**File Directory**

FBA-pipeline\

* Code + Models\ - Everything for generating and running FBA models
  + data\ - Jupyter notebooks and storage of data for FBA models
    - clinical\ - Processing of general information about FBA samples
    - concentration\ - Metabolite concentration ranges that can be used to alter ΔG ranges and reaction directionalities
    - deltag\ - Reaction ΔG ranges from the VMH database
    - idh1\ - Recording FBA samples with IDH1 mutations
    - kcat\ - Kinetic rate pipeline for obtaining turnover numbers from the BRENDA database
    - media\ - Recording metabolites present in cell culture media
    - mutation\ - Processing of FBA sample mutation data and Envision scores
    - protein\ - Protein prediction pipeline for FBA samples
    - recon\ - Editing of Recon3D metabolic reconstruction
    - vmax\ - Calculation of reaction Vmax constraints for FBA samples
  + fba\ - Code for running FBA models
    - input\ - Input folders with desired options for FBA analysis
      * \_create\_drug\_objective\_screen\_\ - code for screening chemotherapy response objective functions
      * \_create\_gene\_knockdown\_screen\_\ - code for performing simulated gene knockdown screens
      * \_create\_objective\_function\_screen\_\ - code for performing metabolome-wide metabolite production screen
    - results\ - FBA outputs
* Instructions\ - Instruction files
* Lewis et al. Datasets\ - Supplemental datasets referenced in Lewis et al.
* Other\
  + cobratoolbox\ - MATALB COBRA toolbox, used for calculation of Vmax values from protein abundances and GPR rules