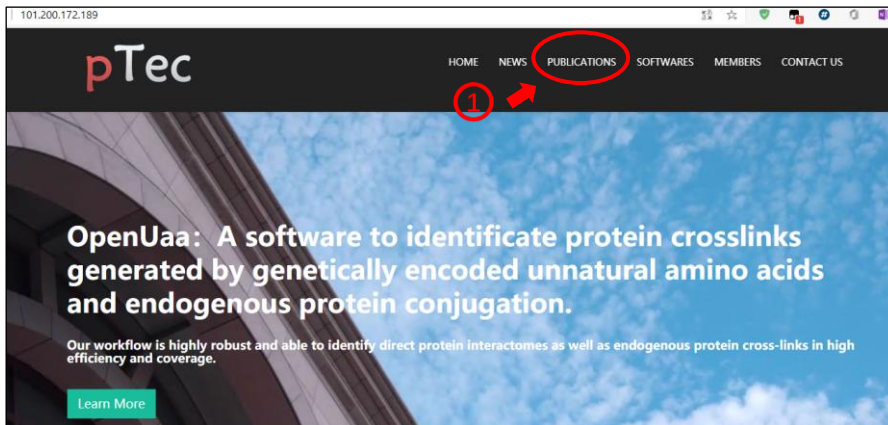


OpenUaa Manual

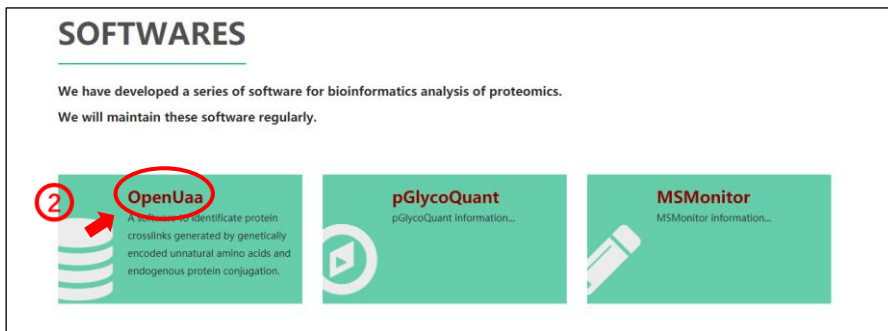
Release date:2020.09.07

1. Get the datasets and the software

① Load the OpenUaa website: <http://101.200.172.189/> and click the “SOFTWARE” to the software page.

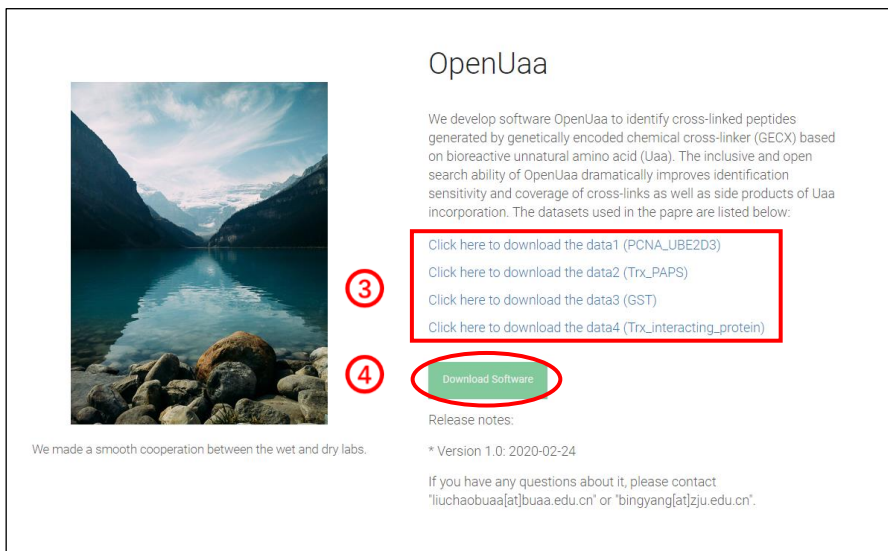


② Click the OpenUaa link.



③ Click the links to download the related datasets.

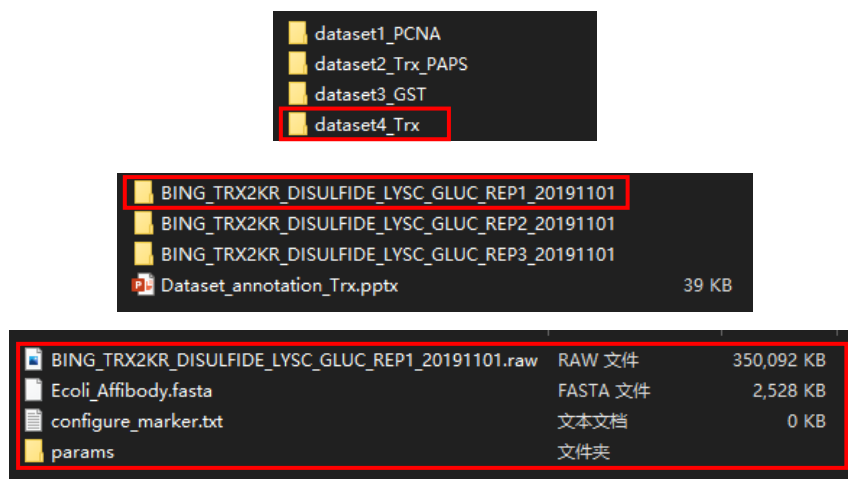
④ Click the “Download Software” button to get the OpenUaa software.



2. The contents of one dataset

Each dataset has one or three raw data files, each raw file was in a separated folder, which also contains one “*.fasta” file, one “configure_marker.txt” file and one “params” folder, each of them is necessary.

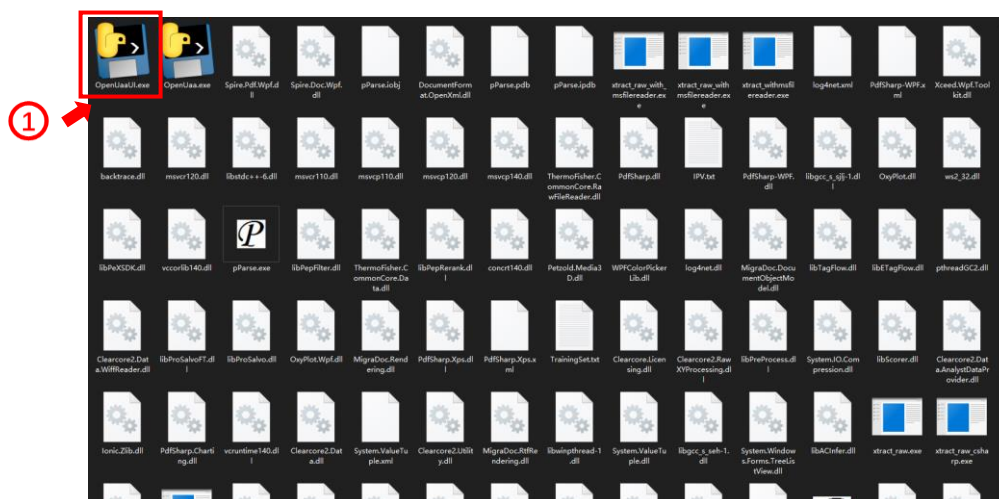
if you want to copy the configure file, choose “configure_marker.txt” and “params” together.



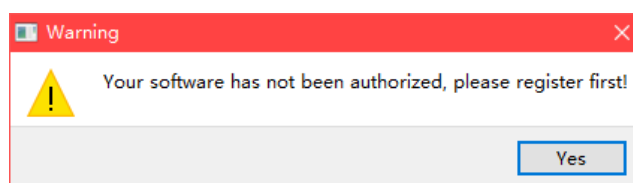
3. The software manual

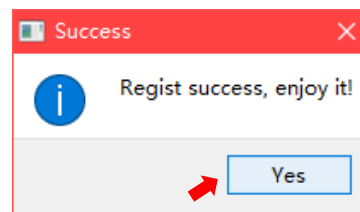
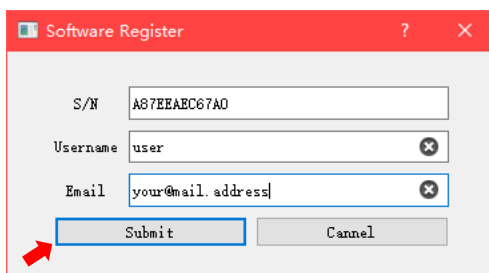
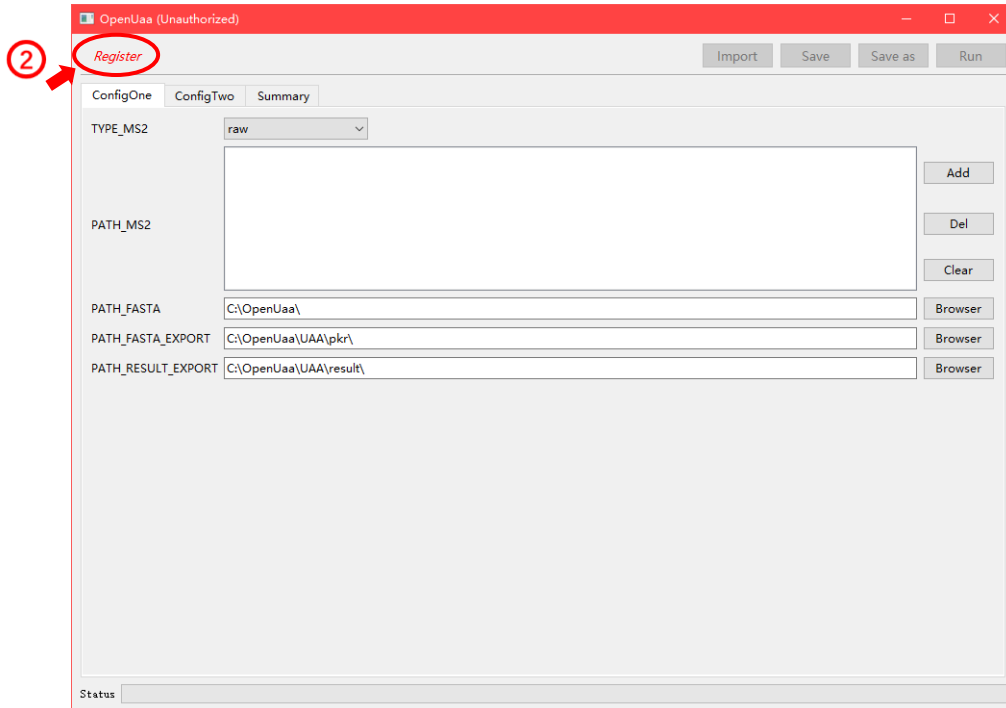
3.1 Register

① After downloading the software, unzip it first, then double click the “OpenUaaUI.exe” file to start the software.

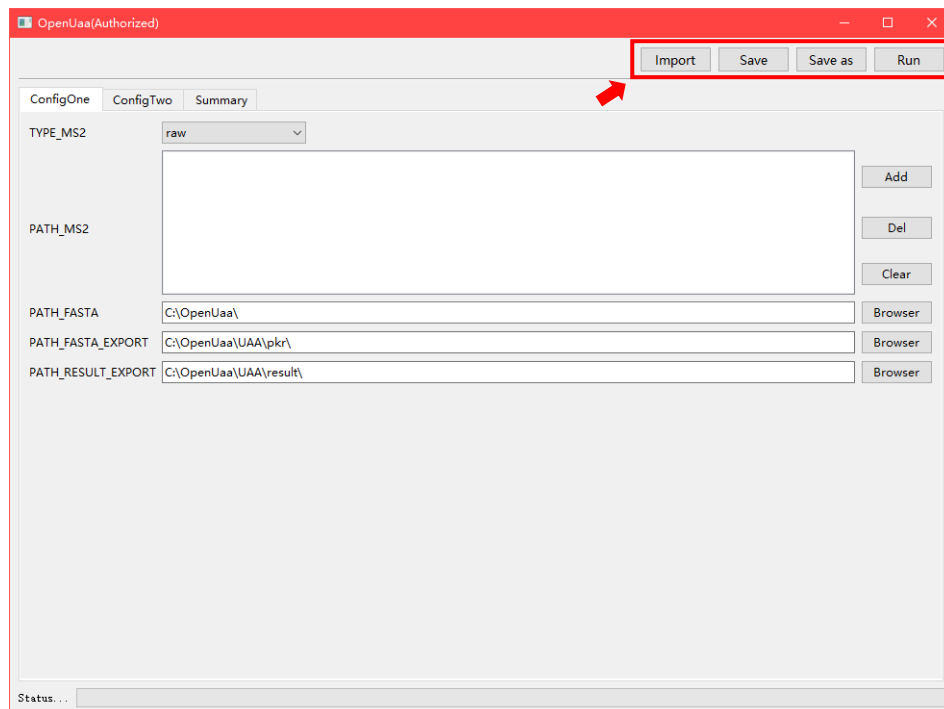


② Make sure that the computer has a good internet connection and register the software to get the license from the server, otherwise the registration operation will be failed. Input your username and email address, then click the “Submit” button.



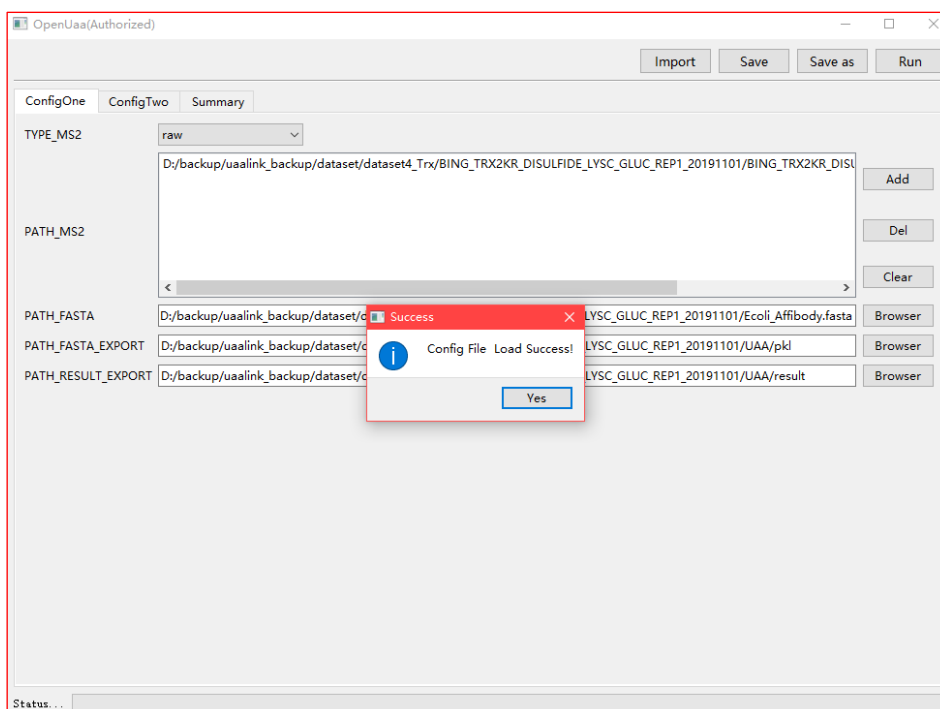
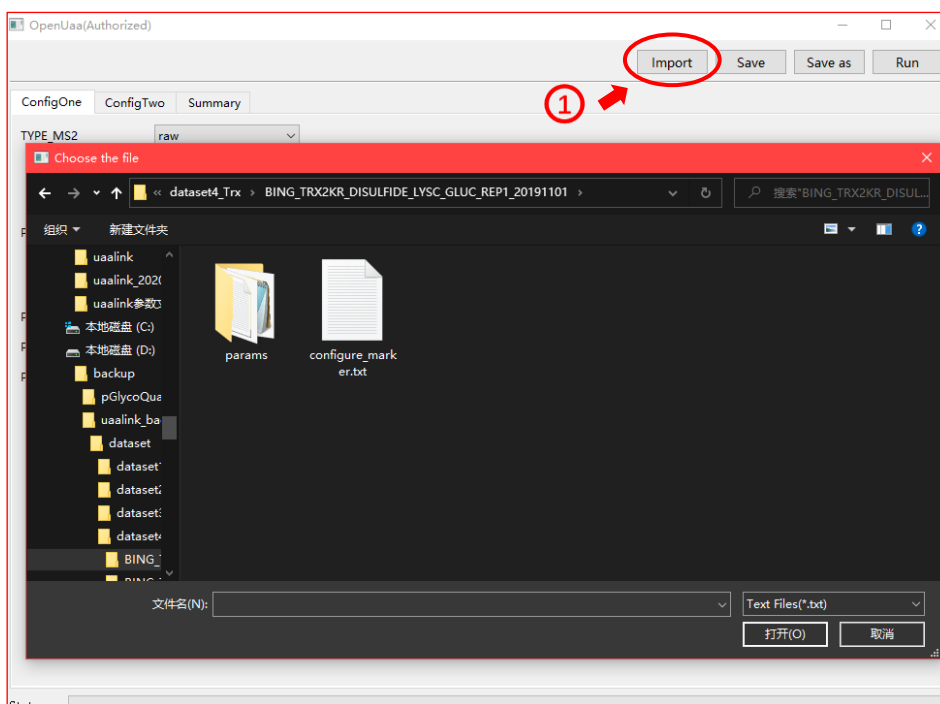


After Submitting the information, you can use the unlimited software.

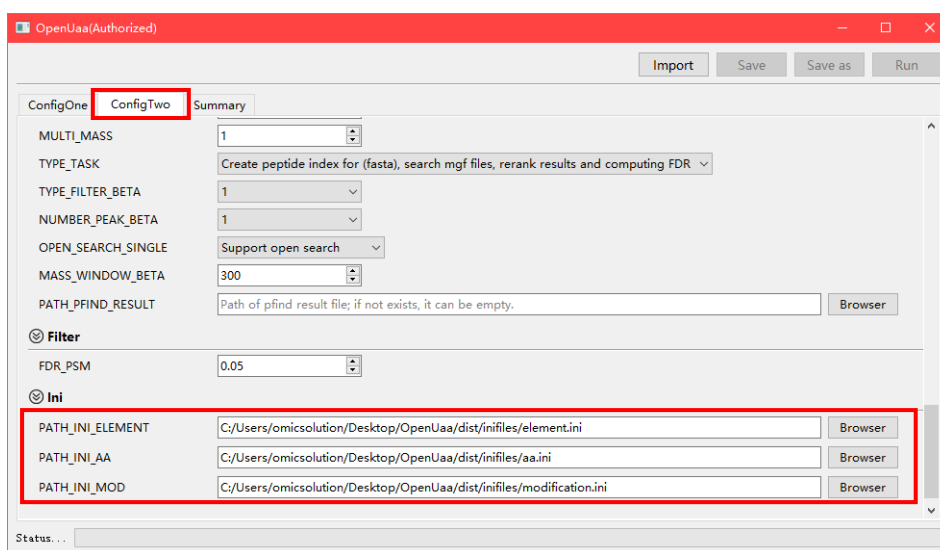
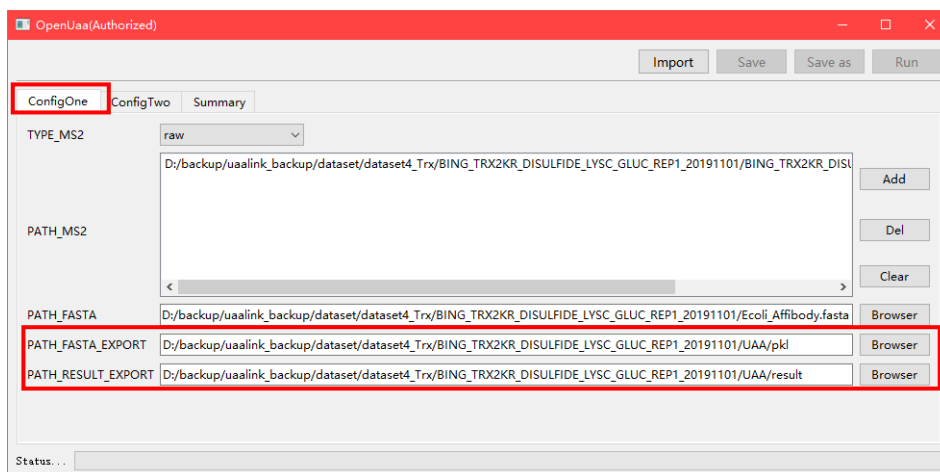


3.2 Run a raw file of the datasets with OpenUaa.

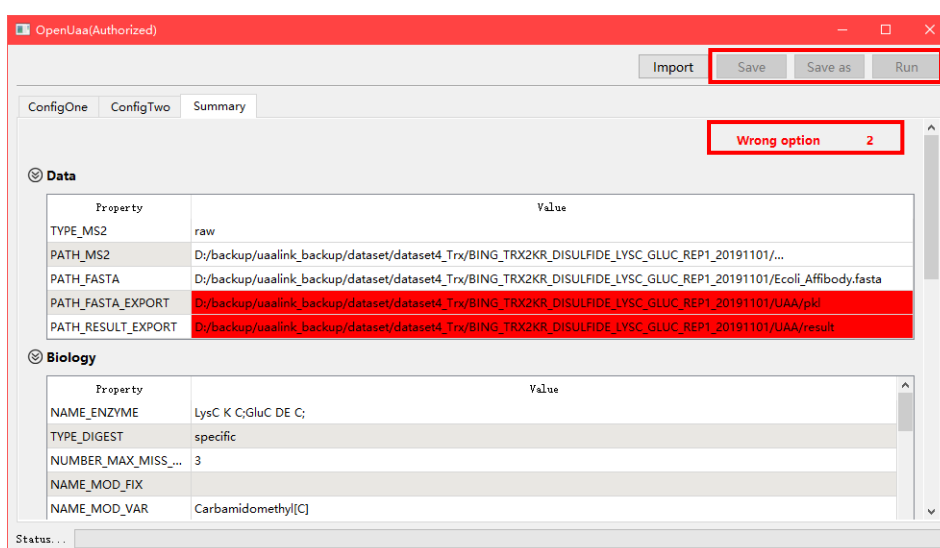
① Start the registered “OpenUaaUI.exe”, click the “Import” button and choose the “configure_marker.txt” from one folder of the datasets.

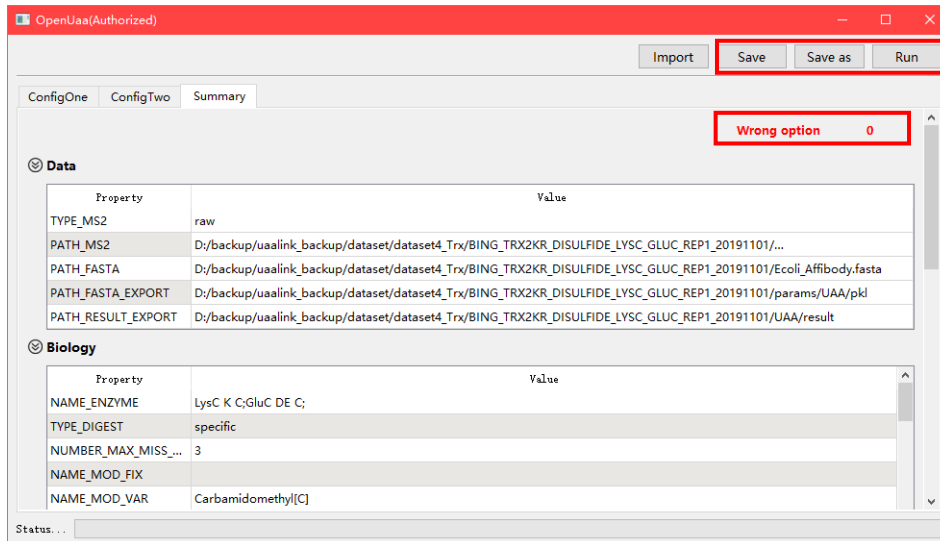


② Change the “PATH_FASTA_EXPORT” and “PATH_RESULT_EXPORT” in “ConfigOne” page and the “PATH_INI_ELEMENT”, “PATH_INI_AA”, “PATH_INI_MOD” at the bottom of “ConfigTwo” page, which will be different between computers. Also, you can change the options you want in the interface.



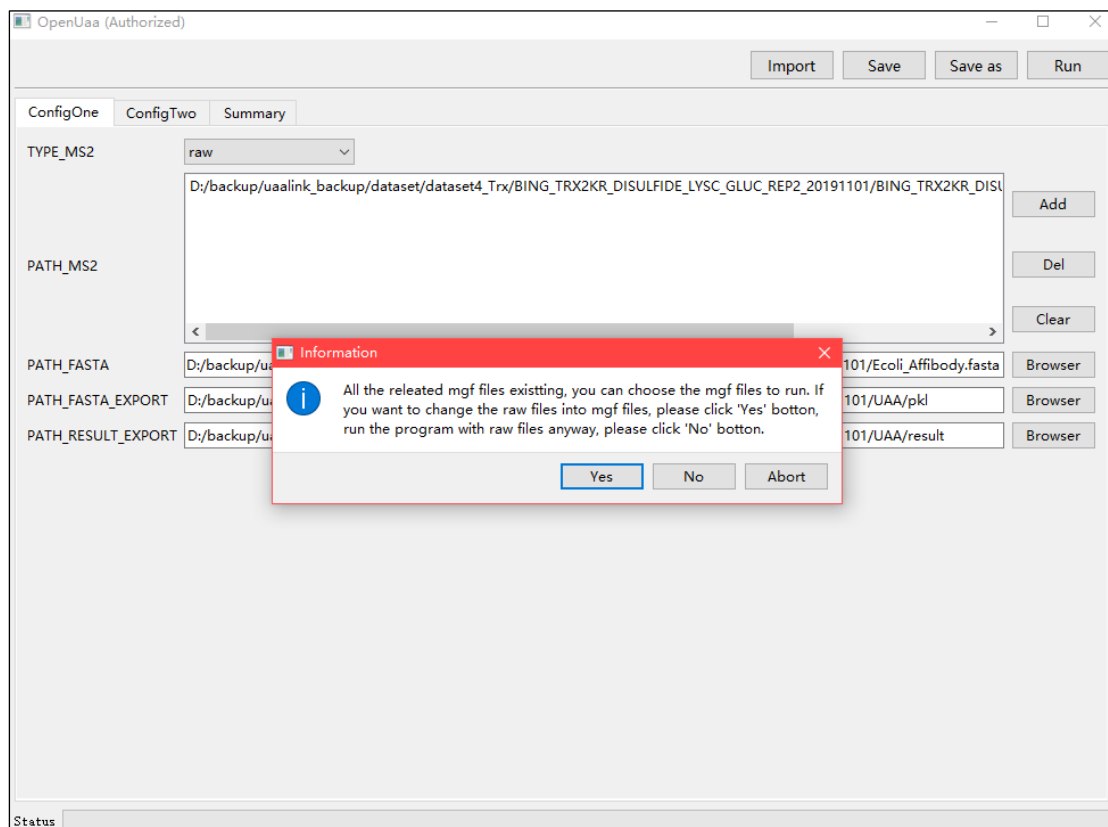
③ Click “Summary” and check the “Wrong option”, Only “0” can you click “Save”, “Save as” and “Run” buttons.





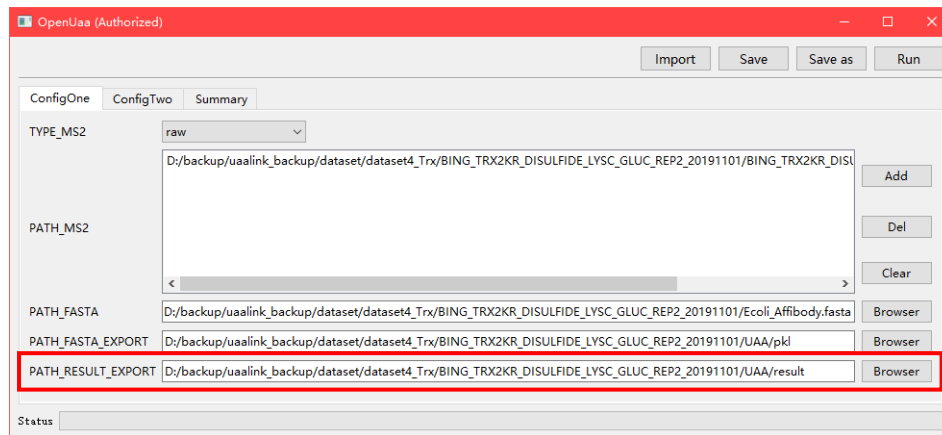
④ Before clicking the “Run” button, make sure to click “Save” or “Save as” button to save the configures you edited, otherwise the progress will be failed.

⑤ When “Run” button clicked, if there is a related “*.mgf” file exists in the same folder, you can choose to skip the first step(file conversion) and use the “*.mgf” file directly.

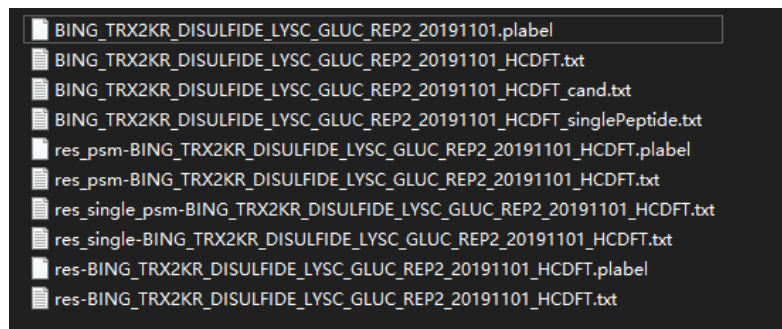


3.4 Results

Switch to the “PATH_RESULT_EXPORT” folder, the progress results are all showed here.



You can choose the result file you need.



Notes:

1. “*.plabel” is the label file of all results.
2. “*_HCDFT.txt” is a text file of all results, one spectrogram corresponds to one result, sorted by the score from high to low.
3. “*_HCDFT_cand.txt” is a text file of all results, one spectrogram keeps the first ten results.
4. “*_HCDFT_singlePeptide.txt” is a text file of all single-peptide results, one spectrogram retains one result.
5. “res_psm*.plabel” is the label file of the result of FDR filtering.
6. “res_psm*.txt” corresponds to the file 5, but the format is a text file.
7. “res_single_psm-*_HCDFT.txt ”: The result after FDR filtering (corresponding to the file 4).
8. “res_single*_HCDFT.txt”: In the open search for single peptides, only one result will be taken if the mass is within 0.5Da (the identification result of a certain mass range in file 7 is considered to be the same peptide).
9. “res-*.plabel” is the peptide level result of FDR filtering(De-redundant peptides in the file 5 and only keep the highest scored result).

10. "res-*.txt" corresponds to the file 9, but the format is a text file.