

2nd French-Russian Workshop on Chemoinformatics and Bioinformatics

Kazan, September 17, 2012

Butlerov Hall, A.M. Butlerov Institute of Chemistry, Kazan Federal University

8:30-9:00	Registration	
9:00-9:30	Opening ceremony Chairman - Prof. I. Antipin Rector I.R. Gafurov, Prof. A. Varnek	
	Session 1. Chairman - A. Varnek	
9:30-9:55	V. Poroikov (Moscow, Russia)	Web-services for prediction of biological activity via Internet
9:55-10:20	D. Horvath (Strasbourg, France)	S4MPLE - Sampler For Multiple Protein-Ligand Entities
10:20-10:45	E. Muratov, V. Kuz'min (Odessa, Ukraine)	<i>Per angusta ad angusta</i> : 10 years of successful application of Simplex approach in antiviral research
10:45-11:10	I. Baskin (Moscow, Russia)	New Approaches to Molecular Alignment and Flexibility Based on Unsupervised Learning and Continuous Molecular Fields
11:10-11:30	Coffee-break	
	Session 2. Chairman - V. Poroikov	
11:30-11:55	A. Varnek (Strasbourg, France)	Condensing chemical reactions to pseudo-molecules: an efficient way of reactions mining
11:55-12:20	P. Vasiliev (Volgograd, Russia)	IT "Microcosm" for property prediction of organic compounds
12:20-12:45	G. Marcou (Strasbourg, France)	QSAR modeling of ADME/Tox properties
12:45-14:30	Lunch	
	Session 3. Chairman - D. Horvath	
14:30-14:55	A. Dejaegere (Strasbourg, France)	Prediction of the methylated histone binding propensities of PHD domains on a genome wide basis
14:55-15:20	M. Gastreich (Bonn, Germany)	An Unsupervised, Visual Affinity Assessment Derived From Physical Principles
15:20-15:45	N. Akberova (Kazan, Russia)	The acetylcholinesterase sites in the active center effect on the interaction of Ser203 with inhibitor
15:45-16:10	R. Stote (Strasbourg, France)	Allotery in nuclear receptor proteins. Molecular mechanisms derived from molecular dynamics simulations
16:10-16:30	Coffee-break	
	Section 4. Chairman - P. Vasiliev	
16:30-16:55	R. Zhdanov (Kazan, Russia)	Molecular mechanics, docking and molecular dynamics study of DNA-lipid complexes
16:55-17:20	E. Katkova (Moscow, Russia)	Docking and postprocessing: application to design of urokinase inhibitors
17:20-17:45	D. Baev (Novosibirsk, Russia)	The integrated approach to the pharmacological screening of some new ursolic triterpenoids
17:45-17:55	T. Madzhidov (Kazan, Russia)	Master in Chemoinformatics at the Kazan University
17:55-18:05	N. Akberova (Kazan, Russia)	Master in Bioinformatics at the Kazan University
18:05-18:15	M. Missarov (Kazan, Russia)	Master program in Data Mining and its Applications at the Kazan University
18:15-18:30	Closing ceremony (I. Antipin, V. Poroikov, A. Varnek)	
19:00	Banquet	