**S3 Code. MATLAB code to perform gene essentiality predictions.**

**Software information:**

MATLAB R2016b

Gurobi 6.5.2

**Required Toolboxes and Software:**

In order to implement the included code, you will first need to download the following:

* Gurobi Optimizer – Can be downloaded from: <http://www.gurobi.com> after acquiring a license. Licenses are free for academic use.
* Cobra Toolbox – Can be downloaded from: https://github.com/opencobra/cobratoolbox/
* Check that your solver and toolbox are installed correctly with the following commands:
  + initCobraToolbox (this command initializes the toolbox)
  + changeCobraSolver(‘solvername’) (where solver name is ‘gurobi5’ or ‘gurobi6’)
  + testAll (note that not all tests will pass with the gurobi solver)

**Scripts:**

* S3\_Code\_Implementation.m – Main script to generate S4 Data
* changeMinimalMedia.m – Function to set the model to minimal media
* addExchangeReaction\_JB.m – Function to add an exchange reaction

\*\* Functions were not originally written by Dunphy et al. Author contributions are listed within the scripts.

**Data files:**

* model\_PA.mat- This workspace contains the model iPau1129 (Bartell, Blazier et al., 2017). The model can also be downloaded from: <http://bme.virginia.edu/csbl/Downloads1.html>

**Instructions:**

* Open MATLAB and change your path to the S3 Code folder (or folder where you have the above scripts and data files stored).
* Add the Cobra Toolbox folder and subfolders to your path.
* If you are using a Windows machine, add the gurobi folder and subfolders to your path.
* Open S3\_Code\_Implementation.m and run it. This will take some time. The script will output a CSV file named geneEssentialityPredictions.csv, which is identical the file of the same name in S2 Code. The output is an unfiltered version of S4 Data.