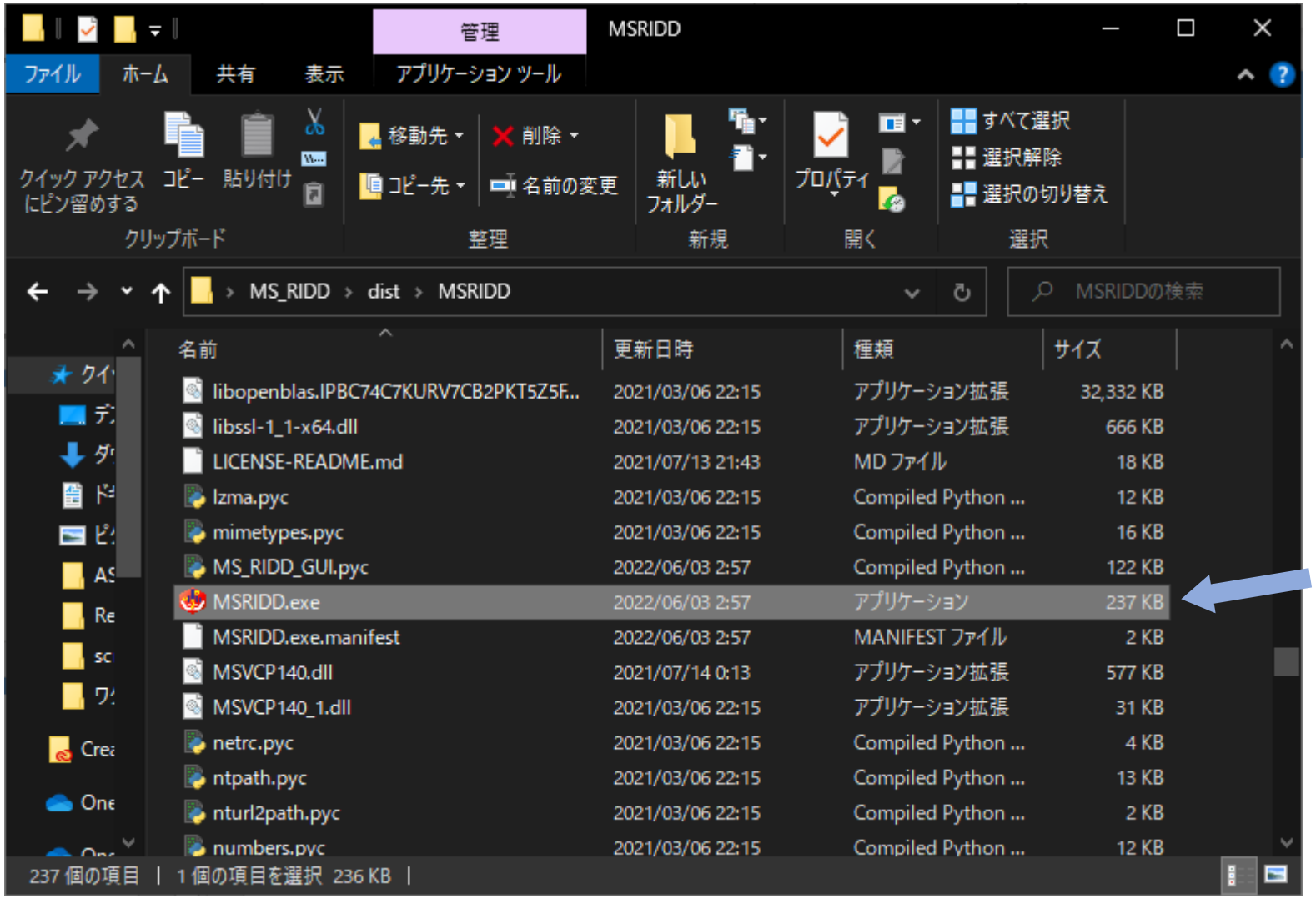
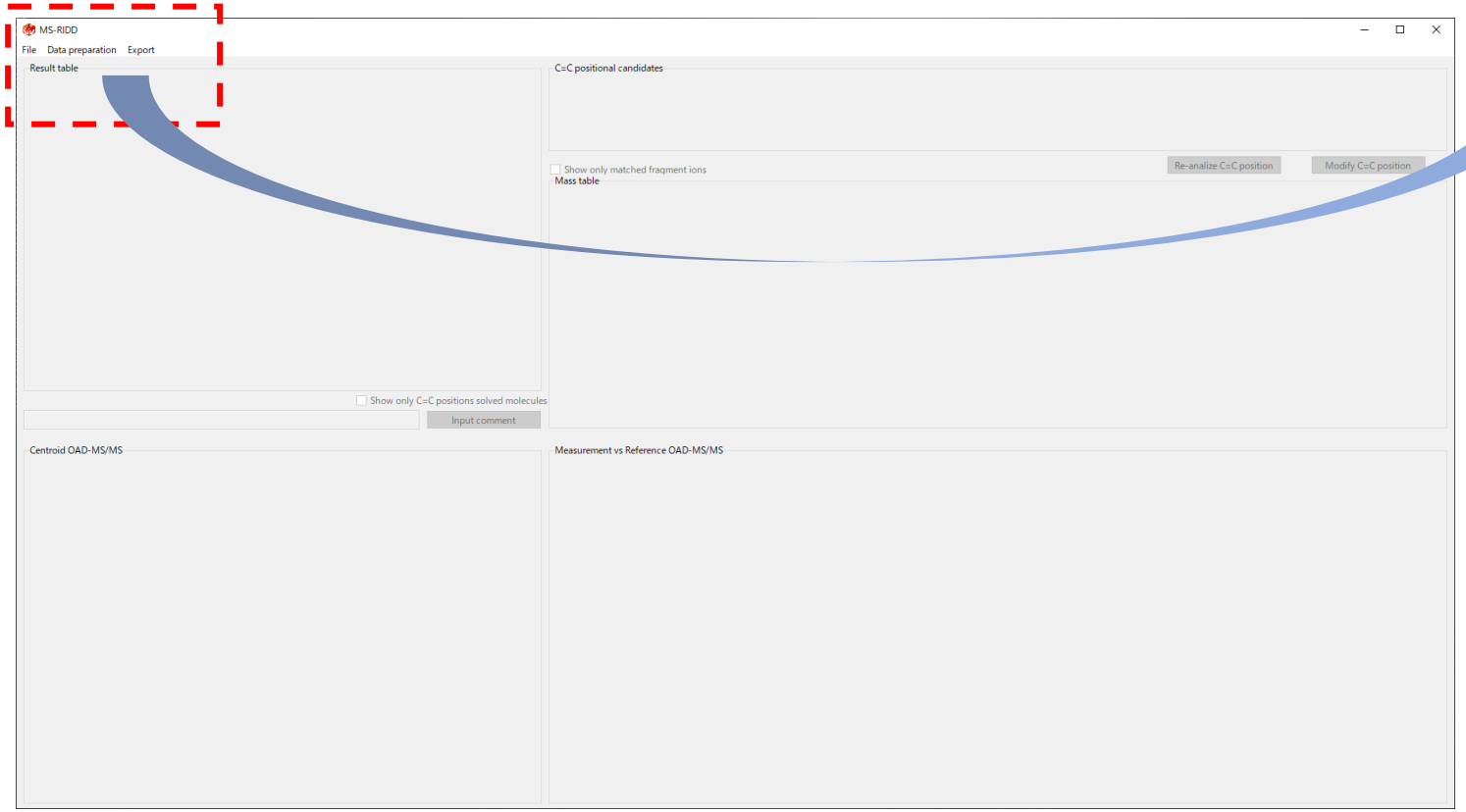
MS-RIDD tutorial

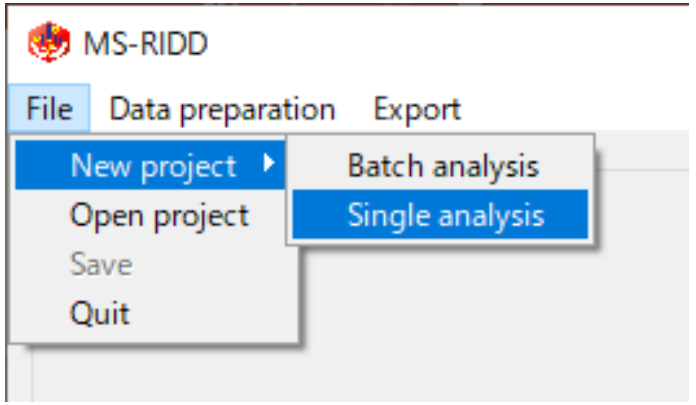
1-1. How to start OAD-MS/MS analysis



Open the folder of MS-RIDD, then double click the .exe file (MS-RIDD.exe)

1-2a-1. How to start OAD-MS/MS analysis (New project / Single analysis)

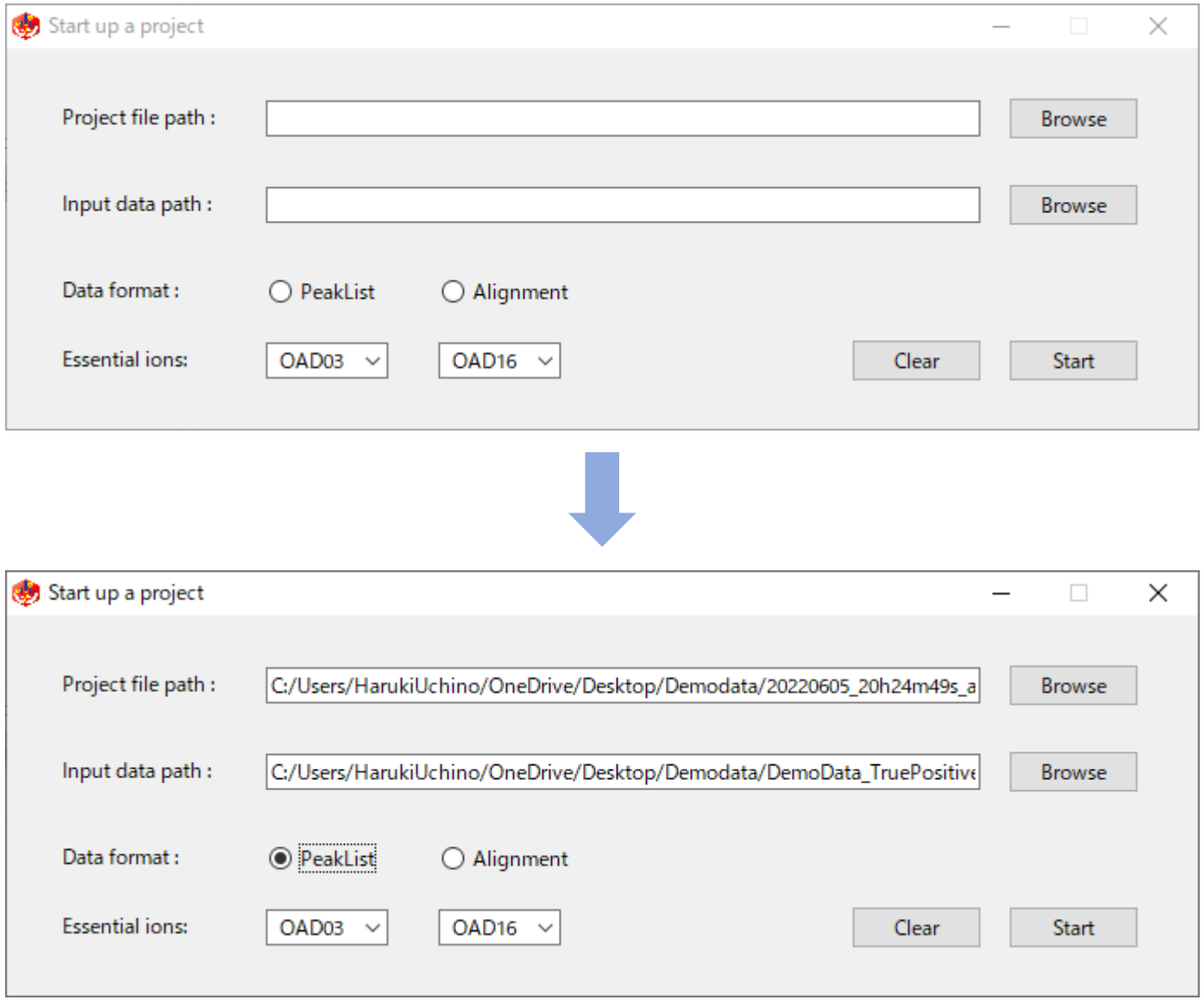




(For a single analysis)
After the GUI shown up, select the below

File > New project > Single analysis

1-2a-2. How to start OAD-MS/MS analysis (New project / Single analysis)



Select the followings and click the start

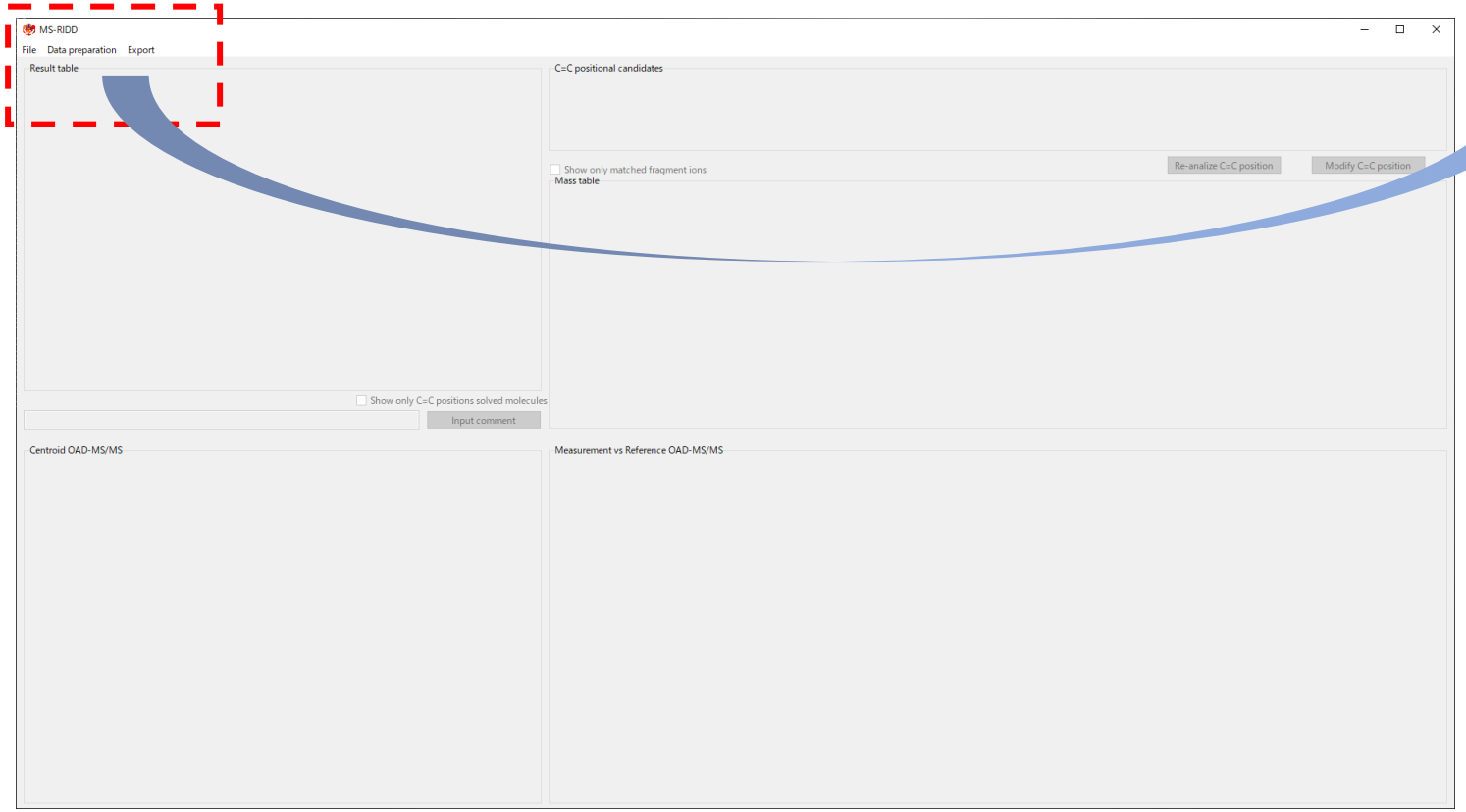
Project file path:
select the folder where the analysis data generated by MS-RIDD locates

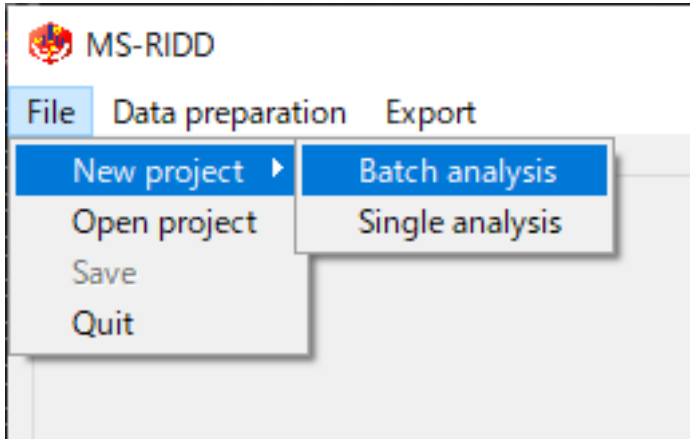
Input data path:
select the data (.txt) from MS-DIAL export containing OAD-MS/MS spectra

Data format:
select the data format in which MS-DIAL exported

Essential ions:
For the current data (doi.org/10.21203/rs.3.rs-727852/v1), select OAD03/OAD16

1-2b-1. How to start OAD-MS/MS analysis (New project / Batch analysis)

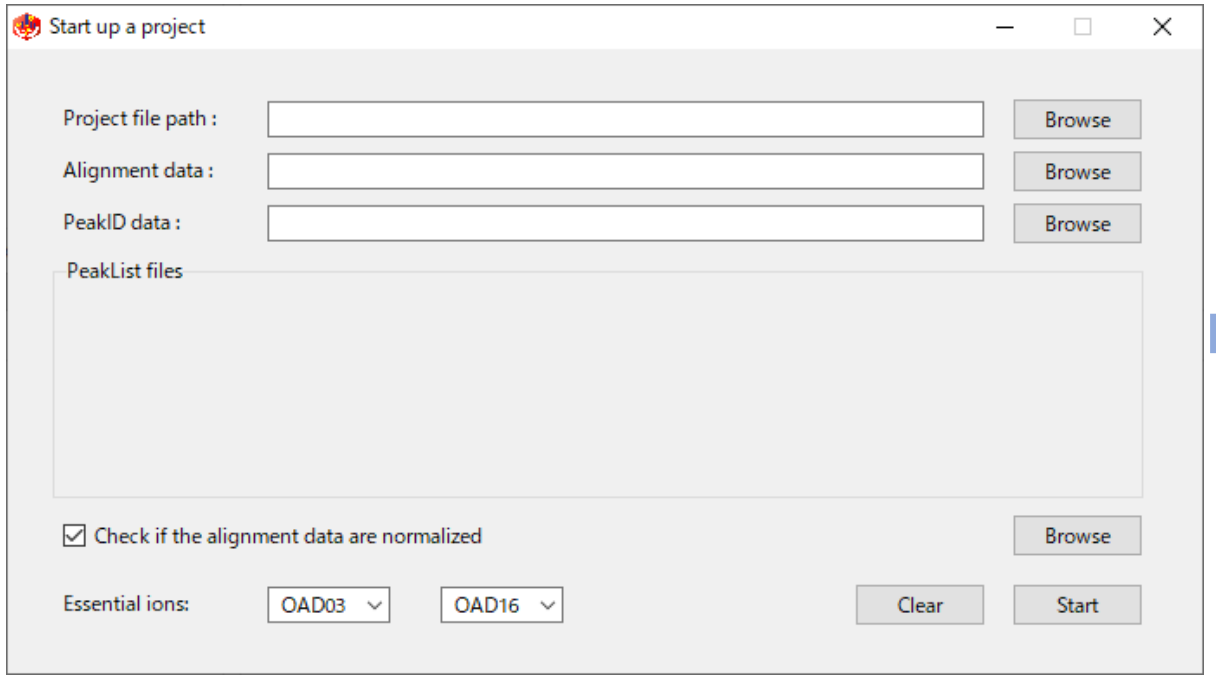


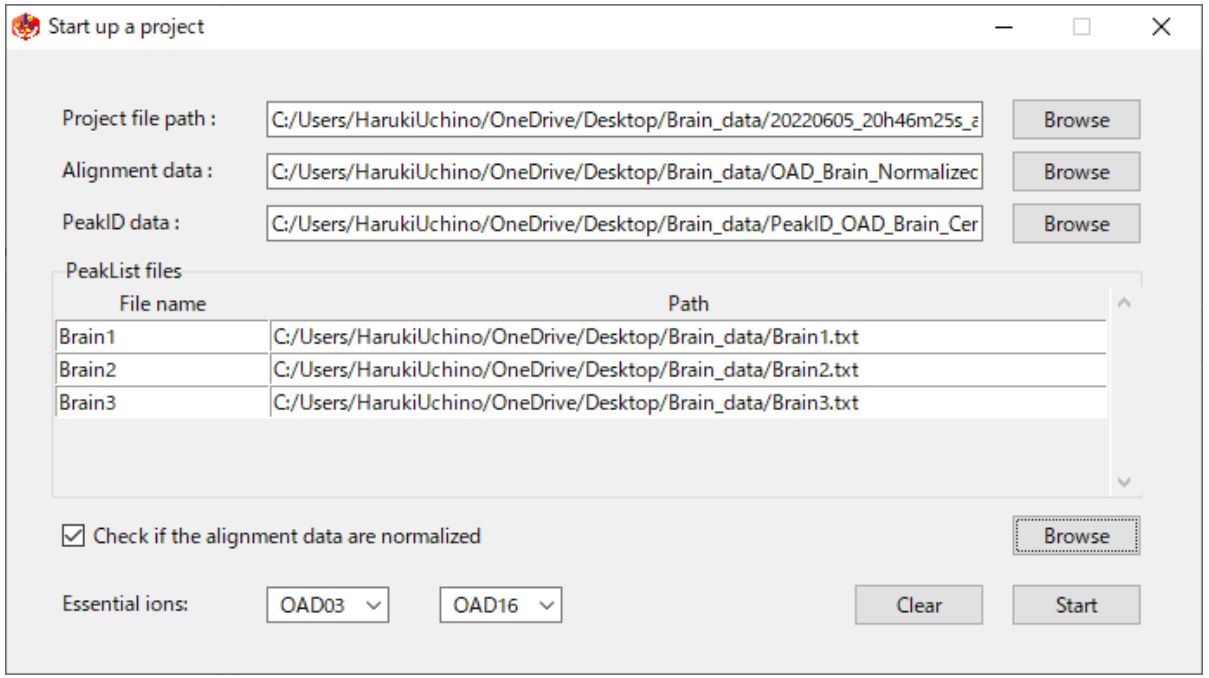


(For a batch analysis)
After the GUI shown up, select the below

File > New project > Batch analysis

1-2b-2. How to start OAD-MS/MS analysis (New project / Batch analysis)





Select the followings and click the start

Project file path:
select the folder where the analysis data generated by MS-RIDD locates

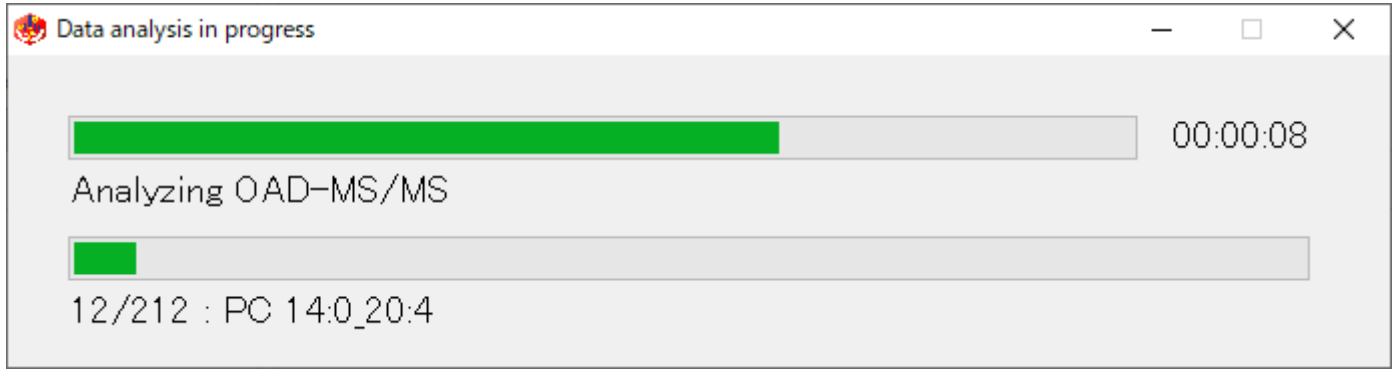
Alignment data path:
select the data (.txt) from MS-DIAL as alignment data format containing OAD-MS/MS spectra

PeakID data:
select the peak ID data from the same alignment data

PeakList files:
select each sample data of the alignment data as PeakList format of MS-DIAL export

Essential ions:
For the current data (doi.org/10.21203/rs.3.rs-727852/v1), select OAD03/OAD16

1-3. How to start OAD-MS/MS analysis (Processing)



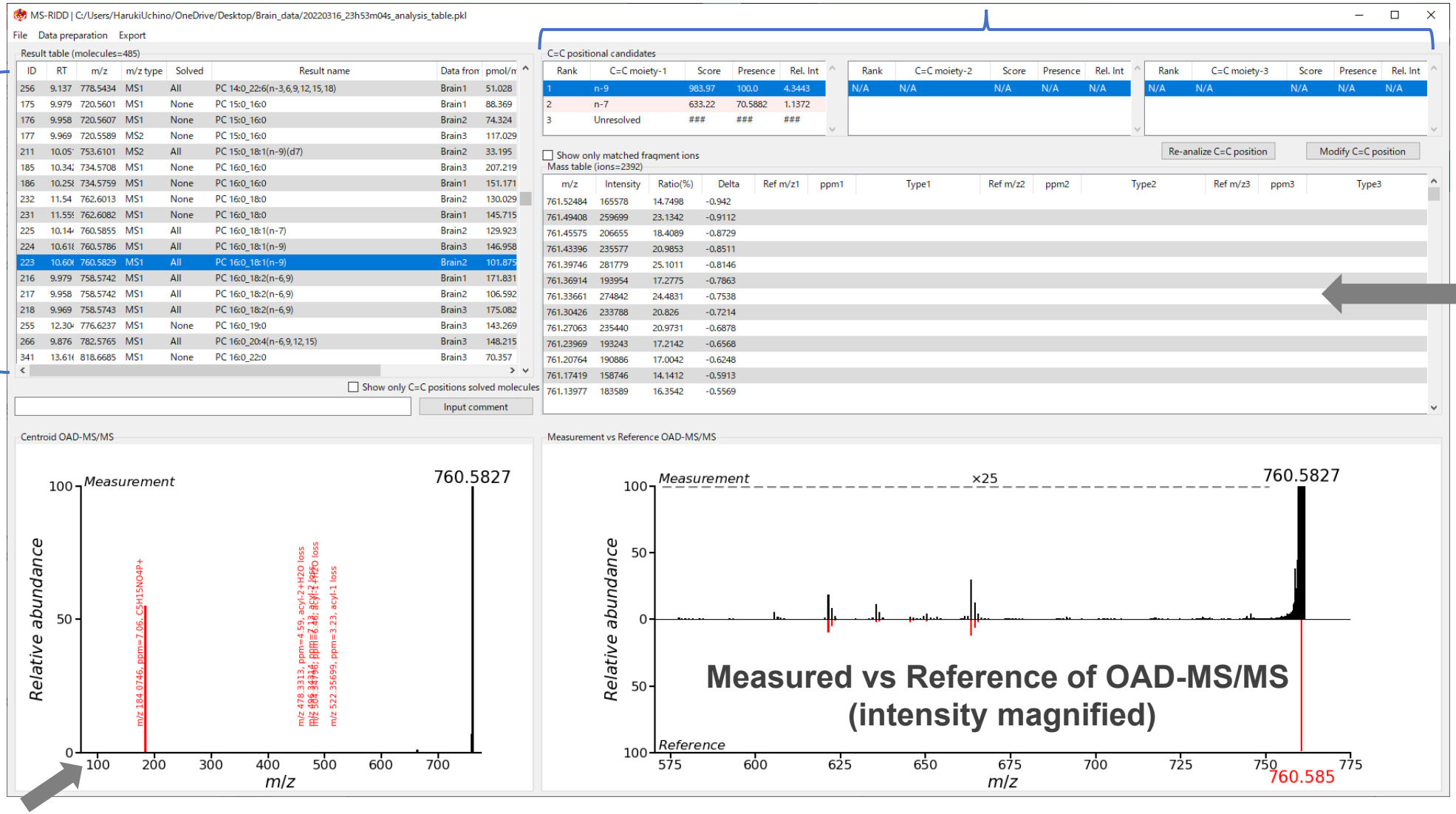
Please wait until the processing finish

*** Error will occur if the data format is not correct**

2-1. How to check the automatic result of OAD-MS/MS analysis

Graphical use interface of MS-RIDD

Candidates of C=C positions for each unsaturated moiety



Metabolite table

Mass table

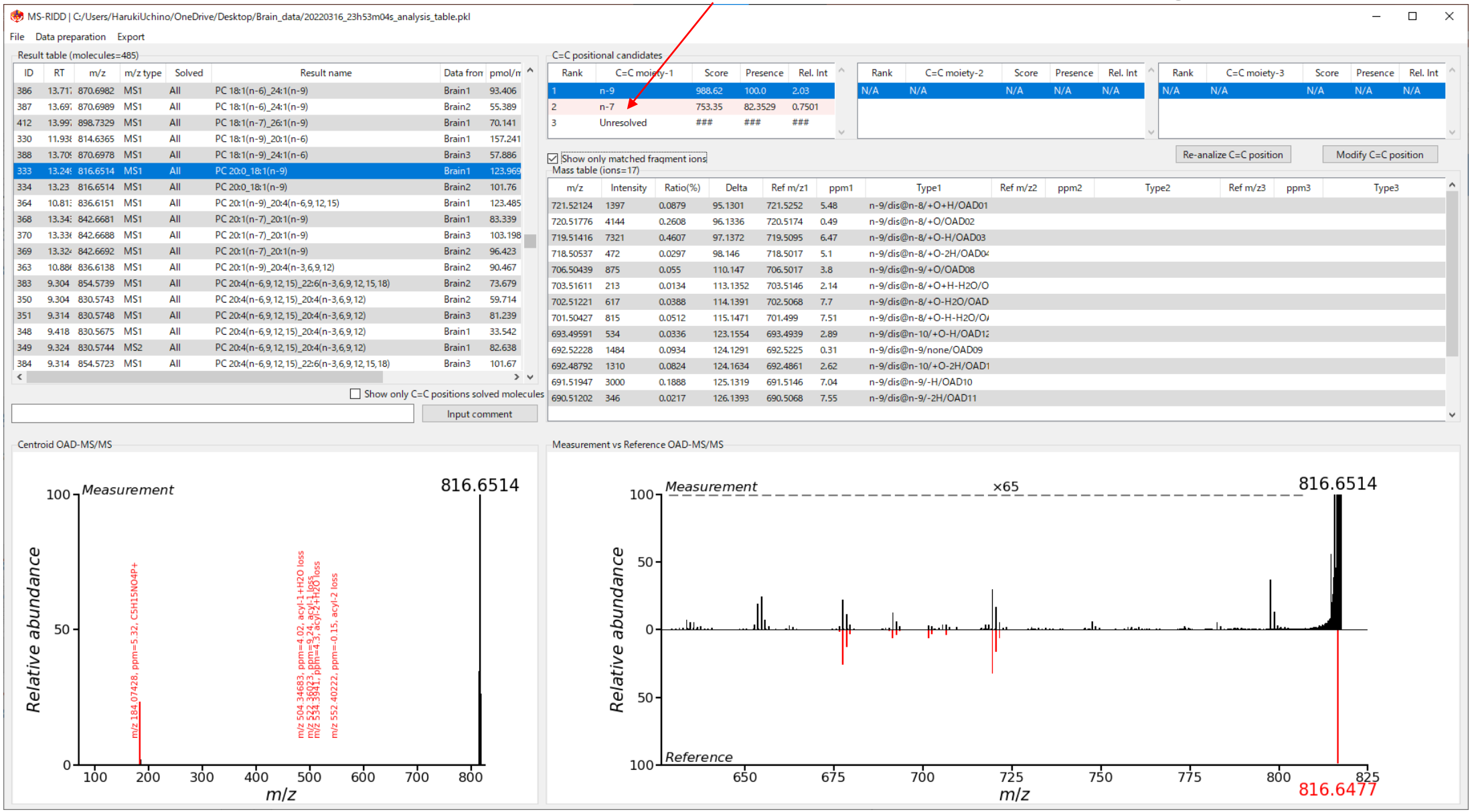
Measured vs Reference of OAD-MS/MS (intensity magnified)

Measured of OAD-MS/MS

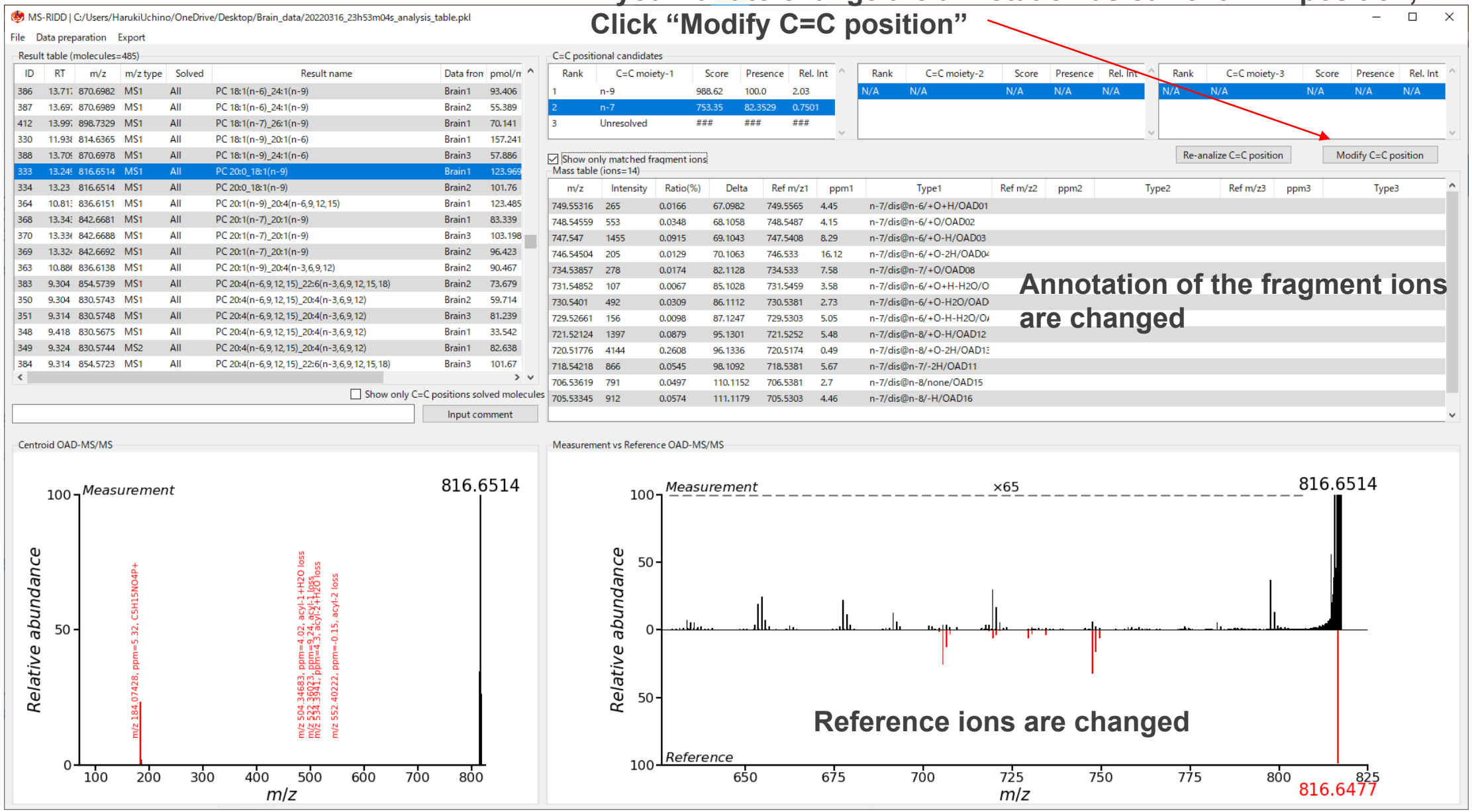
*** If the fragment ions for the annotation of acyl-chain isomer levels are detected (based on the CID), red colored annotation labels will show up**

2-1. How to check the automatic result of OAD-MS/MS analysis (Modify the annotation of C=C position)

Click the other C=C candidates for checking the spectrum matching

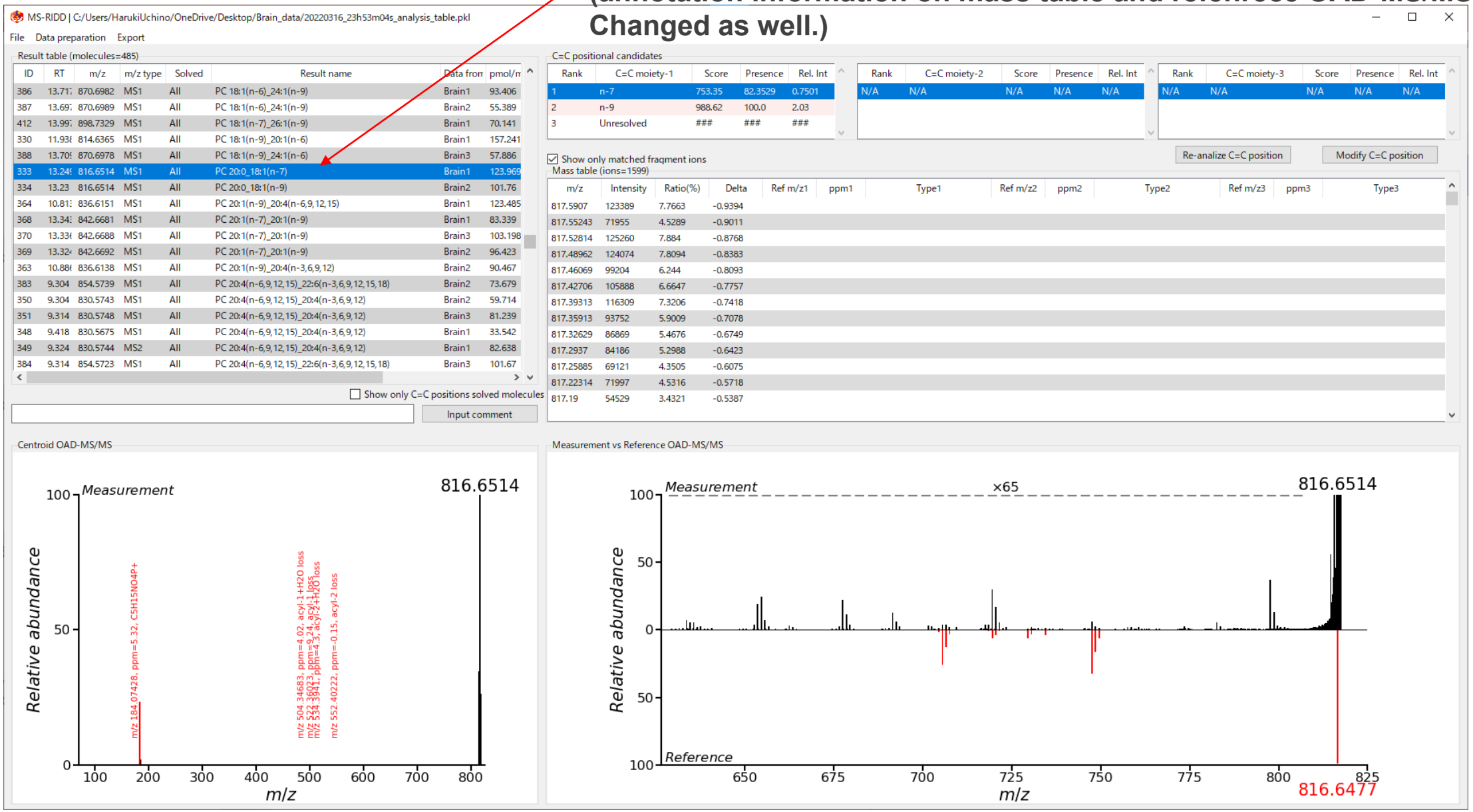


2-1. How to check the automatic result of OAD-MS/MS analysis (Modify the annotation of C=C position)

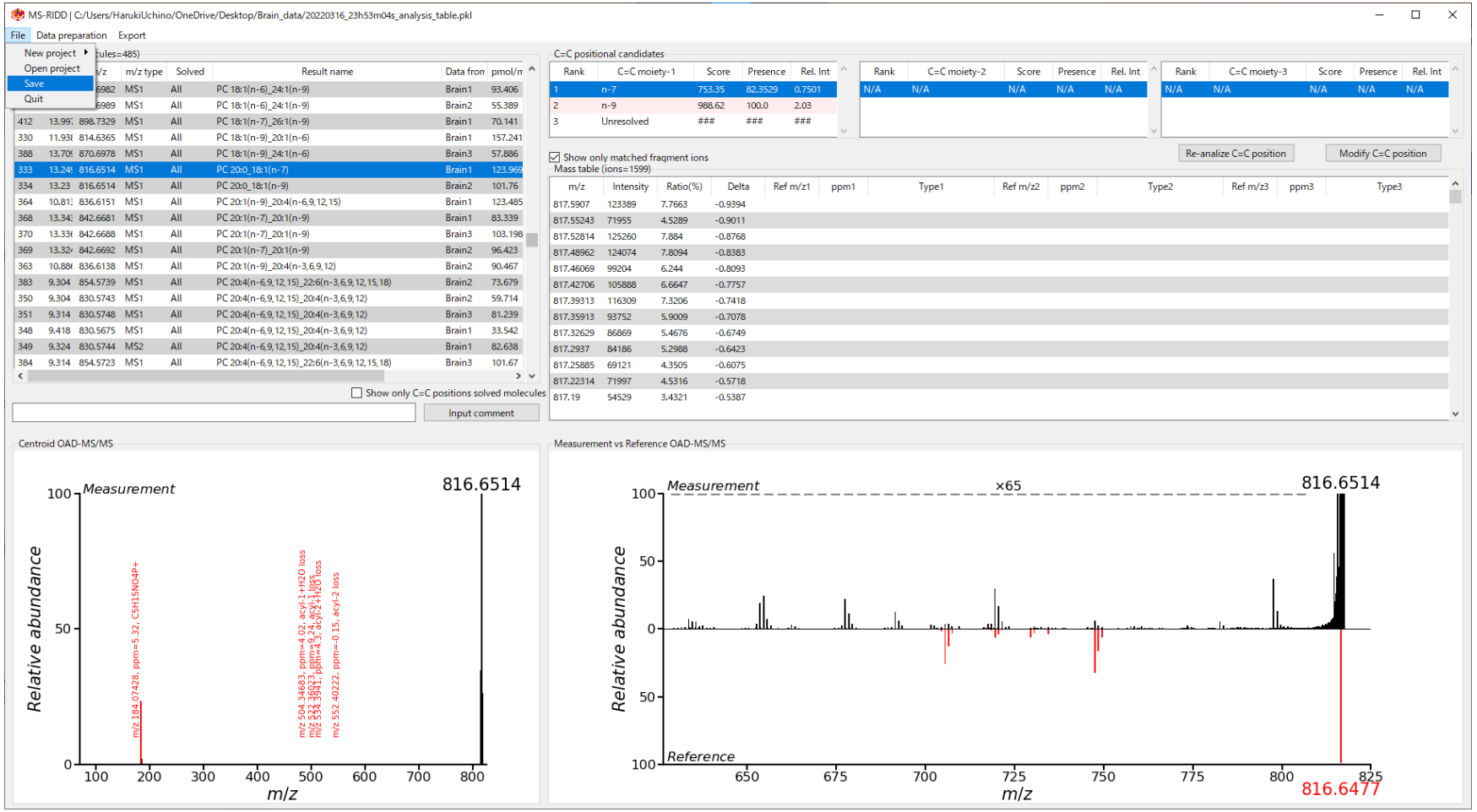


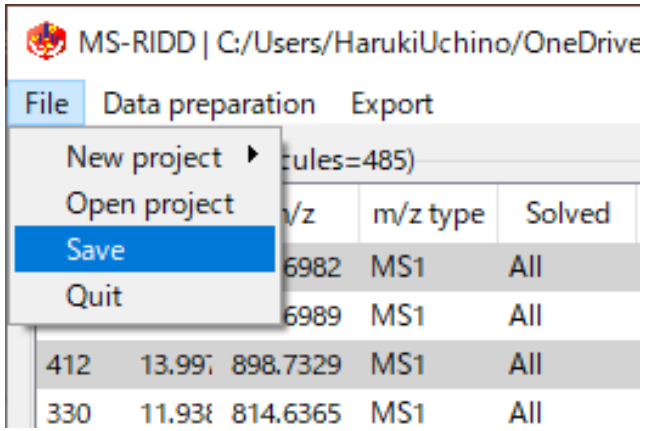
2-1. How to check the automatic result of OAD-MS/MS analysis (Modify the annotation of C=C position)

Then, the annotation name on the metabolite table will change (annotation information on mass table and refenrece OAD-MS/MS are Changed as well.)



3-1. How to save the analysis data

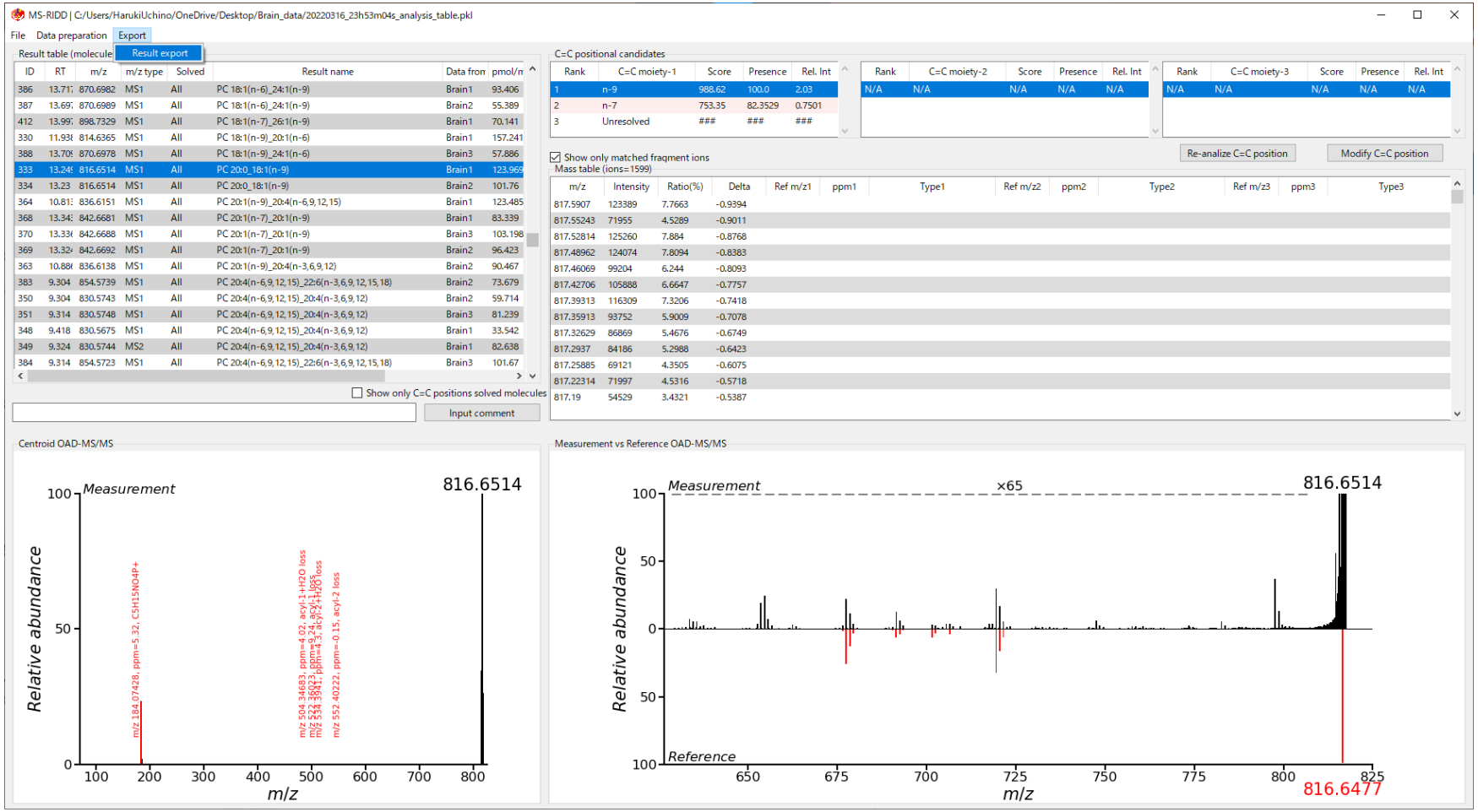


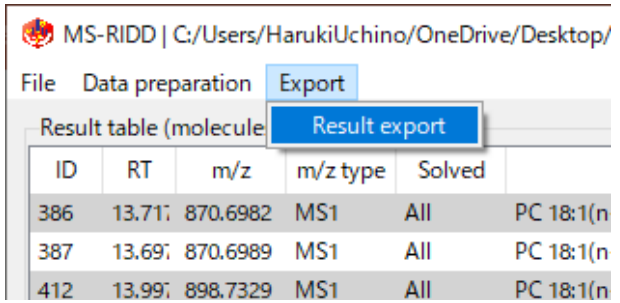


Select: File > Save

*** Saving is needed for the information which user manually modified and/or added.**

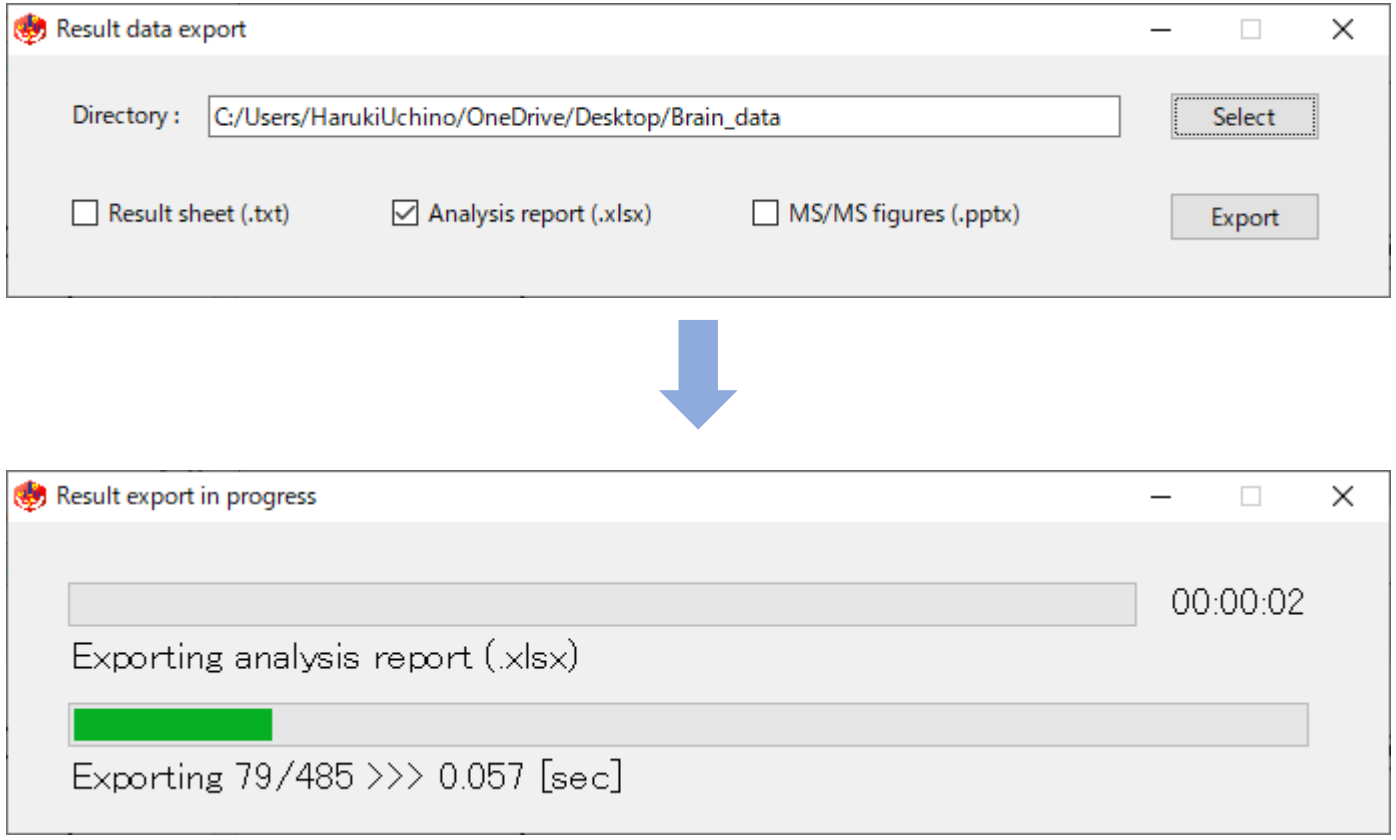
4-1. How to export the analysis data





Select: Export > Result expot

4-1. How to export the analysis data

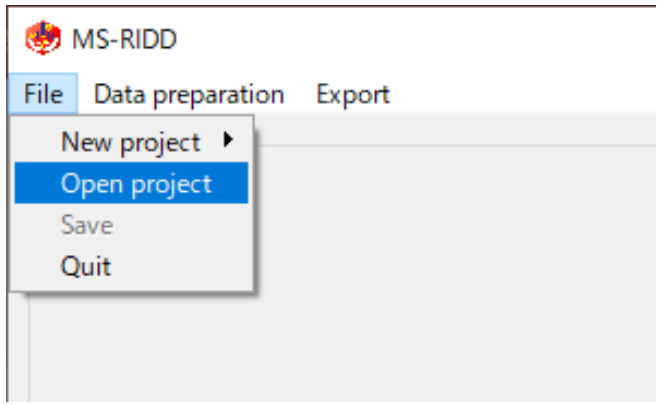


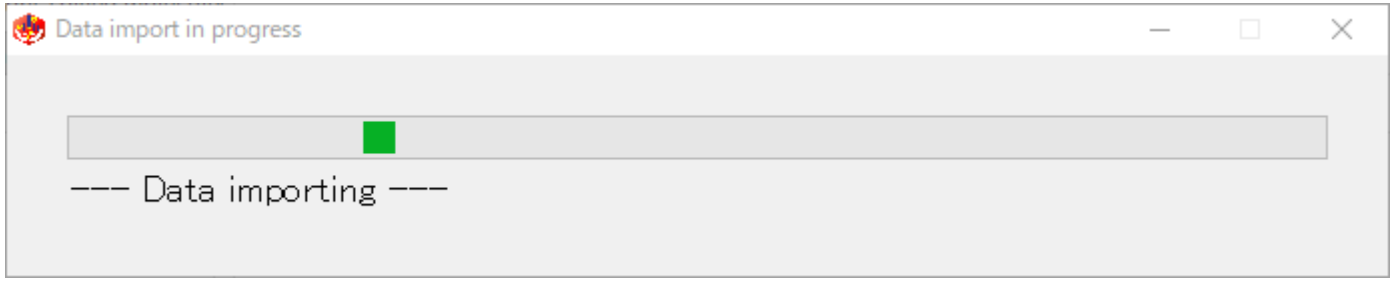
Select the followings and click “Export”

Directory:
select the folder where the selected result data generated by MS-RIDD locates

* For default setting, “Analysis report” is selected. Exporting MS/MS figures (.pptx) takes several minutes.

5-1. How to open the previous analysis data





Select “Open project”,
then select the MS-RIDD data (.pkl).

*** The following data are also required to be in the same folder as the MS-RIDD data (.pkl).**

“ *_cid_result.pickle”
“ *_extracted_msms.pickle”
“ *_graph_info.pickle”
“ *_oad_result.pickle”
“ *_structure_info.pickle”