

Autumn School of Chemoinformatics in Nara  
[http://funatsu.t.u-tokyo.ac.jp/english/autumn\\_school\\_e\\_2013.htm](http://funatsu.t.u-tokyo.ac.jp/english/autumn_school_e_2013.htm)

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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](http://www.pharm.or.jp/index_e.html)

The Chem-Bio Informatics Society

[http://cbi-society.org/index\\_e.html](http://cbi-society.org/index_e.html)

Date: November 27-28, 2013

Location: Nara Prefectural New Public Hall

URL: <http://www.shinkokaido.jp/en/>

[Organizing committee]: Prof. Kimito Funatsu(The University of Tokyo), Prof. Yasushi Okuno(Kyoto University), Prof. Shigehiko Kanaya(Nara Institute of Science and Technology), Dr. Kiyoshi Hasegawa(Chugai Pharmaceutical Co.)

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**[November 27]**

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

[Tutorial session]

**Chair Dr. J. B. Brown**

10:00~11:00 Prof. Juergen Bajorath (Bonn University)

"Exploring Activity Cliffs in Chemoinformatics and Medicinal Chemistry"

**Chair Prof. Juergen Bajorath**

11:00~12:00 Dr. J. B. Brown(Kyoto University)

" Systems Chemical Biology via Computational Compound-Protein Interaction  
Prediction: Core Ideas, Translational Validity, and Important Perspectives "

12:00~13:30 Lunch

**Chair Prof. Alexandre Varnek**

13:30~14:30 Dr. Kiyoshi Hasegawa (Chugai-Pharmaceutical Co.)

"Bayesian statistics for drug design"

**Chair Prof. Kurt Varmuza**

14:30~15:30 Prof. Johann Gasteiger (Erlangen-Nuernberg University )

"Solved and unsolved problems in chemoinformatics"

15:30~16:00 ----- Break -----

[Expert session by Software Vendors]

**Chair** Dr. Hiromasa Kaneko

16:00~16:30 Certara

Dr. Brian Masek (Certara USA)

“Progress in Predicting Off Target and Safety Profiles”

16:30~17:00 OpenEye

Dr. Krisztina Boda (OpenEye Scientific Software, Inc.)

“OEToolkits: The Building Blocks for Software Innovation”

17:00~17:30 BioSolveIT

Dr. Marcus Gastreich (BioSolveIT GmbH)

“Filling a Gap in Computational Lead Optimization:

Proposing Fragments and Visualizing their “Happiness” in Binding Pockets”

17:30~18:00 Schroedinger

Dr. Naotaka Oishi (Schroedinger)

“Free energy calculations and rapid empirical scoring functions: insight into structure based drug design”

18:30~20:30 Banquet: Nara National Museum (5 min. walk from Conference Hall)

URL: [http://www.narahaku.go.jp/english/index\\_e.html](http://www.narahaku.go.jp/english/index_e.html)

**[November 28]**

[Tutorial session]

**Chair Prof. Gisbert Schneider**

9:00~10:00 Prof. Didier Rognan (Strasbourg Univ.)  
"Computational methods to profile bioactive ligands"

**Chair Prof. Didier Rognan**

10:00~11:00 Prof. Gisbert Schneider (ETH Zurich)  
"From chaos to order by adaptive molecular design"

11:00~11:15 ----- Break -----

**Chair Prof. Shigehiko Kanaya**

11:15~12:15 Prof. Takaaki Nishioka (Nara Institute of Science and Technology)  
"Mass spectral database MassBank and its application to chemical structure elucidation"

12:15~13:30 Lunch

**Chair Prof. Johann Gasteiger**

13:30~14:30 Prof. Kurt Varmuza (Technical University of Vienna)  
"Variable selection for multivariate models - myth and reality"

**Chair Dr. Kiyoshi Hasegawa**

14:30~15:30 Prof. Alexandre Varnek (Strasbourg University)  
"Chemography concept in Chemical Space analysis"

15:30~16:00 ----- Break -----

[Expert session by Software Vendors]

**Chair Dr. Kiyoshi Hasegawa**

16:00~16:30 PerkinElmer-Spotfire  
Dr. Naotaka Oishi (PerkinElmer Japan)  
"Accelerating Research Process by Visual Analytics"

16:30~17:00 Accelrys  
Dr. Yuji Takaoka (Accelrys Japan)  
"Chemoinformatics tools in Accelrys Enterprise Platform"

17:00~17:30 Japan Association for International Chemical Information/CCDC  
Dr. Jason Cole (Cambridge Crystallographic Data Centre)  
"A New Knowledge-Informed Methodology for Ligand Based Drug Design"

Closing remarks: Prof. Yasushi Okuno (Kyoto University)