How to use Lipid Class Algorithm

1.) Install Anaconda Navigator if you don't have it in your computer.

The link for download: https://docs.anaconda.com/anaconda/install/

2.) Make sure all the required files are stored under the correct names and placed in one folder:

a) The LC Algorithm: AbundanceQt.py

b) Criteria for lipid class filtering (table saved as text file): ClassSpecs.txt

c) A dataset (table saved as text file): data.txt

Column A: Compound

Column B: m/z

Column C: Retention time (min)

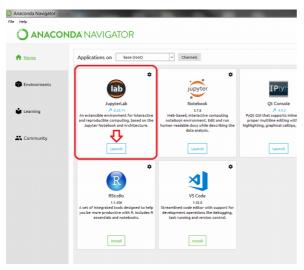
Column D: Sample 1

. Sample 2

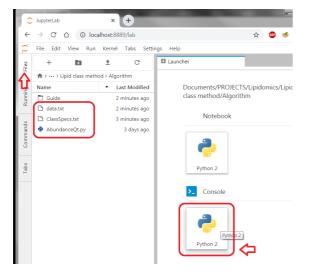
. Sample 3

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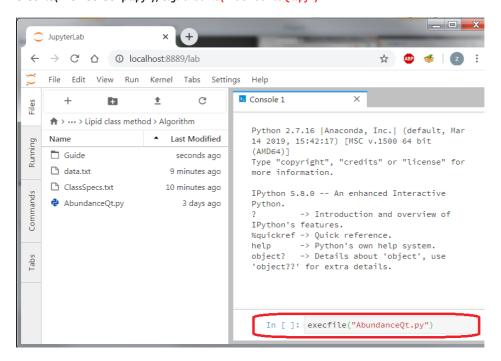
3.) Run Anaconda navigator and launch JupyterLab.



4.) First open the right directory (in the left navigation panel) and then launch Python Console.



5.) Input command in the line In []: execfile("NameOfScript.py"), e.g. execfile("AbundanceQt.py")



6.) Press [Shift]+[Enter] to execute the command.

