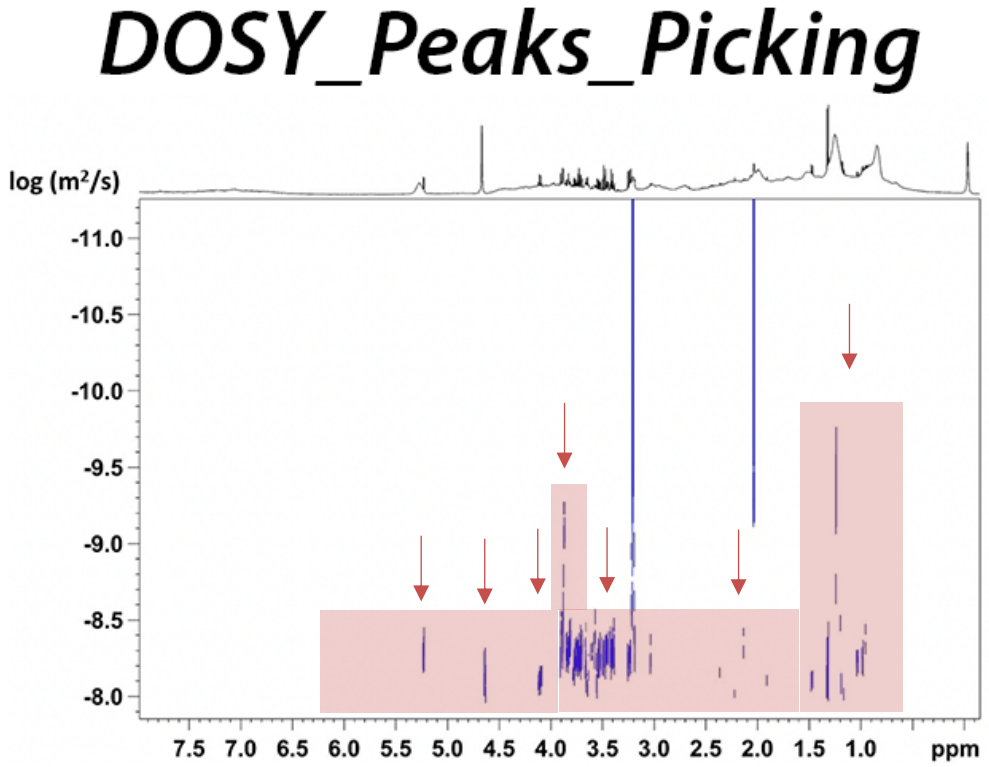
USER'S GUIDE



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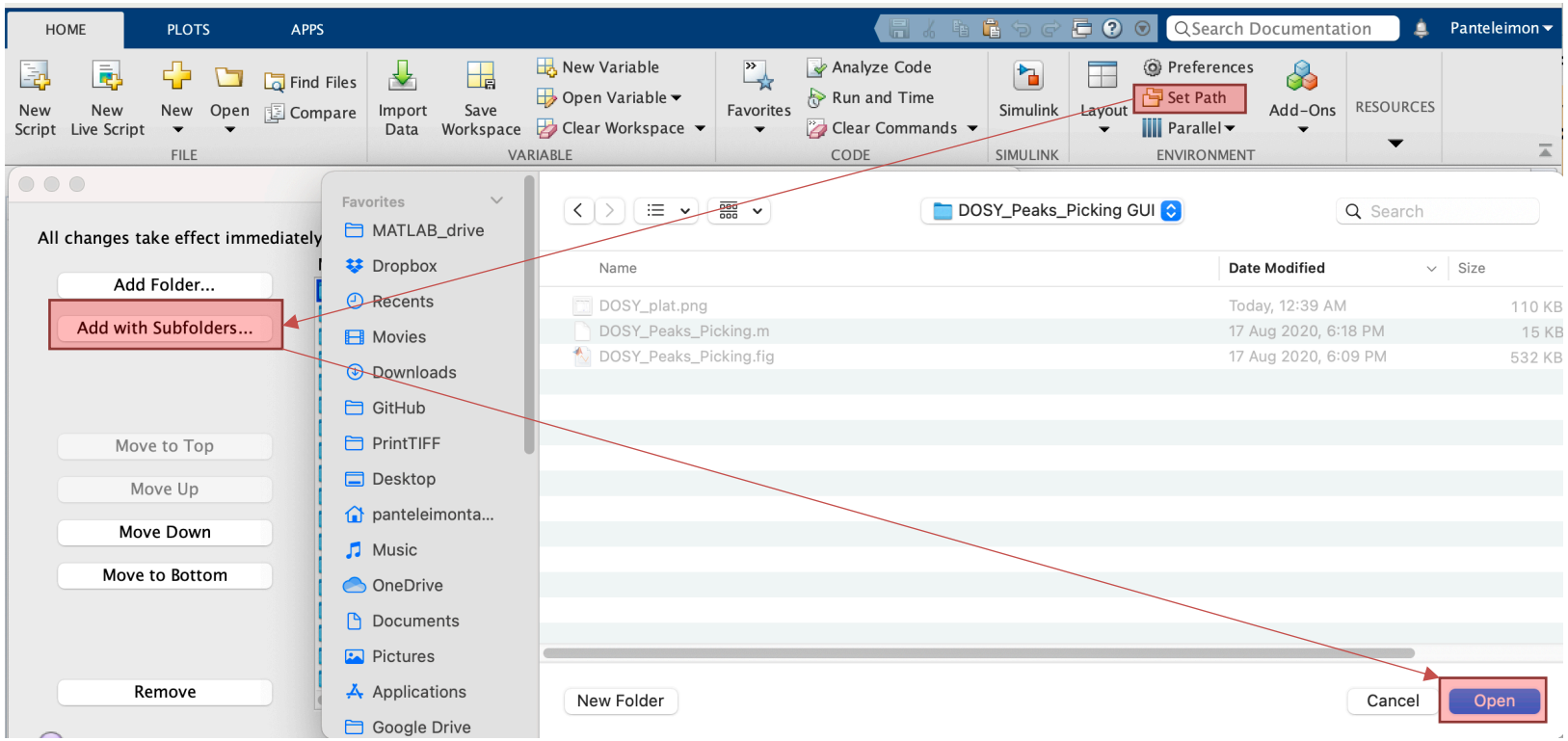
INSTALLATION

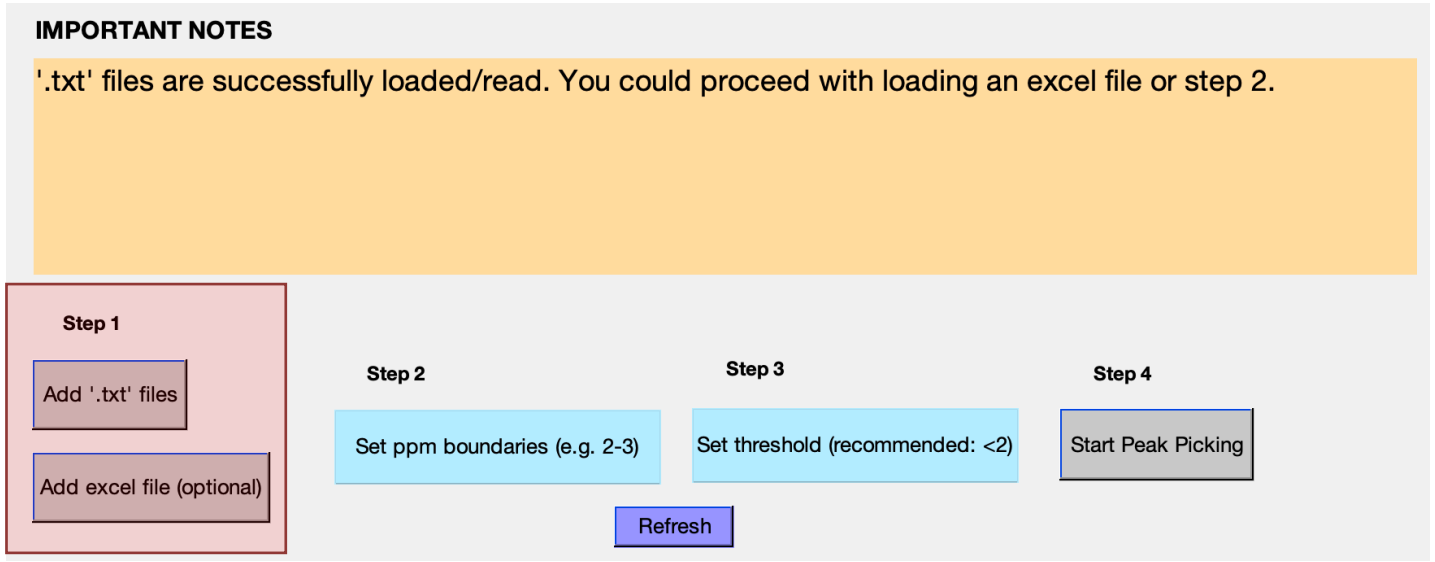
- Choose either the MacOS or Windows compiled software and follow on screen steps to complete installation

- 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:

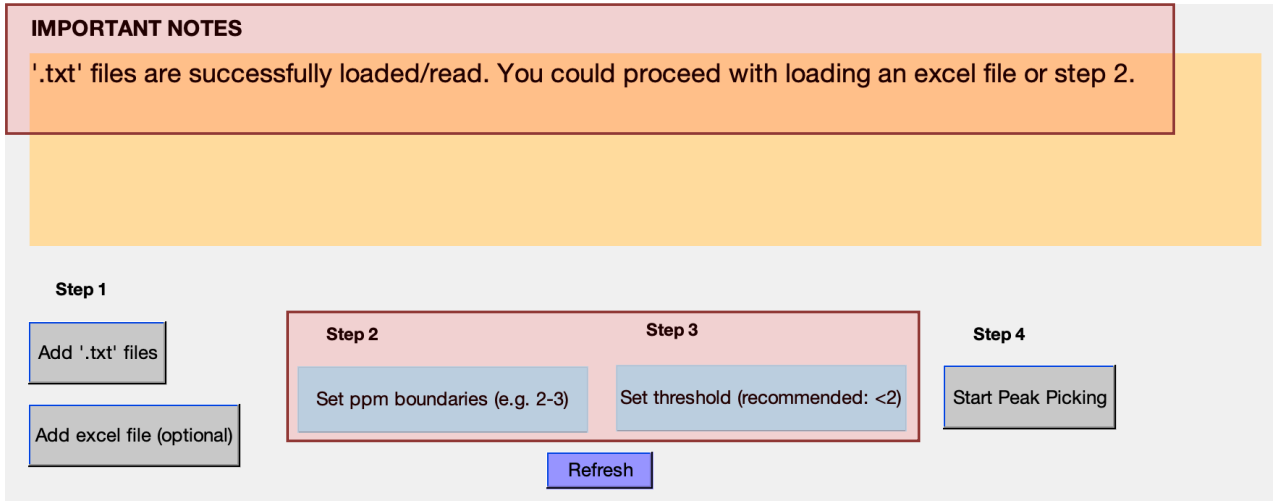
input_template.xlsx Open with Microsoft Excel

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 threshold of peaks detection please set a value (step 3) according to the smallest fitting errors in each spectral bin from the GNAT* files. Usually setting the threshold to ”2 or below” is enough, however, it could be set higher.



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

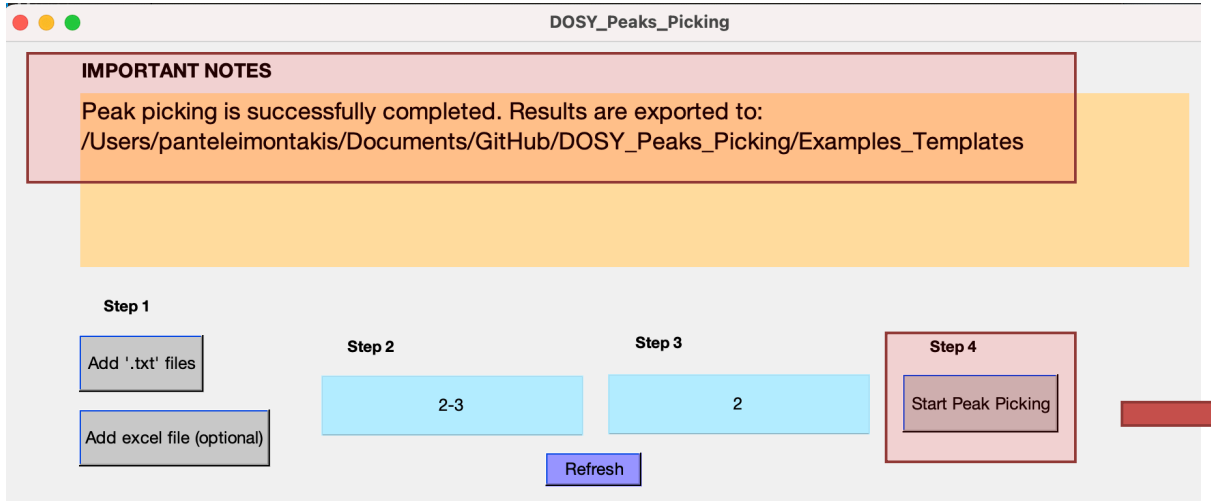
input_template.xlsx — Open with Microsoft Excel

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

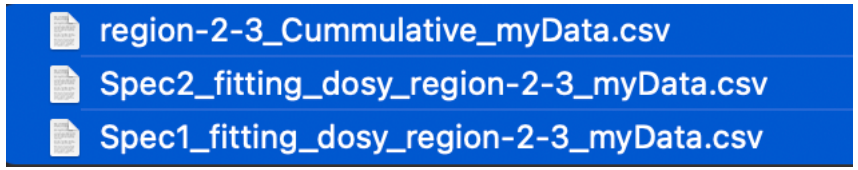
* https://doi.org/10.1002/mrc.4717

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.



Output files for 2 spectra



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

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