**STEP 1. Code Installation**

1. Install MATLAB (any version should work) and Python 3.
2. Install the following Python libraries:

collections, glob, hashlib, json, numpy, os, pandas, pickle, pybel, re, scipy, seaborn, sklearn, SOAPpy, string, time, urllib2, xlrd

* + Not every library is needed for each step. The top of each Jupyter notebook lists the required libraries for each step.
  + The pybel library is not the one installed from “pip install pybel”. Installation instructions can be found here: https://openbabel.org/docs/dev/UseTheLibrary/PythonInstall.html

1. Install Jupyter software and the IPython kernel (https://jupyter.readthedocs.io/en/latest/install.html). Ensure that Python 3 notebooks can be run.
2. Install the MATLAB Engine API for Python (https://www.mathworks.com/help/matlab/matlab\_external/install-the-matlab-engine-for-python.html).
3. Install the MATLAB kernel for Jupyter (https://github.com/Calysto/matlab\_kernel). Ensure that MATLAB notebooks can be run.
4. Download everything from the Github folder “FBA-pipeline\Code + Models”. This folder has all the code for generating and running FBA models.
5. Move the “FBA-pipeline\Other\cobratoolbox” folder into the “C:\Program Files\MATLAB\(Version)\toolbox\” folder. This is the COBRA toolbox (https://opencobra.github.io/cobratoolbox/stable/), but slightly modified to correctly use reaction GPR rules.
6. Install Gurobi version 8.01 (https://www.gurobi.com/). Free academic licenses can be obtained.
7. Add “cobratoolbox” and “gurobi” folders to your MATLAB path:
   * “addpath(genpath(“C:\ Program Files\MATLAB\(Version)\toolbox\cobratoolbox”))”
   * “addpath(genpath(“C:\gurobi801”))
   * “savepath”