**Instructions for using MAGENTA**

**Installation:**

1. Download MAGENTA files and add the folder to the MATLAB path.



1. Download dependencies (to run code as described in the original MAGENTA publication):
   1. Random Forest toolbox for MATLAB (<https://code.google.com/p/randomforest-matlab/downloads/list>)

**Data description:**

* *MAGENTA\_supplementary\_dataset.xlsx* – this file contains the drug interaction training and validation data. Details on each sheet:
  + ‘triplet predictions' – contains the experimental drug interaction validation data for 56 three-way combinations
  + 'media predictions' – contains the experimental drug interaction training data for MAGENTA
  + 'media predictions test' – contains the experimental drug interaction validation data for 55 two-way combinations measured in glycerol media
  + 'acinetobacter' – contains the experimental drug interaction validation data for 15 two-way combinations in three conditions – LB, glucose and glycerol for *A. baumannii*
* *ecoli\_phenotype\_data\_cell.xlsx* – has the chemogenomic data taken from the supplementary information of Nichols et al, 2011.
* *ecoli\_fulldata.xlsx* – has the drug interaction data taken from Chandrasekaran et al, 2016. It contains 171 pairwise combinations of 19 drugs. This data will be used for training MAGENTA.
* *ecoli\_acinetobacter\_orthologs.xlsx* – this file contains the list of orthologs between *E. coli* and *A. baumannii.*
* *identifiers\_match.xlsx* – matches the drug identifiers used in the drug interaction data with the chemogenomic data.

**Code description:**

* *MAGENTA\_tutorial.mlx* – this file reproduces all the results in the manuscript.
  + Also contains a new section on how to use the alternative RF function (MATLAB built-in)
* *process\_chemgen\_v2.m* – takes in the chemogenomic data and identifies significant interactions using the z-score threshold provided as input.
* *MAGENTA\_train.m* – MAGENTA takes in drug interaction scores and chemogenomic data to train the random forest model.
  + Note: default ML method is set to *fitrensemble* (builti-in MATLAB function). To replicate the results reported in the MAGENTA publication, set ML method to *regRF* (see tutorial).
* *MAGENTA\_predict.m* – use the trained model to predict new drug interactions based on chemogenomic data.
  + Note: default ML method is set to *fitrensemble* (builti-in MATLAB function). To replicate the results reported in the MAGENTA publication, set ML method to *regRF* (see tutorial).