

4th Autumn School of Chemoinformatics in Tokyo 2015

Auspice: Funatsu Lab. , The University of Tokyo

<http://funatsu.t.u-tokyo.ac.jp>

Cosponsor: Division of Chemical Information and Computer Sciences, Chemical Society of Japan

<http://cicsj.chemistry.or.jp/index.html>

The Pharmaceutical Society of Japan

http://www.pharm.or.jp/index_e.html

The Chem·Bio Informatics Society

http://cbi-society.org/index_e.html

Date: November 25-26, 2015

Location: Sanjyo-Conference Hall, The University of Tokyo

25 November

9:50 Opening remarks: Prof. Kimito Funatsu (The University of Tokyo)
[Tutorial session]

Chair Prof. Gisbert Schneider

10:00~11:00 Prof. Juergen Bajorath (Bonn University)
 “SAR Visualization, Compound Design, and Activity Prediction”

Chair Prof. Juergen Bajorath

11:00~12:00 Dr. Yasushi Okuno (Kyoto University)
 “Big data and simulation approaches for drug discovery”

12:00~13:30 Lunch

Chair Prof. Shigehiko Kanaya

13:30~14:30 Dr. Kiyoshi Hasegawa(Chugai-Pharmaceutical Co.)
 “Data Mining Methods and Chemical Interpretations in Chemoinformatics”

Chair Dr. Kiyoshi Hasegawa

14:30~15:30 Prof. Gisbert Schneider (ETH Zurich)
 “A Philosophy of Chemical Space”

Chair Prof. Yasushi Okuno

15:30~16:00 Prof. Shigehiko Kanaya(NAIST)
 “KNApSAcK Family DB: Data-driven Nutrition Science from Accessibility of Edible
 Species to Cuisine”

16:00~16:20 ----- Break -----

[Expert session by Software Vendors]

Chair Dr. Matheus Escobar

- 16:20~16:40 OpenEye
 Dr. Krisztina Boda
 “Visualizing Chemical Information”
- 16:40~17:00 BIOVIA
 Dr. Dana Honeycutt (BIOVIA Dassault Systèmes)
 “Validation of Statistical Models and Their Predictions Dr. Dana Honeycutt”
- 17:00~17:20 Schrodinger
 Dr. Osamu Ichihara
 “Application of Free Energy Methods and Molecular Dynamics Simulations
 to Drug Discovery”
- 17:30-19:30 Symposium Banquet (Sanjyo-Conference Hall)

26 November

[Tutorial session]

Chair Prof. Andreas Bender

- 9:30~10:30 Prof. Yoshihiro Yamanishi (Kyushu University)
 “Systematic drug repositioning via omics data analysis with machine
 learning methods”

Chair Prof. Yoshihiro Yamanishi

- 10:30~11:30 Prof. Andreas Bender (Cambridge University)
 “Integrating Chemical and Biological Data for Compound Selection and
 Mode-of-Action Analysis”

11:30~13:00 Lunch

Chair Prof. Alexandre Varnek

- 13:00~14:00 Prof. Didier Rognan (Strasbourg Univ.)
 “PDB-scale detection of ligandable cavities at protein-protein interfaces”

Chair Prof. Didier Rognan

- 14:00~15:00 Prof. Kurt Varmuza (Technical University of Vienna)
 “Selected aspects of 40 years applied chemometrics”

15:00~15:30 ----- Break -----

Chair Prof. Kurt Varmuza

15:30~16:30 Prof. Alexandre Varnek (Strasbourg University)

“Cheminformatics approaches to synthetic organic reactions: from empirical to predictive chemistry”

[Expert session by Software Vendors]

Chair Dr. Hiromasa Kaneko

16:30~16:50 Ryoka System

Seiichi Kobayashi

“CIMPL: A new cheminformatic platform for medicinal chemists”

16:50~17:10 Optibrium Dr. Matthew Segall, Hulinks Dr. Sumie Tajima

“Similarity to SAR - Interactive Navigation of Similarity Relationships to Guide Optimization”

Closing remarks: Prof. Yasushi Okuno (Kyoto University)

Contact: Prof. Kimito Funatsu

http://funatsu.t.u-tokyo.ac.jp/autumn_school_2015.htm

e-mail: funatsu@chemsys.t.u-tokyo.ac.jp

TEL: 03-5841-7751