Third French-Japanese Workshop on Computational Methods in Chemistry

Chemoinformatics - Molecular Dynamics - Quantum Chemistry
18 June 2010

Organizing Committee
Chantal Daniel (CNRS/UdS Strasbourg, France)
Kimito Funatsu (Tokyo University, Japan)
Alexandre Varnek (UdS, Strasbourg, France)

Location: Faculty of Chemistry, 1 rue Blaise Pascal, Strasbourg

Tentative Schedule

9:00 Opening
9:10 - 9:40 Kimito FUNATSU
Development of a method for discovering orphan GPCR ligands

9:40 - 10:10 Annick DEJAEGERE
Computational studies on the molecular mechanisms of transcriptional regulation: methylated histones and their protein recognition modules

10:10 - 10:40 Umpei NAGASHIMA
Too short CN bonds found experimentally in the electronic ground state of FeNC, CoCN, and NiCN: A Possible Interpretation from ab Initio Computational Spectroscopy View Point

10:40 – 11:00 Coffee break

11:00 - 11:30 Dragos HORVATH
Neighborhood Behavior approach: Similar Molecules have Similar Properties… but can you tell whether they’re similar?

11:30 – 12:00 Kenji HORI
Predicting Experimental Yields as an Index to Rank Synthesis Routes: Application to Diels-Alder Reactions and Curtius rearrangements.
12:00 - 12:20  Megumi KAYANUMA  
Theoretical Study of Hydrogen Adsorption and Diffusion in Spillover Process on Curved Surface of Microporous Carbon

12:20 - 14:00  Lunch (Esplanade)

14:00 - 14:30  Didier ROGNAN  
Fingerprinting protein cavities and protein-ligand complexes in rational drug design

14:30 - 15:00  Masanori TACHIKAWA  
Path integral simulation for hydrogen bonded systems: Protonic quantum nature and H/D isotope effect

15:00 - 15:30  Trond SAUE  
A comparative study of covalency in trihalides of lutetium and lawrencium

15:30 – 15:50  Coffee break

15:50 - 16:20  Kazunari YOSHIZAWA  
Frontier Orbital Concept for Conductance of Molecules

16:20 – 16:50  Pascal MULLER  
HSP90 inhibitors: hit finding using Molecular Interaction Fingerprint and non-covalent ESI-MS screening

17:00 – 18:00  POSTER SESSION

19:30  Dinner in the city