PROGRAM
of
Kazan Summer School on Chemoinformatics

Kazan, 2013
Kazan Federal University

August 25, 2013		
Arrival day		
13:00-15:00	**Registration (for Kazan citizens)**	
15:00-19:00	**Excursion Program**	
August 26, 2013		
8:00-9:00	**Registration (for other Participants)**	
9:00-9:15	**Opening ceremony**	
	Lecture Session 1 **Chairman – V. Poroikov**	
9:15-10:15	A. Varnek (Strasbourg, France)	Chemoinformatics: Basic Concepts and Areas of Application
10:15-11:15	T. Madzhidov (Kazan, Russia)	Chemical Databases: Encoding, Storage and Search of Chemical Structures
11:15-11:45	Coffee-break	
11:45-12:30	V.-P. Hyttinen (CAS, Finland)	Basics about CAS and SciFinder
12:30-14:00	**Lunch**	
	Oral Session 1 **Chairman – I. Tetko**	
14:00-14:20	V.S. Abrukov (Cheboksary, Russia)	Artificial neural networks for creation of knowledge bases in scientific and applied research
14:20-14:40	N.I. Baranova (Saint-Peterburg, Russia)	QSAR modeling of calculation IC50 for Xa coagulation factor
14:40-15:00	O.V. Galzitskaya (Moscow, Russia)	How to Determine the Size of the Nucleus of Protofibrils from the Concentration Dependence of the Lag-Time Of Aggregation? Experimental Application: Insulin and Lys-Pro Insulin
15:00-15:30	P. Polishchuk (Odessa, Ukraine)	Development of "non-classical" antagonists of fibrinogen receptors - promising anti-platelet agents
15:30-16:00	Coffee-break	
	Tutorial Session 1	
16:00-18:00	G. Marcou, D. Horvath (Strasbourg, France)	Tutorial with ChemAxon
18:00-20:00	**Welcome party**	

August 27, 2013		
	Lecture Session 2 Chairman – T. Langer	
9:00-10:00	I. Baskin (Moscow, Russia)	Obtaining, Validation and Application of SAR/QSAR Models
10:00-11:00	A. Tropsha (Chapel Hill, USA)	SAR/QSAR Modelling: State of the Art
11:00-11:30	Coffee-break	
11:30-12:30	I. Tetko (Munich, Germany)	ADMET Predictions
12:30-14:00	**Lunch**	
	Tutorial Session 2	
14:00-16:00	I. Tetko (Munich, Germany)	Tutorial with QSAR modeling
16:00-18:00	**Poster Session**	
August 28, 2013		
	Lecture Session 3 Chairman – A. Tropsha	
9:00-10:00	D. Horvath (Strasbourg, France)	Conformational Sampling
10:00-11:00	T. Langer (Strasbourg, France)	Pharmacophores and Its Applications
11:00-11:30	Coffee-break	
11:30-12:30	G. Marcou (Strasbourg, France)	Molecular Docking Methods
12:30-14:00	**Lunch**	
	Tutorial Session 3	
14:00-16:00	S. Bryant (Vienna, Austria)	Tutorial with LigandScout
16:00-16:30	Coffee-break	
16:30-18:30	G. Marcou, D. Horvath (Strasbourg, France)	Tutorial with LeadIt
August 29, 2013		
	Oral Session 2 Chairman – K. Balakin	
9:00-9:20	S.V. Luschekina (Moscow, Russia)	Refining Molecular Modeling Techniques: 2-Amino-5-Halomethyl-Thiazolines Esterase Profile Case Study
9:20-9:40	E. Muratov (Odessa, Ukraine)	Obscurum per obscurius: computer-aided design of novel antivirals using Simplex approach
9:40-10:00	L.A. Uroshlev (Moscow, Russia)	Algorithm for prediction ions in protein structures
10:00-10:30	V. Solovev (Moscow, Russia)	Substructural Molecular Fragments in Consensus QSPR Modeling
10:30-11:00	Coffee-break	

	Lecture Session 4 Chairman – A. Varnek	
11:00-12:00	K. Balakin (Moscow, Russia)	Computational Mapping Tools for Drug Discovery
12:00-13:00	V. Poroikov (Moscow, Russia)	Drug Design & Discovery in Academia
13:00-13:30	**Winner award ceremony, Closure of the School**	

Post-School event (all Participants are welcome to attend)

14:30-16:30	N. Krukovskaya (CAS, Russia)	Basic features how to explore references, structures and reactions with SciFinder

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