

The 4th French-Japanese Workshop on Computational Methods in Chemistry

CHEMOINFOMA TICS - MOLECULAR DYNAMICS - QUANTUM CHEMISTRY

Book of Abstracts and Program



*National Park Resort Village, Sikanosima,
Fukuoka, Japan*
March 5-6, 2012

Organizing Committee

Chantal Daniel (CNRS/UdS Strasbourg)
Kimito Funatsu (University of Tokyo)
Kenzi Hori (Yamaguchi University)
Alexandre Varnek (UdS, Strasbourg)
Kazunari Yoshizawa (Kyushu University)
Yoshihito Shiota (Kyushu University)
Takashi Kamachi (Kyushu University)

Invited Speakers

Prof. Dr. Jürgen Bajorath, University of Bonn
Dr. Sharon Bryant, CEO "Inte:Ligand", Vienna-Strasbourg
Prof. Hiroshi Chuman, The University of Tokushima
Dr. Emmanuel Fromager, University of Strasbourg
Prof. Kimito Funatsu, The University of Tokyo
Prof. Kenzi Hori, Yamaguchi University
Dr. Dragos Horvath, University of Strasbourg
Dr. Takayoshi Ishimoto, Kyushu University
Prof. Thierry Langer, CEO "Prestwick Chemicals", Strasbourg,
Dr. Gilles Marcou, University of Strasbourg
Prof. Luc Morin-Allory, University of Orleans
Prof. Mitsuru Shindo, Kyushu University
Prof. Masanori Tachikawa, Yokohama City University
Prof. Kazunari Yoshizawa, Kyushu University
Prof. Alexandre Varnek, University of Strasbourg

Past workshops

The 1st F-J Workshop (2008) in Strasbourg, France
(<http://infochim.u-strasbg.fr/spip.php?article142>)

The 2nd F-J Workshop (2009) in Nishinomiya, Japan
(<http://www.ph.tokushima-u.ac.jp/article/0015900.html>)

The 3rd F-J Workshop (2010) in Strasbourg, France
(<http://infochim.u-strasbg.fr/spip.php?article62>)

Contact

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Registration Fee

Registration fee : JPY 12,000

Banquet : JPY 4,000 (Student: JPY 2,000)

MAPS



Program

Monday, March 5, 2012

Time for each lecture is about 25 min (including discussion)

13:00-13:10 Opening remarks (Kazunari Oshizawa)

(Chair:)

13:10-13:35 L01 Prof. Mitsuru Shindo, Kiyushu University

Electrocyclic Reactions Controlled by Stereoselectivity

13:35-14:00 L02 Prof. Luc Morin-Allory, University of Orleans

Visual Characterization and Diversity Quantification of Chemical Libraries: The Delimited Reference Chemical Subspaces (DRCS) Methodology.

(Chair:)

14:00-14:25 L03 Dr Takayoshi Ishimoto, Kiyushu University

Molecular Dynamics Simulation with Nuclear Quantum Effect

14:25-14:50 L04 Dr Dragos Horvath, University of Strasbourg

Highly flexible sampling & docking - taking the time to really address relevant degrees of freedom

14:50-15:10 Coffee break

(Chair:)

15:10-15:35 L05 Dr Sharon Bryant, CEO "Inte:Ligand", Vienna-Strasbourg

Bridging the Gap Between Structure- and Ligand-Based Pharmacophore Modeling: Advanced Pharmacophores for Accurate Virtual Screening and Identification of Opioid Lead Compounds

15:35-16:00 L06 Prof. Dr Jürgen Bajorath, University of Bonn

Molecular Scaffold Analysis in Cheminformatics: Assessment of Scaffold Hopping Potential and Systematic Mapping of Protein-Ligand Interactions Using Compound Data

16:00-16:25 L07 Prof. Kimito Funatsu, The University of Tokyo

Design of Alkanolamine Structure for CO₂ Absorption Method

16:25-17:40 Poster presentation

18:30-21:00 Banquet

Program

Tuesday, March 6, 2012

(Chair:)

9:00-9:25 L08 Prof. Masanori Tachikawa, Yokohama City University
Multi Component Molecular Theory for Hydrogen Bonded Systems and Positronic Compounds

9:25-9:50 L09 Dr Emmanuel Fromager, University of Strasbourg
Rigorous Formulation of Double Hybrid Density-Functionals

9:50-10:15 L10 Prof. Kazunari Yashizawa, Kyushu University
Quantum Chemical Studies for Future Energy Sources

10:15-10:40 L11 Prof. Kenzi Hori, Yamaguchi University
Theoretical Study on Keto-Enol Tautomerism using the QM/MC/FEP method

10:40-11:00 **Coffee break**

(Chair:)

11:00-11:25 L12 Prof. Thierry Langer, CEO Prestwick Chemicals, Strasbourg,
Pharmacophore-based Ligand Profiling: An Efficient Tool in Lead Structure Discovery and Optimization

11:25-11:50 L13 Prof. Hiroshi Chuman, The University of Tokushima
Links between Traditional and Modern QSAR Approaches - Linear Expression by Representative Energy (LERE) Terms

11:50-12:15 L14 Alexandre Varnek, University of Strasbourg
Generative Topographic Maps: universal tool for data visualization and structure-activity modeling

12:15-12:40 L15 Dr Gilles Marcou, University of Strasbourg
Interpretability of SAR/QSAR models of any complexity by atomic contributions

12:40-12:50 Closing remarks (Kimito Funatsu)

List of Poster Presentations

Monday, March 5 (16:25 – 17:40)

PP01 Kimichi Suzuki, Masanori Ōchikawa, Hiroshi Ogawa, Somlak Ittisanronnchai, Hirotomo Nishihara, Ōkashi Kiyotani, Umpei Nagashima

Temperature dependence of the hydrogen adsorption sites on Zeolite-templated Carbon

PP02

PP03

PP04

PP05

PP06

PP07

PP08

PP09

PP10

PP11

PP12

PP13

PP14