



University
of Basel

Department
Biozentrum



BIOZENTRUM
The Center for
Molecular Life Sciences

Basel Computational Biology Seminar

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Models, Databases and Computational Methods for Analysis, Synthesis and Design in Synthetic Metabolism

Metabolic engineering, synthetic biology, and management of metabolic networks in health, environmental, and nutrition sciences involve the design, analysis, retrofitting, and repair of genome-scale metabolic networks through the manipulation of enzyme activities and cellular processes. Two of the central problems in the studies of metabolism are the expansion of our current knowledge of biochemical reactions and compounds and the identification of targets for manipulating metabolism with the minimum possible impact on cells physiology. We will present and discuss our work in addressing one of these two problems using concepts and methods from chemoinformatics, chemical reaction engineering, and process systems engineering.

We will present and discuss the development of BNICE.ch, a computational framework for design, evaluation, ranking and visualization of the promising de novo pathways for several applications ranging from metabolic gap-filling to metabolic engineering and drug design. BNICE.ch has several components that are integrated in a computational framework, namely: a database of generalized enzymatic reaction rules, integrated biological and chemical databases, metabolic network generation and pathway enumeration algorithms, and several cheminformatics and bioinformatics tools for the pathway feasibility studies.

We used BNICE.ch for the development of ATLAS of biochemistry, a database of all the biochemically plausible reactions between compounds reported to occur in living organisms. ATLAS uses KEGG as the reference database with 16,000 metabolites and 10,000 reactions and it contains more than 130,000 new reactions. The mining of ATLAS will undoubtedly offer new opportunities for the design of synthetic pathways and metabolic engineering.

Date: **Monday, March 25th, 2019**
Time: **16:00 h**
Room: **Lounge (level 13), Klingelbergstrasse 61**
(vis-à-vis Pharmazentrum)
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