

Instructions for Matlab program running.

MATLAB version 7.1 service pack 3 was used to run the program. Later version of MATLAB should also be fine.

Three files are included: Calculator.m and PlotChemSpace.m are MATLAB file, drug.dat is text file. Calculator.m and drug.dat should be put in the same folder since Calculator.m needs to read data from drug.dat for calculation.

drug.dat is to store drug information. Drugs' name and properties can be changed but the format of this file should be unchanged.

Calculator.m is to calculate intracellular concentration and permeability.

PlotChemSpace.m is to generate the plot of permeant-nontoxic physicochemical properties space.

To calculate drug permeability, open Calculator.m through MATLAB and the shortcut key is 'F5'. Or go to the menu 'Debug', pull down the menu and click 'run'. If the drugs number is less than thousands it should take less than one minute for the program to give results. A new file named 'Peff\_all.dat' will be generated in the same folder, which is a text file and includes the calculated intracellular concentration and permeability.

To generate the plot of permeant-nontoxic physicochemical properties space, open PlotChemSpace.m through MATLAB and click 'F5' to run it. It would take a while for this program to give results (It took about three to four hours on a PC with 1.8GHz CPU and 2GB RAM).