pGlycoQuant Manual

version.2021.12

Version: pGlycoQuant_V1.1

Release Date: 2021.11.19

Computer configuration

CPU: Intel or AMD processor with 64-bit support; 2.3 GHz or faster processor with at least 2 cores is recommended

RAM: 16G or higher is recommended

ROM: for one raw data (1G) 5G or higher is recommended

OS: Windows 10 (x64) or Windows 11 (x64)

Other: MSFileReader 3.0 Sp1 or higher is needed. If MSFileReader 3.0 has not been installed, please download MSFileReader.3.0.Sp1.zip and install it.

Description

At present, pFind, pGlyco, Byonic and MSFragger software glycosylation identification results can be used for quantification by pGlycoQuant.

Notes for running Byonic result

1. It is found that the name of mass spectrum data recorded by Byonic software is inconsistent with the original data, when running pGlycoQuant in Byonic mode, it should be guaranteed that the name of the mass spectrum data recorded in the Byonic result file is the same as that of the entered mass spectrum data.
2. Byonic glycosylation modification reliable results screening commonly used scores are Score and LogProb, rather than FDR. FDR cannot be modified on the pGlycoQuant interface. To modify B4_THRESHOLD_SCORE_BYONIC and B5_THRESHOLD_PROB_BYONIC in the config file (default: 200 and 2, indicating score≥200 and absolute value of LogProb ≥2).
3. Byonic ini files are required for quantification, in the ./ini/ini_Byonic directory.

Notes for running MSFragger result

MSFragger ini files are required for quantification, in the ./ini/ini_MSFragger directory.

Cite us

Weiqian Cao, et. al. pGlycoQuant with a deep residual network for precise and minuscule-missing-value quantitative glycoproteomics enabling the functional exploration of site-specific glycosylation. bioRxiv 2021.11.15.468561.
doi: https://doi.org/10.1101/2021.11.15.468561

CONTENTS

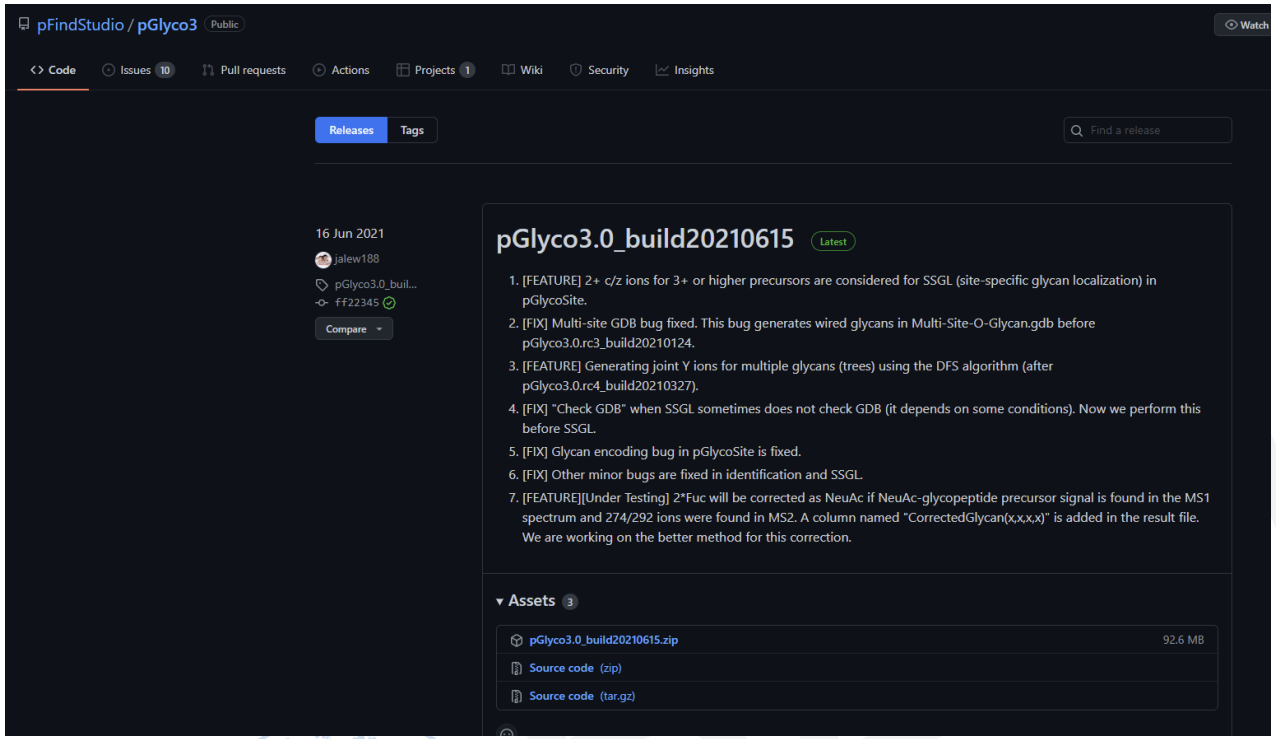
pGlyco & pGlycoQuant

Download and Regist

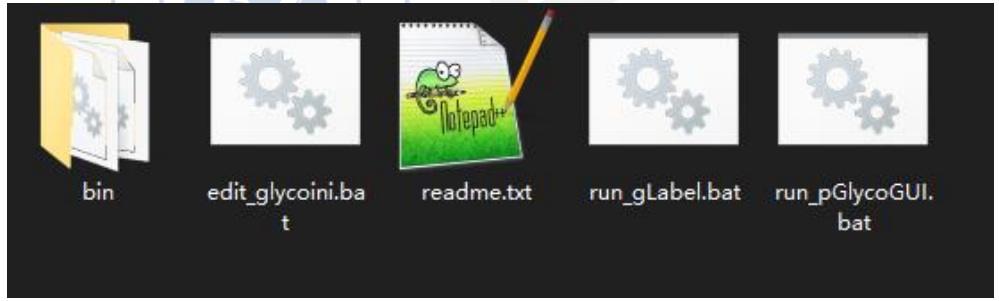
1 Identification with pGlyco

1.1 pGlyco download

①



② The unzipped pGlyco files.

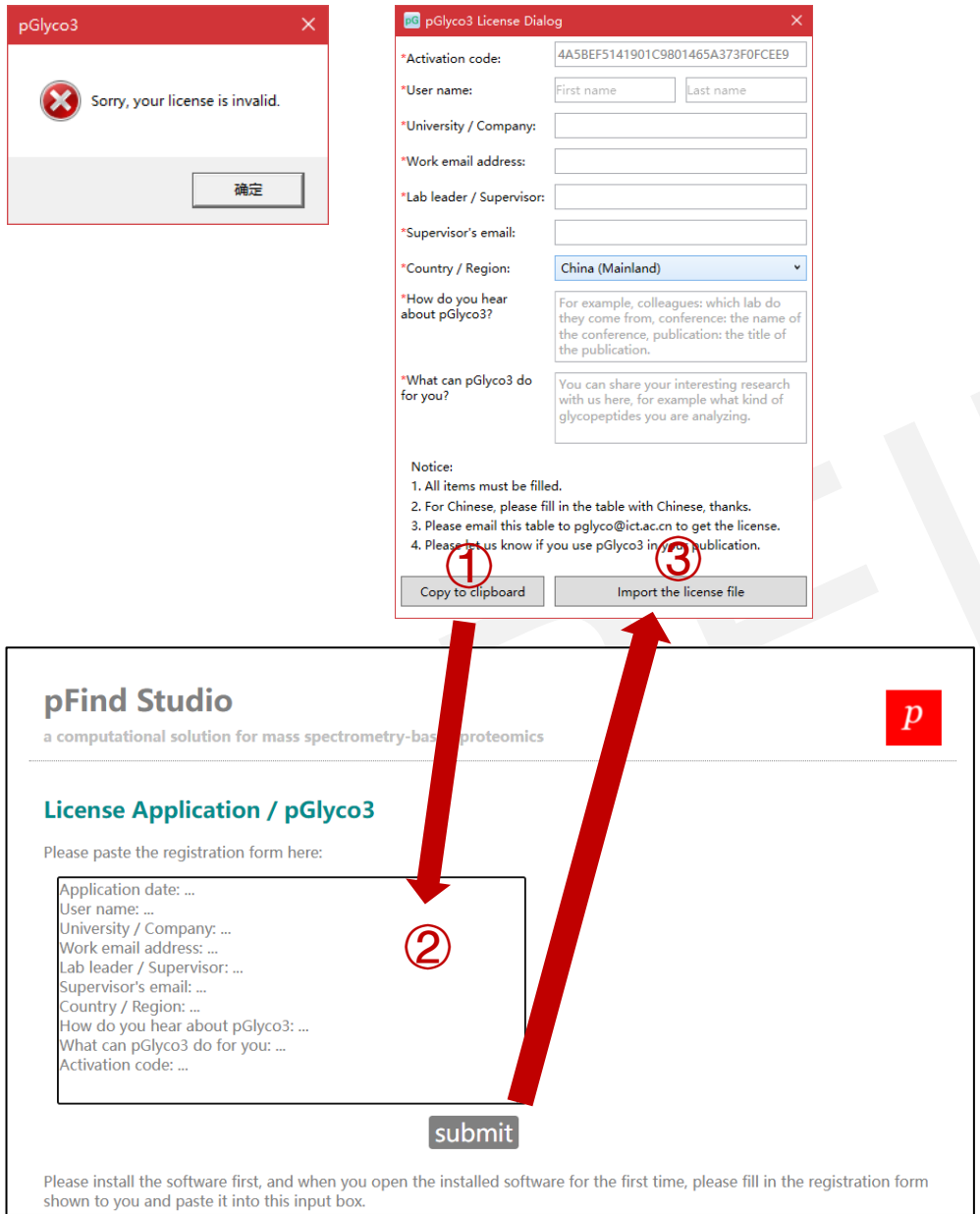


① Login https://github.com/pFindStudio/pGlyco3/releases and download the latest version at the top of the page.

② The unzipped pGlyco files.

1 Identification with pGlyco

1.2 pGlyco register



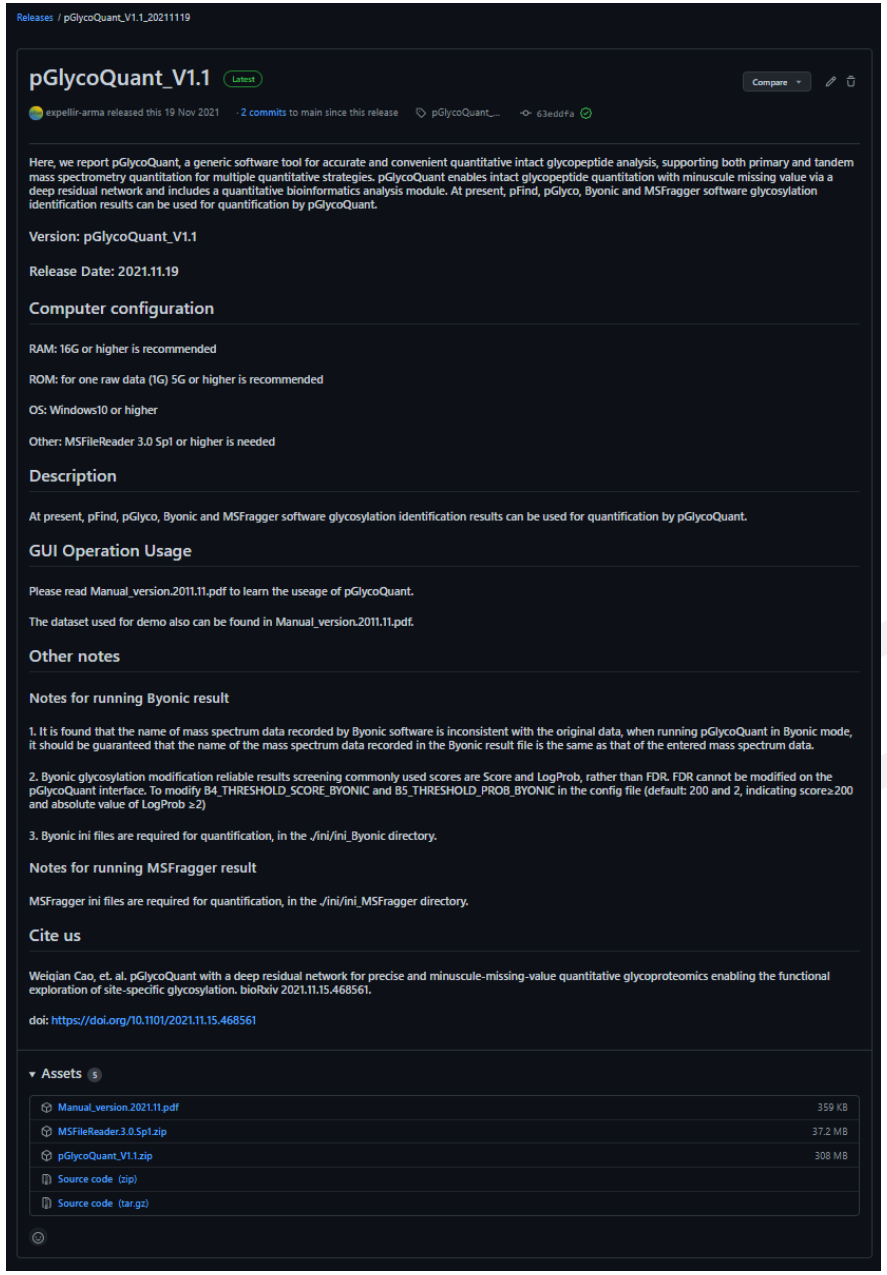
① Run **run_pGlycoGUI.bat**, fill in the forms, and then click **Copy to clipboard** button in the pGlyco3 License Dialog.

② Login http://i.pfind.org/license/pGlyco3, paste the information and **submit**.

③ Import the replied license (**pGlyco3.license**) file to the pGlyco3 License Dialog.

1 pGlycoQuant download

①



Releases / pGlycoQuant_V1.1_20211119

pGlycoQuant_V1.1

Latest

Compare

expellir-arma released this 19 Nov 2021 · 2 commits to main since this release · pGlycoQuant_... · 63eddfa

Here, we report pGlycoQuant, a generic software tool for accurate and convenient quantitative intact glycopeptide analysis, supporting both primary and tandem mass spectrometry quantitation for multiple quantitative strategies. pGlycoQuant enables intact glycopeptide quantitation with minuscule missing value via a deep residual network and includes a quantitative bioinformatics analysis module. At present, pFind, pGlyco, Byonic and MSFragger software glycosylation identification results can be used for quantification by pGlycoQuant.

Version: pGlycoQuant_V1.1

Release Date: 2021.11.19

Computer configuration

RAM: 16G or higher is recommended

ROM: for one raw data (1G) 5G or higher is recommended

OS: Windows10 or higher

Other: MSFileReader 3.0 Sp1 or higher is needed

Description

At present, pFind, pGlyco, Byonic and MSFragger software glycosylation identification results can be used for quantification by pGlycoQuant.

GUI Operation Usage

Please read Manual_version.2011.11.pdf to learn the useage of pGlycoQuant.

The dataset used for demo also can be found in Manual_version.2011.11.pdf.

Other notes

Notes for running Byonic result

1. It is found that the name of mass spectrum data recorded by Byonic software is inconsistent with the original data, when running pGlycoQuant in Byonic mode, it should be guaranteed that the name of the mass spectrum data recorded in the Byonic result file is the same as that of the entered mass spectrum data.

2. Byonic glycosylation modification reliable results screening commonly used scores are Score and LogProb, rather than FDR. FDR cannot be modified on the pGlycoQuant interface. To modify B4_THRESHOLD_SCORE_BYONIC and B5_THRESHOLD_PROB_BYONIC in the config file (default: 200 and 2, indicating score≥200 and absolute value of LogProb ≥2)

3. Byonic ini files are required for quantification, in the ./ini/ini_Byonic directory.

Notes for running MSFragger result

MSFragger ini files are required for quantification, in the ./ini/ini_MSFragger directory.

Cite us

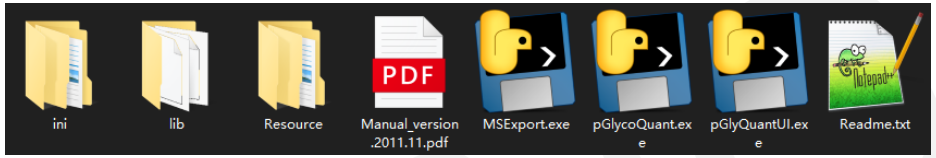
Weiqian Cao, et. al. pGlycoQuant with a deep residual network for precise and minuscule-missing-value quantitative glycoproteomics enabling the functional exploration of site-specific glycosylation. bioRxiv 2021.11.15.468561.

doi: https://doi.org/10.1101/2021.11.15.468561

▾ Assets 5

Manual_version.2021.11.pdf	359 KB
MSFileReader.3.0.Sp1.zip	37.2 MB
pGlycoQuant_V1.1.zip	308 MB
Source code (zip)	
Source code (tar.gz)	

②



① Login https://github.com/expellir-arma/pGlycoQuant/releases and download the latest version at the top of the page.

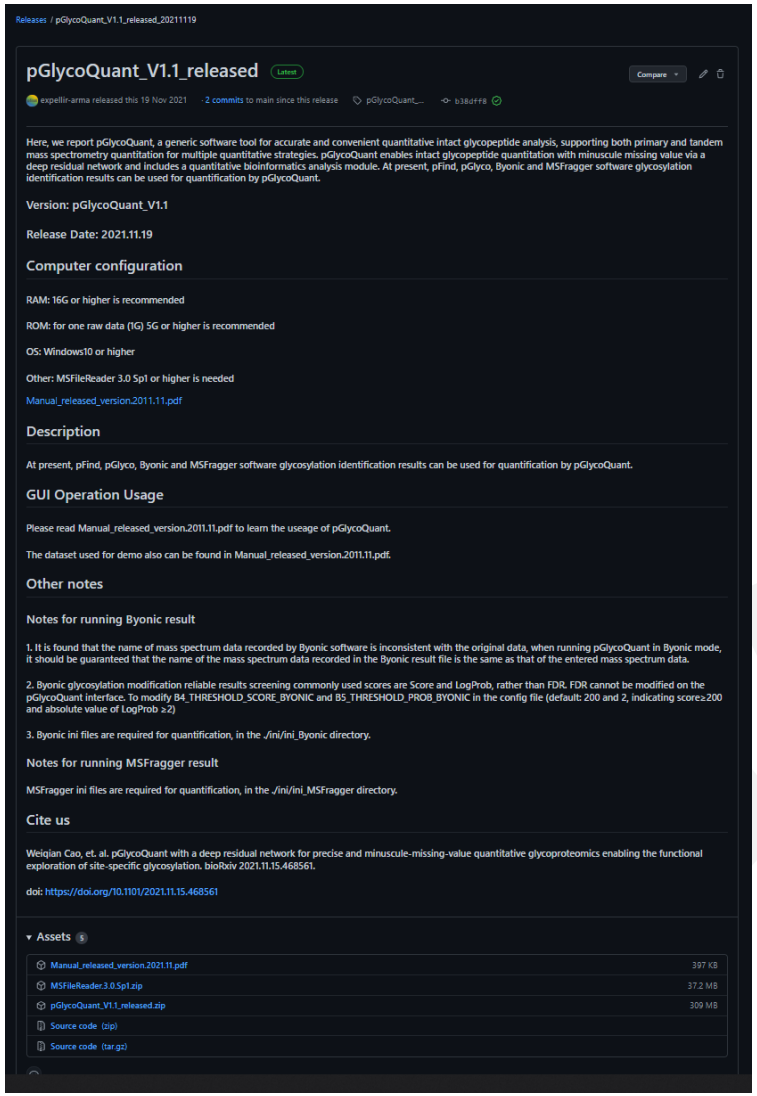
If MSFileReader 3.0 has not been installed, please download **MSFileReader.3.0.Sp1.zip** and install it.

② The unzipped pGlycoQuant files.

For editor

1 pGlycoQuant download

①



pGlycoQuant_V1.1_released

Here, we report pGlycoQuant, a generic software tool for accurate and convenient quantitative intact glycopeptide analysis, supporting both primary and tandem mass spectrometry quantitation for multiple quantitative strategies. pGlycoQuant enables intact glycopeptide quantitation with minuscule missing value via a deep residual network and includes a quantitative bioinformatics analysis module. At present, pFind, pGlyco, Byonic and MSFragger software glycosylation identification results can be used for quantification by pGlycoQuant.

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Computer configuration

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ROM: for one raw data (1G) 5G or higher is recommended

OS: Windows10 or higher

Other: MSFileReader 3.0 Sp1 or higher is needed

Manual_released_version.2011.11.pdf

Description

At present, pFind, pGlyco, Byonic and MSFragger software glycosylation identification results can be used for quantification by pGlycoQuant.

GUI Operation Usage

Please read Manual_released_version.2011.11.pdf to learn the useage of pGlycoQuant.

The dataset used for demo also can be found in Manual_released_version.2011.11.pdf.

Other notes

Notes for running Byonic result

1. It is found that the name of mass spectrum data recorded by Byonic software is inconsistent with the original data, when running pGlycoQuant in Byonic mode, it should be guaranteed that the name of the mass spectrum data recorded in the Byonic result file is the same as that of the entered mass spectrum data.

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3. Byonic ini files are required for quantification, in the ./ini/ini_Byonic directory.

Notes for running MSFragger result

MSFragger ini files are required for quantification, in the ./ini/ini_MSFragger directory.

Cite us

Weiqian Cao, et. al. pGlycoQuant with a deep residual network for precise and minuscule-missing-value quantitative glycoproteomics enabling the functional exploration of site-specific glycosylation. bioRxiv 2021.11.15.468561.

doi: https://doi.org/10.1101/2021.11.15.468561

Assets

Manual_released_version.2021.11.pdf 397 KB

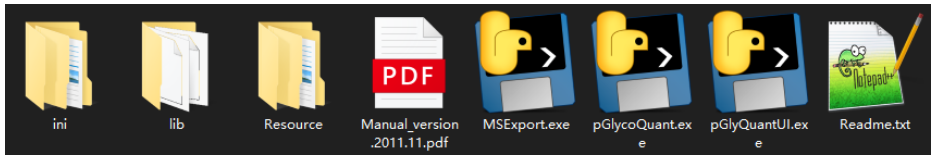
MSFileReader.3.0.Sp1.zip 37.2 MB

pGlycoQuant_V1.1_released.zip 309 MB

Source code (zip)

Source code (tar.gz)

②



① Login https://github.com/expellir-arma/pGlycoQuant_V1.1_released/releases and download **pGlycoQuant_V1.1_released.zip** at the bottom of this page.

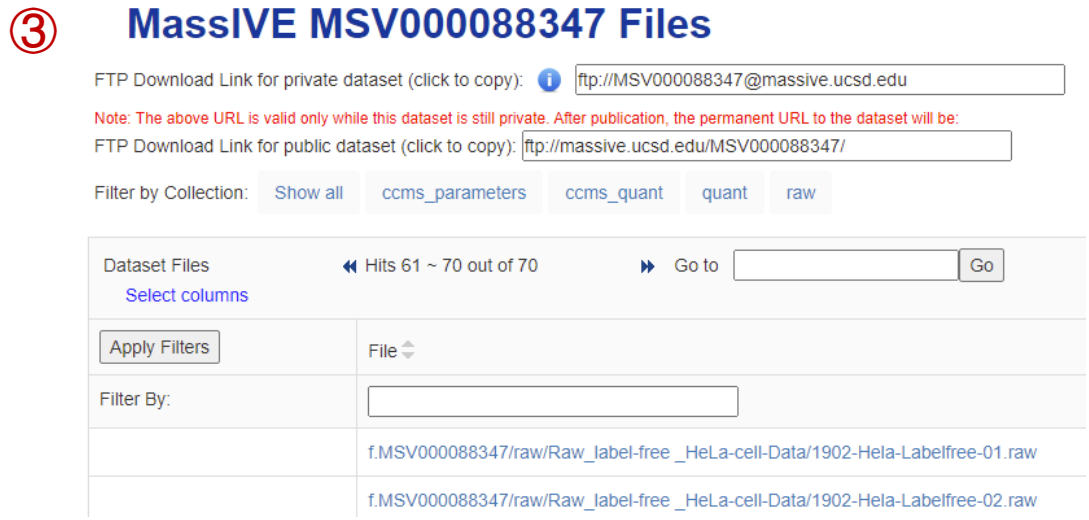
If MSFileReader 3.0 has not been installed, please download **MSFileReader.3.0.Sp1.zip** and install it.

② The unzipped pGlycoQuant files.

③ The dataset to test the software could be downloaded from MassIVE (https://massive.ucsd.edu/) with identifier MSV000088347. The login name of the dataset's web page (including title, description, and metadata) is MSV000088347_reviewer and password is a.

For Label Freedata, the dataset ftp://massive.ucsd.edu/raw/Raw_label-free%20_HeLa-cell-Data/1902-Hela-Labelfree-01.raw and 1902-Hela-Labelfree-02.raw could be used for testing.

③



MassIVE MSV000088347 Files

FTP Download Link for private dataset (click to copy): ftp://MSV000088347@massive.ucsd.edu

Note: The above URL is valid only while this dataset is still private. After publication, the permanent URL to the dataset will be:

FTP Download Link for public dataset (click to copy): ftp://massive.ucsd.edu/MSV000088347/

Filter by Collection: Show all | ccms_parameters | ccms_quant | quant | raw

Dataset Files | Hits 61 ~ 70 out of 70 | Go to | Go

Select columns

Apply Filters | File

Filter By:

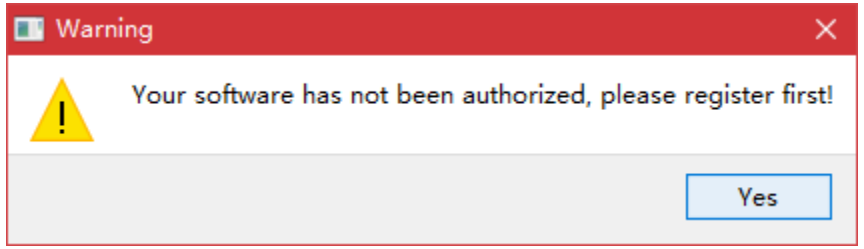
f.MSV000088347/raw/Raw_label-free _HeLa-cell-Data/1902-Hela-Labelfree-01.raw

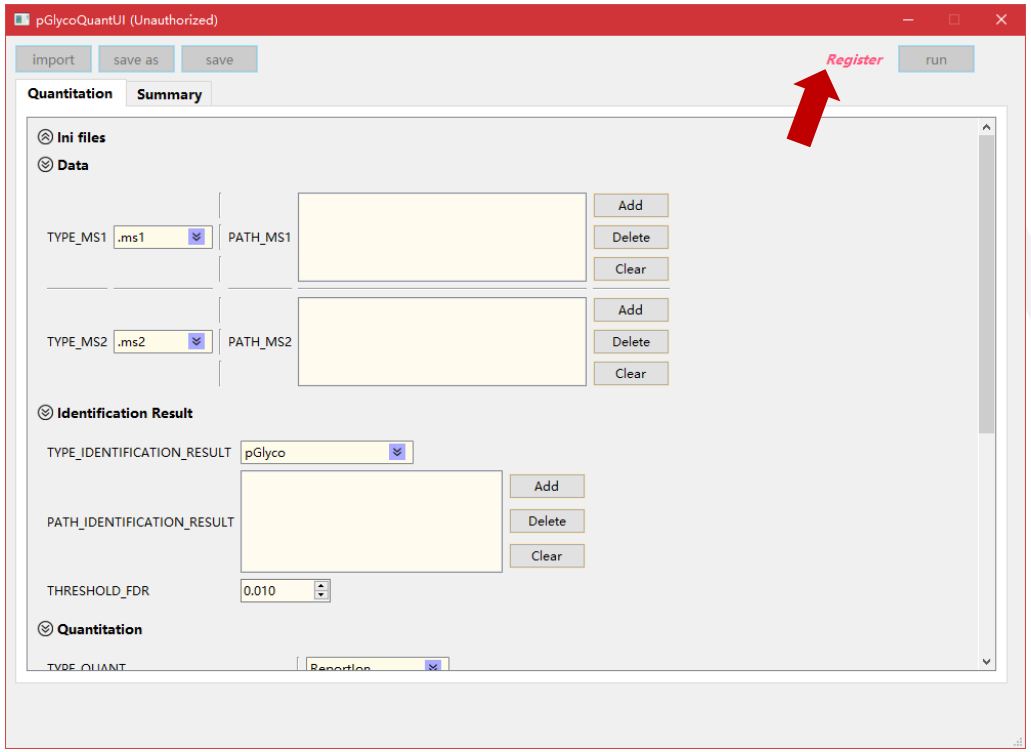
f.MSV000088347/raw/Raw_label-free _HeLa-cell-Data/1902-Hela-Labelfree-02.raw

2 Quantitation with pGlycoQuant

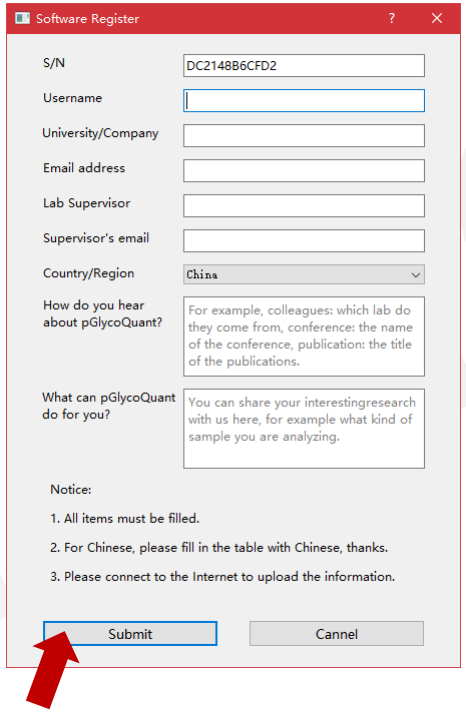
2.2 pGlycoQuant register

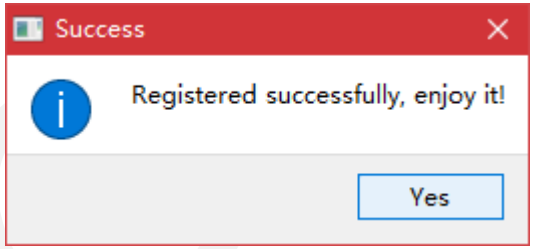
①





②





① Double click **pGlycoQuantUI.exe**, if software has not been authorized, click **Register** button, before that, make sure that your PC is linked to the Internet.

② Fill the register information and click **Submit**, then pGlycoQuant will be authorized.

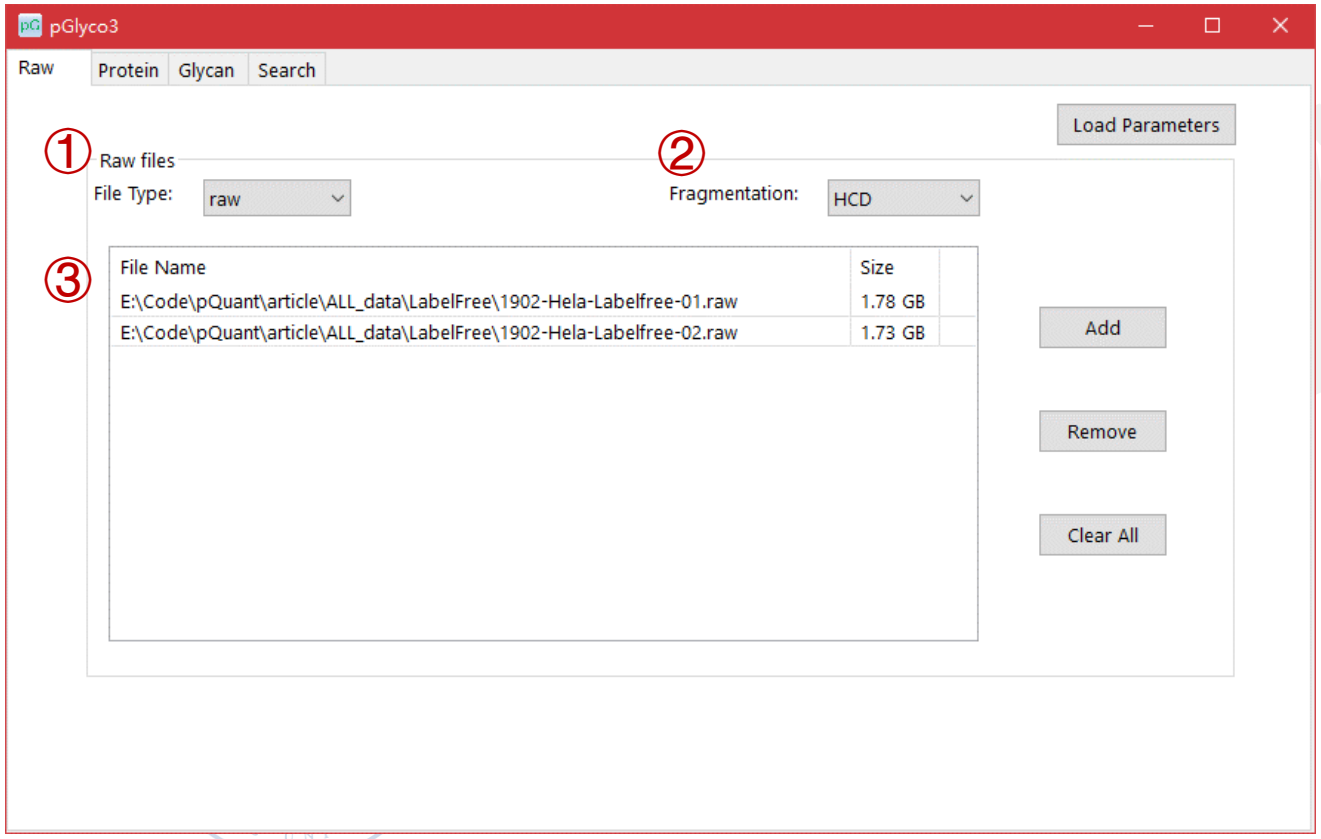
pGlyco & pGlycoQuant

Manual for DDA Label Free Data

1 Identification with pGlyco

1.1 pGlyco identification

Label Free



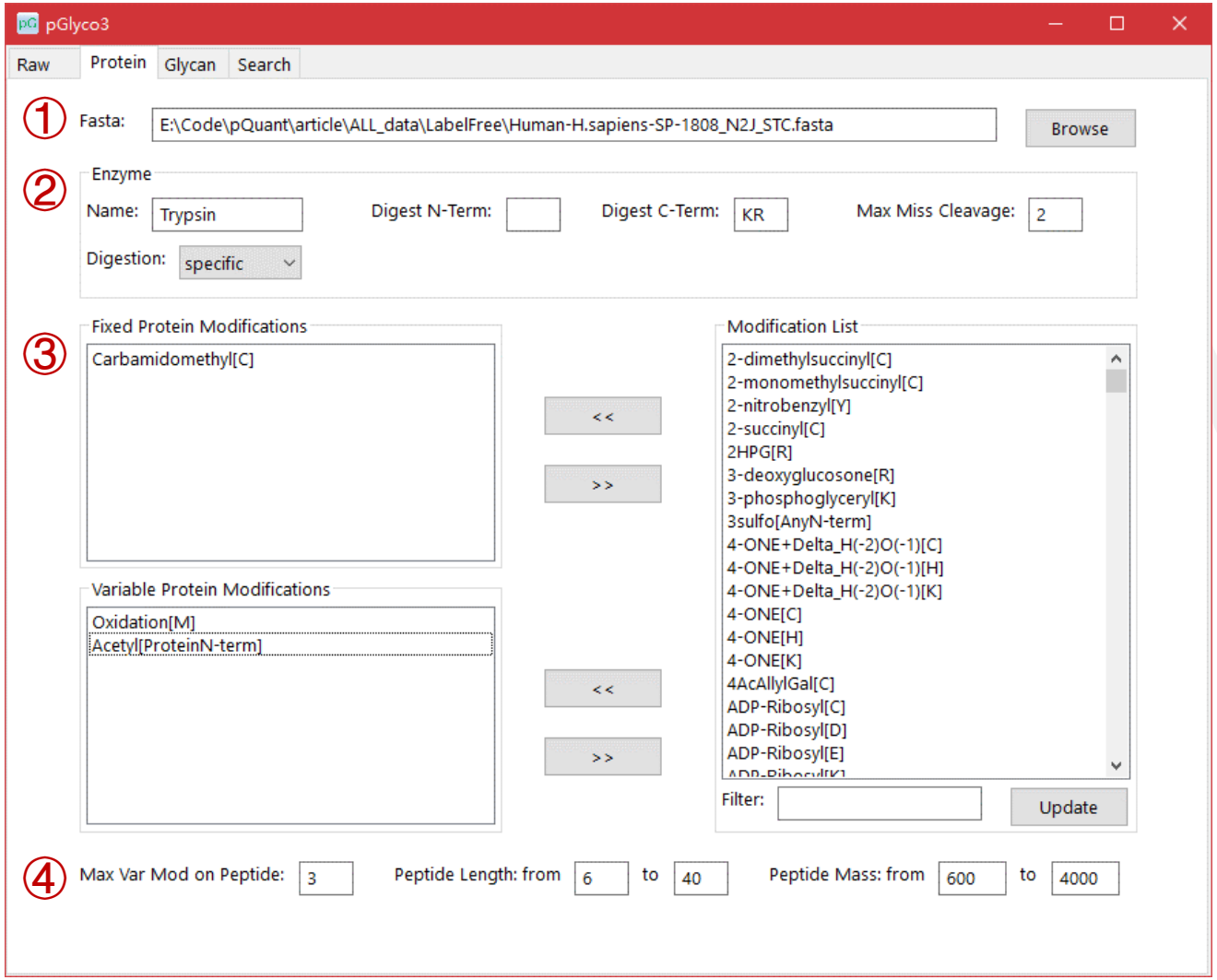
① Load raw files.

② Set the **Fragmentation** as **HCD**.

③ Add the **Label Free** file.

1 Identification with pGlyco

1.1 pGlyco identification



① Set the fasta database (The file could be downloaded from https://github.com/expellir-arma/pGlycoQuant/).

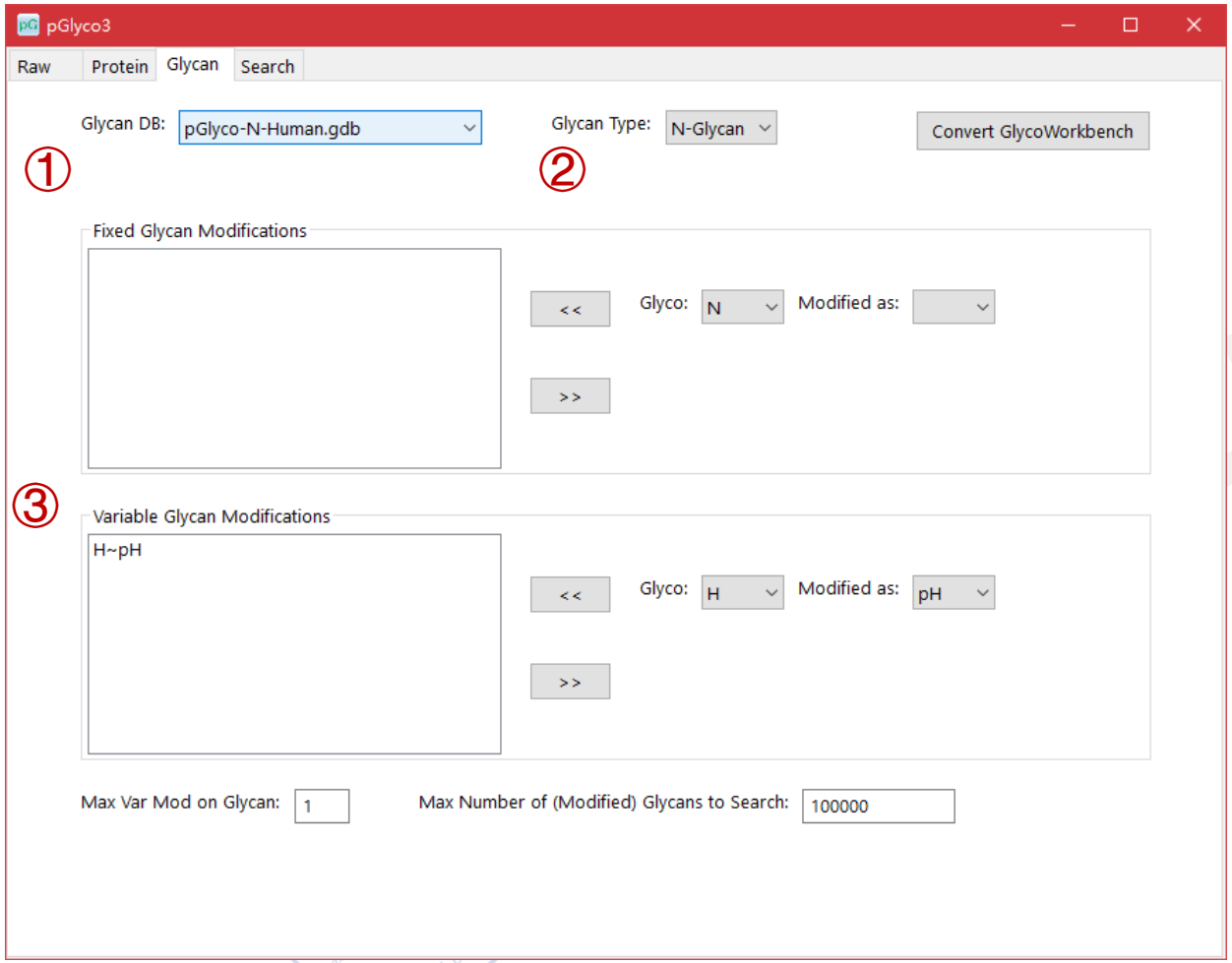
② Set the trypsin enzyme.

③ Set the fixed modification as Carbamidomethyl on Cys site. Set the variable modification as Acetyl on Protein N-Term and Oxidation on Met site.

④ Set the filter information.

1. Identification with pGlyco

Label Free



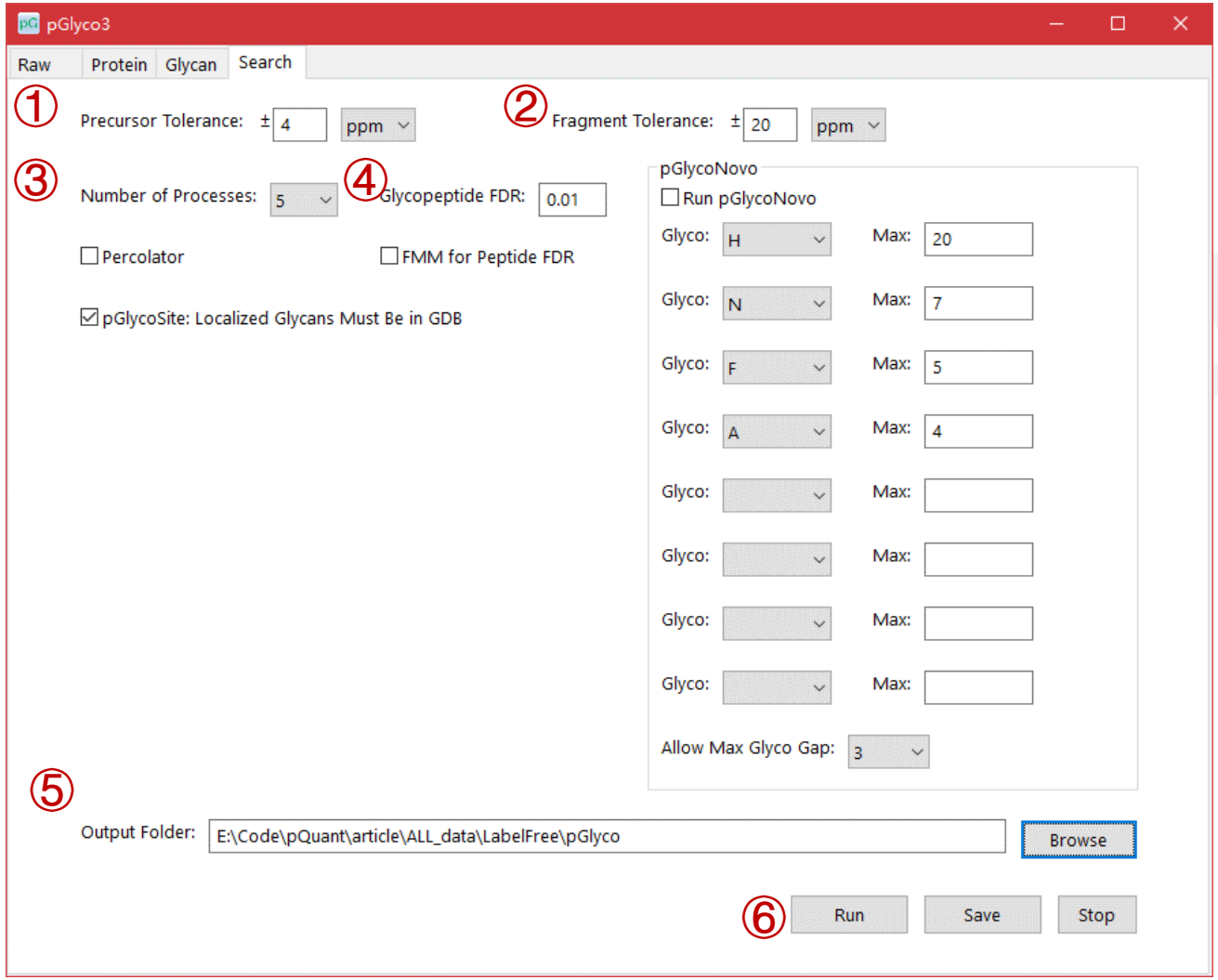
① Set the **Glycan DB** as **pGlyco-N-Human.gdb**.

② Set the **Glycan Type** as **Glycan**.

③ Set the Glycan modification information.

1 Identification with pGlyco

1.1 pGlyco identification



① Set the **Precursor Tolerance** as ±**4** ppm.

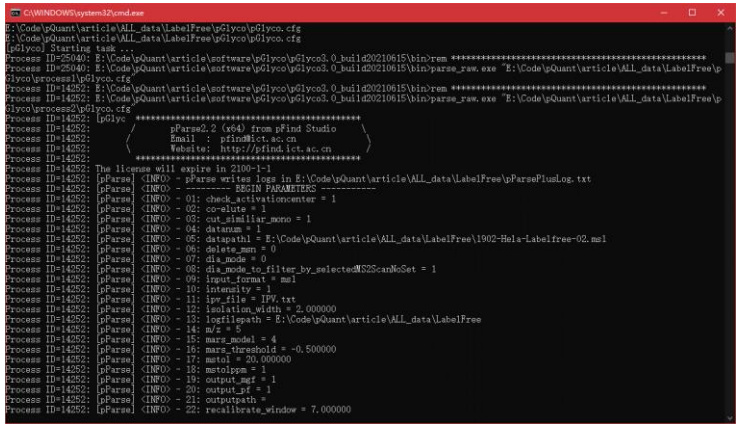
② Set the **Fragment Tolerance** as ±**20** ppm.

③ Set the **Number of Processes** according to your PC.

④ Set the **Glycopeptide FDR** as **0.01**.

⑤ Set the **Output Folder** for saving the identification results.

⑥ Click **Save** and **Run** buttons, the progress information will be shown in the command-line interface.

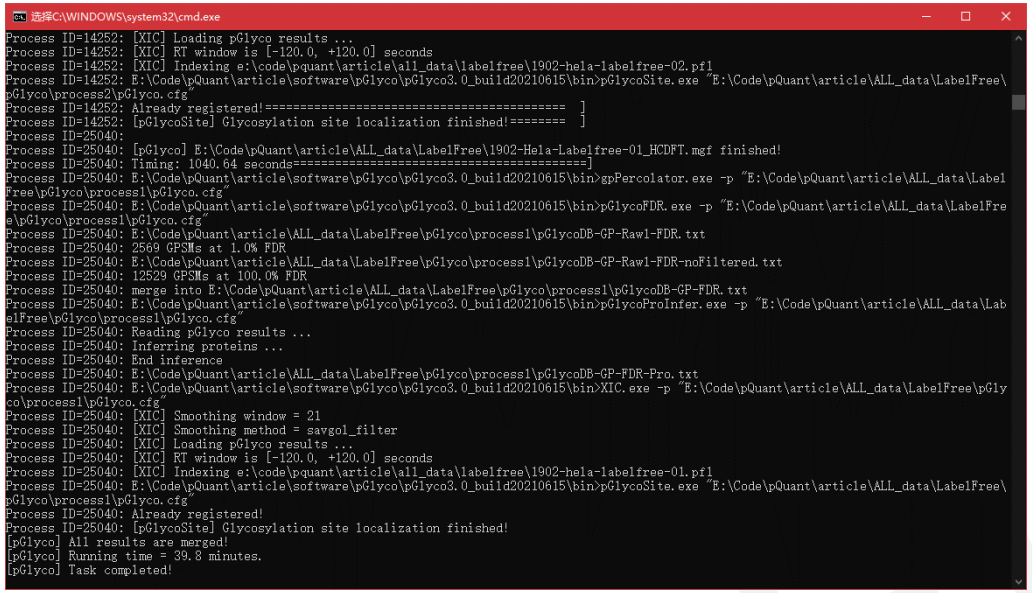


1 Identification with pGlyco

1.2 identification results

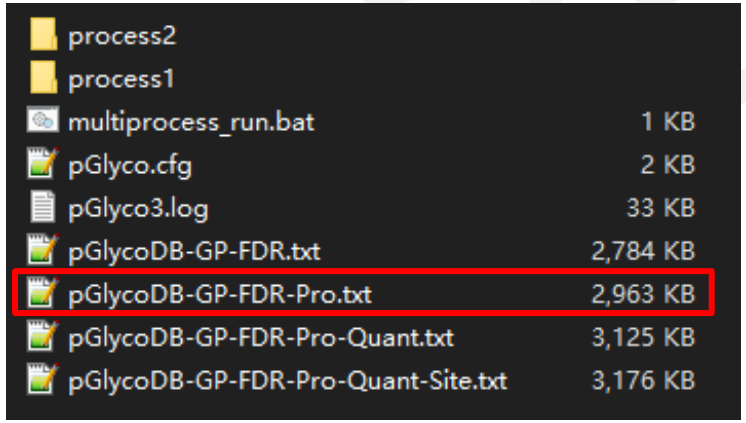
Label Free

①



②

③



① The completed information in the command-line interface.

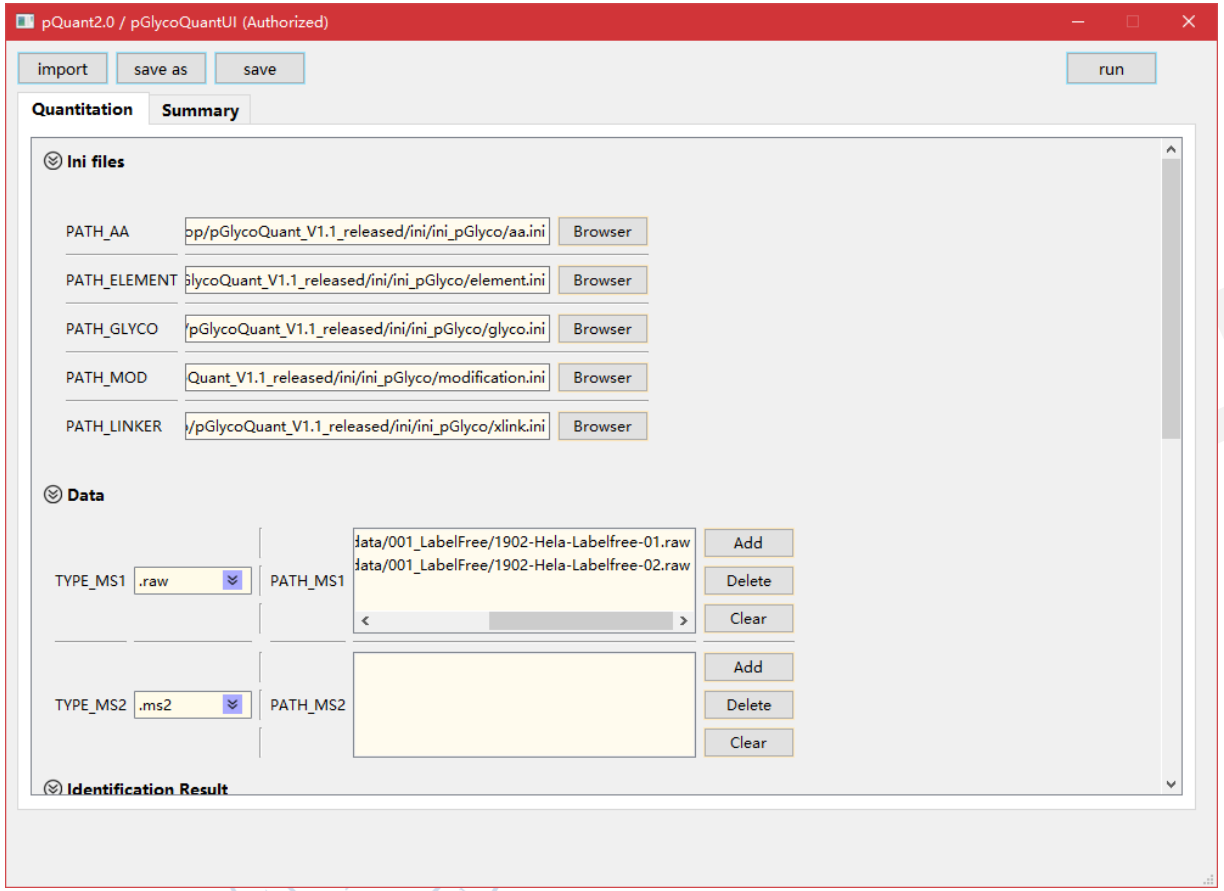
② The identification results.

③ The identification result file used for quantitation.

2 Quantitation with pGlycoQuant

2.1 pGlycoQuant quantitation

Label Free



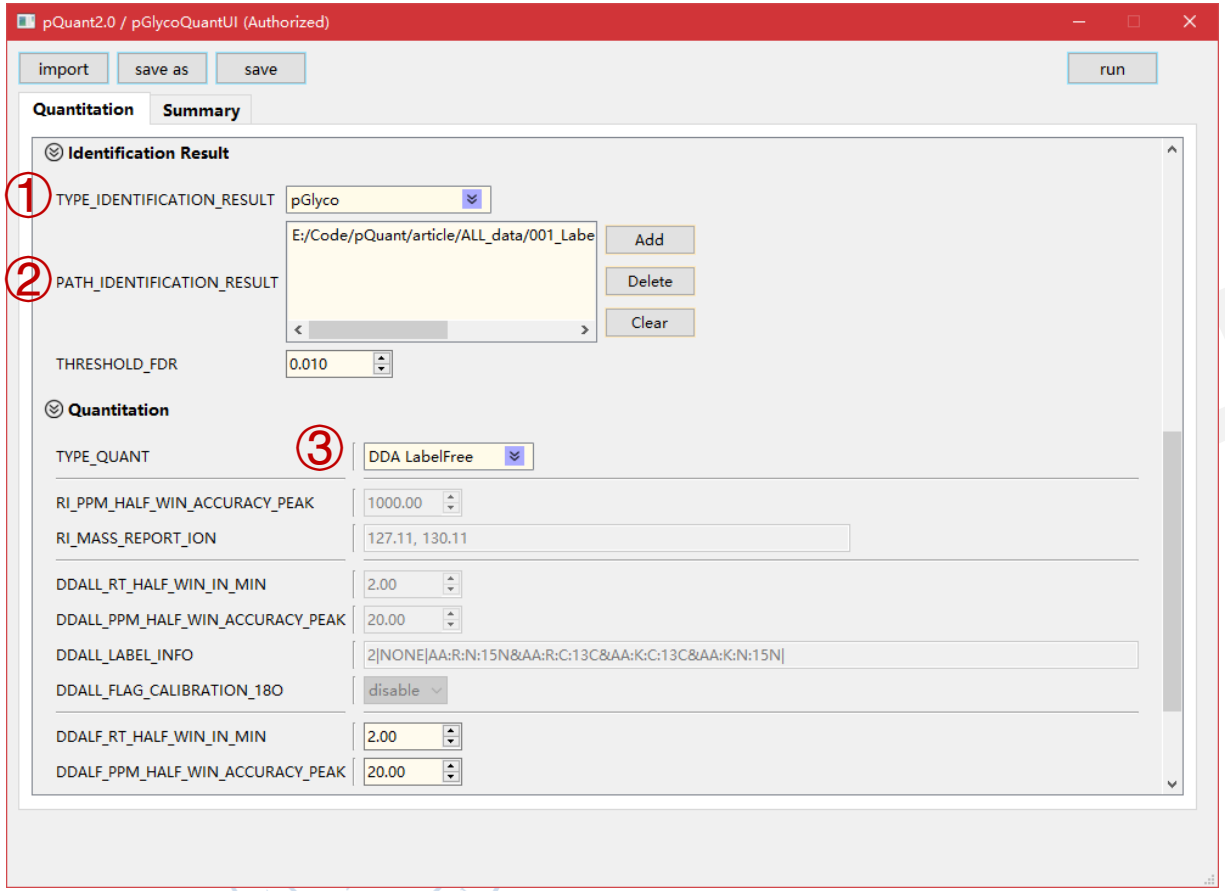
① Ensure that the ini file paths are valid.

② Set the TYPE_MS1 as .raw and fill the raw files into the PATH_MS1 blank.

2 Quantitation with pGlycoQuant

2.1 pGlycoQuant quantitation

Label Free



① Set **TYPE_IDENTIFICATION_RESULT** as **pGlyco** (For other identification software results like Byonic and MSFragger, Byonic and MSFragger glyco-N options also can be chosen).

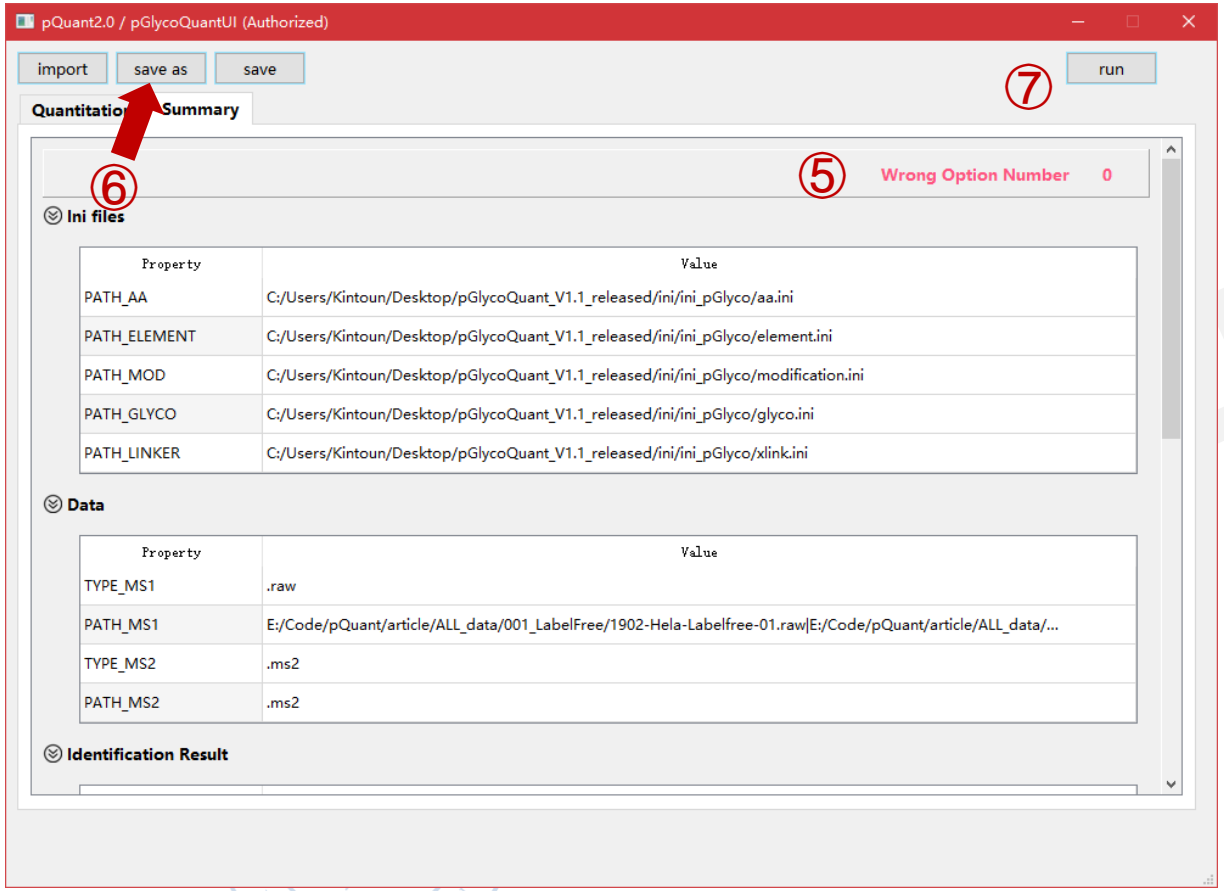
② Put the identification result file **pGlycoDB-GP-FDR-Pro.txt** here and set **FDR** as **0.01**.

③ Set **TYPE_QUANT** as **DDA LabelFree**.

④ Set the Output Folder for saving the quantitation results.

2 Quantitation with pGlycoQuant

2.1 pGlycoQuant quantitation

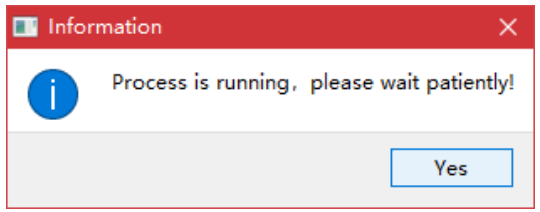


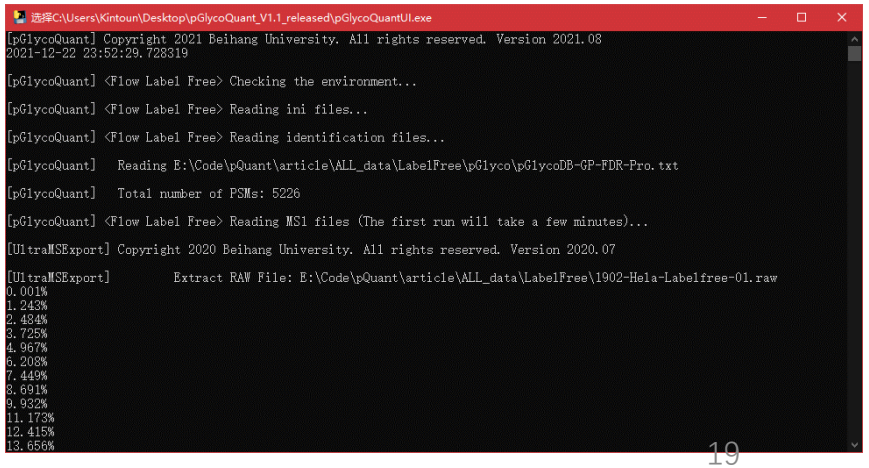
⑤ Click **Summary** button and make sure that the **Wrong Option Number** is **0**.

⑥ Then click **save as** button to save the config file.

⑦ Click **run** button to start the quantitation, the progress information will be shown in the command-line interface.

⑦



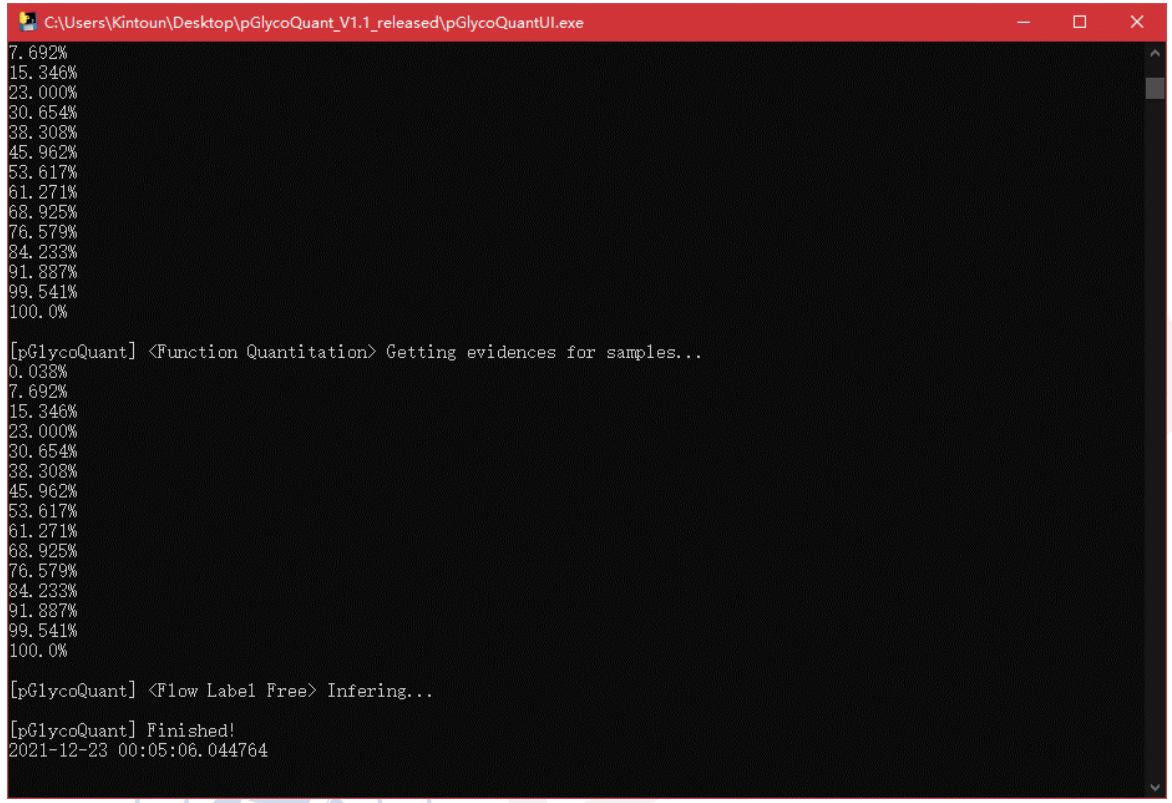


2 Quantitation with pGlycoQuant

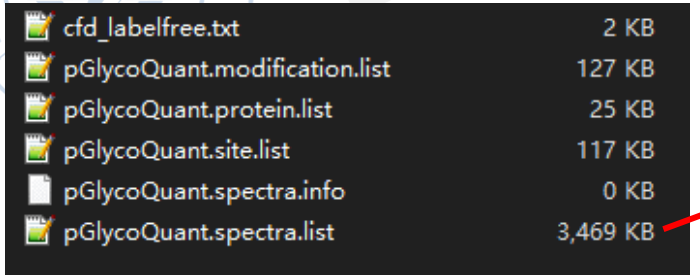
2.2 quantitation results

Label Free

①

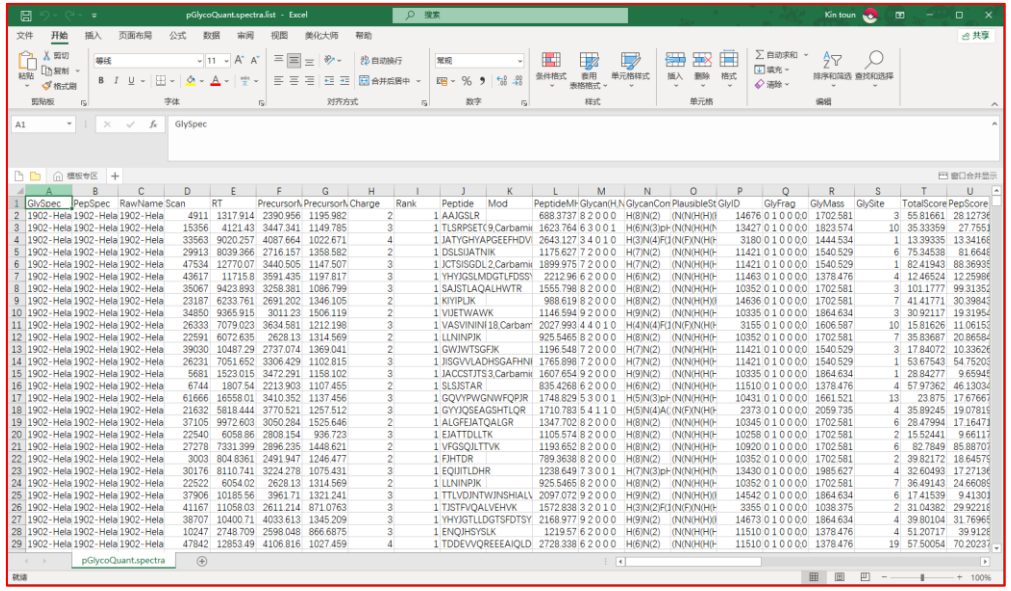


②



① The completed information.

② The quantitation results. Please open the files with Excel.

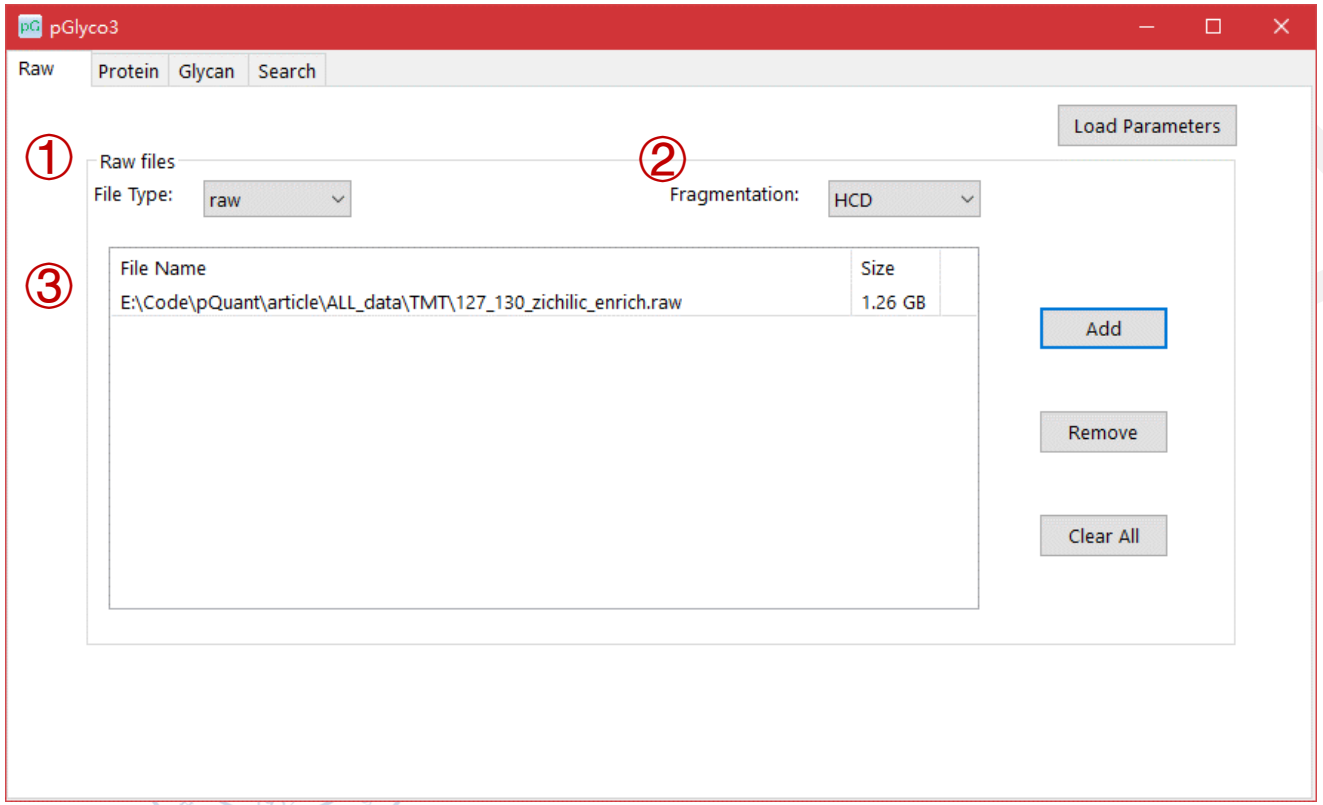


pGlyco & pGlycoQuant

Manual for TMT Data

1. Identification with pGlyco

TMT



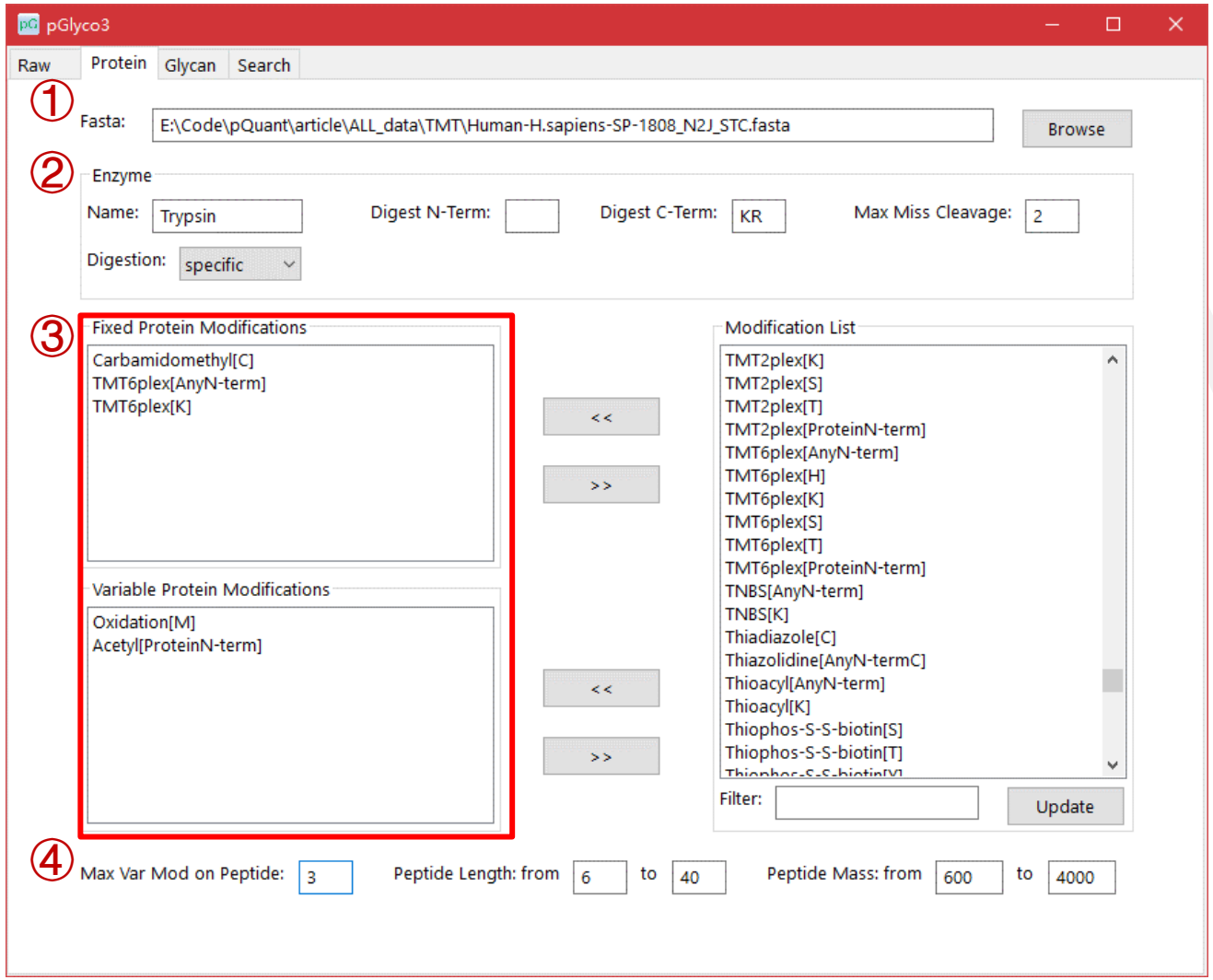
① Load raw files.

② Set the **Fragmentation** as **HCD**.

③ Add the **TMT** raw file.

1. Identification with pGlyco

TMT



① Set the fasta database (The file could be downloaded from https://github.com/expellir-arma/pGlycoQuant/).

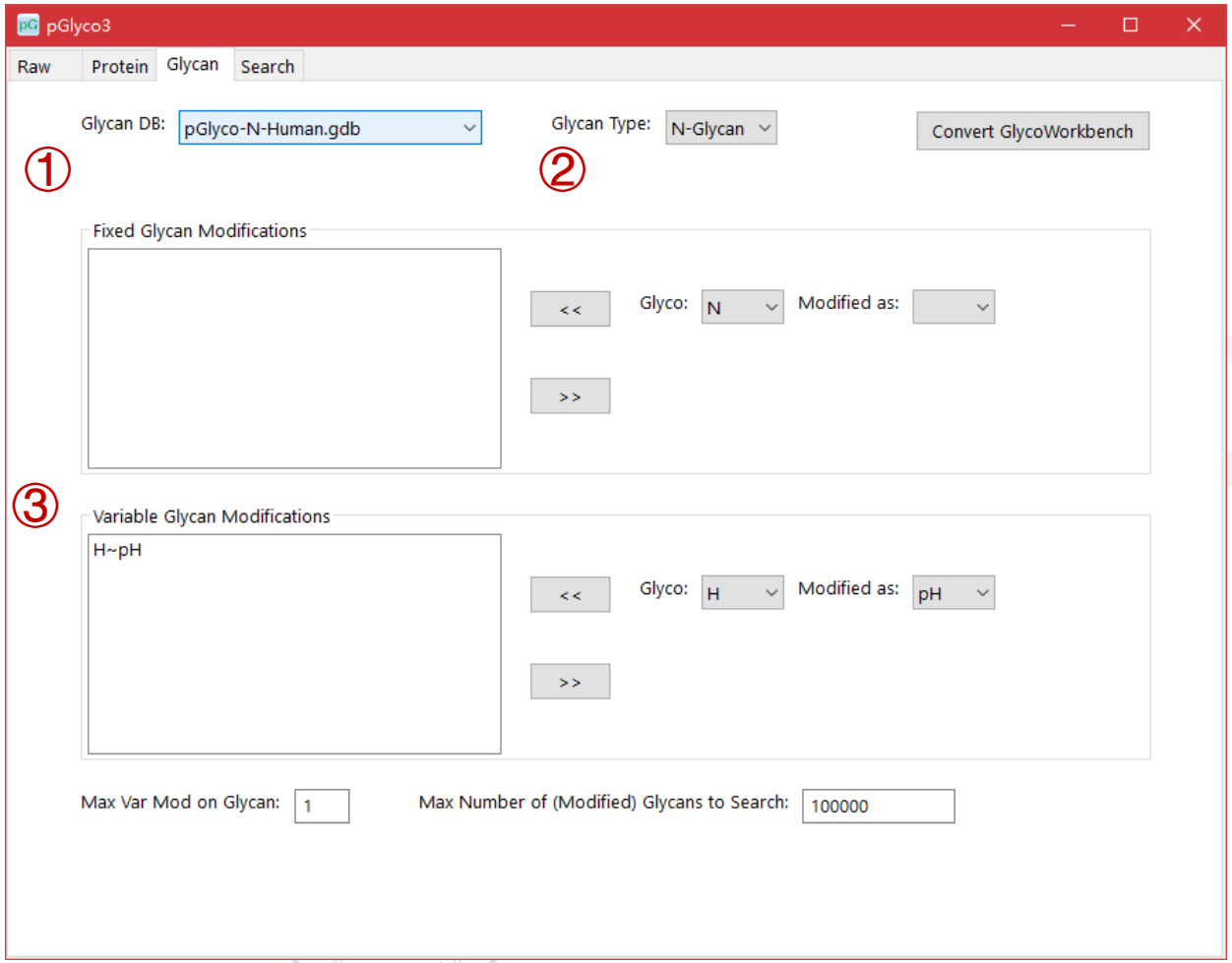
② Set the trypsin enzyme.

③ Set the modification information like the left panel.

④ Set the filter information.

1. Identification with pGlyco

TMT



① Set the **Glycan DB** as **pGlyco-N-Human.gdb**.

② Set the **Glycan Type** as **Glycan**.

③ Set the Glycan modification information.

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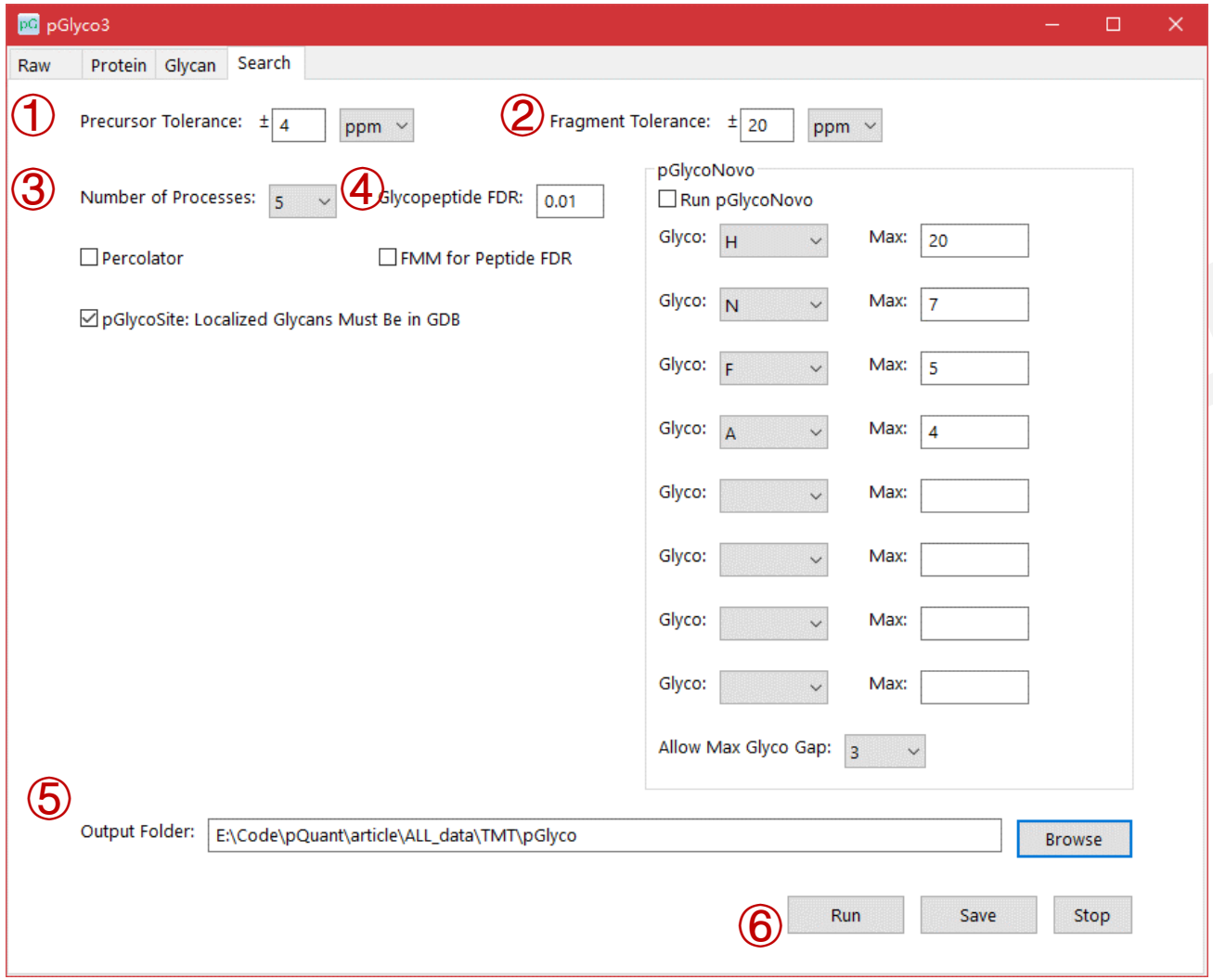


① Set the **Precursor Tolerance** as ±**4** ppm.

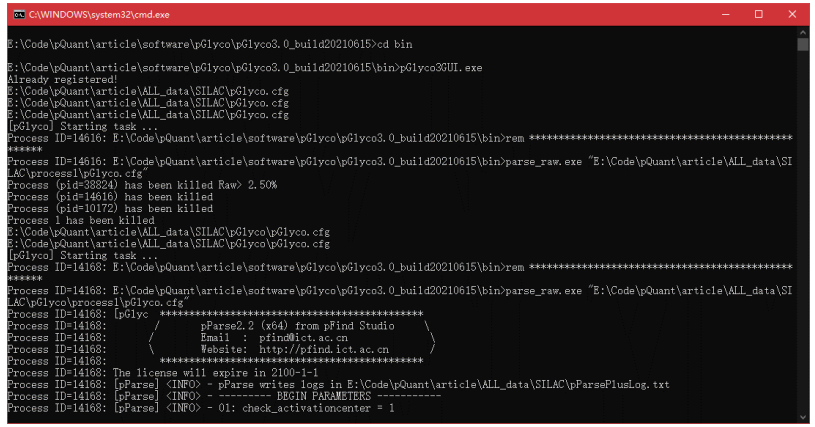
② Set the **Fragment Tolerance** as ±**20** ppm.

③ Set the **Number of Processes** according to your PC.

④ Set the **Glycopeptide FDR** as **0.01**.

⑤ Set the **Output Folder** for saving the identification results.

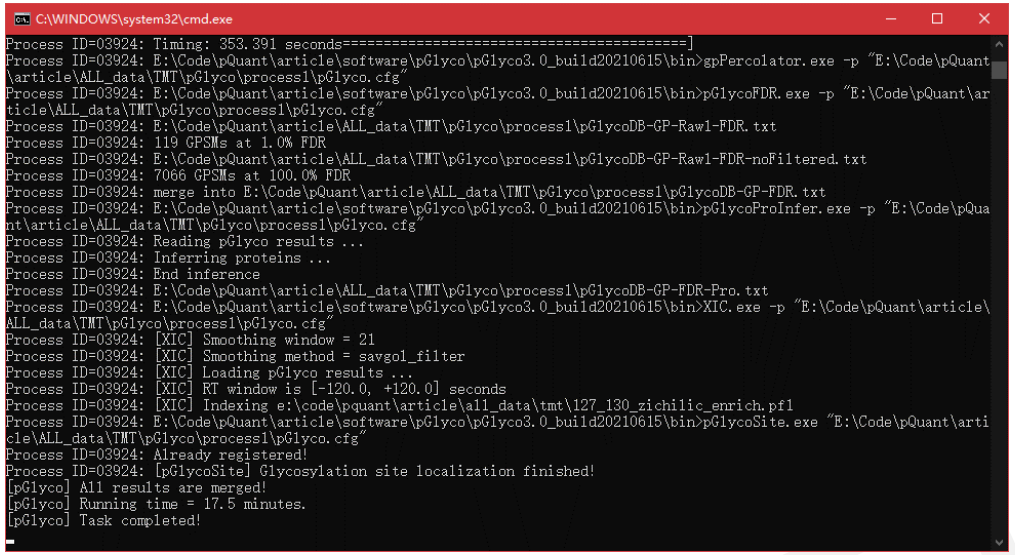
⑥ Click **Save** and **Run** buttons, the progress information will be shown in the command-line interface.



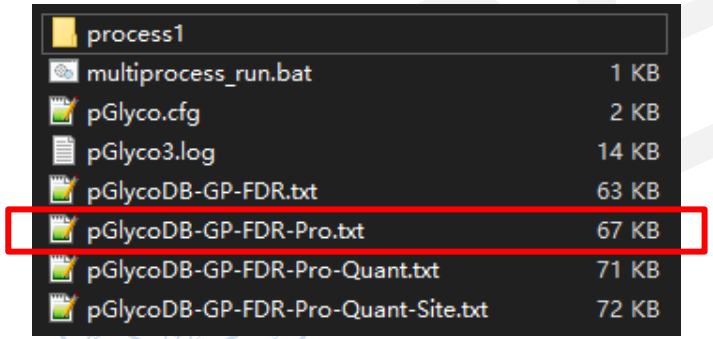
1. Identification with pGlyco

TMT

①



②



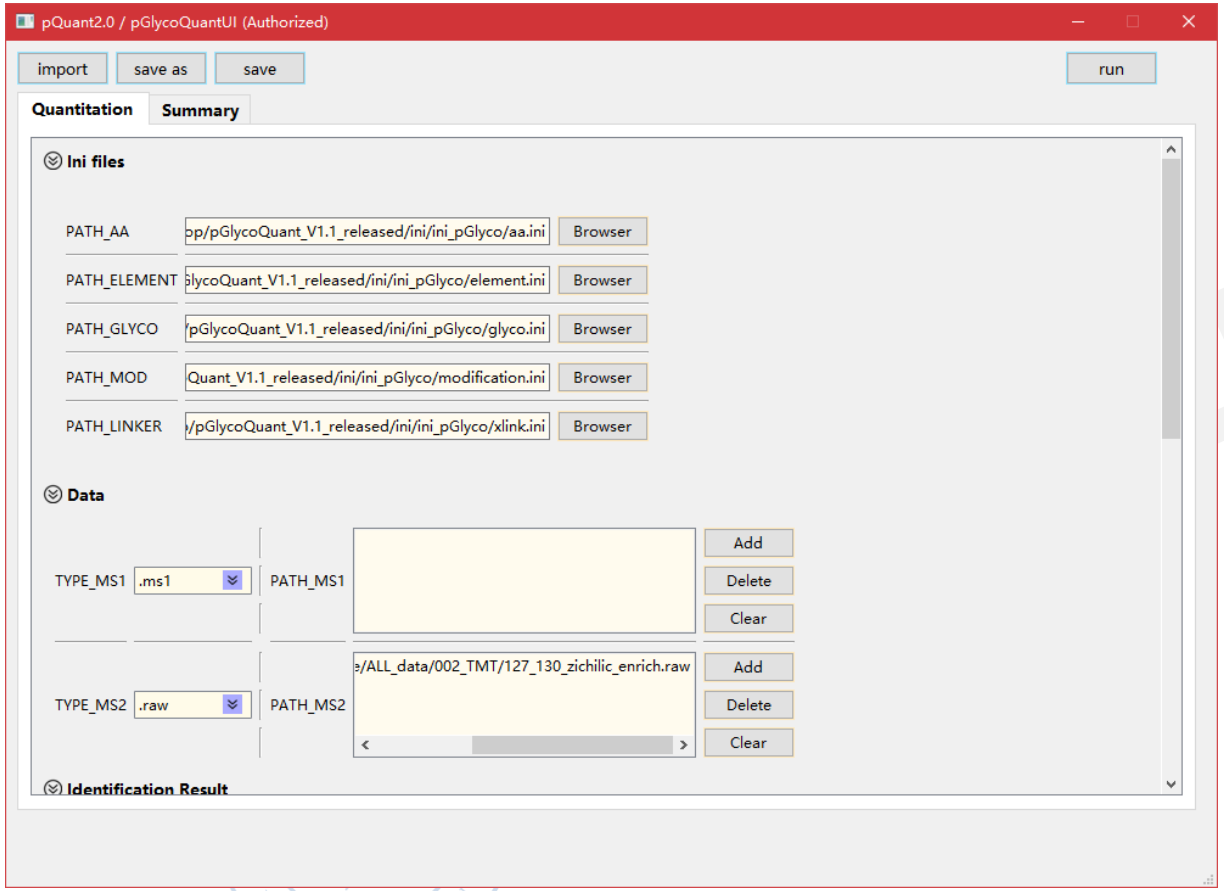
① The completed information in the command-line interface.

② The identification results.

2 Quantitation with pGlycoQuant

1.3 pGlycoQuant quantitation

TMT



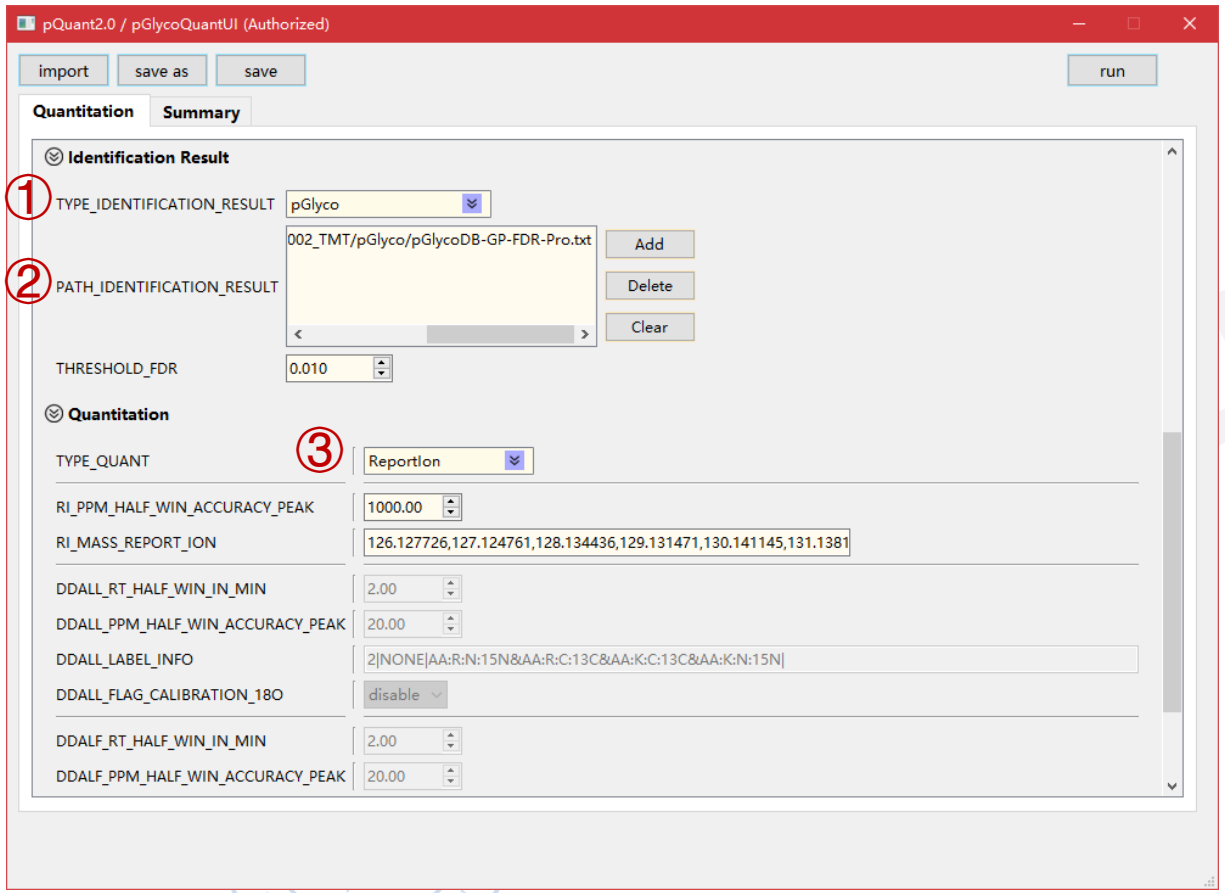
① Ensure that the ini file paths are valid.

② Set the TYPE_MS2 as .raw and fill the raw files into the PATH_MS2 blank.

2 Quantitation with pGlycoQuant

1.3 pGlycoQuant quantitation

TMT



① Set **TYPE_IDENTIFICATION_RESULT** as **pGlyco**.

② Put the identification result file **pGlycoDB-GP-FDR-Pro.txt** here and set **FDR** as **0.01**.

③ Set **TYPE_QUANT** as **ReportIon**.

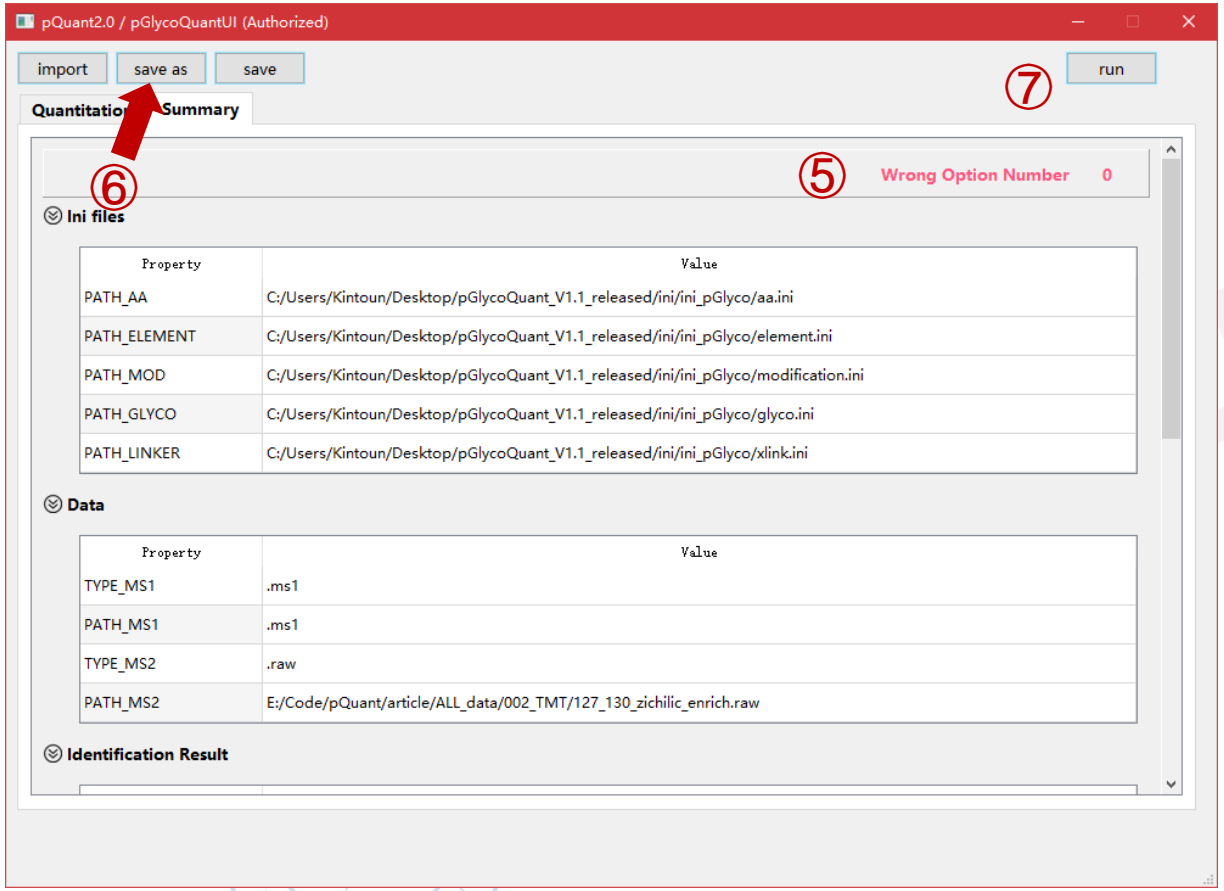
The **RI_MASS_REPORT_ION** could be 126.127726,127.124761,128.134436,129.131471,130.141145,131.138180.

④ Set the Output Folder for saving the quantitation results.

2 Quantitation with pGlycoQuant

1.3 pGlycoQuant quantitation

TMT

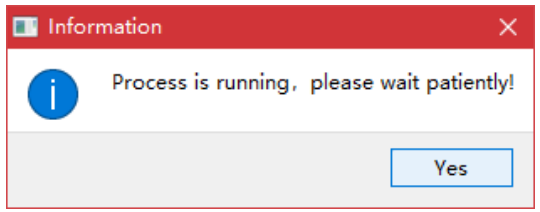


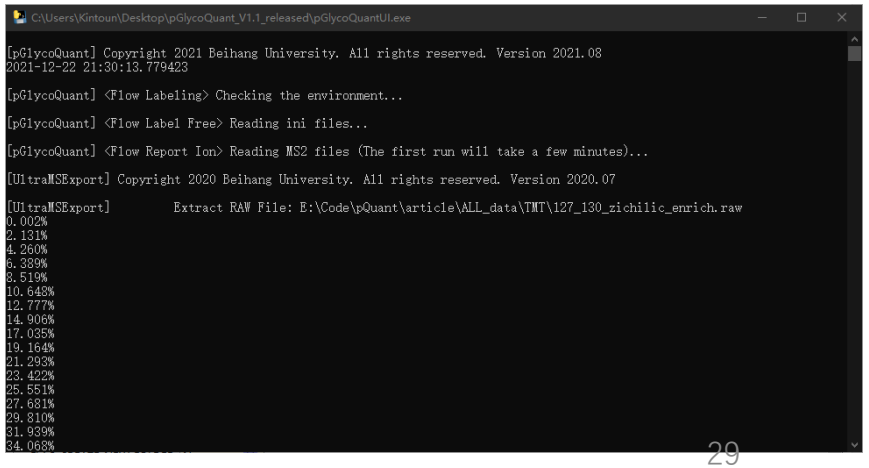
⑤ Click **Summary** button and make sure that the **Wrong Option Number** is **0**.

⑥ Then click **save as** button to save the config file.

⑦ Click **run** button to start the quantitation, the progress information will be shown in the command-line interface.

⑦



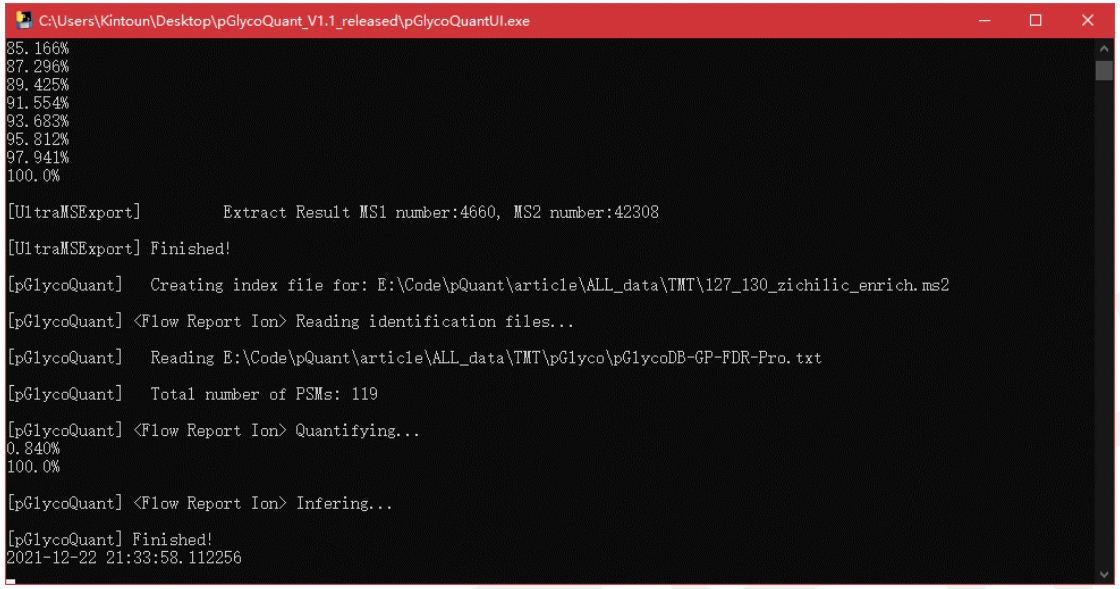


2 Quantitation with pGlycoQuant

1.4 quantitation results

TMT

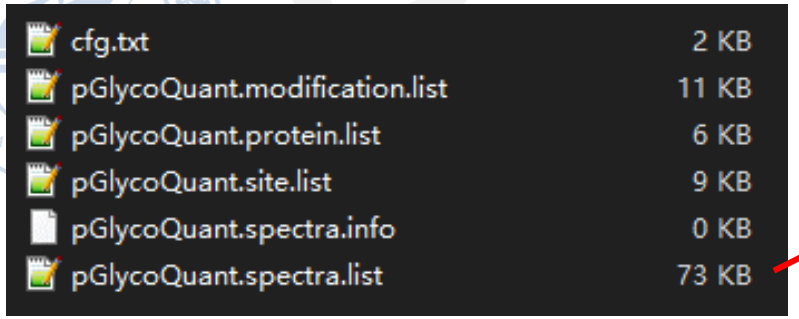
①

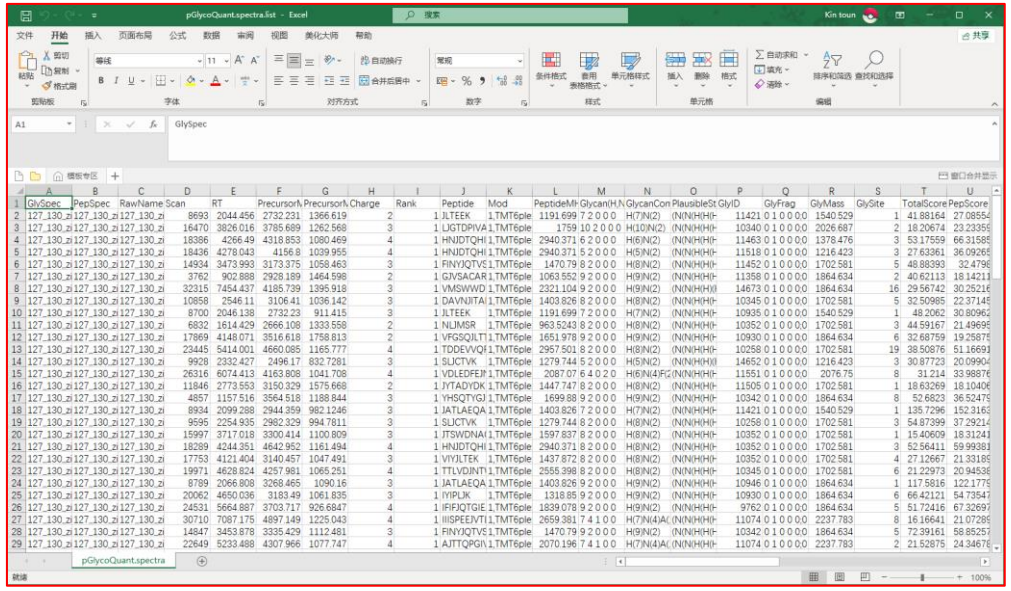


② The completed information.

② The quantitation results. Please open the files with Excel.

②



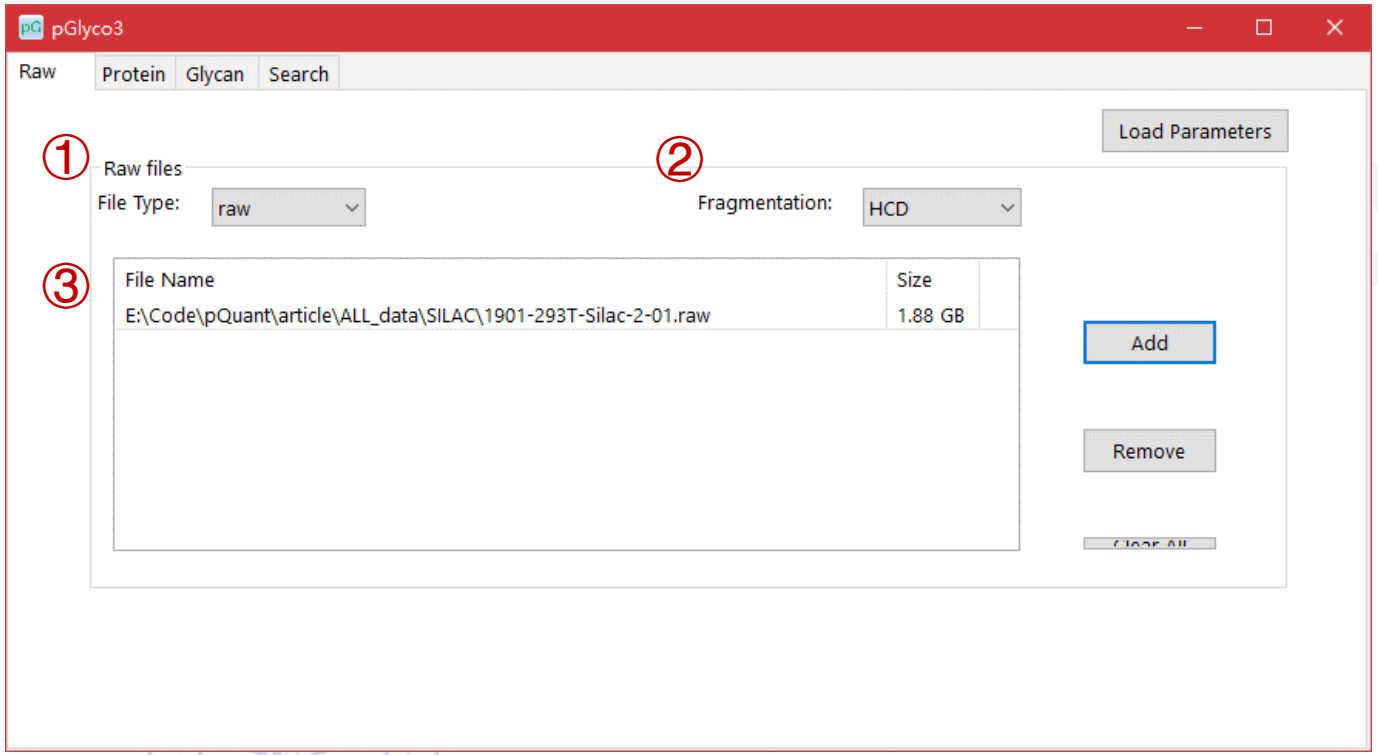


pGlyco & pGlycoQuant

Manual for SILAC Data

1. Identification with pGlyco

SILAC



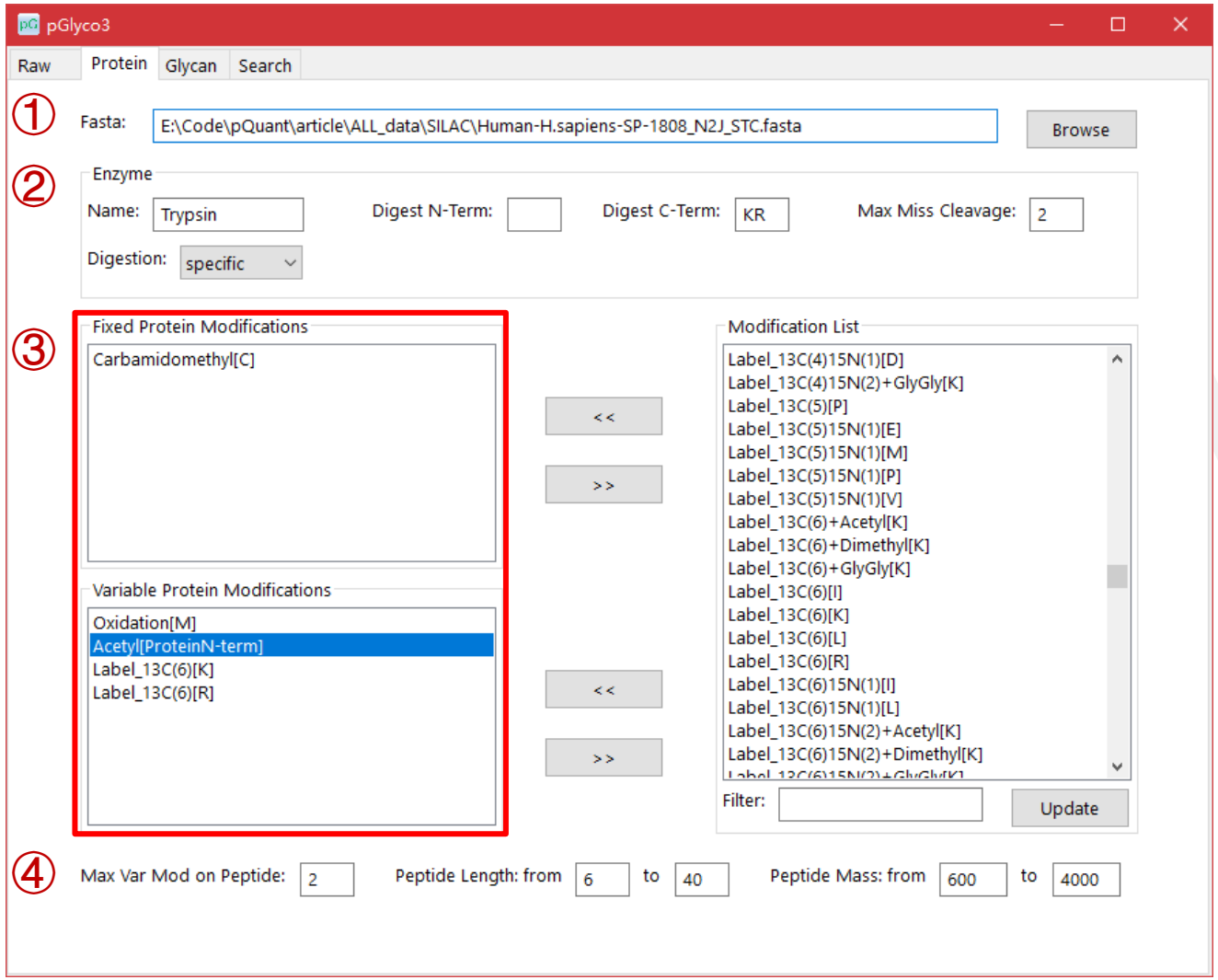
① Load raw files.

② Set the **Fragmentation** as **HCD**.

③ Add the **SILAC** raw file.

1. Identification with pGlyco

SILAC



① Set the fasta database (The file could be downloaded from https://github.com/expellir-arma/pGlycoQuant/).

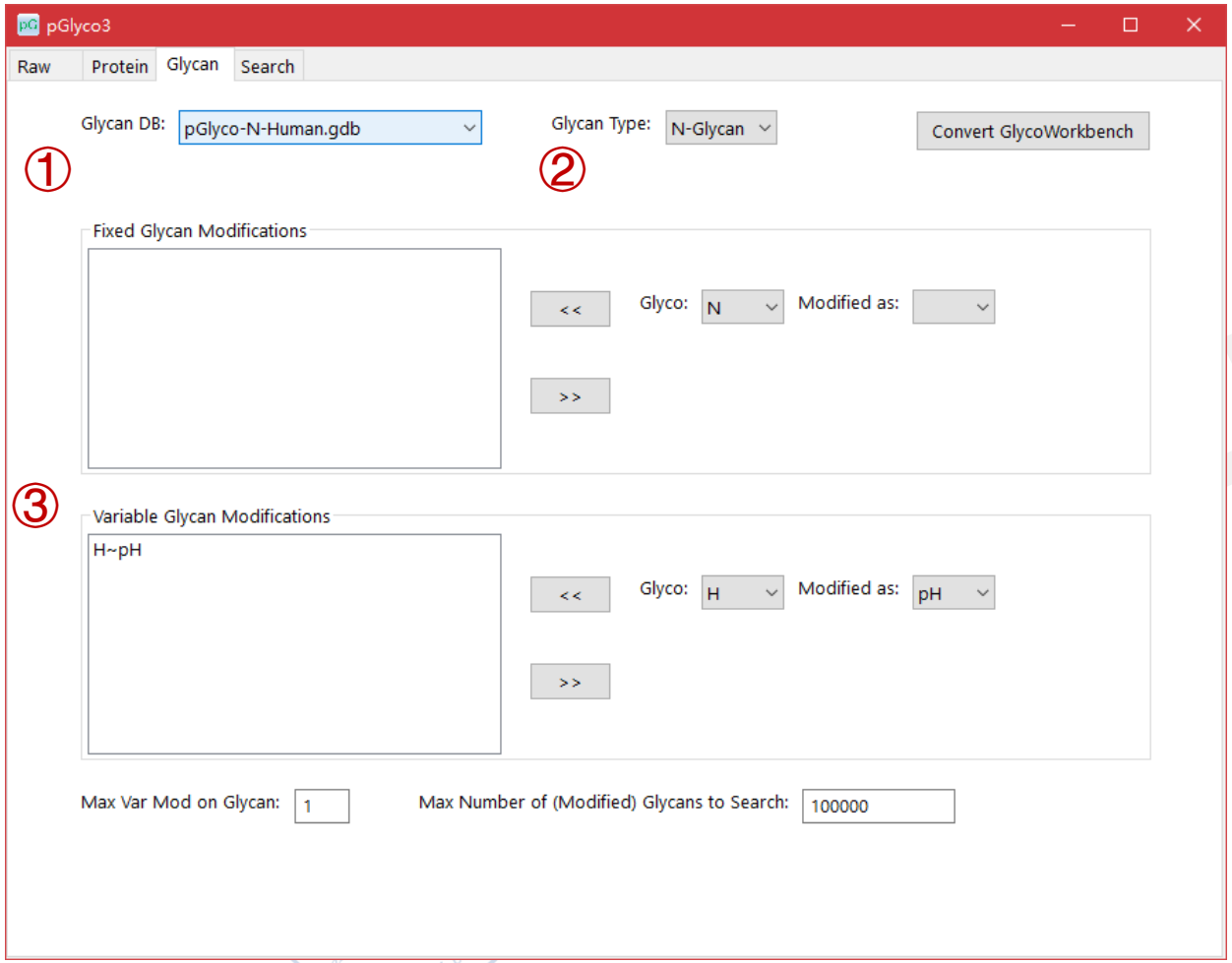
② Set the trypsin enzyme.

③ Set the fixed modification as Carbamidomethyl on Cys site. Set the variable modification as Acetyl on Protein N-Term, Oxidation on Met site, Label_13C(6)[K] on Lys site and Label_13C(6)[R] on Arg site.

④ Set the filter information.

1. Identification with pGlyco

SILAC



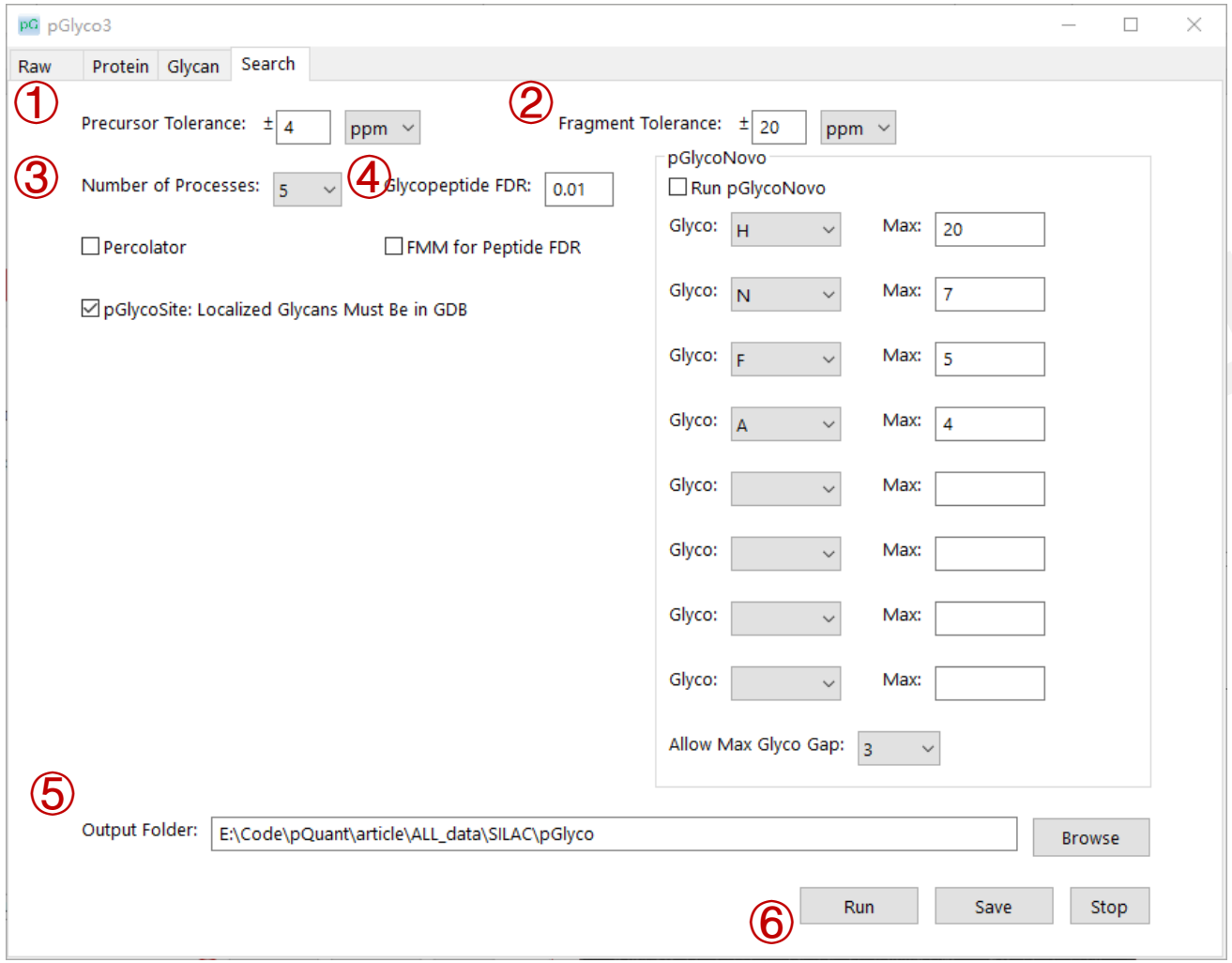
① Set the **Glycan DB** as **pGlyco-N-Human.gdb**.

② Set the **Glycan Type** as **Glycan**.

③ Set the Glycan modification information.

1. Identification with pGlyco

SILAC



① Set the **Precursor Tolerance** as ±**4** ppm.

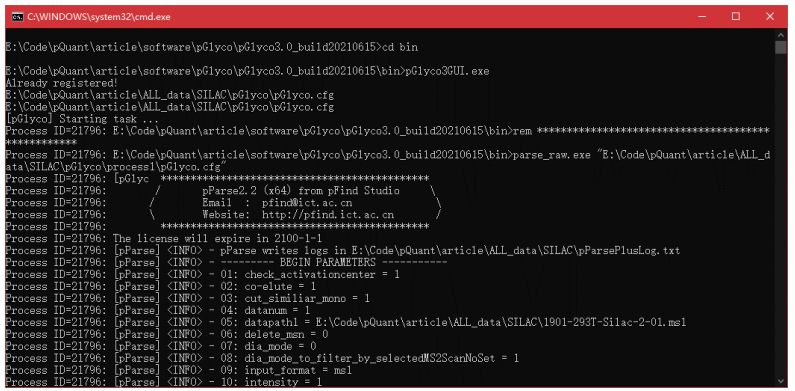
② Set the **Fragment Tolerance** as ±**20** ppm.

③ Set the **Number of Processes** according to your PC.

④ Set the **Glycopeptide FDR** as **0.01**.

⑤ Set the **Output Folder** for saving the identification results.

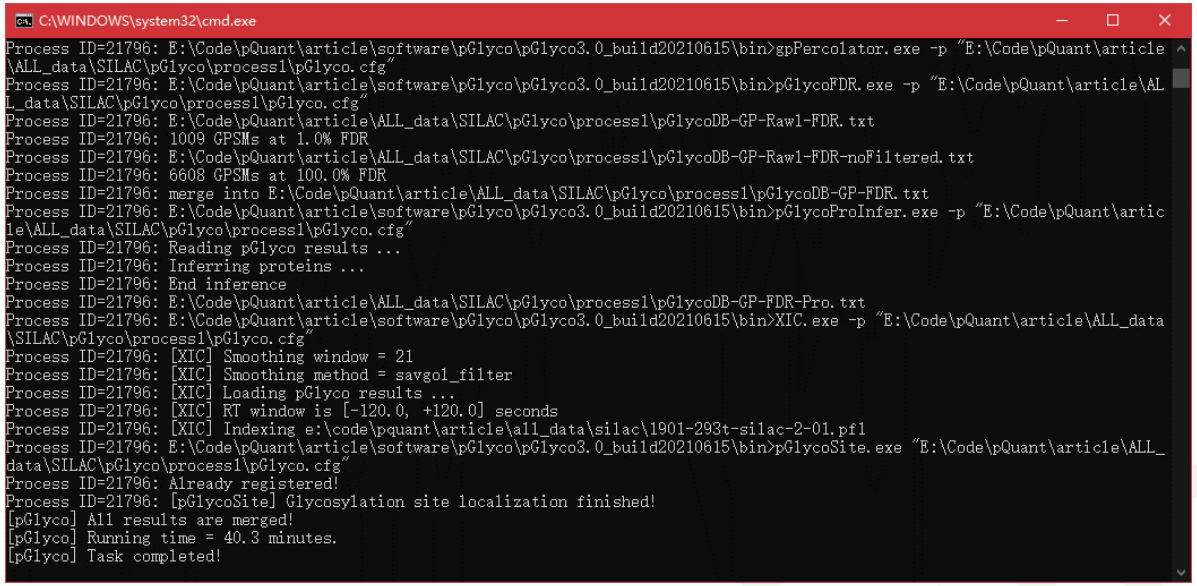
⑥ Click **Save** and **Run** buttons, the progress information will be shown in the command-line interface.



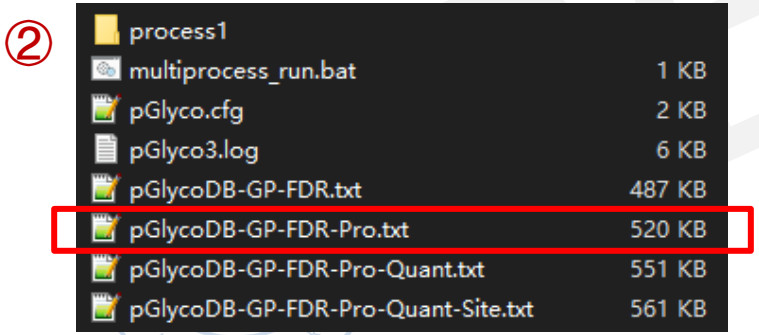
1. Identification with pGlyco

SILAC

①



②



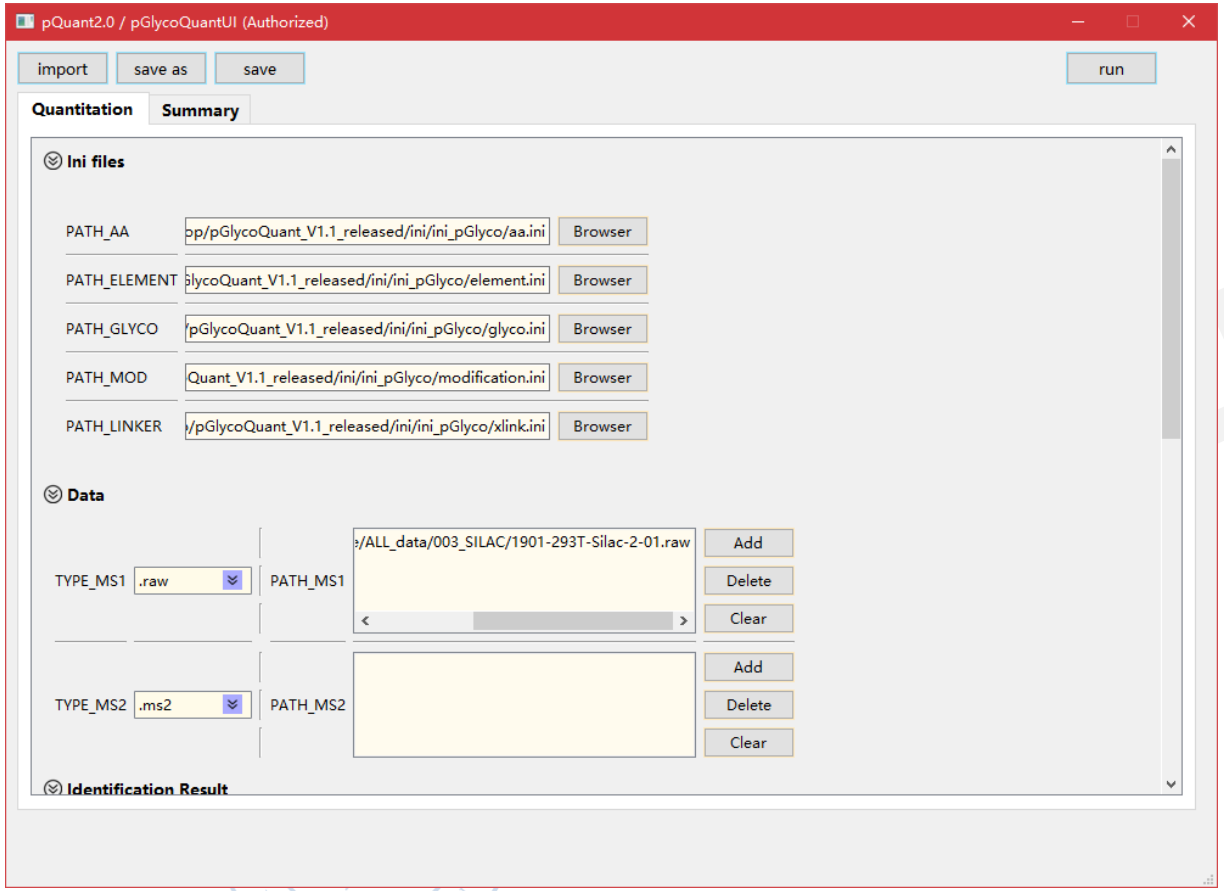
① The completed information in the command-line interface.

② The identification results.

2 Quantitation with pGlycoQuant

1.3 pGlycoQuant quantitation

SILAC



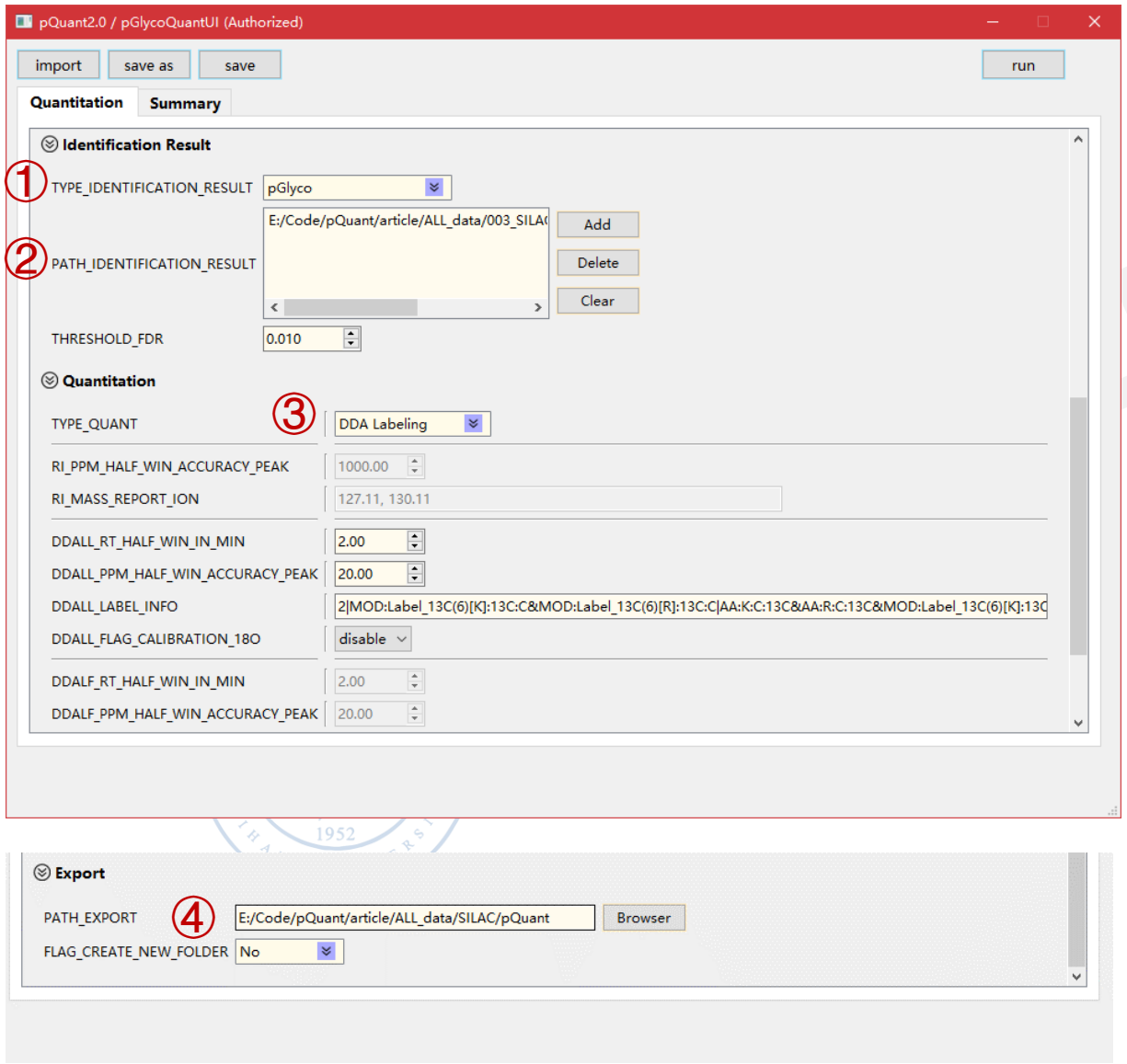
① Ensure that the ini file paths are valid.

② Set the TYPE_MS1 as .raw and fill the raw files into the PATH_MS1 blank.

2 Quantitation with pGlycoQuant

1.3 pGlycoQuant quantitation

SILAC



① Set **TYPE_IDENTIFICATION_RESULT** as **pGlyco**.

② Put the identification result file **pGlycoDB-GP-FDR-Pro.txt** here and set **FDR** as **0.01**.

③ Set **TYPE_QUANT** as **DDA Labeling**.

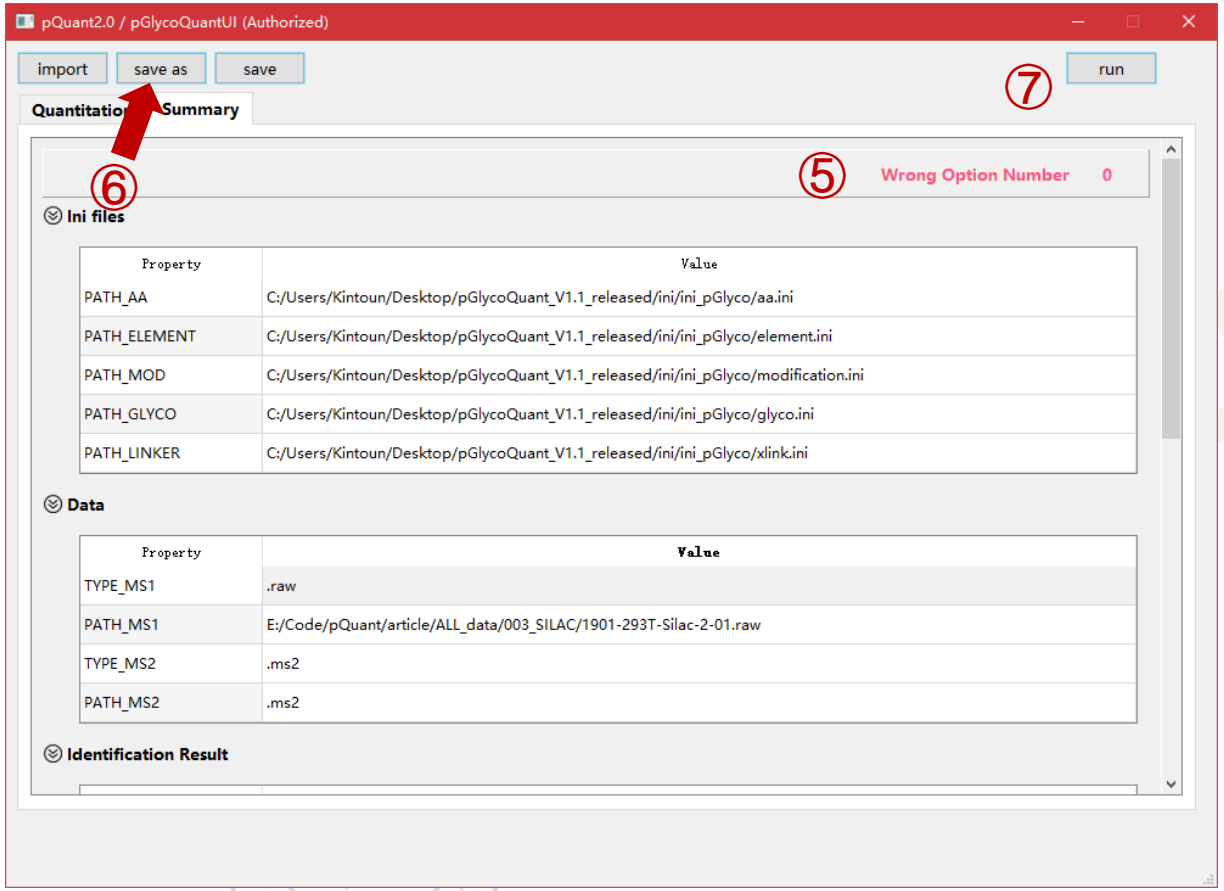
The DDALL_LABEL_INFO could be 2|MOD:Label_13C(6)[K]:13C:C&MOD:Label_13C(6)[R]:13C:C|AA:K:C:13C&AA:R:C:13C&MOD:Label_13C(6)[K]:13C:C&MOD:Label_13C(6)[R]:13C:C|.

④ Set the Output Folder for saving the quantitation results.

2 Quantitation with pGlycoQuant

1.3 pGlycoQuant quantitation

SILAC

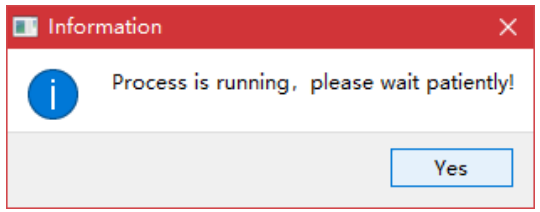


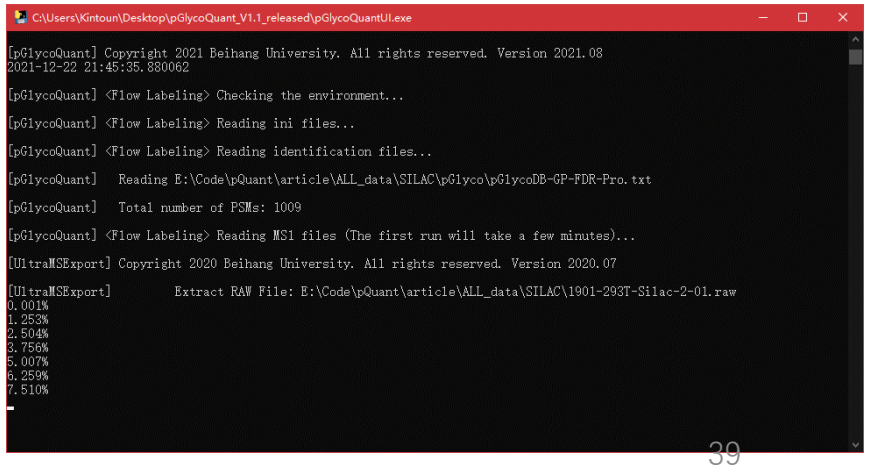
⑤ Click **Summary** button and make sure that the **Wrong Option Number** is **0**.

⑥ Then click **save as** button to save the config file.

⑦ Click **run** button to start the quantitation, the progress information will be shown in the command-line interface.

⑦



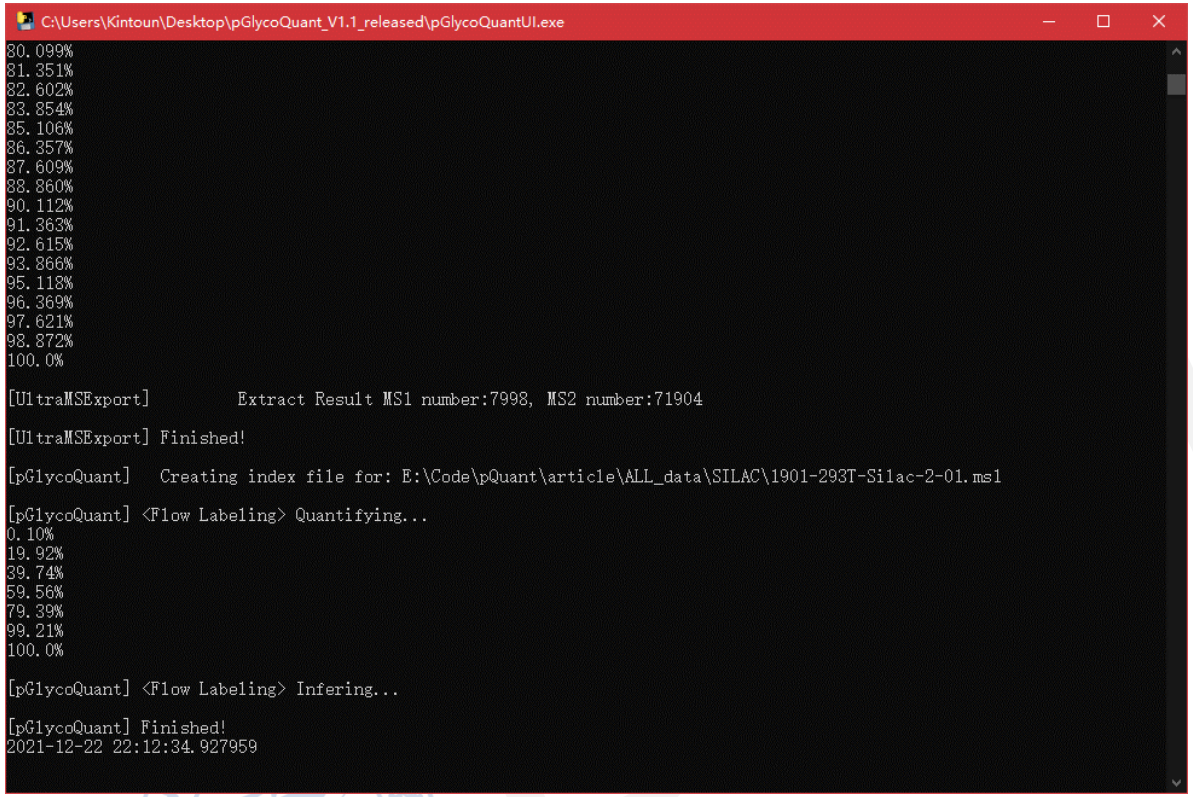


2 Quantitation with pGlycoQuant

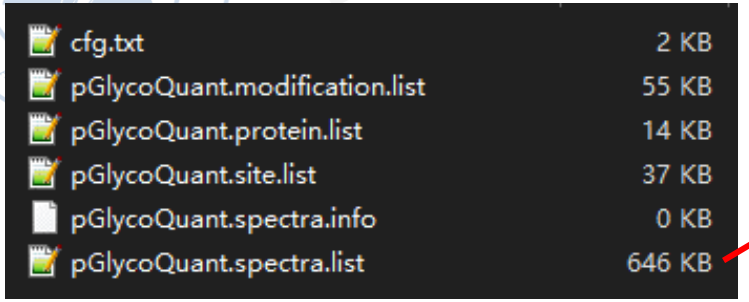
1.4 quantitation results

SILAC

①

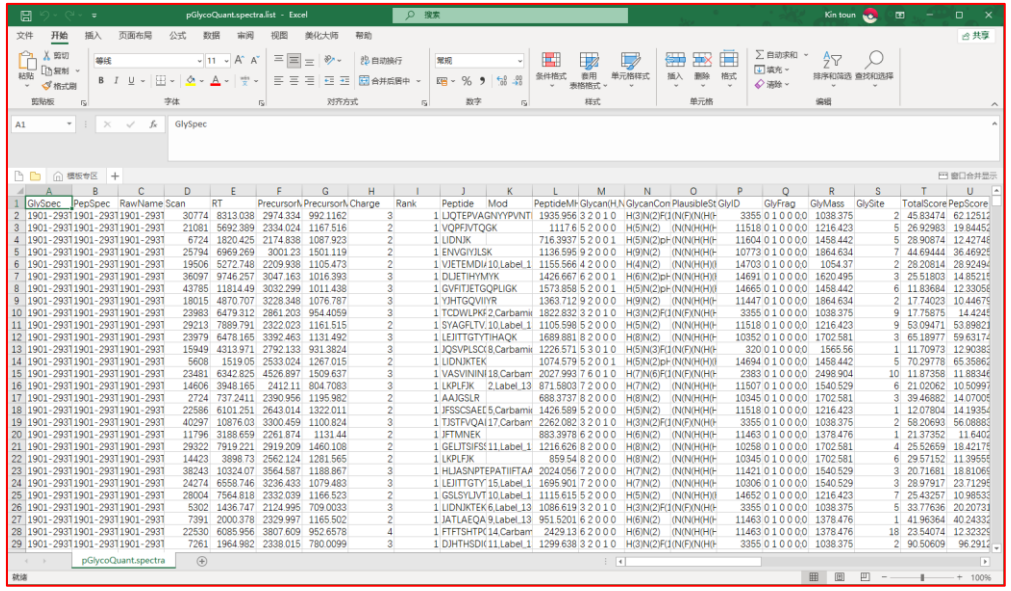


②



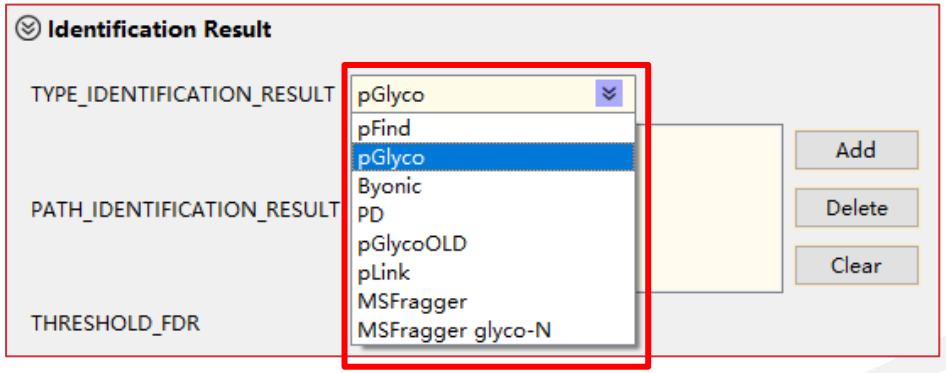
① The completed information.

② The quantitation results. Please open the files with Excel.

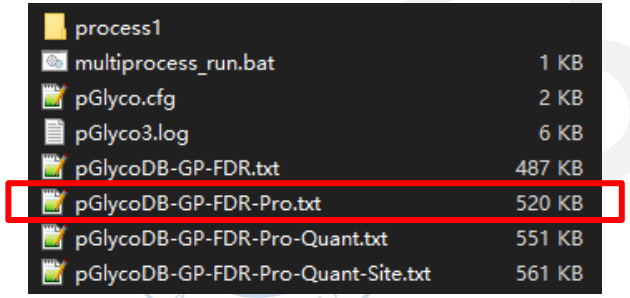


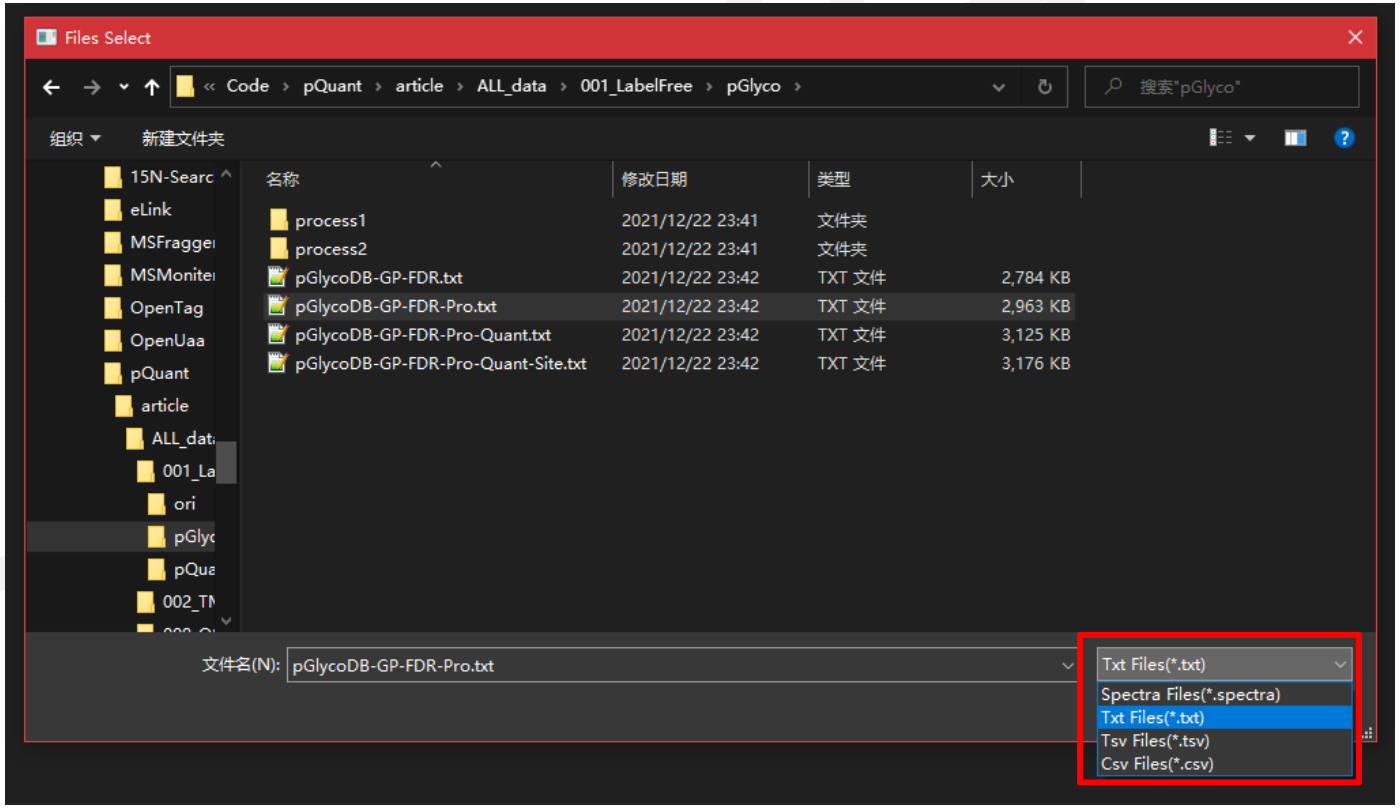
Notes for Choosing the Input File for pGlycoQuant

Choose the related type of identification result for quantitation

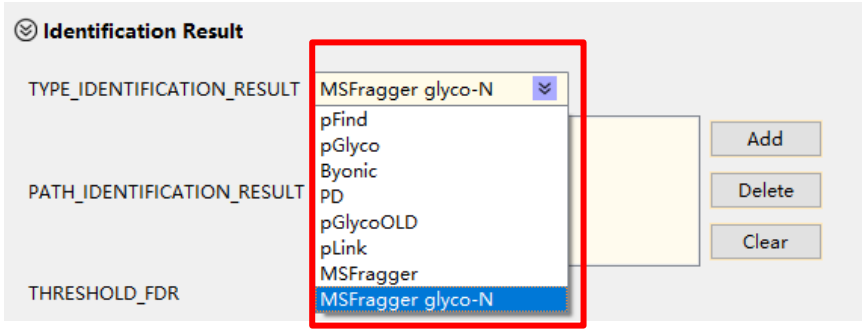


pGlyco results

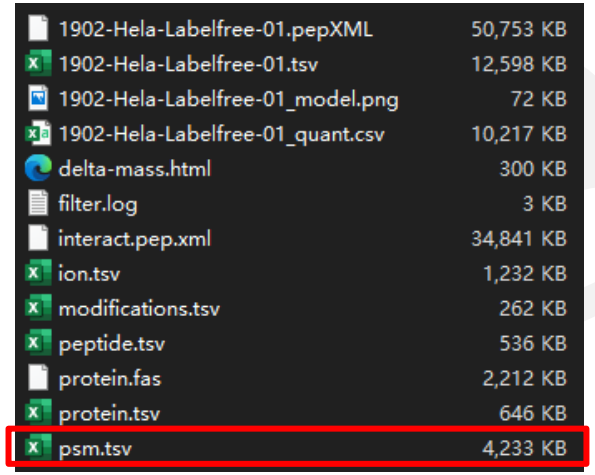


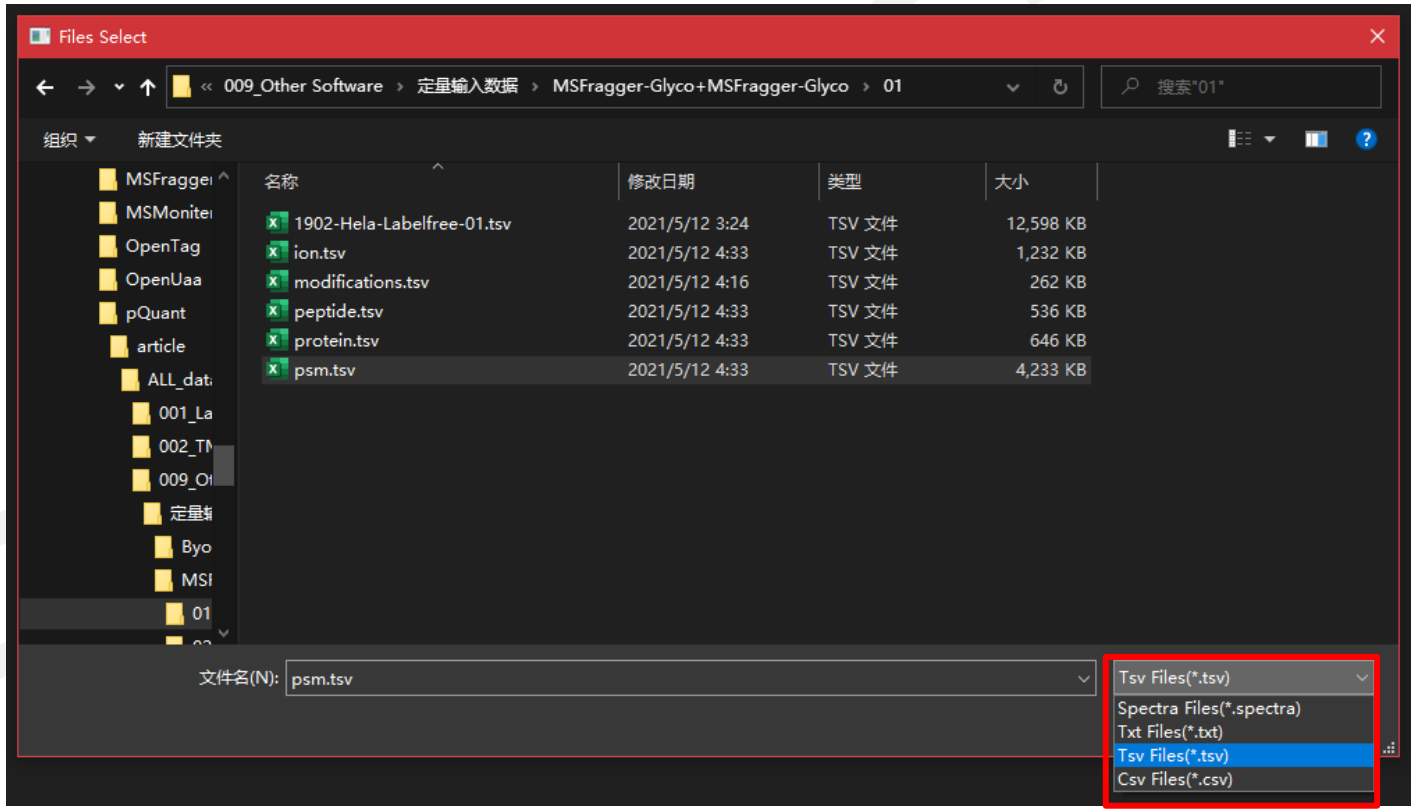


Choose the related type of identification result for quantitation

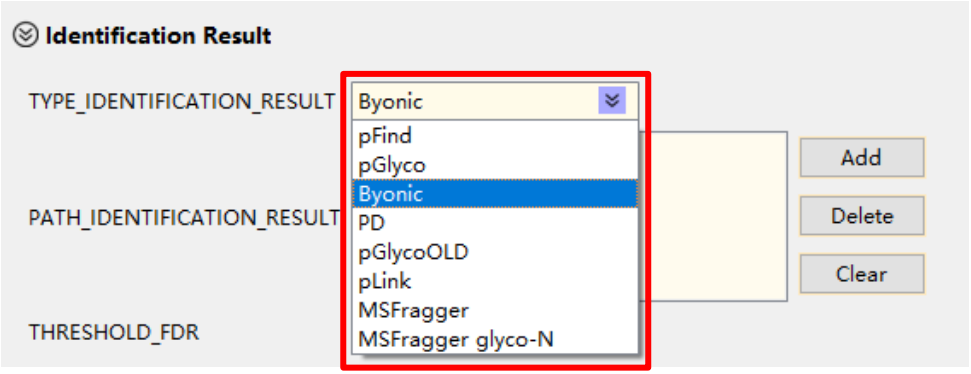


MSFragger results

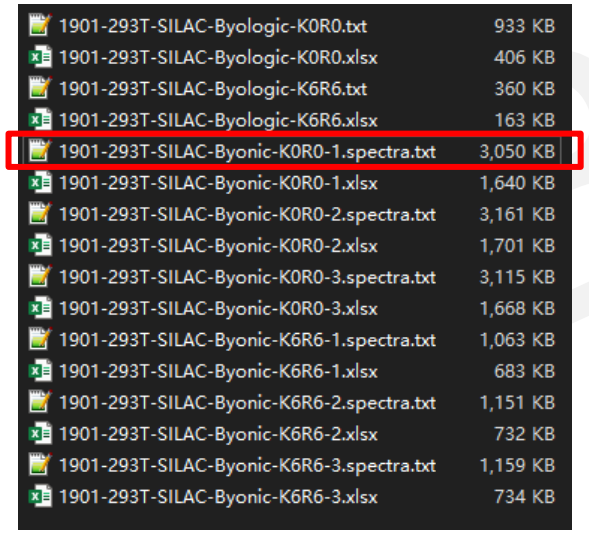


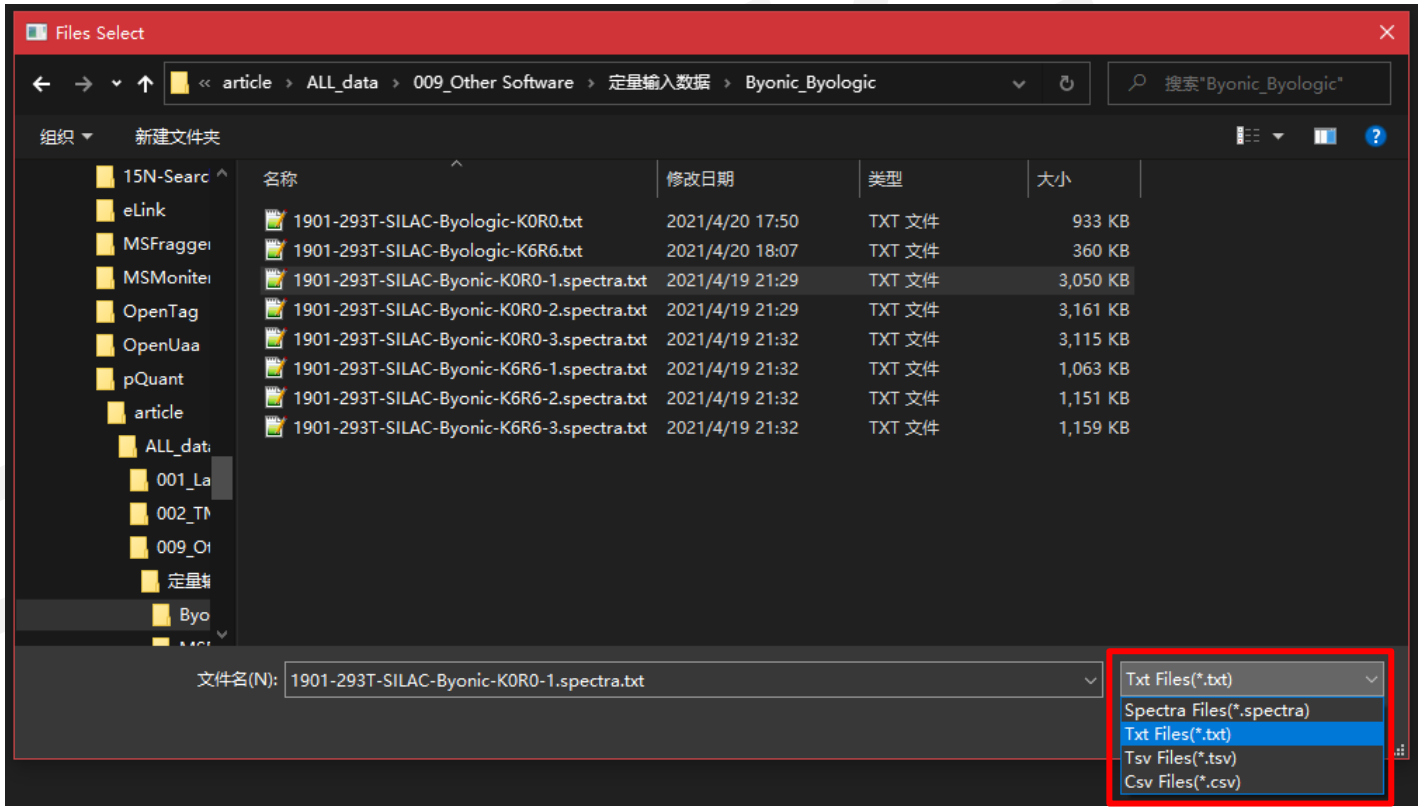


Choose the related type of identification result for quantitation



Byonic results





Thanks!