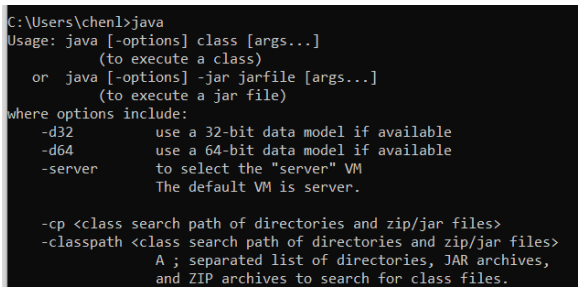
User manual of the GUI version of PCprophet

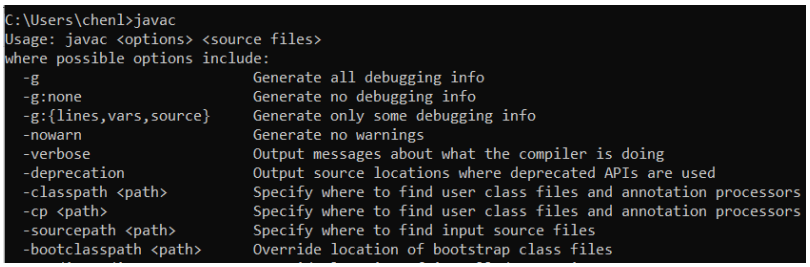
1. Monitor resolution

   If you are running the GUI version of PCprophet using Apple products, such as laptop or PC, there is no requirement for the resolution as the resolution of GUI has been optimised. However, if you are using Windows system, the GUI version works best with the resolution of 1920*1080.

2. Installing PCprophet and Java

   In order to run the GUI version of PCprophet, the command line version must be successfully installed. Please follow the instructions for installing the command line version of PCprophet and required dependencies on our GitHub repository (https://github.com/anfoss/PCprophet). Besides, Java (version >= 1.8) needs to be installed and the Java paths need to be appropriately configured. To test if Java has been successfully installed, please try 'java', 'javac' to see if the help document can display in the console, as demonstrated in the following figures:



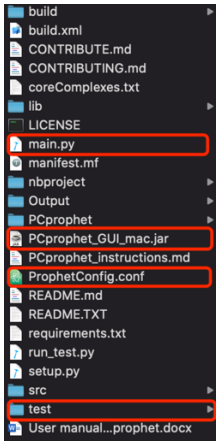


3. Updating the PCprophet folder

   As the GUI version is dependent on the original command line version of PCprophet, it is therefore crucial to keep the "**PCprophet**" folder (see the figure below) up to date. To do so, before running the GUI version, please copy and paste the most up to date PCprophet source code folder to the GUI folder. Note that this folder doesn't exist in the initial GUI folder, please copy the "**PCprophet**" folder to the GUI folder before running.

4. Folder structure

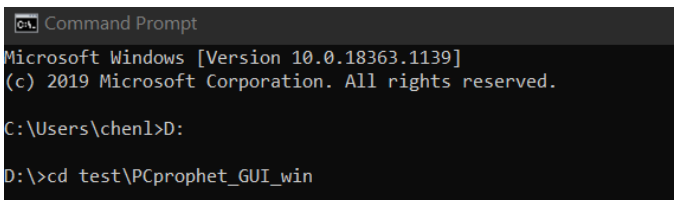
   In general, after unzipping the file, the structure of PCprophet GUI folder will be shown as the following:



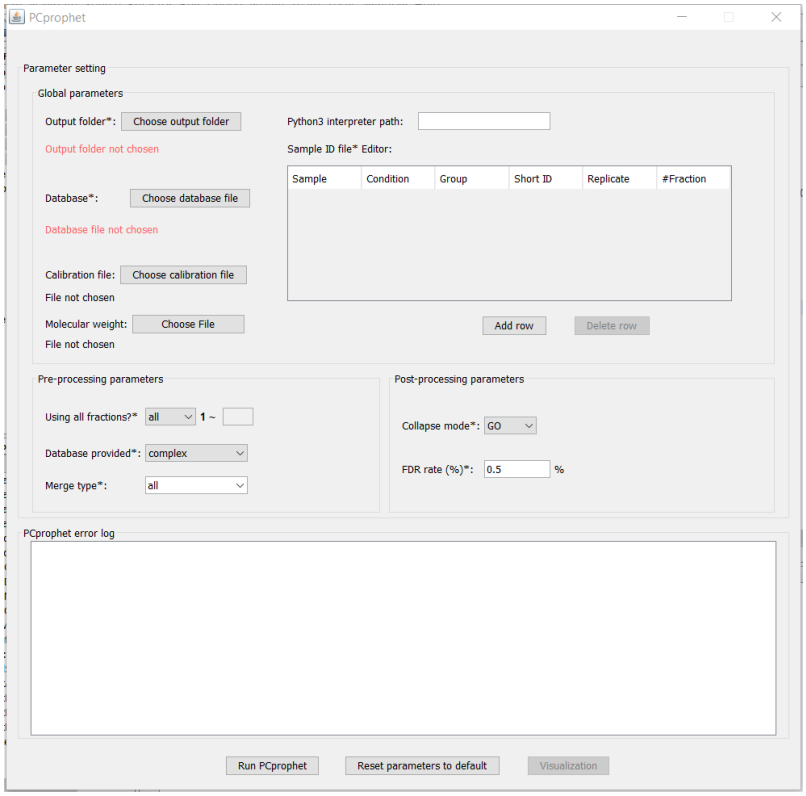
In this folder, there are four important files/folders, including (i) PCpropehet_GUI_win.jar, which is the main executable file of the GUI version of PCprophet; (ii) main.py, which is the main program of PCprophet; (iii) ProphetConfig.conf, which contains all parameter settings for PCprophet; and (iv) the test folder, which is for input files and sample description file. As PCprophet is able to deal with co-elution profiles of different replicates and conditions, we need users to provide a descriptive file for these replicates and conditions, the details of which will be described in the following section. In addition, there is no need to manually change the ProphetConfig.conf file. Once the parameters are configured via the GUI version of PCprophet, the parameters will be written and updated to the ProphetConfig.conf file by the main.py, for your future reference. Note that during the prediction by PCprophet, a temporary folder (termed 'tmp') will be generated to store the intermediate files during the prediction and analysis. It is suggested that before running PCprophet, this folder should be deleted.

5. Running the GUI version of PCprophet using provided example

To run the GUI version of PCprophet, please use the console of your operating system and locate to the PCprophet folder. For example, in Windows, when the console (i.e. the Command Prompt) has started, type the 'cd' command to relocate to the PCprophet folder. In this example, the folder is in "D:\test\PCprophet_GUI_win":

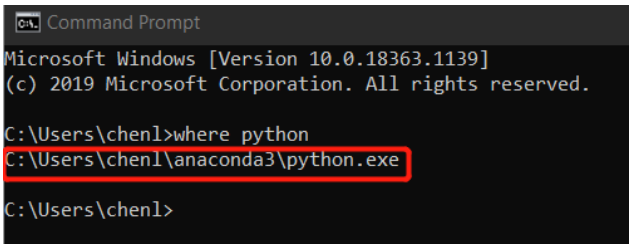


Then type "java -jar PCprophet_GUI_win.jar" to initiate the GUI version of PCprophet. The main interface should display as shown in the following figure:



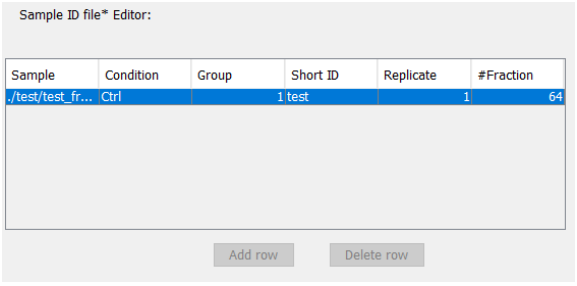
All the mandatory parameters are marked with a '*' and must be provided. As can been from the figure, some of the parameters have been provided using their default values. Please refer to our GitHub repository for the detailed explanation of these parameters.

Due to the fact that the macOS system also has built-in Python (version 2.x), PCprophet may have problem using the right version of Python (i.e. version >3.0). Therefore, we would like users to provide the location of the Python 3 interpreter. This path can be easily obtained by the console of Windows and macOS. For example, in Windows, simply type 'where python3', the path of the Python 3 interpreter will be shown as follows:



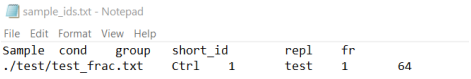
Users can just copy the content in the red rectangle and paste into the text box of 'Python 3 interpreter path'.

The 'Sample file ID editor' is designed for users to provide the basic information of their experiment. A file named 'sample_ids.txt' will be generated based on the input to this editor and the file will be saved to the test folder, where all the co-elution files of the experiment should be stored as well. The following figure demonstrate the information we have put for the example test file (i.e. test_frac.txt) we provided in the 'test' folder:

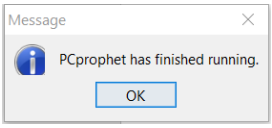


There are six columns of information to provide by clicking the 'Add row' button in the 'Sample' column, the co-elution file of current condition and replicate should be provided using the relative file path: "./test/test_frac.txt". Notice that the "test" folder is the one for storing the replicate and condition information. Please make sure that the file name is correct otherwise PCprophet will have problems recognising and locating the file. All the co-elution files should be described using this editor. After you click the 'Run PCprophet' button, you will be able to see a 'sample_ids.txt' file has been generated in the 'test' folder:

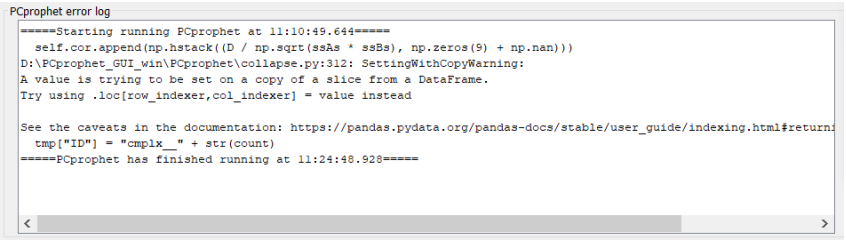
And the 'sample_ids.txt' file should content the following information:



After the 'Run PCprophet' button has been clicked, the prediction process will be initiated. When the process is over (either successfully finished or interrupted by errors), a dialog box will show as follows:



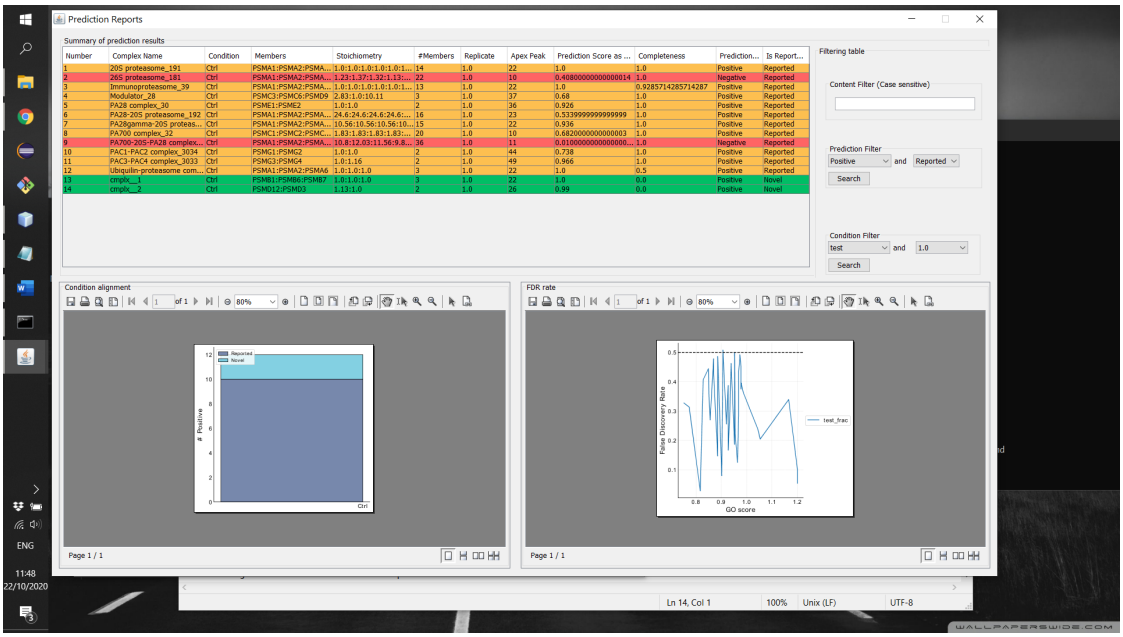
The 'PCprophet error log' was designed to pass the error message to the users to indicate anything that goes wrong during the prediction. However, the warning messages, which do not affect the prediction and analysis processes, are also shown here:



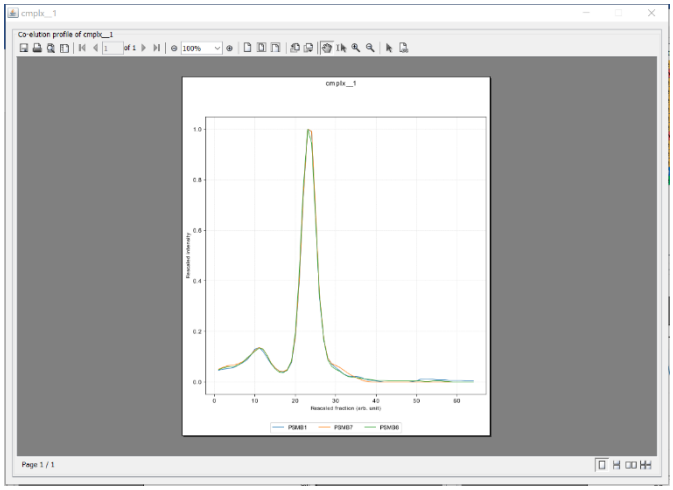
We recommend users not to close the program when PCprophet is still running at the backstage. This is due the mechanism of Java invoking other non-Java programs (Python program in our case). If

you would like to kill the running PCprophet, simply go to the Task Manager (for Windows) or Activity Monitor (for macOS). Based on the security consideration, the current GUI version of PCprophet does not provide the option for parallel processing, which will be offered in our future versions once the security issue is tackled.

After PCprophet has successfully finished the prediction, users can click the 'Visualization' button to review the prediction results:



Users can further filter the prediction results using the options provided in the top-right panel. If users would like to come back to all the results after filtering, simply go to the text input area of 'Content Filter' and hit the 'backspace' key on the keyboard. Users can also click any row in the table to closely examine the co-elution profile of selected complex. For example, if the 'cmplx_1' (i.e. #13) is clicked, users will be able to see the following dialog box for its co-elution profiles:



6. <u>Contact</u>

For questions, bug reports and suggestions, please feel free to contact Dr Andrea Fossati (Andrea.Fossati@ucsf.edu) and Dr Chen Li (Chen.Li@monash.edu).