

Time Table

Wednesday, 27th November 2019

17:30-20:00	Registration	King Skyfront Tokyu REI Hotel, 1st floor
18:00-20:00	Reception Presentations from AHeDD representatives	

Thursday, 28th November 2019

10:00-10:20	Opening address Yutaka Akiyama Professor, Department of Computer Science, Tokyo Institute of Technology, Japan Shengyong Yang Professor, Department of Medicinal Chemistry, Sichuan University, China Kyoung Tai No Professor, Department of Biotechnology, Yonsei University, Korea	LISE, Conference room, 1st floor
10:20-12:00	Session 1: Chemoinformatics and ADMET prediction (Chairs: Liu Hong, and Kyoung Tai No) 10:20-10:45 <i>In silico ADMET prediction and optimization</i> Yun Tang Professor, School of Pharmacy, East China University of Science and Technology, China 10:45-11:10 <i>Systems chemo-informatics and fragment based lead discovery</i> Gyoonhee Han Professor, Department of Biotechnology, Yonsei University, Korea 11:10-11:35 <i>Prediction of membrane permeability and plasma protein binding of cyclic peptides</i> Yutaka Akiyama Professor, Department of Computer Science, Tokyo Institute of Technology, Japan 11:35-12:00 <i>A protechemometric approach for beta-lactam antibiotic response prediction in Staphylococcus aureus</i> Jae Hong Shin Senior Scientist, Standigm Inc., Korea	
12:00-13:00	Lunch	
13:00-13:20	Move to PeptiDream (5 min. on foot)	
13:30-14:30	Plenary Talk (Chair: Yutaka Akiyama) <i>Constrained peptides in drug discovery and development - various therapeutic applications offered by PeptiDream</i> Keiichi Masuya Vice President, PeptiDream Inc., Japan	PeptiDream, Auditorium, 1st floor
14:30-14:50	Coffee Break	
14:50-16:30	Session 2: Structures of Key Drug Targets (Chairs: Takatsugu Hirokawa, and Yun Tang) 14:50-15:15 <i>CryoEM analysis of the GPCR neurotensin receptor 1-G protein complex for the future engineering of biased allosteric modulator</i> Hideaki E. Kato Associate Professor, Komaba Institute for Science, The University of Tokyo, Japan 15:15-15:40 <i>Discovery and development of novel CCR5 antagonists</i> Hong Liu Professor, Shanghai Institute of Materia Medica, CAS, China 15:40-16:05 <i>Molecular modeling study for identification of binding site of AIMP2-DX2 inhibitor</i> Yuno Lee Senior Scientist, Korea Research Institute of Chemical Technology (KRICT), Korea 16:05-16:30 <i>Computer aided drug discovery with natural compounds</i> Kyoung Tai No Professor, Department of Biotechnology, Yonsei University / Director, BMDRC, Korea	
16:30-16:40	Break	
16:40-18:20	Session 3: Artificial Intelligence for Drug Discovery (Chairs: Weiliang Zhu, and Gyoonhee Han) 16:40-17:05 <i>Drug discovery with artificial intelligence: advances and challenges</i> Shengyong Yang Professor, Department of Medicinal Chemistry, Sichuan University, China 17:05-17:30 <i>Multiple approaches to discover human DDX3 inhibitors for cancer therapeutics</i> Keun Woo Lee Professor, Department of Biochemistry, Gyeongsang National University, Korea 17:30-17:55 <i>Visualizations within chemogenomic active learning reveal how protein descriptors are used and underlying truths about chemogenomic and</i> J. B. Brown Junior Associate Professor, Graduate School of Medicine, Kyoto University, Japan 17:55-18:20 <i>Target discovery facilitated by machine learning</i> Feng Zhu Professor, College of Pharmaceutical Sciences, Zhejiang University, China	
18:20-18:35	Move to King Skyfront Tokyu REI Hotel (5 min. on foot)	
18:45-20:30	Banquet	King Skyfront Tokyu REI Hotel, Restaurant, 5th floor

Friday, 29th November 2019

9:00-10:30	Flash Talk Session: Presentations by Young Researchers in Asia-Pacific Regions (Chair: Masahito Ohue) (4 min + 1 min Q&A) 9:00-9:05 <i>Systematic construction of the cosolvents sets for cosolvent MD (CMD) with the large-scale simulation</i> Keisuke Yanagisawa JSPS Research Fellow, Department of Biotechnology, The University of Tokyo, Japan 9:06-9:11 <i>Investigation of protein-protein interactions and hot spot region between PD-1 and PD-L1 by fragment molecular orbital method</i> Hocheol Lim Researcher, Bioinformatics & Molecular Design Research Center, Korea 9:12-9:17 <i>Metagenome analysis implies bacterial community and gene category composition disorder in periodontal disease sites</i> Kazuki Izawa Researcher, Department of Computer Science, Tokyo Institute of Technology, Japan 9:18-9:23 <i>In silico drug discovery targeting Hippo pathway and YAP-TEAD protein protein interactions for small molecules anti cancer agent</i> Jongwan Kim Researcher, Bioinformatics & Molecular Design Research Center, Korea 9:24-9:29 <i>Discovery of leucyl-tRNA synthetase (LRS) PPI inhibitor for modulating mTORC1 pathway via the chemical biology approach</i> Chulho Lee Research Associate, Department of Biotechnology, Yonsei University, Korea 9:30-9:35 <i>Novel computational approach for natural product (NP) research: development of natural compound molecular fingerprint (NC-MFP) for exploring new NP-based drugs</i> Myungwon Seo Graduate Student, Department of Biotechnology, Yonsei University, Korea 9:36-9:41 <i>Predicting membrane permeability for cyclic peptides</i> Yasushi Yoshikawa Specially Appointed Assistant Professor, Department of Computer Science, Tokyo Institute of Technology, Japan 9:42-9:47 <i>Development of a prediction model for the onset of disease and risk factor analysis</i> Atsuyoshi Matsuda CEO, Logbii, Inc., Japan 9:48-9:53 <i>GCMQA: a novel single-protein structure model quality assessment method using graph convolution</i> Rin Sato Graduate Student, Department of Computer Science, Tokyo Institute of Technology, Japan 9:54-9:59 <i>Contest-based compound screening enables identification of chemically diverse inhibitors of target proteins</i> Shuntaro Chiba Researcher, MIH, RIKEN, Japan 10:00-10:05 <i>Underestimated non-covalent interactions in protein data bank</i> Zhijian Xu Associate Professor, Shanghai Institute of Materia Medica, CAS, China 10:06-10:11 <i>Evaluation of a self-balanced force field for biomolecule simulations</i> Sungbo Hwang Graduate Student, Department of Biotechnology, Yonsei University, Korea 10:12-10:17 <i>Application of informatics approaches to compound library design for intractable target chemical spaces</i> Kazuyoshi Ikeda Specially Appointed Associate Professor, Division of Physics for Life Functions, Keio University, Japan 10:18-10:23 <i>Learning-to-rank for ligand-based virtual screening</i> Masahito Ohue Assistant Professor, Department of Computer Science, Tokyo Institute of Technology, Japan	LISE, Conference room, 1st floor
10:30-10:50	Coffee Break	
10:50-12:30	Session 4: High-Performance Molecular Simulation (Chairs: Keun Woo Lee, and Shengyong Yang) 10:50-11:15 <i>Development of the rapid QM/MM molecular dynamics techniques aimed at medium molecular drug discovery</i> Hiroaki Nishizawa Assistant Professor, Center for Computational Sciences, University of Tsukuba, Japan 11:15-11:40 <i>New methods for highly efficient MD simulation</i> Weiliang Zhu Professor, Shanghai Institute of Materia Medica, CAS, China 11:40-12:05 <i>Next generation accelerated supercomputing: Cygnus system at University of Tsukuba</i> Taisuke Boku Director, Center for Computational Sciences, University of Tsukuba, Japan 12:05-12:30 <i>In silico Drug Discovery using Molecular Modeling and Simulation</i> Takatsugu Hirokawa Professor, University of Tsukuba / Team Leader, molprof, AIST, Japan	
12:30-13:30	Lunch	
AMED BINDS project special sessions		
13:30-14:15	Plenary Talk (Chair: Takatsugu Hirokawa) <i>Perspectives of computational drug discovery: AMED-BINDS activities in Japan</i> Shigenori Tanaka Professor, Department of Computational Science, Kobe University / AMED BINDS Project Officer, Japan	
14:15-15:30	BINDS Achievements 1 (Chair: Takatsugu Hirokawa) 14:15-14:40 <i>In silico drug discovery based on structural informatics and FMO method</i> Teruki Honma Group Leader, BDR, RIKEN, Japan 14:40-15:05 <i>Molecular simulation studies on protein functions and improvement of the efficiency of cryo-EM data collection by machine learning</i> Tohru Terada Associate Professor, Interfaculty Initiative in Information Studies, The University of Tokyo, Japan 15:05-15:30 <i>Structural modeling of the entire EHV-ATPase in multiple states using cryo-EM data and homology modeling</i> Yu Yamamori Research Scientist, AIRC, AIST, Japan	
15:30-15:50	Coffee Break	
15:50-17:30	BINDS Achievements 2 (Chair: Teruki Honma) 15:50-16:15 <i>Finding a drug candidate regulating protein function at an allosteric site</i> Yuko Ito Research Scientist, molprof, AIST, Japan 16:15-16:40 <i>MD simulations and QM/MM analysis to gain insight into protein functions</i> Yoshitaka Moriwaki Assistant Professor, Department of Biotechnology, The University of Tokyo, Japan 16:40-17:05 <i>Improving the virtual screening ability using machine learning</i> Masakazu Sekijima Unit Leader, ACDD / Associate Professor, IIR, Tokyo Institute of Technology, Japan 17:05-17:30 <i>Combination of molecular dynamics simulations and small-angle X-ray scattering experiments</i> Mitsunori Ikeguchi Professor, Graduate School of Medical Life Science, Yokohama City University, Japan	
17:30-17:45	Closing Remarks	

Saturday, 30th November 2019

9:00-10:30	AHeDD Steering Committee Meeting	King Skyfront Tokyu REI Hotel, 1st floor
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