Time Table

Wednesday, 27th November 2019

17:30-20:00 Location : King Skyfront Tokyu REI Hotel, 1st floor

17:30-20:00 **Registration**
18:00-20:00 **Reception** Presentations from AHeDD representatives

Thursday, 28th November 2019

10:00-13:00 Location : LiSE, Conference room, 1st floor

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

10:20-12:00 **Session 1: Chemoinformatics and ADMET prediction** (Chairs: Liu Hong, and Kyong Tai No)

10:20-10:45 *In silico ADMET prediction and optimization*
Yun Tang Professor, School of Pharmacy, East China University of Science and Technology, China

10:45-11:10 *Syetems chemo-informatics and fragment based lead discovery*
Gyoonhee Han Professor, Department of Biotechnology, Yonsei University, Korea

11:10-11:35 *Prediction of membrane permeability and plasma protein binding of cyclic peptides*
Yutaka Akiyama Professor, Department of Computer Science, Tokyo Institute of Technology, Japan

11:35-12:00 *A proteochemometric approach for beta-lactam antibiotic response prediction in Staphylococcus aureus*
Jae Hong Shin Senior Scientist, Standigm Inc., Korea

12:00-13:00 **Lunch**

13:00-13:20 Move to PeptiDream (5 min. on foot)

13:30-18:20 Location : PeptiDream, Auditorium, 1st floor

13:30-14:30 **Plenary Talk 1** (Chair: Yutaka Akiyama)
Constrained peptides in drug discovery and development - various therapeutic applications offered by PeptiDream
Keiichi Masuya Executive Vice President, PeptiDream Inc., Japan

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 *CryoEM analysis of the GPCR neurotensin receptor 1-G protein complex for the future engineering of biased allosteric modulator*
Hideaki E. Kato Associate Professor, Komaba Institute for Science, The University of Tokyo, Japan

15:15-15:40 *Discovery and development of novel CCR5 antagonists*
Hong Liu Professor, Shanghai Institute of Materia Medica, CAS, China

15:40-16:05 *Molecular modeling study for identification of binding site of AIMP2-DX2 inhibitor*
Yuno Lee Senior Scientist, Korea Research Institute of Chemical Technology (KRICT), Korea

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16:05-16:30 *Computer aided drug discovery with natural compounds*
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 *Drug discovery with artificial intelligence: advances and challenges*
Shengyong Yang Professor, Department of Medicinal Chemistry, Sichuan University, China

17:05-17:30 *Multiple approaches to discover human DDX3 inhibitors for cancer therapeutics*
Keun Woo Lee Professor, Department of Biochemistry, Gyeongsang National University, Korea

17:30-17:55 *Visualizations within chemogenomic active learning reveal how protein descriptors are used and underlying truths about chemogenomic and single target QSAR model utility*
J. B. Brown Junior Associate Professor, Graduate School of Medicine, Kyoto University, Japan

17:55-18:20 *Bioinformatics-Facilitated Therapeutic Target discovery*
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 Location : King Skyfront Tokyu REI Hotel, Restaurant, 5th floor

18:45-20:30 **Banquet**

Friday, 29th November 2019

8:30-17:45 Location : LiSE, Conference room, 1st floor

8:30- 9:00 Coffee and Donuts

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 *Systematic construction of the cosolvents sets for cosolvent MD (CMD) with the large-scale simulation*
Keisuke Yanagisawa JSPS Research Fellow, Department of Biotechnology, The University of Tokyo, Japan

9:06-9:11 *Investigation of protein-protein interactions and hot spot region between PD-1 and PD-L1 by fragment molecular orbital method*
Hocheol Lim Researcher, Bioinformatics & Molecular Design Research Center, Korea

9:12-9:17 *Metagenome analysis implies bacterial community and gene category composition disorder in periodontal disease sites*
Kazuki Izawa Researcher, Department of Computer Science, Tokyo Institute of Technology, Japan

9:18-9:23 *In silico drug discovery targeting Hippo pathway and YAP-TEAD protein protein interactions for small molecules anti cancer agent*
Jongwan Kim Researcher, Bioinformatics & Molecular Design Research Center, Korea

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9:24-9:29 *Discovery of leucyl-tRNA synthetase (LRS) PPi inhibitor for modulating mTORC1 pathway via the chemical biology approach*
Chulho Lee Research Associate, Department of Biotechnology, Yonsei University, Korea

9:30-9:35 *Novel computational approach for natural product (NP) research: development of natural compound molecular fingerprint (NC-MFP) for exploring new NP-based drugs*
Myungwon Seo Graduate Student, Department of Biotechnology, Yonsei University, Korea

9:36-9:41 *Predicting membrane permeability for cyclic peptides*
Yasushi Yoshikawa Specially Appointed Assistant Professor, Department of Computer Science, Tokyo Institute of Technology, Japan

9:42-9:47 *Development of prediction model for onset of disease and risk factor analysis*
Atsuyoshi Matsuda CEO, Logbii, Inc., Japan

9:48-9:53 *GCMQA: a novel single-protein structure model quality assessment method using graph convolution*
Rin Sato Graduate Student, Department of Computer Science, Tokyo Institute of Technology, Japan

9:54-9:59 *Contest-based compound screening enables identification of chemically diverse inhibitors of target proteins*
Shuntaro Chiba Researcher, MIH, RIKEN, Japan

10:00-10:05 *Underestimated non-covalent interactions in protein data bank*
Zhijian Xu Associate Professor, Shanghai Institute of Materia Medica, CAS, China

10:06-10:11 *Evaluation of a self-balanced force field for biomolecule simulations*
Sungbo Hwang Graduate Student, Department of Biotechnology, Yonsei University, Korea

10:12-10:17 *Application of informatics approaches to compound library design for intractable target chemical spaces*
Kazuyoshi Ikeda Specially Appointed Associate Professor, Division of Physics for Life Functions, Keio University, Japan

10:18-10:23 *Learning-to-rank for ligand-based virtual screening*
Masahito Ohue Assistant Professor, Department of Computer Science, Tokyo Institute of Technology, Japan

10:24-10:29 *Multiple virtual screening strategies for the discovery of novel compounds active against dengue virus: a hit identification study*
Kowit Hengphasatporn, Researcher, University of Tsukuba / Chulalongkorn University

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 *Development of the rapid QM/MM molecular dynamics techniques aimed at medium molecular drug discovery*
Hiroaki Nishizawa Assistant Professor, Center for Computational Sciences, University of Tsukuba, Japan

11:15-11:40 *New methods for highly efficient MD simulation*
Weiliang Zhu Professor, Shanghai Institute of Materia Medica, CAS, China

11:40-12:05 *Next generation accelerated supercomputing: Cygnus system at University of Tsukuba*
Taisuke Boku Director, Center for Computational Sciences, University of Tsukuba, Japan

12:05-12:30 *In silico Drug Discovery using Molecular Modeling and Simulation*
Takatsugu Hirokawa Professor, University of Tsukuba / Team Leader, molprof, AIST, Japan

12:30-13:30 **Lunch**

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Friday, 29th November 2019

9:00-17:45 Location : LiSE, Conference room, 1st floor

13:30-17:30 **AMED BINDS project special sessions**

13:30-14:15 **Plenary Talk 2** (Chair: Takatsugu Hirokawa)
Perspectives of computational drug discovery: AMED-BINDS activities in Japan
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 *In silico drug discovery based on structural informatics and FMO method*
Teruki Honma Group Leader, BDR, RIKEN, Japan

14:40-15:05 *Molecular simulation studies on protein functions and improvement of the efficiency of cryo-EM data collection by machine learning*
Tohru Terada Associate Professor, Interfaculty Initiative in Information Studies, The University of Tokyo, Japan

15:05-15:30 *Structural modeling of the entire EhV-ATPase in multiple states using cryo-EM data and homology modeling*
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 *Finding a drug candidate regulating protein function at an allosteric site*
Yuko Ito Research Scientist, molprof, AIST, Japan

16:15-16:40 *MD simulations and QM/MM analysis to gain insight into protein functions*
Yoshitaka Moriwaki Assistant Professor, Department of Biotechnology, The University of Tokyo, Japan

16:40-17:05 *Improving the virtual screening ability using machine learning*
Masakazu Sekijima Unit Leader, ACDD / Associate Professor, IIR, Tokyo Institute of Technology, Japan

17:05-17:30 *Combination of molecular dynamics simulations and small-angle X-ray scattering experiments*
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 Location : King Skyfront Tokyu REI Hotel, 1st floor

9:00-10:30 AHeDD Steering Committee Meeting