BLANKA v1 Quick Guide

New Features

- GUI for better usability
- Input/output to/from .mzXML format and new data structure to accommodate
- Removal of .mgf output (temporary)
- Consensus spectrum for MALDI DD control spots generated before being compared/removed form sample spots
- Consensus spectrum generated LC-MS/MS spectra with matching/very similar retention times/precursor m/z values
- New intensity threshold option: spectrum is not included in final output file if blank removal has occurred and $\frac{\text{total ion current (blank removed spectrum)}}{\text{total ion current (raw spectrum)}} <=$ threshold value (threshold value <= 1)

Check if Python is Set to PATH (Windows)
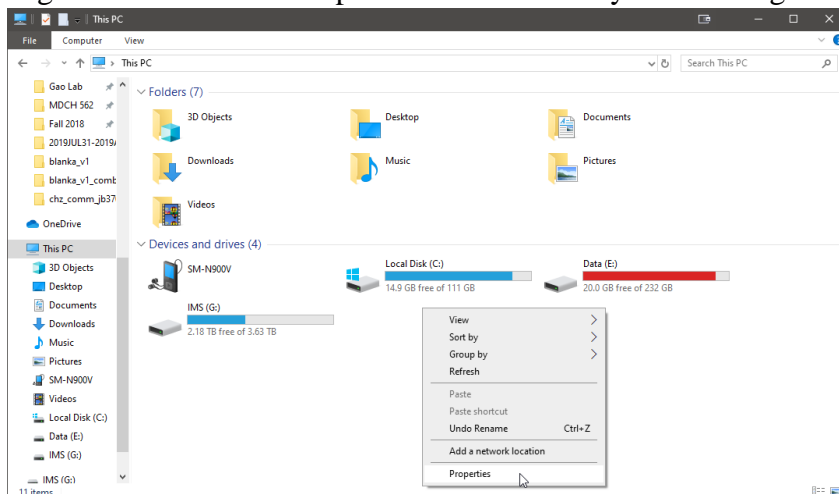
1. Open Command Prompt.

2. Type "python" and hit "Enter".
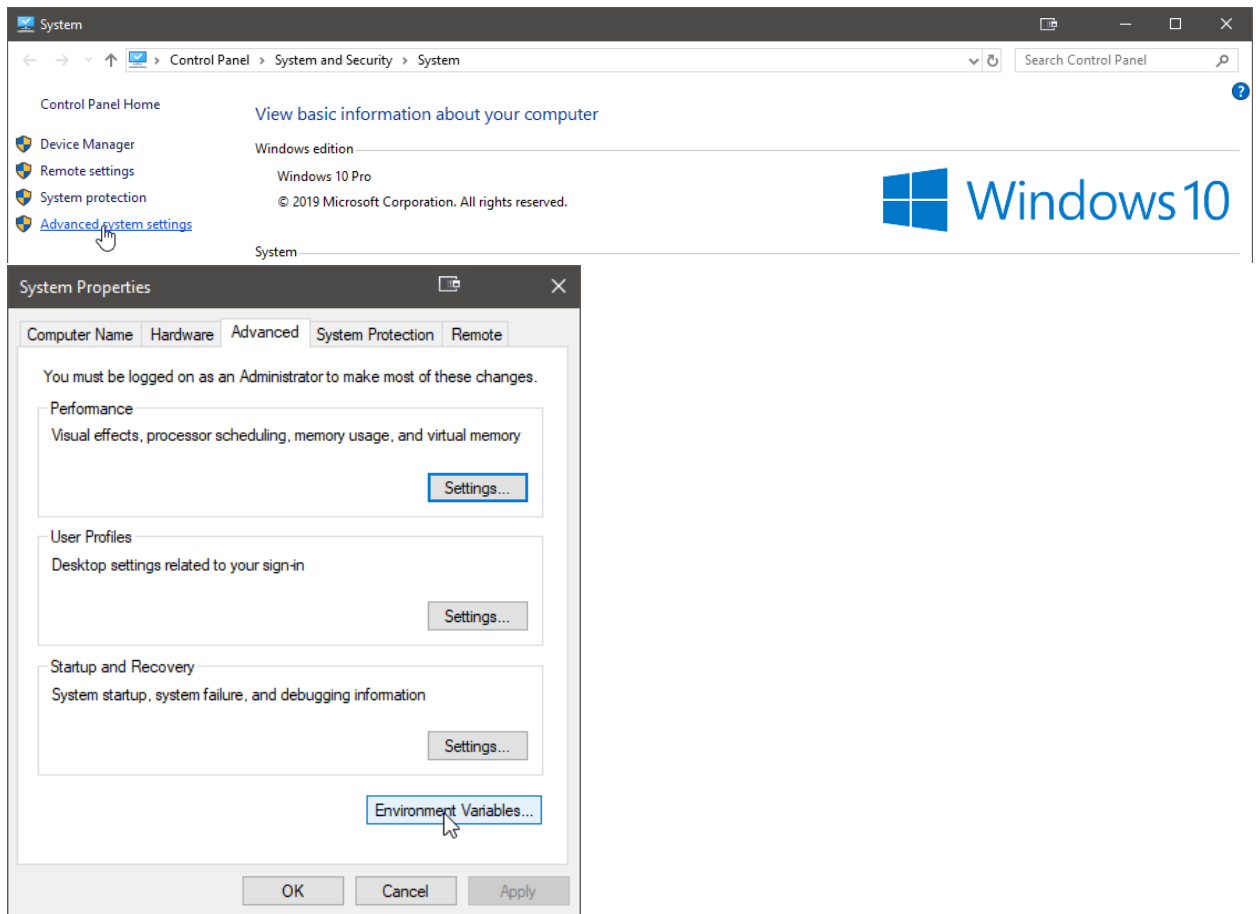3. Python 2 should now start in the Command Prompt Window.
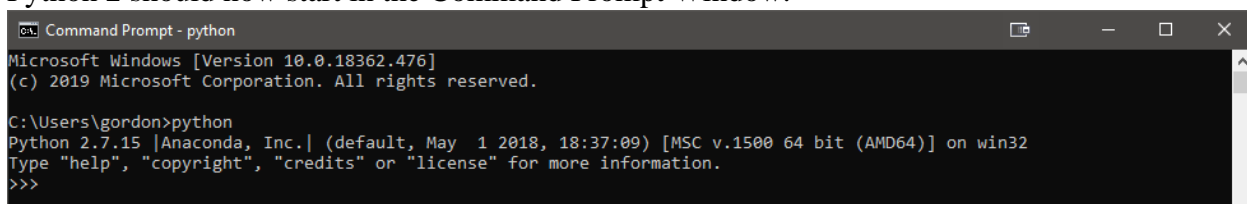
4. If it does not start, proceed to the next section; if it does, you can skip this next section.
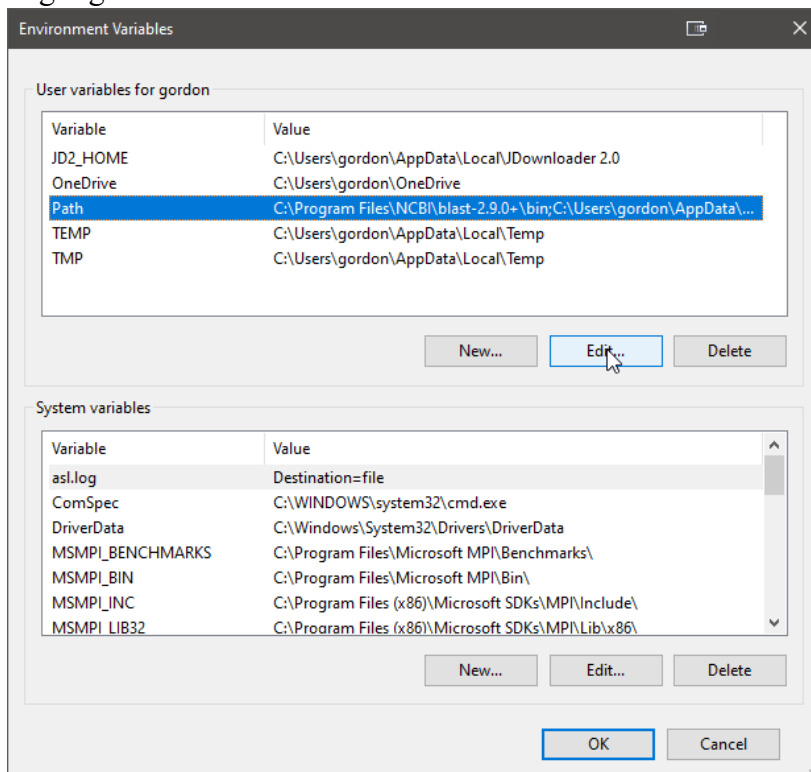
Add python.exe to PATH (Windows)

1. Open File Explorer > This PC.
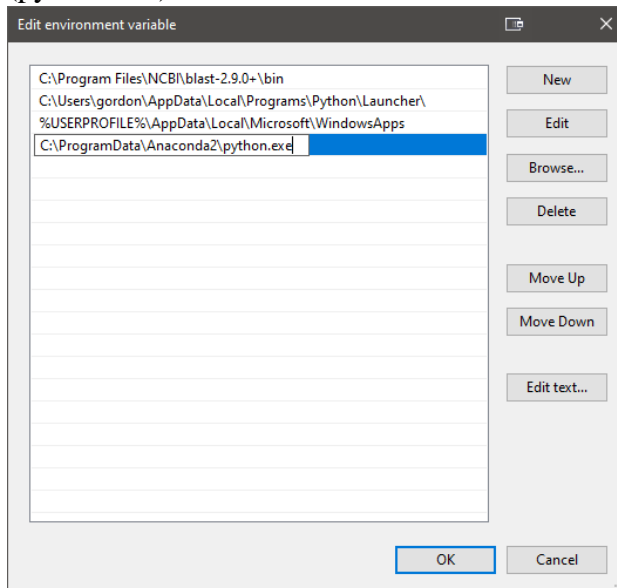2. Right click and select Properties > Advanced System Settings > Environment Variables.

3. Highlight "Path" and select Edit.

4. Click "New" and add the directory containing the executable file for Python 2 (python.exe).

    a. Here the Anaconda2 version of python.exe is used as an example.

5. Click Ok on all previous menus to ensure that all settings are saved.
6. Open Command Prompt.
7. Type "python" and hit "Enter".
8. Python 2 should now start in the Command Prompt Window.

Running BLANKA

You should now have 4 files (3 Python files and 1 batch script file): run_blanka.py, functions.py, gui.py, and run_blanka_gui.bat. BLANKA can be run in either the command line or a GUI. All 4 files should always be kept in the same folder/directory.

Command Line

1. Open Command Prompt/Anaconda Prompt/Powershell/terminal of your choice.
2. Type in "python C:\path\to\run_blanka.py" followed by arguments.
    a. For a list of arguments and a short description of each, type "python C:\path\to\run_blanka.py --help".

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b. Examples can be found on the BLANKA Github page (NOTE: short versions of parameters such as -s and -c have been removed; --sample --control should be used instead).
3. Status updates will be output as BLANKA runs and the total runtime will display.

Note: Logging in Command Line

- To output a text log in addition to the command line output in Windows, run your BLANKA command in Windows PowerShell and add "|& filename.txt" to the end of your command.

GUI

1. Double click the run_blanka_gui.bat file to run BLANKA with a GUI.
2. Click on the box with three dots next to "Sample" or "Control" to select a dataset.
   a. Checking the "Multiple Sample/Control Files" will allow you to select a folder containing multiple sample or control datasets.
   b. If non-.mzXML files are selected as input, MSConvert will be used to convert them to .mzXML format.
3. Choose type of data (LCQ, QTOF, or MALDI DD).

4. Change other parameters as needed based on instrument used.
5. Choose whether or not to perform noise/blank removal only.
6. Change number of CPU threads to use (the recommended maximum amount is total number of threads – 1).
7. Currently, a verbose option is present in the GUI but is still under development and should be ignored.
8. Click Run.
9. A new window will popup and BLANKA will run.
10. Once complete, a popup window will appear saying BLANKA has completed.
    a. Note: Error handling is still under development in the GUI version of BLANKA. Therefore, whether BLANKA exits with an error or completes successfully, the popup will say BLANKA has completed successfully. The GUI version so far is easier to use if there are no errors in the data but still very buggy at the moment.