

# MatLab Code User Guide:

## In silico modelling of liver metabolism in a human disease reveals a key enzyme for histidine and histamine homeostasis

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## 1 Introduction

In this document, we briefly describe how to use the MatLab code that we implemented in order to simulate the effects of primary hyperoxaluria type 1 on liver metabolism. By using it, we obtained the results reported in **Table S3** of our manuscript, in particular the complete lists of ranked metabolites and reactions. From this list of metabolites, it is possible to obtain the result of **Table 1**.

## 2 Using the code

The main file is *creatingRankedLists.m*, that allows the user to obtain the results reported in **Table S3** of our manuscript, in particular the complete lists of ranked metabolites and reactions.

```
[MeanFluxesWT, MeanFluxesPH1] = creatingRankedLists(CreatingModel, OutString)
```

The inputs and outputs are described in the following.

- Input:
  - CreatingModel = string that allows to create objective functions or to upload the existent models. If CreatingModel = 'Y' then the function creates the 442 metabolic objective functions starting from the extended version of HepatoNet1 (see manuscript for details about the extension of Hepatonet1), otherwise the function uploads existent models;
  - OutString = string for final txt output.

Example: if OutString = 'PH1' then the output will be *ReactionsRank\_PH1.txt* and *MetabolitesRank\_PH1.txt*.

- Output =
  - Two vectors containing mean fluxes in wild-type and loss of function simulations plus the textual files storing the ranked lists.

### 3 Equipment

- The COBRA Toolbox (<http://systemsbiology.ucsd.edu/Home>);
- Version 7.0 or above of MatLab (MathWorks Inc., <http://www.mathworks.com>);
- A linear programming solver. Currently the COBRA Toolbox supports:
  - Gurobi (Gurobi Optimization, <http://www.gurobi.com>) through Gurobi Mex ([http://www.convexoptimization.com/wikimization/index.php/Gurobi\\_mex](http://www.convexoptimization.com/wikimization/index.php/Gurobi_mex));
  - CPLEX (ILOG Inc.) through Tomlab (Tomlab Optimization Inc., <http://tomopt.com>);
  - GLPK (<http://www.gnu.org/software/glpk>) through glpk mex (<http://glpkmex.sourceforge.net>).

In our simulation we used the GLPK through glpk mex.

#### 3.1 Example

In the following, it is possible to find how we set the paths for the COBRA toolbox and GLPK in order to run the code on a MacBook Pro (OS X Yosemite, Processor 2.5 GHz Intel Core i5, Memory 4 GB 1600 MHz DDR3):

- `addpath(genpath('/Applications/MATLAB_R2012a.app/toolbox/glpkmex'));`
- `addpath(genpath('/Applications/MATLAB_R2012a.app/toolbox/cobra'));`
- `changeCobraSolver('glpk','LP');`