FOSBE 2019 Workshop Proposal

Analyzing and redesigning metabolic networks with *CellNetAnalyzer*

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Duration: ca. 3 hours

Target audience: Students and researchers interested in constraint-based and stoichiometric modeling of metabolic networks. Some basic experiences in constraint-based modeling would be of advantage but is not an absolute requirement. The workshop will focus on the use of the software *CellNetAnalyzer*. If the participants want to follow the live demonstration or/and take part in the hands-on session, then they should bring their laptops (with MATLAB installed) along.

Abstract: *CellNetAnalyzer* (CNA) is a widely used MATLAB package for analyzing biological (metabolic, signaling and regulatory) networks. CNA and supports both command-line based operations as well as a graphical user interface with embedded network visualizations. In the first part of this workshop (1,5h) we will demonstrate key features of CNA for stoichiometric and constraint-based modeling of metabolic networks including flux (balance) analysis, flux and yield optimization, phase plane analysis, elementary mode analysis, computational (re)design of metabolic networks based on minimal cut sets, and many more. The second part of the tutorial (1,5h) will consist of hands-on exercises with example networks where the participants will learn how to use *CellNetAnalyzer* in practice.

Tentative Schedule:

First part (1,5h):

- Introduction to *CellNetAnalyzer*

- Overview of key methods of constraint-based modeling and how they can be used in *CellNetAnalyzer* to analyze metabolic networks (including live demonstrations):

- Fundamentals of constraint-based modeling of metabolic networks (relevant constraints and the resulting solution spaces)
- Metabolic flux analysis
- Flux balance analysis and optimal flux distributions
- Flux Variability analysis
- Phase planes and Yield spaces
- Elementary flux modes and metabolic pathway analysis
- Minimal cut sets and computational design of metabolic networks

- Introduction to Application Programming Interface in *CellNetAnalyzer*

Second part (1,5h):

- Guided hands-on exercises with *CellNetAnalyzer:* participants may either built and analyze small example models or/and solve exercises with existing (larger and realistic) network models in *CellNetAnalyzer*