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Pathway Assistant: a web portal for metabolic modelling

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PATHWAY ASSISTANT portal

Metabolic modelling

- 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

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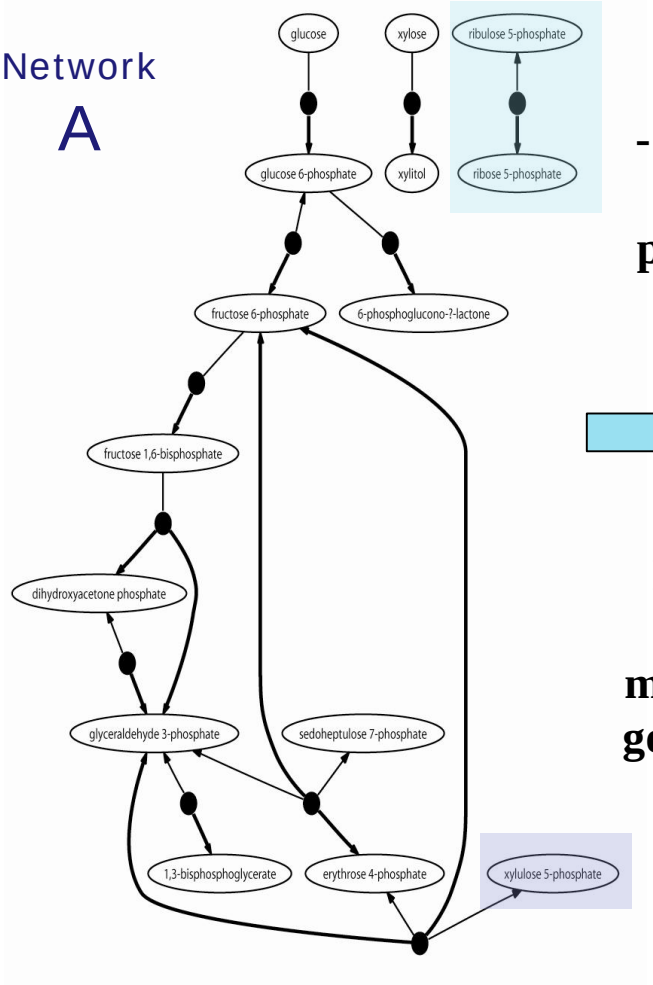
Automated generation of metabolic networks

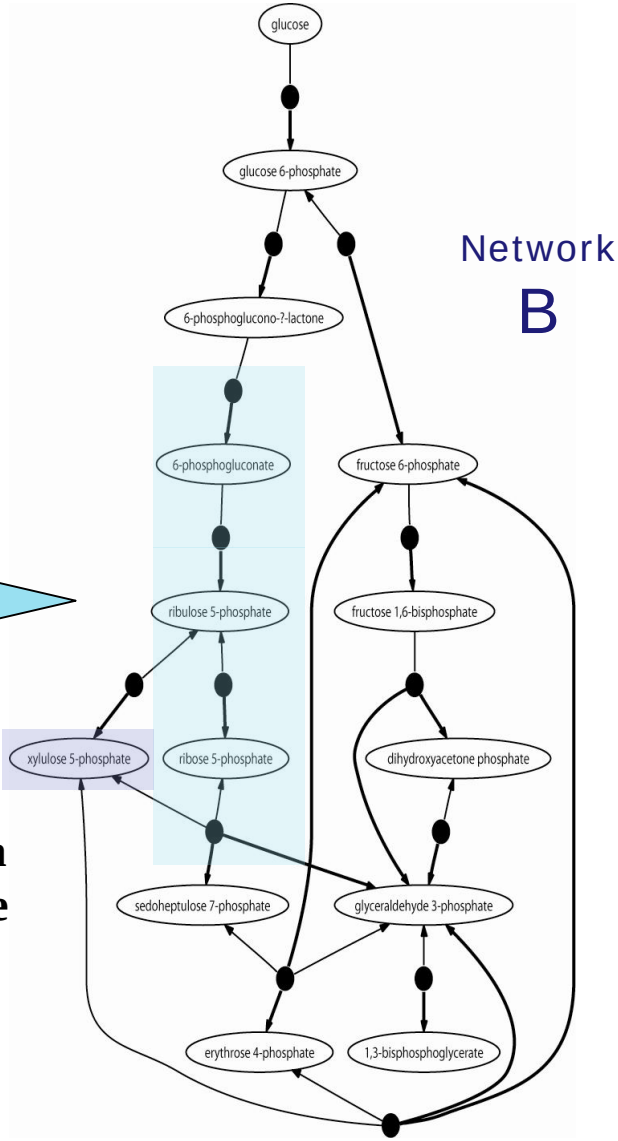
Network A



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

Network B



PATHWAY ASSISTANT portal

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.

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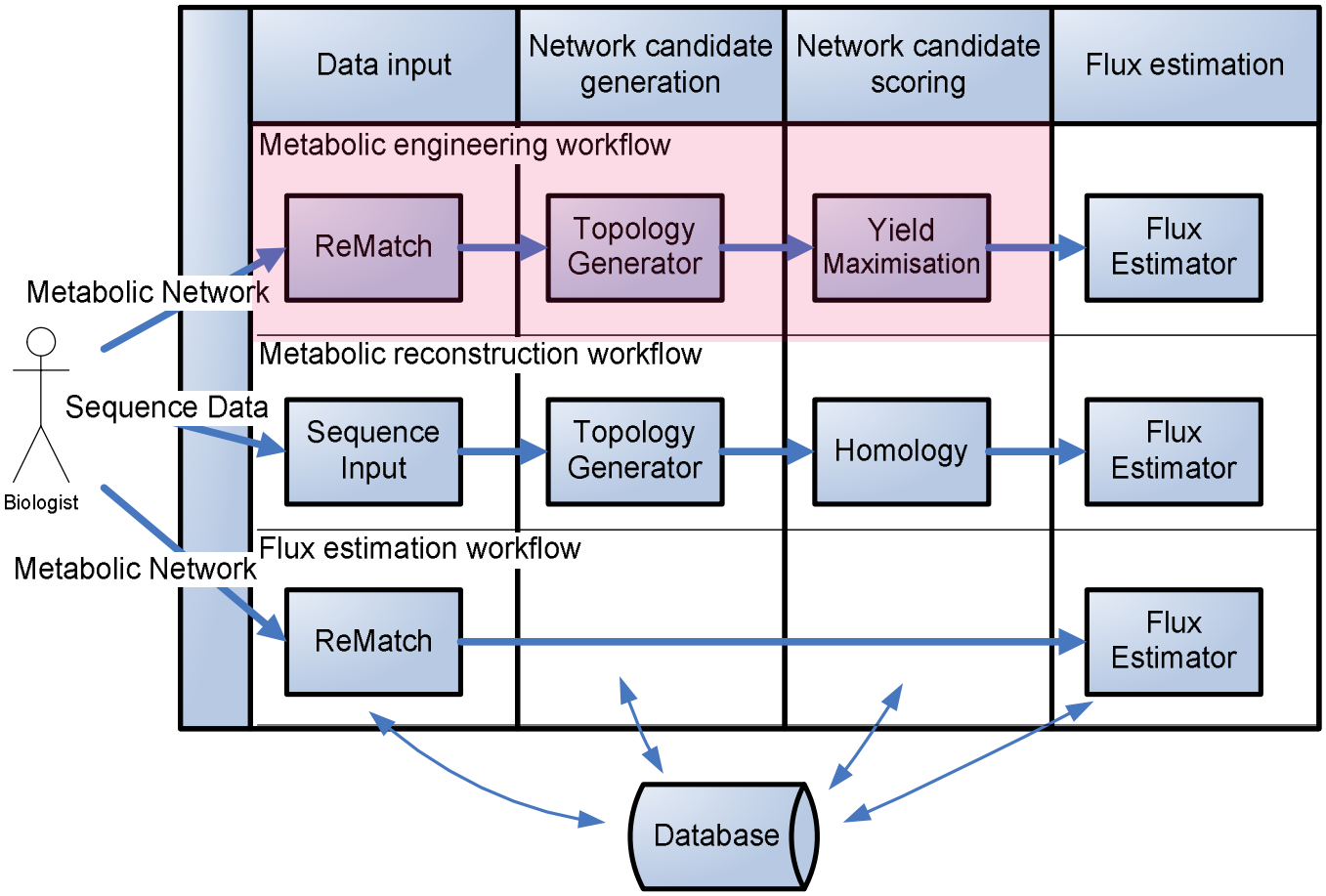
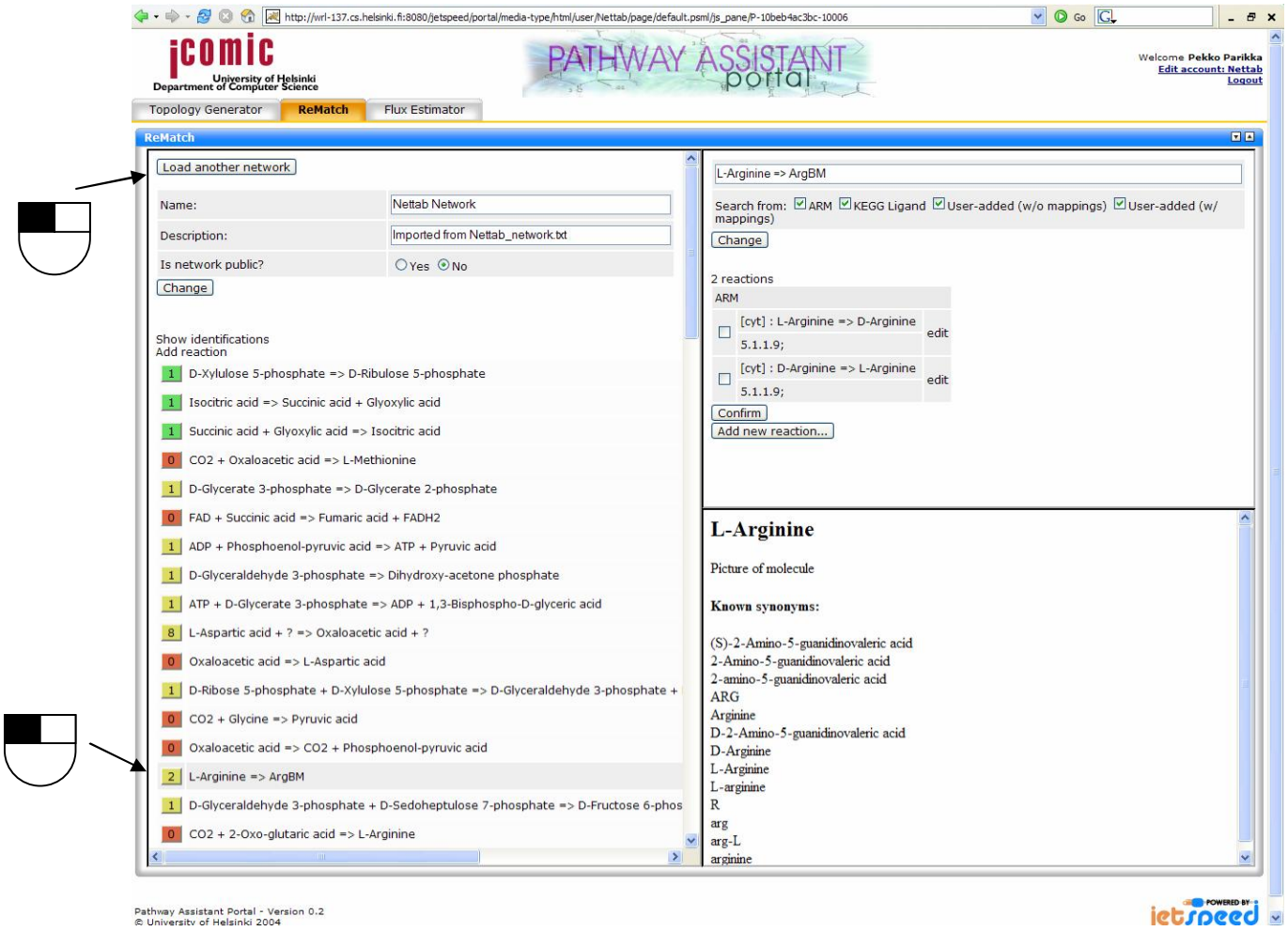
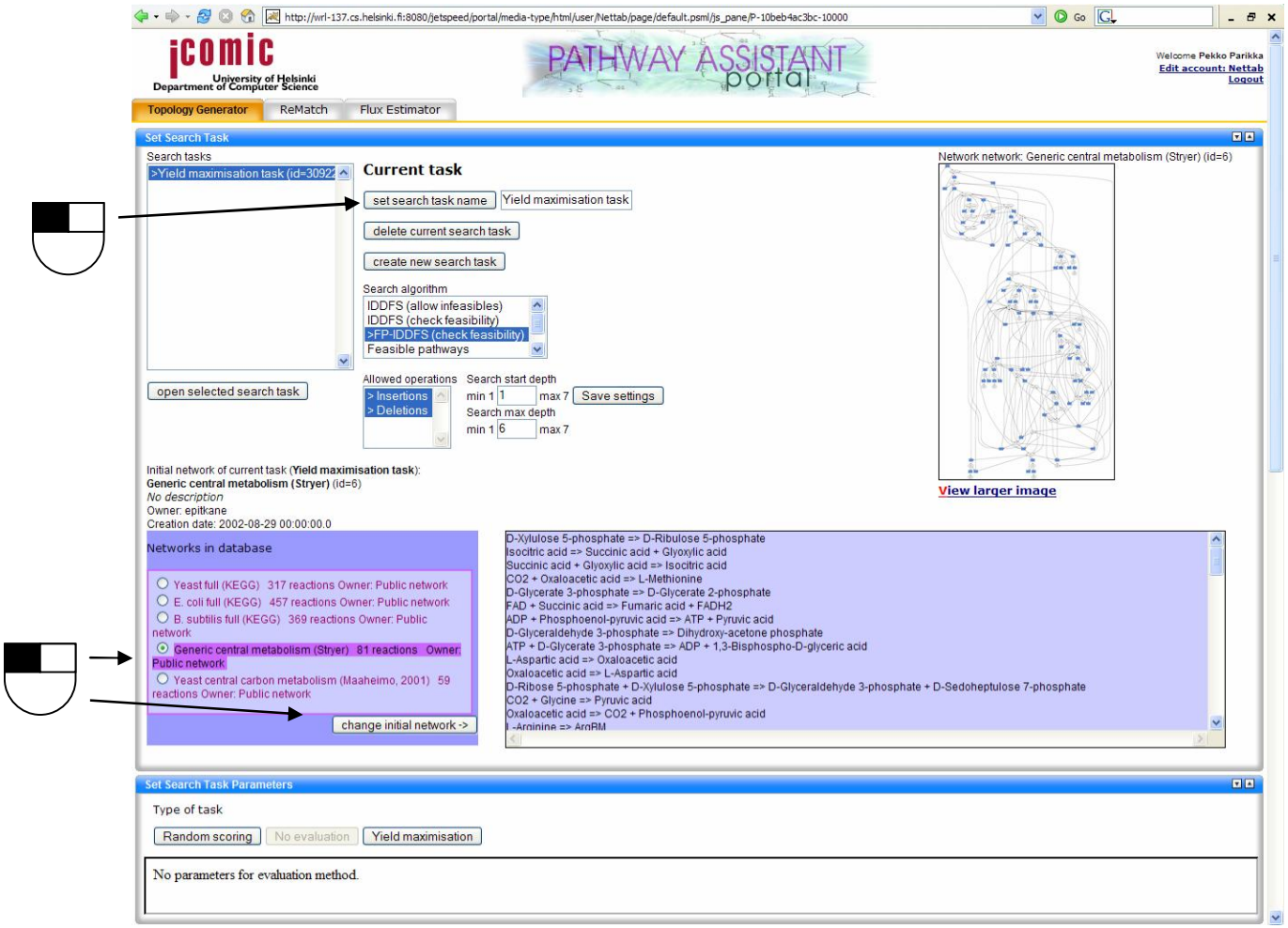
Pathway Assistant tools and supported workflows



Metabolic Engineering
Phase 1 importing network with ReMatch



Phase 2 Open the network in Topology Generator



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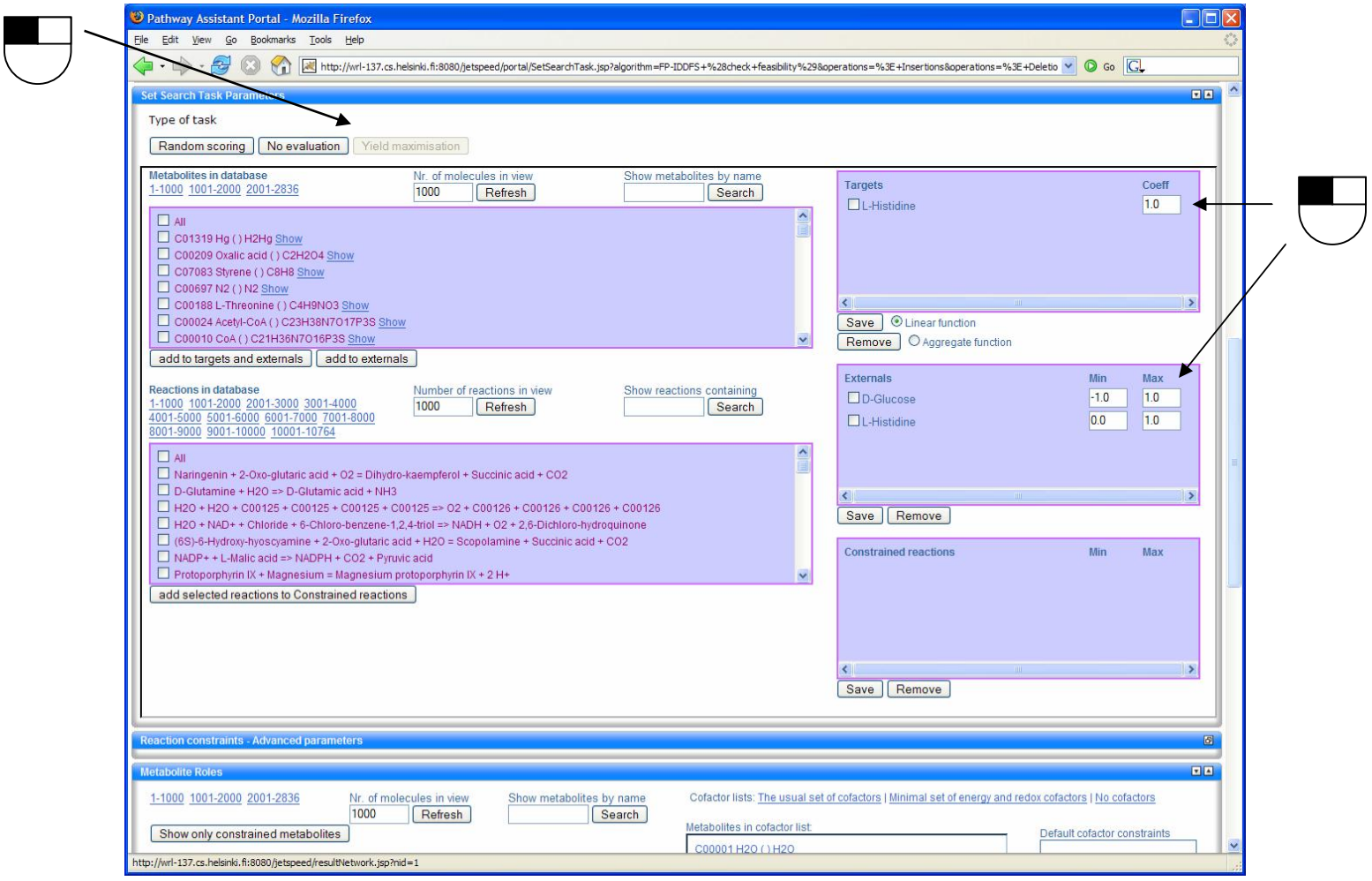
Phase 3 set up basic parameters for Yield maximisation



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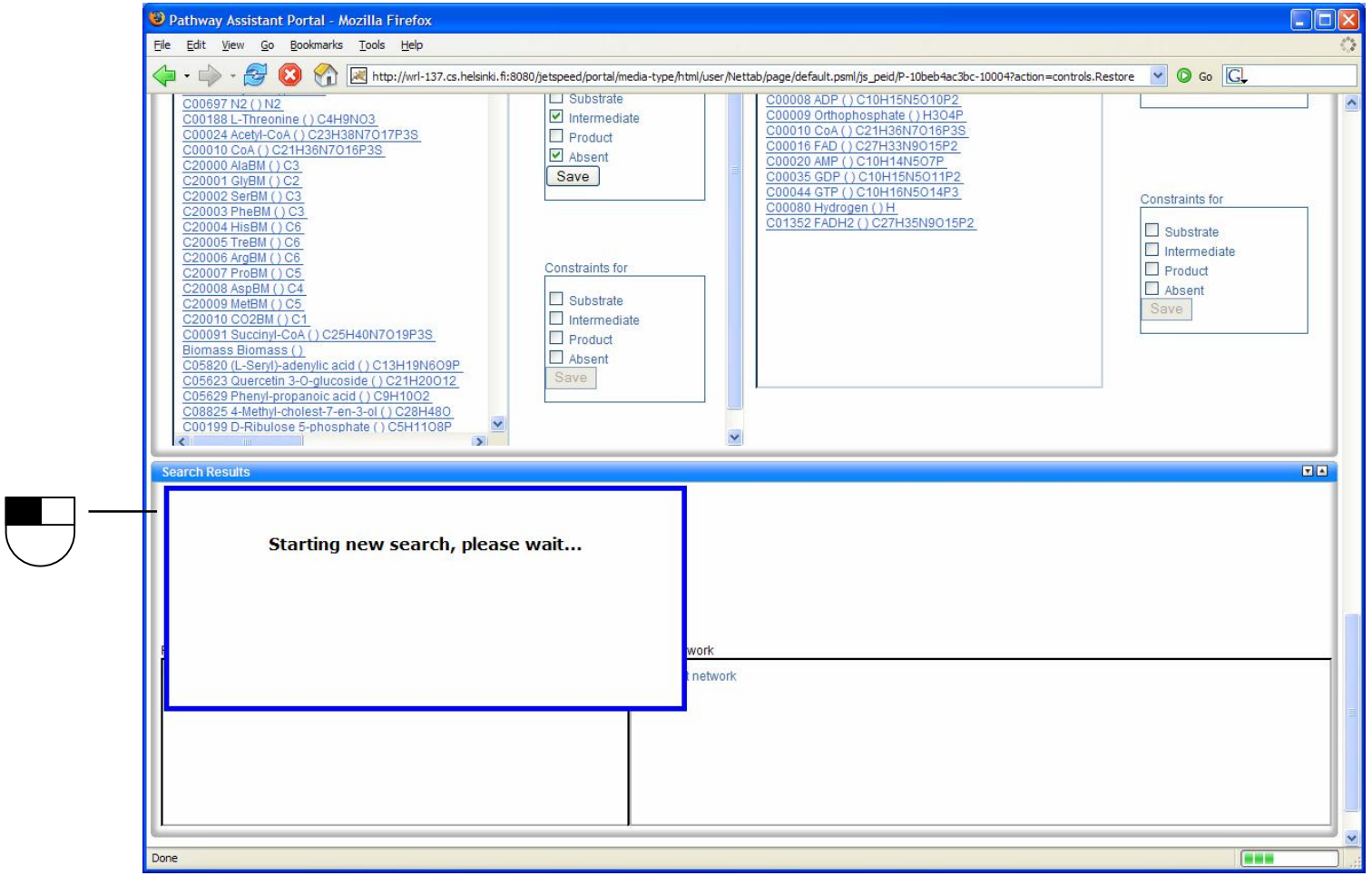
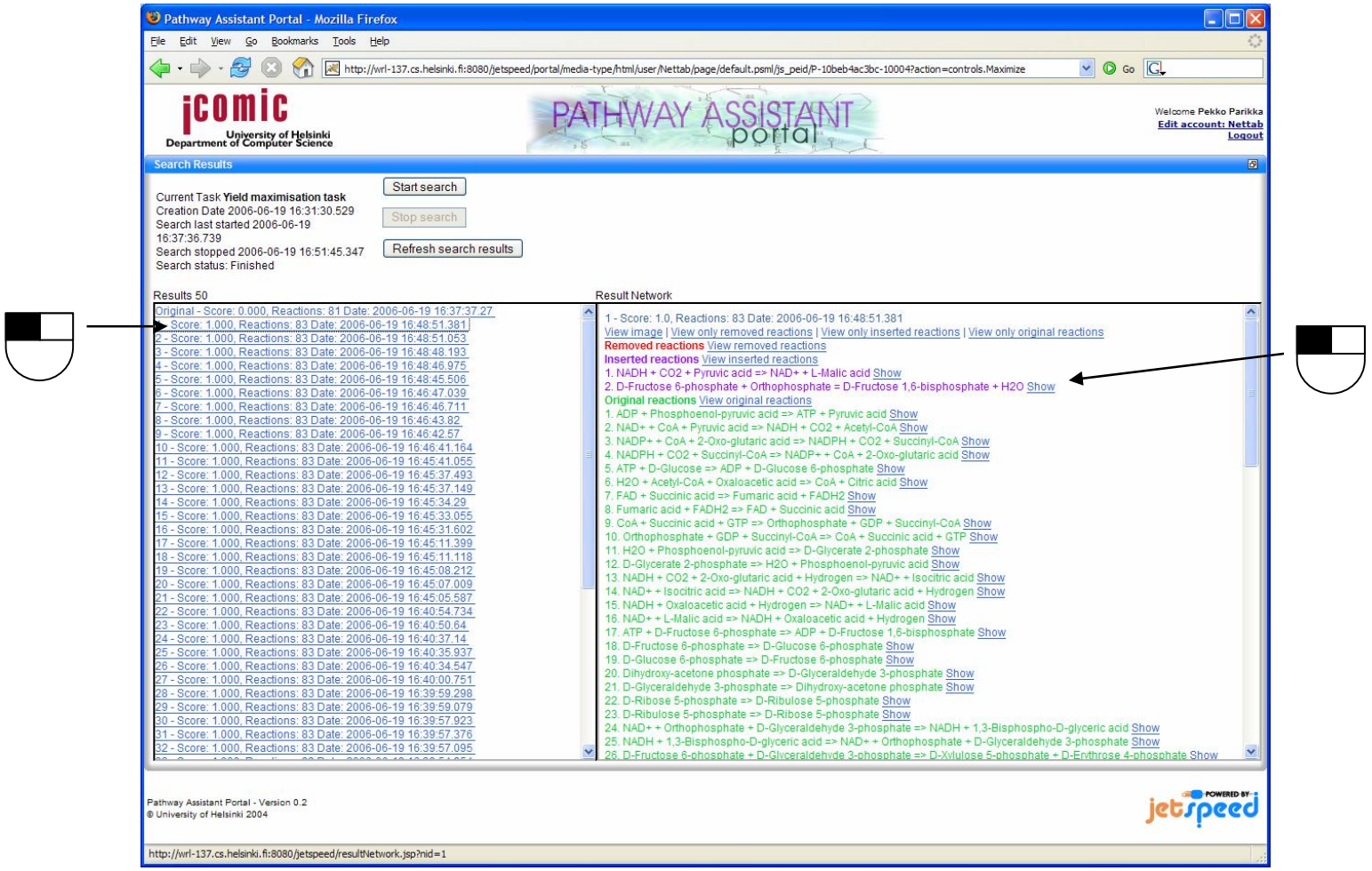
Phase 4 start the search of alternative metabolic networks



Phase 5 browse alternative networks



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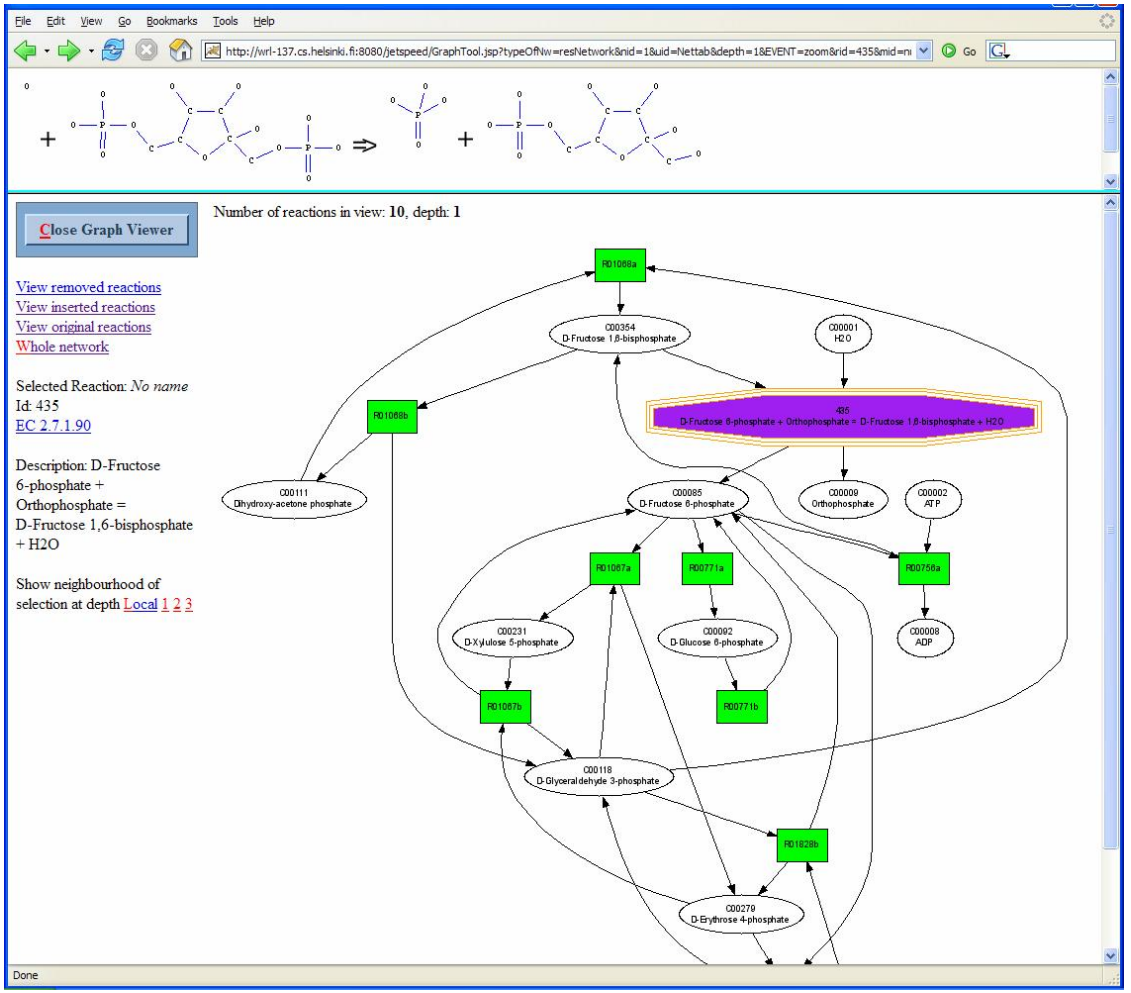
Last phase: visualization of modifications in a candidate network



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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/