

Tutorial: The COBRA Toolbox for visualisation and map manipulation through CellDesigner and MatLab environment

Jennifer Modamio¹, Nicolas Sompairac², Andrei Zinovyev², Inna Kuperstein² and Ronan Fleming¹

Luxembourg Centre for Systems Biomedicine, Luxembourg, Luxembourg¹, Institut Curie, 26 rue d'Ulm, F-75005 Paris, France, PSL Research University, F-75005 Paris, France, Inserm, U900, F-75005, Paris France, Mines Paris Tech, F-77305 cedex Fontainebleau, France²

Visualisation of data on top of biochemical pathways is an important tool for interpreting constrained-based modelling results. Biochemical network maps permit the visual integration of model predictions with the underlying biochemical context. Patterns that are very difficult to appreciate in a simple vector can be better appreciated by studying a generic map contextualised with model predictions. No currently available software satisfies all the requirements that might be desired for visualisation of predictions from genome-scale models. Here we present a tool for the visualisation of computational predictions from The Constraint-based Reconstruction and Analysis Toolbox (COBRA Toolbox) to available metabolic maps developed in Cell Designer (CD). Furthermore, online visualization is also possible in ReconMap3.0, a virtual visualisation of human metabolism derived from Recon3D. In this tutorial, basic map manipulations and data visualisation in the context of a metabolic network will be explained. Furthermore, visualisation of some common COBRA methods such as Flux Balance Analysis (FBA) and Flux Variability Analysis (FVA) would be also approached.

The COBRA Toolbox is a MATLAB software suite for quantitative prediction of cellular and multicellular biochemical networks with constraint-based modelling. The COBRA Toolbox can be freely downloaded from (<https://opencobra.github.io/>). MATLAB environment would be therefore required; a trial can be freely downloaded from (<https://nl.mathworks.com/downloads/>). If you are already familiarized with MATLAB and you want to test some analyses like FBA on your own, you will need a mathematical solver such as the GUROBI Optimizer solver (<http://www.gurobi.com>). However, during this workshop, we will provide you with some examples. For map visualisation, the diagram editor for drawing gene-regulatory and biochemical networks Cell Designer would be required, which is also freely available at (<http://www.celldesigner.org>). The latest version of ReconMap3 and Recon3.0 model can be found and downloaded from (VMH.uni.lu). At last, online visualisation trough the VMH website would be also approached.

After this tutorial, you would be able to understand the structure of a constraint-based model, the structure of a CD metabolic map parsed to MATLAB environment, and more important the crosslink between both structures. Furthermore, you will be able to automatically manipulate CD metabolic maps through MATLAB environment and visualise the output of some COBRA methods in Cell Designer. As for last, you will also visualise these outputs in an online version of the map through VMH website.