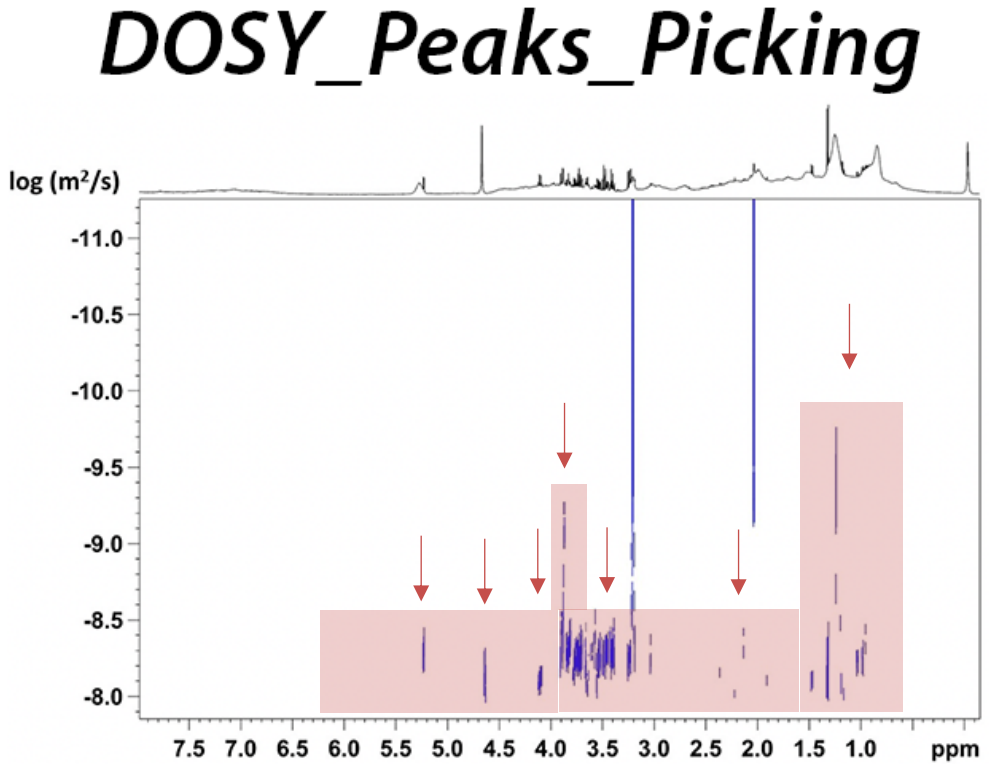
USER'S GUIDE



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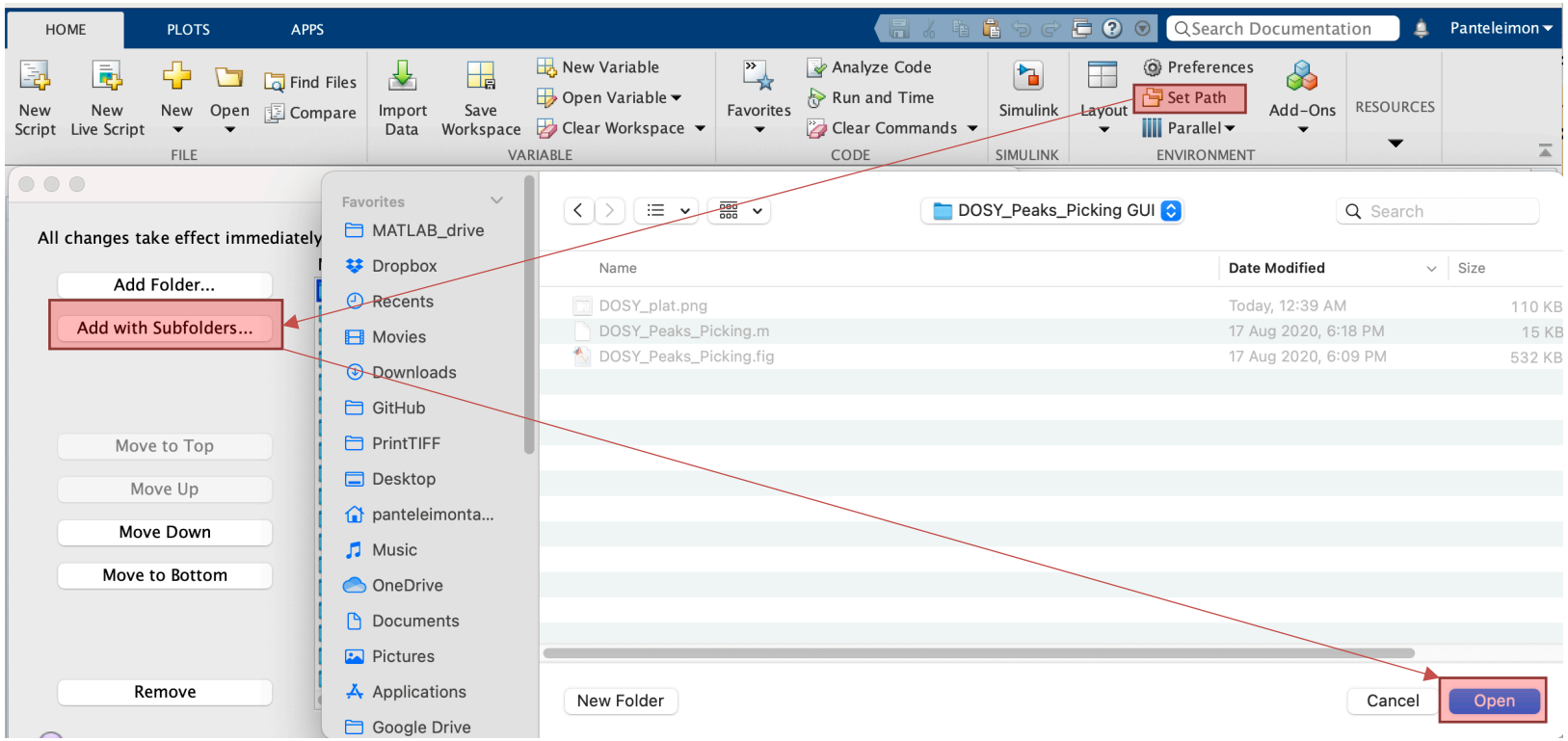
INSTALLATION

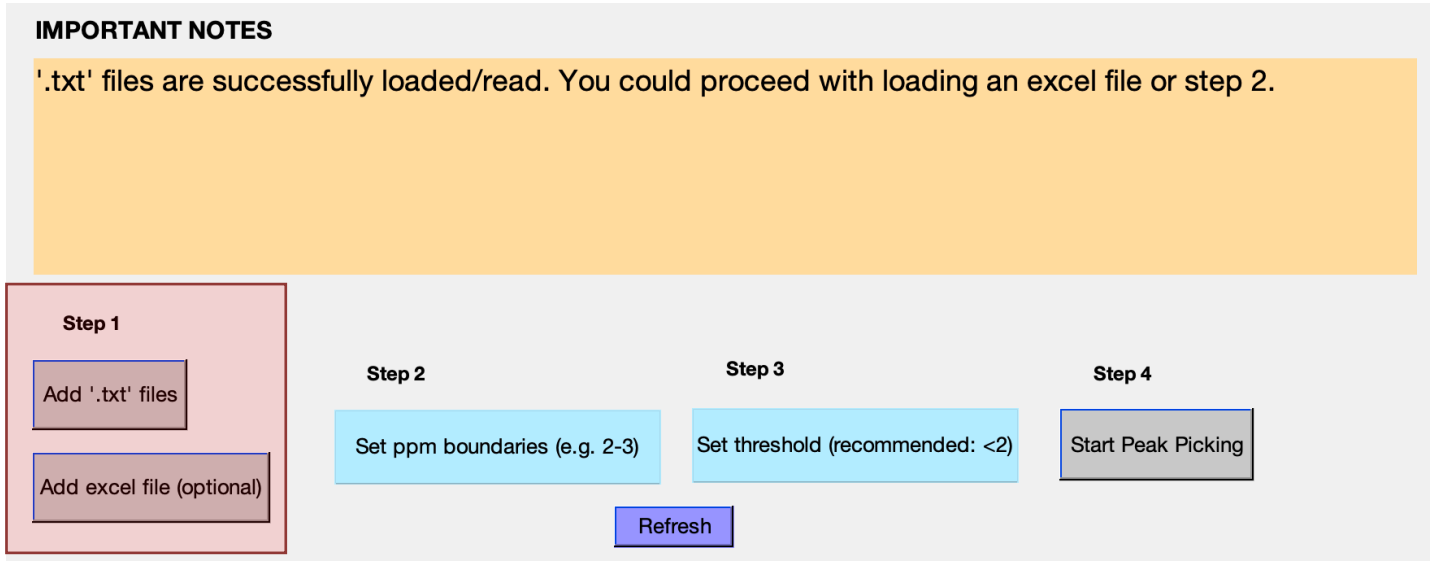
- Choose either the MacOS or Windows compiled software and follow steps to complete installation

- You could run the software via Matlab, by cloning the software from Github (https://github.com/pantakis/DOSY_Peaks_Picking) and add the parent folder with subfolders into the Matlab path (see figure below):



RUN THE SOFTWARE

- Step 1: Import the DOSY fitted peaks .txt files (by defining the parent folder containing all txt files for all spectra) generated by GNAT*



- Optional: you could load an excel file defining multiple ppm spectral regions to perform peak picking:

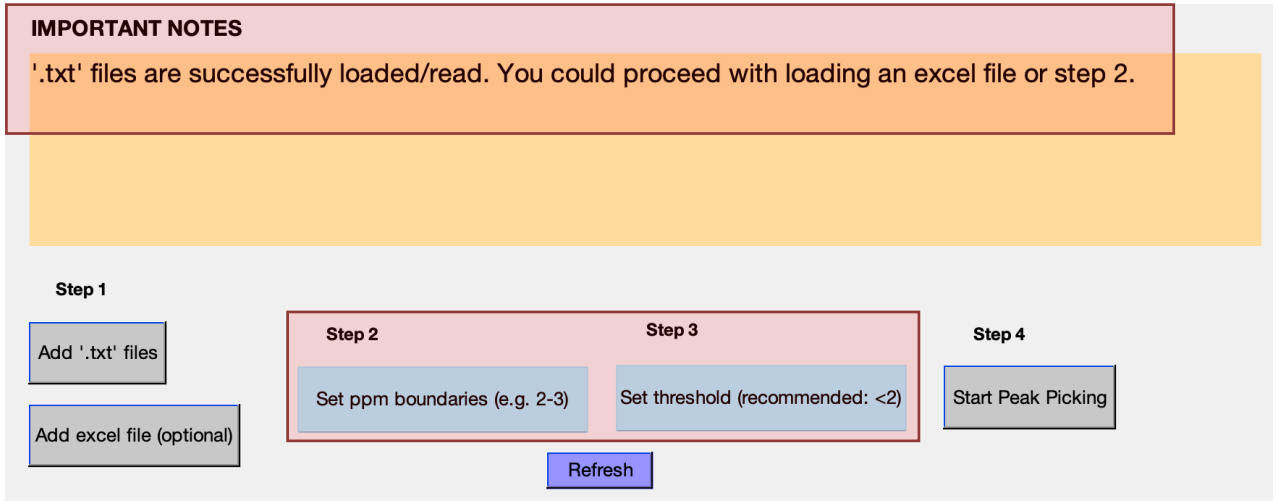
input_template.xlsx Open with Microsoft Excel

Metabolites	Min_window (ppm)	Max_window (ppm)	Threshold (fitting error)
Region1	2.7	3.5	2
Region2	3	4.07	1.5
Region3	0.9	2.5	1

* https://doi.org/10.1002/mrc.4717

RUN THE SOFTWARE

- Steps 2-3: Manually set only one spectral ppm region for all spectra to be peak picked. To define the threshld of peaks detection you could set a value (step 3) according to the smallest fitting errors in each spectral bin from the GNAT* files. Usually settoing the threshold to ”2” is enough, however, it could be set higher.



- Optional: you could omit steps 2,3 if the excel file is used see below:

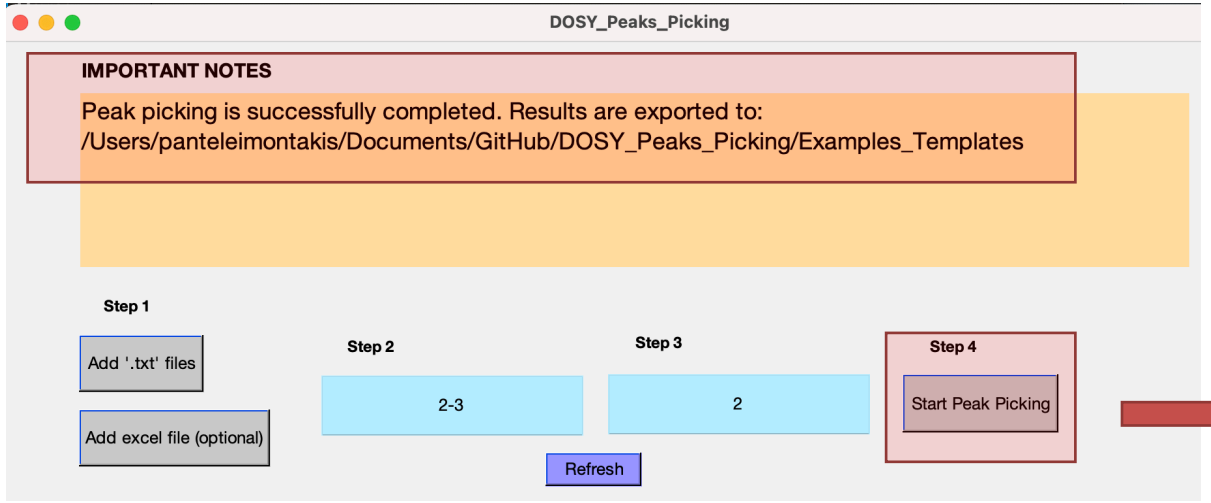
input_template.xlsx — Open with Microsoft Excel

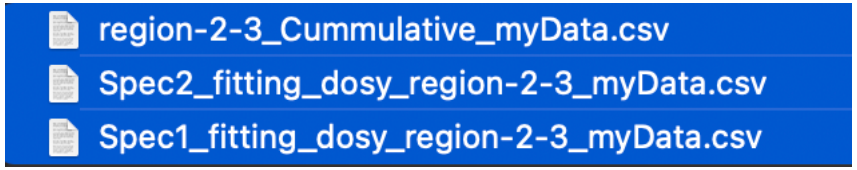
Metabolites	Min_window (ppm)	Max_window (ppm)	Threshold (fitting error)
Region1	2.7	3.5	2
Region2	3	4.07	1.5
Region3	0.9	2.5	1

* https://doi.org/10.1002/mrc.4717

RUN THE SOFTWARE

- Step 4: Press the “start peak picking” button and the results will be automatically exported as .csv files for all spectra in the parent folder containing the loaded .txt files.





region-2-3_Cummulative_myData.csv

Peaks / Spectra -->	spec_Spec1_fitting_dosyPPM	spec_Spec1_fitting_dosyDiffCoef	spec_Spec2_fitting_dosyPPM	spec_Spec2_fitting_dosyDiffCoef
Peak-1	2.53766	7.709267	2.13778	9.262495
Peak-2	2.56315	5.899619	2.37431	11.158717
Peak-3	0	0	2.44215	8.968256
Peak-4	0	0	2.45425	8.656717
Peak-5	0	0	2.53786	7.290462

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