Jia Liang

ModelPK

The pharmacokinetic profile of a drug refers to how a drug moves into, through, and out of the body, and is a critical piece of knowledge in calculating drug doses for clinical or translational projects.

The goal of this package is to make it easier for a bench scientist who is not familiar with PK modeling to visualize and extract basic information about the pharmacokinetic profile of a drug from experimental data. This package can enable the development of PK models that would better inform experimental or clinical drug dosing.

User profile:
This package was designed for bench scientists with a background in chemical or bioengineering who want to visualize and extract information about the pharmacokinetic profile of a drug from experimental data.

Users should have experimental data on in vivo drug concentrations over time and will have knowledge on the route of administration and how the drug is distributed or partitioned throughout the body. Users should be familiar with Python and calling Python functions.

Use case 1: Scientist would like to extract PK parameters of interest from experimental data.

1. Users would input Excel or CSV file containing experimental data (drug concentrations over time) and select most relevant model based on prior knowledge of route of administration and drug distribution in the body.
2. System will load data into dataframe, remove any null values, and log transform concentration data.
3. System will extract PK parameters Co, k, Cmax, Tmax, and half life.

Use case 2: Scientist would like to find the time it takes for drug concentrations to reach subtherapeutic levels.

1. User would select most relevant model based on prior knowledge of route of administration and drug distribution in the body.
2. System will generate base model based on selected model and update initial conditions to reflect previously extracted parameters.
3. System will simulate change in drug concentrations, find the time it takes for drug concentrations to reach subtherapeutic levels, and generate a plot of the final simulation.

Use case 3: Scientist would like to understand how changing PK parameters changes the time it takes for drug concentrations to reach subtherapeutic levels.

1. User would select most relevant model based on prior knowledge of route of administration and drug distribution in the body.
2. User would input values of interest for PK parameters (currently only Co and k supported).
3. System will generate base model based on selected model and update initial conditions to reflect chosen values for parameters.
4. System will simulate change in drug concentrations, find the time it takes for drug concentrations to reach subtherapeutic levels, and generate a plot of the final simulation.