Mathematical modelling workshop

Current and Future Perspectives of micro- and macro modelling of infectious diseases: from system biology to control and dynamics

Rīga Stradiņš University, Dzirciema iela 16, Rīga, Latvia
Senate Hall, Block K

13 – 15 January 2016

PRELIMINARY AGENDA

Wednesday, 13 January 2016	
12.30 - 13.00	Registration and welcome coffee
13.00-13.10	**Welcome and opening** **Modra Murovska**, *BALTINFECT* coordinator
	Session 1 **Mathematical tools for infectious disease modeling: current state and perspectives** Chairs: **Mikhail Barishev, Natal van Riel**
13.10 - 13.50	**Natal van Riel,** Department of Biomedical Engineering, Technische Universiteit Eindhoven, Netherlands **Using mathematical and computational modelling to study human disease**
13.50 - 14.30	**Rimantas Eidukevicius,** Department of Mathematical Statistics, Faculty of Mathematics and Informatics, Vilnius University, Lithuania **Estimating of Durations of Cell Cycle Phases Using a Stochastic Model and Flow Cytometry Data**
14.30 - 15.10	**Nuno Sepúlveda,** London School of Hygiene and Tropical Medicine, United Kingdom; Centre for Statistics and Applications of University of Lisbon, Portugal **Serology and mathematical modelling as joint tools to inform the epidemiology of infectious diseases on the cusp of elimination**
15.10 - 15.30	*Coffee break*
15.30 - 16.10	**Sofia Johansson**, Department of Microbiology, Tumor and Cell Biology, Karolinska Institutet **Natural Killer cell receptor dynamics investigated with novel quantitative techniques**
16.10 - 16.50	**Yoram Louzoun,** Department of Mathematics, Bar-Ilan University, Ramat Gan, Israel **Impact of bacterial load and spatio-temporal population structure on epidemiology of infectious diseases**

Thursday, 14 January 2016	
	Session 2 **Systems Biology and Biological Networks** Chairs: **Uldis Berķis, Vladimir Poroykov**
10.00 - 10.40	**Alexander Kel,** GeneXplain GmbH, Wolfenbüttel, Germany **Walking pathways" and personalized medicine**
10.40 – 11.20	**Vladimir Poroykov,** Department for Bioinformatics, Institute of Biomedical Chemistry, Moscow, Russia **Discovery of new pharmaceutical agents using *in-silico* approaches: PASS, GUSAR, PharmaExpert and Way2Drug platform**
11.20 - 11.40	*Coffee break*
11.40 - 12.20	**Jürgen Borlak,** Institute for Pharmaco- and Toxicogenomics, Centre of Pharmacology and Toxicology, Hannover Medical School, Germany **Immunogenomics reveals molecular circuits of diclofenac induced immune-mediated liver injury in mice**
12.20 - 13.00	**Marzio Pennisi,** Department of Drug Sciences, University of Catania, Italy **Coloured petri nets for modelling immune response**
13.00 - 13.40	**Athina Geronikaki,** Laboratory of Pharm. Chemistry, School of Pharmacy, Aristotle University of Thessaloniki, Greece **Computer-aided finding of new pharmaceutical agents with multitargeted action**
13.40 - 14.40	*Lunch break*
	Session 3 **Modelling of Cell interactions** Chairs: **Mārtiņš Kālis, Olga Kel-Margoulis**
14.40 - 15.20	**Alexey Chernobrovkin,** Department of Medical Biochemistry and Biophysics, Karolinska Institutet, Sweden **In-silico structure optimization and MoA characterization of novel antibacterial agents.**
15.20 - 16.00	**Olga Tikhonova,** Laboratory of Systems Biology, Institute of Biomedical Chemistry, Moscow, Russia **Proteome and transcriptome analysis of retinoic acid-induced differentiation of human promyelocytic leukemia HL-60 cells**
16.00 - 16.40	**Olga Kel-Margoulis,** Director Applied Life Science informatics, GeneXplain GmbH, Wolfenbüttel, Germany **Upstream analysis with the geneXplain platform: a bioinformatics approach to OMICS data**
Friday, 15 January 2016	
	Session 4 **Modelling Platforms** Chairs: **Šimons Svirskis, Jürgen Borlak**

10.00 - 10.40	**Šimons Svirskis,** A.Kirchenstein Institute of Microbiology and Virology, Riga Stradiņš University, Latvia **Matlab as a platform for analysis and modelling in molecular biology: MBET, SBET, PGET, Simulink**
10.40 - 11.00	**Vladimirs Kozlovs,** A.Kirchenstein Institute of Microbiology and Virology, Riga Stradiņš University, Latvia **Matlab usage in data analysis**
	Case studies
11.00 - 11.40	**Agnieszka Kaczor,** Faculty of Pharmacy with the Department of Medical Analytics, Medical University of Ljublin, Poland **Molecular modeling for cannabinoid receptors**
11.40 - 12.20	**Jürgen Borlak**, Institute for Pharmaco- and Toxicogenomics, Centre of Pharmacology and Toxicology, Hannover Medical School, Germany **Advanced computational biology methods identify molecular switches for malignancy in an EGF mouse model of liver cancer**
12.20 – 13.30	*Lunch break*
13.30 – 14.30	Group work – Demonstration of software updates (platforms)
	Group 1: Presentation of geneXplain **Presenters: Olga Kel-Margoulis, Alexander Kel** **Group 2**: Drug design **Presenters: Vladimir Poroykov, Jürgen Borlak** **Group 3**: Schrodinger suite **Presenters: Diāna Zeļencova**
14.30 – 14.45	Presentations of results from the group work to the all audience by the rapporteurs Conclusions and perspectives
15.00 - 15.10	Closing of the Workshop **Modra Murovska**, *BALTINFECT* coordinator