French-Russian Workshop on Chemoinformatics

Moscow, Russia - 11-12 May 2010

	11 May 2010 Department of Chemistry, Moscow State University	
	Nikolay ZEFIROV, Head of the Division of Organic Chemistry, MSU **Introductory Remarks**	09:15-09:30
1.	Vladimir PALYULIN, Moscow State University **Molecular Modelling of Neuroreceptors and QSAR Studies of Their Ligands**	09:30-10:00
2.	Alexandre VARNEK, University of Strasbourg **ISIDA Platform For Virtual Screening Based on Fragment and Pharmacophoric Descriptors**	10:00-10:30
3.	Oleg RAEVSKY, Institute of Physiologically Active Compounds **Classification and Regression Models of Rodent Acute Toxicity**	10:30-10:50
	Coffee-break	*10:50-11:10*
4.	Jason THEODOSIOU, Aureus Pharma, France **Ligand Based Virtual Screening Using Aureus' Knowledge Platform**	11:10-11:40
5.	Dmitry OSOLODKIN, Moscow State University **Virtual Screening Workflow for GSK3b Inhibitors**	11:40-11:55
6.	Gilles MARCOU, University of Strasbourg **Exploring Linearly Separable Problems in Chemoinformatics**	11:55-12:15
7.	Eugene RADCHENKO, Moscow State University **Antiesterase Selectivity of Organophosphorus Compounds: an MFTA Study**	12:15-12:35
8.	Peter FEDICHEV, Quantum Pharmaceuticals, Russia. **"Quantum" Approach to Computational Drug Discovery**	12:35-13:00
	Lunch	*13:00-14:00*
	Visit the laboratories of the Department of Chemistry, MSU	*14:00-16:00*
	Cultural program	*16:00–19:00*

12 May 2010	**Institute of Biomedical Chemistry of Russ. Acad. Med. Sci.**	
	Vladimir POROIKOV, Head of the Department for Bioinformatics, Institute of Biomedical Chemistry **Introductory Remarks**	09:15-09:30
9.	Anne-Claude CAMPROUX, Christelle REYNÈS, University Paris-7 **Rationalizing the Chemical Space of Protein-Protein Interaction Inhibitors Using Statistical Approaches**	09:30-10:00
10.	Dmitry FILIMONOV, Institute of Biomedical Chemistry **Local Correspondence Concept in Bio- And Chemoinformatics**	10:00-10:30
11.	Dragos HORVATH, University of Strasbourg **Neighborhood Behavior Approach: Global and Local Similarity Principle and Consequences for Virtual Screening**	10:30-10:50
	Coffee-break	*10:50-11:10*
12.	Andrey LISITSA, Ekaterina ILGISONIS. Institute of Biomedical Chemistry **Personal Reference Dashboard as a Tool for Chemoinformatics**	11:10-11:30
13.	Vitaly SOLOV'EV, Institute of Physical Chemistry **CoMet Project: Prediction of Stability Constants of Metal - Ligand Complexes in Solutions**	11:30-11:50
14.	Alexey LAGUNIN, Institute of Biomedical Chemistry **Computer-Aided Analysis of Biological Activity Spectra for Phytoconstituents**	11:50-12:05
15.	Daria TSAREVA, Moscow State University **Atomic Charges in 3D QSAR: Comparison of Different Calculation Schemes**	12:05-12:20
16.	Alexey ZAKHAROV, Institute of Biomedical Chemistry **QSAR Modelling of Rodent Acute Toxicity**	12:20-12:35
17.	Ghermes CHILOV, MolTech, Russia. **Lead Finder Software for Ligand Docking and Virtual Screening**	12:35-13:00
	Lunch	*13:00-14:00*
	Visit the laboratories of the Institute of Biomedical Chemistry	*14:00-16:00*
	Cultural program	*16:00–19:00*