Pathway Assistant: a web portal for metabolic modelling

Pekko Parikka
with Esa Pitkänen, Ari Rantanen, Esko Ukkonen and Arto Åkerlund

University of Helsinki
Department of Computer Science
The metabolism of an organism consists of a complex network of biochemical reactions transforming small molecules (i.e., metabolites) into others.

Metabolic modelling is a study of metabolism:
- the discovery of the topology of the metabolic network
- the estimation of the pathway velocities
- the modelling of regulation of metabolism

Computational metabolic modelling is:
- about automating above examples
- a relatively new and strongly progressing discipline
Automated generation of metabolic networks

Metabolic engineering
- Alterations to the current metabolic network that produce target metabolites more efficiently

Metabolic reconstruction
- Construction of the metabolic network based on genome data and a database of metabolic reactions
Pathway Assistant: a web portal for metabolic modelling

- Pathway Assistant portal is a collection of related metabolic modelling tools supporting multiple workflows.
- The design of Pathway Assistant is based on two main principles:
  - We want to deploy and update tools rapidly and iteratively based on the feedback given by the domain experts.
  - We want to present all modelling tools as an integrated user interface for end users.
- We aim to attain these goals with using SaaS software delivery model and a portal environment.
- We use web techniques like Java portlets and AJAX.
Pathway Assistant tools and supported workflows

Metabolic engineering workflow:
- ReMatch
- Topology Generator
- Yield Maximisation
- Flux Estimator

Metabolic reconstruction workflow:
- Sequence Input
- Topology Generator
- Homology
- Flux Estimator

Flux estimation workflow:
- ReMatch
- Flux Estimator

Database

Biologist

Metabolic Network

Sequence Data
Metabolic Engineering
Phase 1 importing network with ReMatch
Phase 2 Open the network in Topology Generator
Phase 3 set up basic parameters for Yield maximisation
Phase 4 start the search of alternative metabolic networks
Phase 5 browse alternative networks
Last phase: visualization of modifications in a candidate network
Preliminary results of Pathway Assistant project

- SaaS model suits well for productisation of bioinformatics methods
- Portal environment and portlets offers certain benefits:
  - Rapid distribution of new tools for portal users
  - Eases expandability of the system
  - Eases integration of the tools inside the portal
- AJAX is a good way to improve usability of user interface
- Combining of portlet and AJAX techniques has challenges
- Pathway Assistant is available in Internet:
  http://www.cs.helsinki.fi/group/sysfys/software/pa/