LiP-MS Data Processing Program

General Notes:

- All input files must be in .csv format
- If you have never used a terminal before, see instructions on last page

Using the program:

1. Open up a terminal, navigate to the folder where the program is housed, and type:
   `python LiP-MS_v3pt1.py`
2. The first step will prompt you to input your working directory. This is the path to a folder where you would like all results exported to.
3. Input path to proteingroup.csv and peptidegroup.csv files
   **Example files are packaged with the distribution for reference*
4. A message will appear that will let you know that the first stage of processing is complete
5. Open these files from your working directory
6. Add a column entitled "p value"
7. In the first row of that column, add this formula:

   `=TTEST(A2:E2,F2:J2,2,2)`

8. Double click the bottom right corner of the box to apply that formula to all the cells in that column
9. Click "find and replace". Select to search for "#DIV/0!" and leave the replace field empty. Click replace all.
10. Save, ensuring file is still saved as .csv
    **An example file is packaged with the distribution as "MCIvCtrl_nofilter_updated.csv" for reference*
11. In terminal, again navigate to folder housing the program, and type:

    `python LiP-MS_v3pt2.py`

12. Follow onscreen prompts as before
13. All output data will appear in the working directory specified

Troubleshooting:

Converting to .csv format:

The easiest way to accomplish this is to open the file of interest in Excel. From there go to:

File > Save As > CSV (Comma delimited) (*.csv)

Please note, .csv files can only be one sheet. If you have multiple sheets in your Excel file, all but the first sheet will be lost when converting file types.

Getting file path:

(Windows) In File Explorer, highlight the file or folder of interest. In the top “home” toolbar, click copy path. The path is now copied to the clipboard.

Note: when adding path to terminal prompt, make sure no quotations around path

Error message:

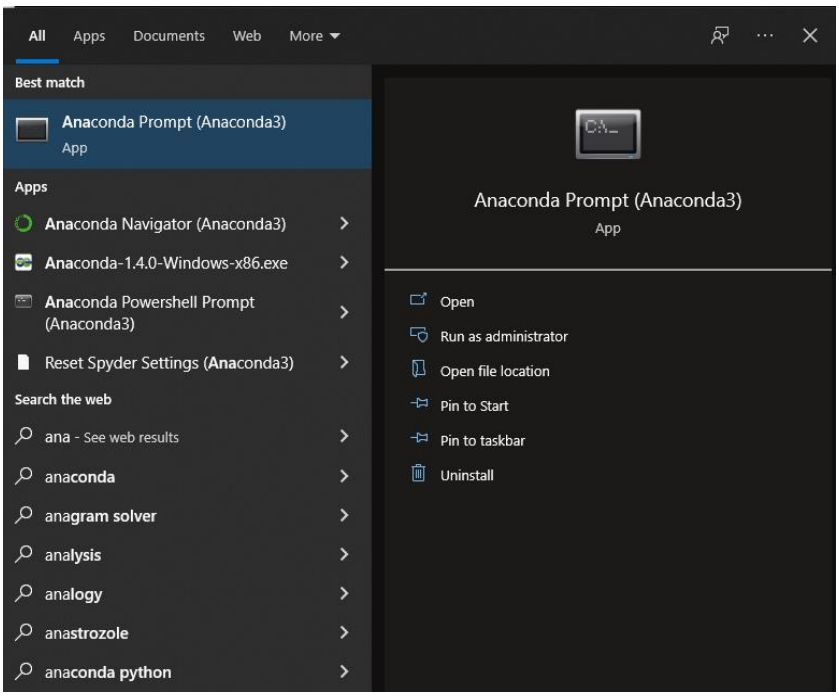
An error message will occur if the files you are trying to access are open. Close all necessary files prior to running.

You will also likely get an error message if you do not follow the template formatting. Please see all sample data in the supplied folder so the templates match.

Running a program through the terminal:

My favorite way to run a homebuilt program is through Anaconda. Anaconda provides a terminal and houses all necessary python packages. Anaconda also is cross platform, and commands are generally universal across operating systems.

1. Install anaconda: https://www.anaconda.com/products/individual
2. From the search bar, search for the anaconda prompt:



3. Open the anaconda prompt:

4. Navigate to the folder where the program is stored. For example, if the path to my folder is `C:\Users\lawashburn\documents\LiP-MS:`

   I see that I am already in the folder `C:\Users\lawashburn` (this is what is written on the screen when you first open anaconda)

   I can change the directory to documents by typing:

   `cd documents`

   Press enter

   And then I can change the directory again to the LiP-MS folder by typing:

   `cd LiP-MS`

   It should look like this:

5. From here we can jump into step 1 of the first set of instructions by typing: `python LiP-MS_v3pt1.py`

General anaconda/command prompt notes:

- To rerun the last command, simple press the up button and the last command will appear, and press enter to run