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***