Component Specifications:

extractPKparam: This module will take experimental data from the user saved in a CSV or Excel file and convert it to a Pandas dataframe. It will perform any necessary cleanup of the data prior to analysis, then extract PK parameters of interest.

- LoadData: Load data into dataframe
- PrepData: Remove null values and log transforms data
- findCo: Fits line to log transformed data based on model chosen and extracts drug concentration at time=0 (Co) and slope (elimination constant k)
- findCmax: Scans data to find peak drug concentration (Cmax) and the time that Cmax is reached (Tmax)
- findT_half: Scans data to find half life of drug
- findPK: combines functions findCo(), findCmax(), and findT_half() to generate a single output with all PK parameters of interest

simulatePK: This module will load an Antimony model based on user input on the relevant route of administration and pharmacokinetic model, such as a drug administered as an IV bolus which follows a 1 component model. It will update PK parameters in the model with either experimentally derived values or values chosen by the user. It will then simulate PK curves to help scientists with experimental or clinical dose planning.

- findSubtherapeuticTime: Loads Antimony model from library of models. Updates initial conditions either based on results from extractPKparam module or based on user input. Simulates change in drug concentration over time, then outputs time it takes for drug to reach subtherapeutic concentrations.