Tools-4-Metatool. Online suite of web-tools to process stoichiometric network analysis data from METATOOL

Federico Morán, Francisco Montero, Sara Vázquez, Daniela Xavier, Alessio Gamba, Paola Bettinelli.

Department of Biochemistry and Molecular Biology I. Universidad Complutense de Madrid. 28040 Madrid.

METATOOL [1] [2] is widely used for stoichiometric analysis (SNA) of metabolic networks. The output of Metatool provides information on the stoichiometric matrix, the convex basis, elementary modes, and enzyme subsets. For systems with large number of reactions, this output is hard to process and visualize, specially for users who have no experience with this software. We have developed suite of web-tools called Tools-4-Metatool (t4m) (http://solea.quim.ucm.es/t4m/) as an online platform that analyses, parses, and manipulates files related with Metatool. It has two major options: Analysis and Compare. Analysis facilitates the visualization of the results of the SNA. This option has five tools: (i) MDigraph that draws bipartite directed graphs of Metatool's metabolic network, its subsets and the subsets' pathways; (ii) MetaMatrixTXT visualizes the convex basis and elementary modes of Metatool's output in function of subsets, in vectorial or matrix format; (iii) CBGraphs draws bipartite directed graphs of Metatool's convex basis and its pathways; (iv) EMGraph draws bipartite directed graphs of Metatool's elementary modes and its pathways; and (v) SortEModes orders Metatool's elementery modes that contain a given metabolite (or a list of metabolites) in a certain side of its reaction. Compare was developed to compare different Metatool's results from two species, using subsets or elementary modes comparison. It is composed by: (i) Compara tool compares distincts Metatool's outputs and shows the identical subsets, (ii) ComparaSub compares different Metatool's outputs and shows the first output in function of the subsets of the second, and (iii) ComparaEM compares distincts Metatool's outputs and shows the identical elementary modes.

The suite t4m also include scripts that generate Metatool's input based on COBRA [3] SBML files, Cobra2Metatool, or based on a Metatool's output file that is filtered by a list of convex basis' enzymes, CBasis2Metatool.

All these tools have been tested with several metabolic networks. In this contribution we will present some examples to illustrate the use and t4m possibilities.

[1] T. Pfeiffer, I. Sanchez-Valdenebro, J. C. Nuno, F. Montero and S. Schuster: METATOOL: For Studying Metabolic Networks, Bioinformatics 15 (1999) 251-257.

[2] A. von Kamp and S. Schuster: Metatool 5.0: fast and flexible elementary modes analysis. Bioinformatics 22 (15), 2006, 1930-1931.

[3] Becker SA, Feist AM, Mo ML, Hannum G, Palsson BO, et al. (2007) Quantitative prediction of cellular metabolism with constraint-based models: the COBRA Toolbox. Nat Protoc 2: 727–738.

Contact author: Federico MORÁN
Department of Biochemistry and Molecular Biology I
Universidad Complutense de Madrid. 28040 Madrid
e-mail: fmoran@bio.ucm.es