Synthetic datasets for the 3 case studies**: Simulation\_data.xlsx**

Case study 1**:** threonine synthesis model in *E. coli* [1]

* SBML file of original mechanistic model: **chassagnole1.xml**
* SBML file of hybrid mechanistic/FFNN model: **chassagnole1hyb.xml**

Case study 2**:** P58IPK signal transduction pathway [2]

* SBML file of original mechanistic model: **goodman.xml**
* SBML file of hybrid mechanistic/FFNN model: **goodmanhyb.xml**

Case study 2**:** Yeast glycolytic oscillations [3]

* SBML file of original mechanistic model: **dano1.xml**
* SBML file of hybrid mechanistic/FFNN model: **dano1hyb.xml**