Standard Time, KST)

### January 14 (Fri) - 15 (Sat), 2022

Offline venue: Sookmyung Women's University

Sihyun Ham Lecture Hall (Fri) and Room 104, Building Prime (Sat)

Online link: <https://snu-ac-kr.zoom.us/j/3907204837>

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### January 14 (Friday)

8:30 - 9:00 Registration

Opening Remarks (Seokmin Shin)

8:50 - 9:00 Jinho Lee, Dean of College of Science, Sookmyung Women's University

9:00 - 9:10 Seokmin Shin, on behalf of the organizing committee

9:10 - 9:20 Chang-Dae Ham, on behalf of Sihyun's family

Chair (Yuji Sugita)

9:20 - 9:45 Peter Rossky Rice University

**Understanding the Message from a Sensing Fluorescent Protein**

9:45 - 10:10 Songi Han UC Santa Barbara

**Water and proteins, an inseparable relationship**

10:10 - 10:35 Matthias Heyden Arizona State University

**Solvation Free Energy Arithmetic and Solvent-Mediated Interactions**

10:35 - 10:50 Break

Chair (Song-Ho Chong)

10:50 - 11:15 Michael Feig Michigan State University

**Protein diffusion in concentrated environments**

11:15 - 11:40 Yuji Sugita RIKEN

**Reduced efficacy of a Src kinase inhibitor in crowded protein solution**

11:40 - 12:05 Yuko Okamoto Nagoya University

**The early stage of secondary nucleation of Abeta fibril**

12:05 - 12:30 Wookyoung Yu DGIST

**Exploring ensemble structures of Alzheimer's amyloid  $\beta$  (1-42) monomer using linear regression for the MD simulation and NMR chemical shift**

12:30 - 13:30 Lunch

Chair (Yangmee Kim)

13:30 - 13:55 Fumio Hirata IMS (retired)

**Realization of the structural fluctuation of biomolecules in solution:**

**Generalized Langevin Mode Analysis**

13:55 - 14:20 Song-Ho Chong RIKEN

|                   |   |
|-------------------|---|
|                   | <b>Time-dependent communication between multiple amino acids during protein folding</b>   |
| 14:20 - 14:45     | Changbong Hyeon                      KIAS<br><b>Generalized iterative annealing mechanism for the action of molecular chaperones</b>  |
| 14:45 - 15:10     | Chaok Seok                              SNU<br><b>Computational protein research: hers and mine</b>   |
| 15:10 - 15:25     | Break   |
| Chair (Wonpil Im) |   |
| 15:25 - 15:50     | Juyong Lee                              Kangwon U<br><b>Finding reaction pathways using the Gaussian process</b>  |
| 15:50 - 16:15     | Hyun-Suk Lim                          POSTECH<br><b>Development of alpha-helix mimetics based on the triazine-piperazine scaffold as protein-protein interaction modulators</b> |
| 16:15 - 16:40     | Yangmee Kim                          Konkuk U<br><b>Elucidation of mechanism underlying fatty acid and aryl polyene biosynthesis of <i>Acinetobacter baumannii</i></b>          |

### January 15 (Saturday)

|                      |  |
|----------------------|--|
| Chair (Chaok Seok)   |  |
| 9:00 - 9:25          | Xuhui Huang                          University of Wisconsin-Madison<br><b>Memory Kernels of Protein Conformational Dynamics</b>   |
| 9:25 - 9:50          | Bernie Brooks                          NIH<br><b>Using machine learning for predicting protonation states and understanding protein landscape</b>  |
| 9:50 - 10:15         | Charles Brooks                      University of Michigan<br><b>Novel, high-throughput free-energy methods for drug design</b>  |
| 10:15 - 10:40        | Sun Choi                                  Ewha WU<br><b>Computational mechanistic studies of membrane proteins and drug discovery</b>  |
| 10:40 - 10:55        | Break  |
| Chair (Hyun-Suk Lim) |  |
| 10:55 - 11:20        | Ayyalusamy Ramamoorthy          University of Michigan<br><b>Nanodiscs for Probing Protein-Protein Structural Interactions at the Membrane Interface</b>   |
| 11:20 - 11:45        | John Straub                              Boston University<br><b>Curious orientational behavior of a modified cholesterol in lipid bilayers</b>  |
| 11:45 - 12:10        | Guipeun Kang                          UT Southwestern<br><b>Probing structural determinants for partial agonism and allosteric modulation at human <math>\alpha 4\beta 2</math> nicotinic receptor</b> |
| 12:10 - 12:35        | Weontae Lee                              Yonsei U  |

**Structure and Dynamics of Membrane Proteins by Cryo-EM and Serial Femtosecond X-ray Crystallography (SFX)**

12:35 - 13:30

Lunch

Chair (Juyong Lee)

13:30 - 13:55

Myung Keun Cho SNU

**Site-Specific Backbone and Side-Chain Contributions to Thermodynamic Stabilizing Forces of the WW Domain**

13:55 - 14:20

Wonpil Im Lehigh U

**What can CHARMM-GUI do for you?**

14:20 - 14:45

Myungjin Lee NIH

**Extended antibody-framework-to-antigen distance observed exclusively with broad HIV-1-neutralizing antibodies recognizing glycan-dense surfaces**

14:45 - 15:00

Closing Remark (Fumio Hirata)