



COST Action OpenMultiMed
BioModelling Spring Riga 2019
August 11-13, 2019

Mechanistic modelling of human metabolism

Academic Center for Natural Sciences

University of Latvia <https://www.tornakalns.lv/eng/>

Room 501

Jelgavas iela 1

LV 1004, Riga

Latvia

Speakers:

Prof. Egils Stalidzans, Computational Systems Biology group, University of Latvia, director of Institute of Microbiology and Biotechnology.

Research interests: kinetic and stoichiometric modeling of metabolism, modeling of pharmacokinetics, user of COPASI and COBRA.

Iñigo Apaolaza, Department of Biomedical Engineering and Sciences, TECNUN School of Engineering, University of Navarra, Spain.

Research interests: Systems Biology, Constraint-Based Modeling, drug target identification, user and developer of COBRA.

Prof. Adil Mardinoglu, Systems Medicine group, King's College London, UK and KTH-Royal Institute of Technology, Sweden.

Research interests: Systems Medicine, Integration of multi-omics using biological networks, Biomarker and drug target discovery, user/developer of RAVEN and user of COBRA.

Prof. Dr. Harald Schmidt, Head of Department of Pharmacology & Personalised Medicine Faculty of Health, Medicine & Life Science, Maastricht University, Chair of COST action [OpenMultiMed](#).

Research interests: systems medicine, network pharmacology, drug repurposing.

Participants are expected to have own computers and installed COPASI (<http://copasi.org/>) and COBRA (<https://opencobra.github.io/cobratoolbox/stable/installation.html>) software if they want to follow tutorials.

Day 1 (Sunday, August 11, 2019)

Ordinary differential systems based model development and parametrisation using COPASI

12:30-13:00 Welcome coffee and tea

13:00-14:30 Building and validating dynamic toy model by COPASI (hands-on tutorial), Prof. [Egils Stalidzans](#)

- definition of reactions (hands-on tutorial),
- definition of reaction kinetics (hands-on tutorial),
- parameter estimation (hands-on tutorial).

14:30-15:00 Coffee break

15:00-17:00 Optimising a kinetic model by COPASI, Prof. [Egils Stalidzans](#)

- objective function (hands-on tutorial),
- total amino acid constraint and homeostatic constraint (hands-on tutorial),
- total optimization potential approach.

Day 2 (Monday, August 12, 2019)

Stoichiometric modelling based model development

9:00-10:30 Constraint-Based Modelling with The COBRA Toolbox v3.0 ([Iñigo Apaolaza](#))

- genome scale metabolic networks.
- -omics data integration.
- constraints and models.

10:30-11:00 Coffee break

11:00-12:30 Applications of Constraint-Based Modelling in medicine ([Iñigo Apaolaza](#))

- generation of a COBRA model (hands-on tutorial).
- Flux Balance Analysis (hands-on tutorial).
- Gene Essentiality Analysis (hands-on tutorial).

12:30-14:00 Lunch

14:00-15:30 The use of human tissue metabolic models in the analysis of the omics data (Prof. [Adil Mardinoglu](#))

- generation of human adipose, liver and muscle tissue GEMs.
- Analysis of the omics data using tissue-specific GEMs.
- Revealing the underlying molecular mechanisms of obesity related diseases

15:30-16:00 Coffee break

16:00-17:30 The use of Systems Medicine in treatment of liver diseases (Prof. [Adil Mardinoglu](#))

- Integration of GEMs with other biological networks
- Discovery of liver specific drug targets for NAFLD
- Drug development from target discovery to pre-clinical studies.

18:00 -18:45 Drug repurposing ([Prof. Dr. Harald Schmidt](#))

Day 3 (Tuesday, August 13, 2019)

Network analysis in systems medicine

9:00-9:40 The use of systems biology in treatment of liver diseases (Prof. [Adil Mardinoglu](#))

9:40-10:30 Metabolic Pathway Analysis conference (MPA2019) talks (<https://events.lu.lv/MPA2019>)

10:30-11:00 Coffee break

11:00-11:40 TBA (Prof. [Kathrin Thedieck](#))

11:40-12:30 Metabolic Pathway Analysis conference (MPA2019) talks (<https://events.lu.lv/MPA2019>)