

## 89. Constraint-based reconstruction and analysis toolbox extensions for parallel network reconstruction and CellDesigner interoperability

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**Project Goals:** This project aims at developing software packages for easy metabolic network reconstruction, annotation and visualization and extending the functionality of the established constraint-based modeling software for analysis and bioengineering of cellular metabolisms at systems level.

In the past decade, constraint-based modelling, as implemented in the COBRA toolbox [1], has emerged as an important tool to study the mechanisms behind biological phenotypes and understand physiological and perturbed metabolic states at genome-scale for organisms. However, application of this novel approach to systems biology for different use scenarios is still hindered by the functionality of the current version of the COBRA toolbox. For instances, constraint-based modelling desires a high-quality reconstruction that can demand extensive manual efforts of contributors with different background knowledge, but the existing reconstruction software does not allow synergizing people's efforts in real time towards a reconstruction. In addition, CellDesigner (CD) is a diagram editor commonly utilized to render the network layout and annotate metabolite and reactions, but there are no COBRA functions available to parse and edit the network files created by CD.

To extend the scope of the established COBRA methods for reconstruction, visualization and annotation of a metabolic network, we have developed two COBRA extensions. The first extension is a collaborative metabolic reconstruction platform, rBioNetServer, stemming from a previously published network reconstruction package rBioNet [2]. Different from the ordinary rBioNet, rBioNetServer adopts a client/server model in which the client program communicates with a remote database server, where stores and manages different versions of reconstructions. Based on this architecture, rBioNetServer enables different people to work on the same metabolic reconstruction simultaneously, to inert reaction, metabolites and relevant annotations, and perform quality control procedures according to the established protocol [3]. The second extension is an interface package that can parse an XML file created by CD, change the thickness of reaction links and colours of nodes in the XML file according to the flux values obtained from constraint-based modelling. There are also auxiliary functions not only to compare a network model stored in the CD XML file and a COBRA model in the Matlab file and correct the discrepancies between them, but also integrate different types of omics data into the XML file in line with the Miriam standard. In the future, we envisage that these extensions can facilitate a community-driven effort to ensure a high quality reconstruction of the cellular metabolism for an organism and serve as a bridge between constraint-based modelling and the popular process diagram editor, CellDesigner, for visualisation and annotation of metabolic networks.

### References

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