A User Friendly Platform to Simulate and Assess Generic Drug Pharmacokinetics

Abigail Strand[1], Kelsey Cribari[1]
Mentors: Brad Reisfeld[2], Sudipto Ghosh[1]
[1]Department of Computer Science, [2]Department of Chemical and Biological Engineering, Colorado State University

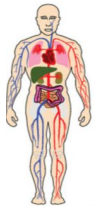
Background

Importance of Generic Drugs

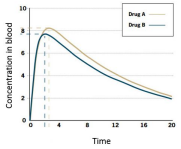
- Represent a large percentage (88%) of all prescriptions dispensed in the US
- Cost much less than name-brand drugs: account for only 28% of total drug spending ((http://www.gphaonline.org/media/wysiwyg/PDF/GPhA_Savings_Report_2015.pdf))

Generic Drug Evaluation

To enter the market, generic drugs must be shown to be ***bioequivalent*** to the corresponding brand-name drugs. Bioequivalence is often evaluated by examining the concentration of the drug in the bloodstream and assuring that the rate and extent of absorption of the drug do not show a significant difference from the rate and extent of absorption of the listed drug when administered at the same molar dose of the therapeutic ingredient.



Pharmacokinetic (PK) simulations are an important component of the assessment of bioequivalence. With appropriate tools, scientists can predict drug PK in individuals and populations and estimate important PK parameters



Objectives

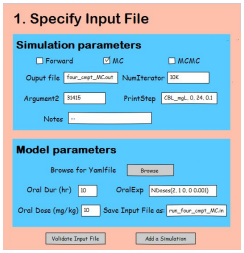
- Design, build, and test a user-friendly, open source computational platform to conduct population-based pharmacokinetic analyses
- Utilize the MCSim simulation package for the computational engine of the platform
- Tailor the interface for the requirements of scientists seeking to perform rigorous bioequivalence studies.

Research Progress to Date

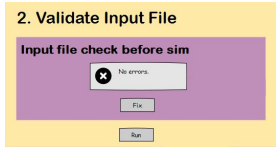
- Modeled user workflow to understand overall goal
- Created prototypes
- Received feedback from researchers on prototypes
- Learned how to use Jupyter Notebook
- Created sample user interface screens using the Jupyter notebook platform
- Modified prototypes
- Started using the QT toolkit to create user interface samples

Workflow for population PBPK modeling

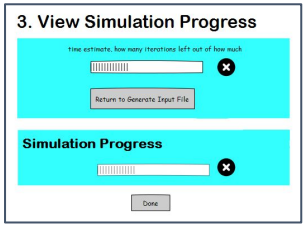
Stage 1: Creating/Modifying Input File



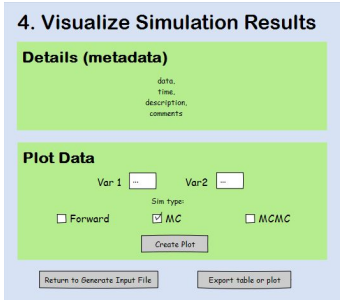
Stage 2: Validating Input File



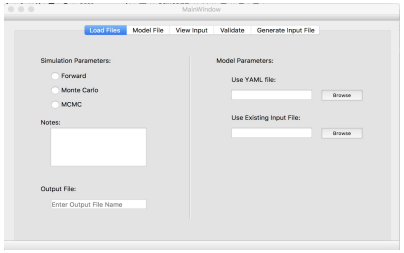
Stage 3: Running Simulation

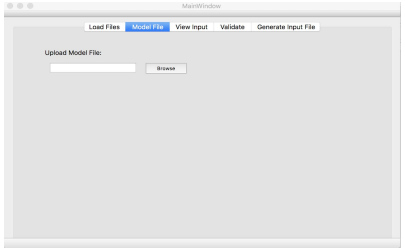


Stage 4: Displaying Results

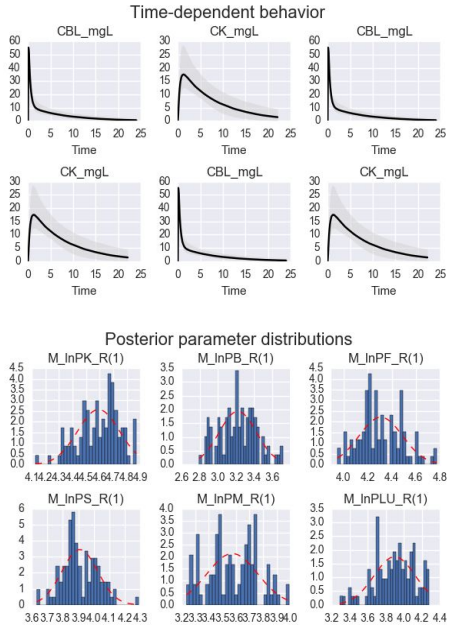


Results: An Initial Graphical User Interface Prototype





Results: Output of the MCSim Simulation Post-processing Code



Future Work

- Complete user interface prototype
- Receive feedback from simulation users
- Modify prototype
- Create walk-through demo to present to FDA

Research reported in this poster was supported by the Center for Drug Evaluation and Research of the U.S. Food and Drug Administration under award number 1U01FD005838-01.

This presentation reflects the views of the authors and should not be construed to represent FDA's views or policies.