5th Autumn School of Chemoinformatics in Nara, 2017

November 15-16, 2017
Nara Kasugano International Forum
http://www.i-ra-ka.jp/iraka/access/

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 Chem-Bio Informatics Society
http://cbi-society.org/index_e.html

November 15
10:00 Opening remarks: Prof. Kimito Funatsu (The University of Tokyo)
[Tutorial session]
10:10~11:00 Prof. Juergen Bajorath (Bonn University)
"Extending Fundamental Concepts for Chemoinformatics: From First to Second Generation Scaffolds, from Activity Cliffs to Promiscuity Cliffs"
11:00~11:50 Dr. Kiyoshi Hasegawa (Chugai Pharmaceutical Co.)
"Activity Landscape and Its Application to Molecular Design"

12:00~13:30 Lunch

13:30~14:20 Prof. Gisbert Schneider (ETH Zurich)
"Automating drug discovery"
14:20~15:10 Prof. Manabu Sugimoto (Kumamoto University)
"Electronic-Structure Informatics for Discovery/Design of Functional Molecules"

15:10~15:40 ------- Break -------

15:40~16:30 Prof. Johann Gasteiger (Erlangen-Nuernberg University)
"Chemoinformatics - From Synthesis Design to the Prediction of Material Properties"
16:30~17:20 Dr. Yoshifumi Fukunishi (Advanced Industrial Science and Technology (AIST))
"Some prediction models for protein-compound interactions in computer-aided drug development

[Expert session by Software Venders]
17:20~17:40 OpenEye

"Visualizing ligand-protein interactions"
Dr. Krisztina Boda

17:40~18:00 DS BIOVIA KK
"Effective Machine Learning for Big Data and Small Data."
Dr. Dana Honeycutt

18:30-20:30 Banquet :Nara national Museum
URL: http://www.narahaku.go.jp/english/index_e.html

11 月 16 日(木)
[Big data session]
9:00~9:20 Prof. Kimito Funatsu (The University of Tokyo)
9:20~9:40 Prof. Yasushi Okuno (Kyoto University)
9:40~10:00 Dr. Makoto Taiji (RIKEN)
10:00~10:20 Prof. Kenji Hori (Yamaguchi University)

10:20~10:50 -------- Break ---------

[Tutorial session]
10:50~11:40 Prof. Didier Rognan (Strasbourg University)
"PDB-scale identification of druggable cavities at or nearby protein-protein Interfaces"
11:40~12:30 Prof. Yoshihiro Yamanishi (Kyushu University)
"Data-driven drug discovery and repositioning by machine learning"

12:30~14:00 Lunch

14:00~14:50 Prof. Alexandre Varnek (Strasbourg University)
"Generative Topographic Mapping: an universal tool for chemical data visualization and modeling"

14:50~15:40 Prof. Thierry Langer (Vienna University)
"Dynamic Pharmacophores: A New Way to Enhance Virtual Screening Screening Efficacy in Early Drug Discovery"

15:40~16:00 -------- Break ---------

16:00~16:50 Prof. Shigehiko Kanaya (Nara Institute of Science and Technology)
"Integration of data-intensive science between chemo- and bio-informatics based on

KNApSAcK DB"

[Expert session by Software Venders]

16:50~17:10 MOLSIS

"MOEsaic: Integrated Web Application for SAR Analysis"

Mr. Takashi Ikegami

17:10~17:30 CONFLEX

"Predictions of conformational and packing polymorphs for organic Molecules"

Mr. Shigeaki Obata

17:30~17:50 Affinity Science

"Modern approaches for hit finding and molecular design in early drug discovery research"

Dr. Sharon Bryant(Inte:Ligand)

Closing remarks: Prof. Kimito Funatsu (The University of Tokyo)

Registration fee: 5,000JPY (Student:2,000JPY) Please pay at registration desk.
Banquet fee: 7,000JYP (Studen:5,000JPY) Please pay at registration desk.
Registration: Deadline: October 30, 2017
Please send e-mail to the following address with 1) Name, 2) Affiliation, 3) e-mail, 4) Tel number, 5) Banquet participation Yes or No.

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