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pXtract User Guide

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Program Introduction

pXtract creates DTA, MGF and MS2 input files directly from Thermo Scientific RAW LC-MS/MS data files.

For each fragmentation spectrum, pXtract first attempts to determine the precursor charge

state using the information recorded in the scan header. If this information is available, only a single spectrum is written using that precursor charge. If it is not available (could not be determined by the instrument firmware), two spectra are generated for +2 and +3 state, respectively. The precursor $[M + H]^+$ value is written with its corresponding charge state, followed by every centroid m/z and intensity pair from the MS2 scan.

Environment Requirement

Hardware:

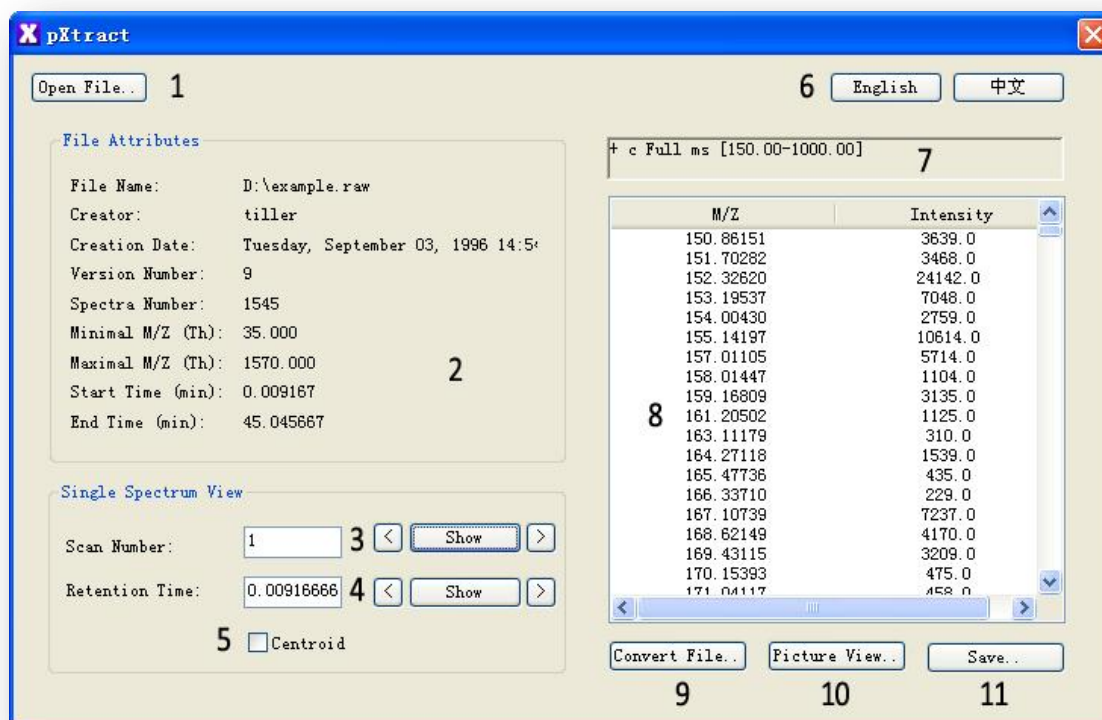
Memory: 256MB or higher
CPU: Pentium 233 or higher
Hard Disk Space: 5M at least

Software:

Microsoft Windows Operating System, Windows 2000 or above
Thermo Scientific Xcalibur 2.0 or later needed

Interface Description

Main Interface



- 1-1: Open file button, click the button to choose the needed raw file.
- 1-2: Area of file attributes, show the attributes of the raw file.
- 1-3: Single spectrum view control, it is used to show the data for the specified scan number.
- 1-4: Single spectrum view control, it is used to show the data for the specified retention time.
- 1-5: Centroid control, select the selection box to show the data after centralization.
- 1-6: Language control, click the two buttons to switch between English and Chinese.
- 1-7: Area of single-spectrum attributes, such as instrument type, activation type, precursor mass, etc.
- 1-8: Area of spectrum data, mass and intensity is shown.
- 1-9: Raw data exporting button, click it to show the exporting dialog. This is used to convert the raw file to other formats.
- 1-10: Picture view for the raw file, click this button to show the spectrum.
- 1-11: Save single-spectrum data, click the button to save the current spectrum as a DTA file.

Export raw data

The image shows a 'Convert File' dialog box with the following elements and annotations:

- 1** File Path: D: [Browse]
- 2** Centroid
- 3** Convert into different folders for different activation type
- 4** File Type: *.ms1, *.ms2, *.ms3, *.ms4 *.dta *.mgf
- 5** Precision: M/Z [5] Intensity [1]
- 6** MSn: MS1 MS2 MS3 MS4
- 7** [Convert]

At the bottom of the dialog box is an empty text input field.

2-1: Choose a path to save the exported files.

2-2: Choose to export the centroid data. The data that has been in the centroid mode will not be centralized again.

2-3: Choose to convert the raw file data into different folders for corresponding activation type.

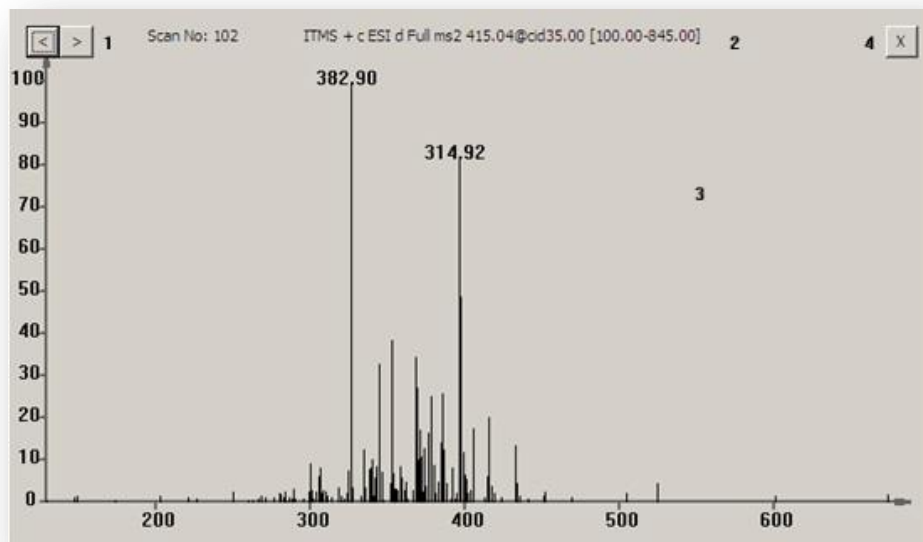
2-4: Choose the exported file format. Currently, MGF, DTA and MSn are supported.

2-5: Write or choose the precision of the exported data.

2-6: When choosing the MSn file format, you can choose to export MS1, MS2, MS3, MS4, or all.

2-7: Click the button to start the exporting procedure.

Spectra View



3-1: Click the two buttons to view the previous or the next spectrum.

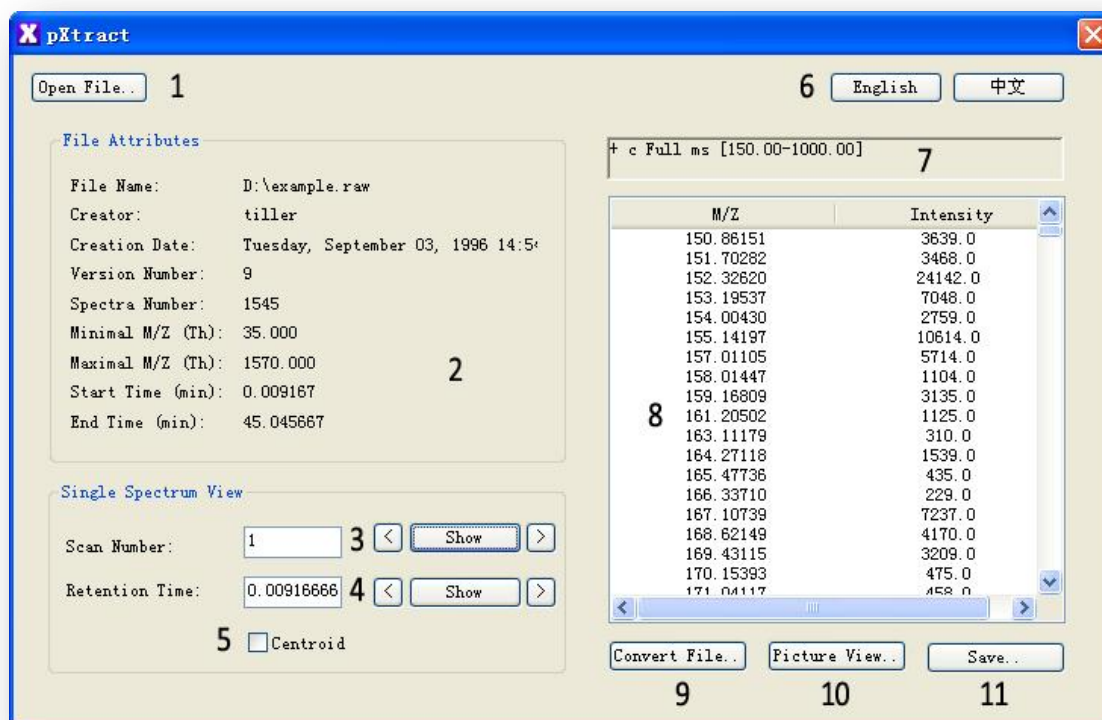
3-2: This part shows the basic information of the spectrum such as scan number, activation type, precursor mass, etc.

3-3: This area is used to view the figure of the spectrum. The peaks that have a relative intensity larger than 70% of the most abundant peak are annotated.

3-4: The button to quit, click it to close the spectra view dialog.

Operation Guide

View the experiment time, spectrum count information and so on



Click the button 1-1, choose the raw file, then the information will appear at 1-2.

View the spectrum with scan number "n"

Input "n" at the text box 1-3, click the button "show". The information will appear at 1-7 and 1-8. "<" and ">" are used to view the previous or the next spectrum information. The text box 1-4 will show the retention time of the spectrum at the same time.

View the spectrum with retention time "t"

Input "t" at the text box 1-4, click the button "show". The information will appear at 1-7 and 1-8. "<" and ">" are used to view the previous or next spectrum information. The text box 1-3 will show the scan number of the spectrum at the same time.

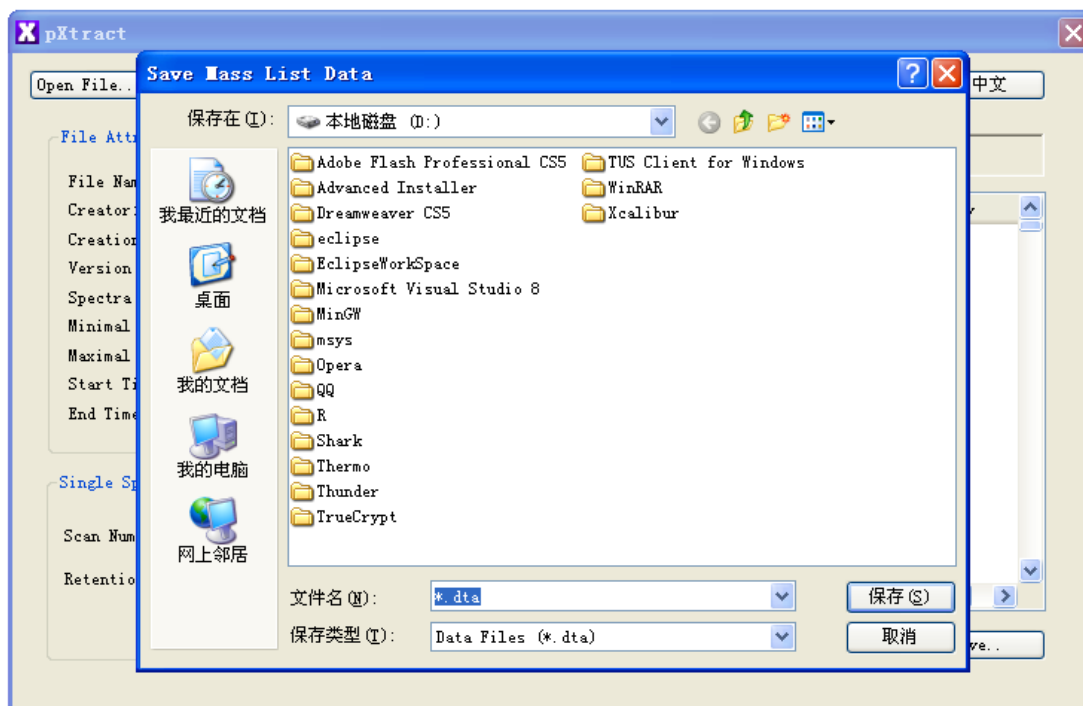
View the data after centralization

Select the selection box 1-5 before click 1-3 or 1-4 "show" button. Deselect 1-5 to view the profile data.

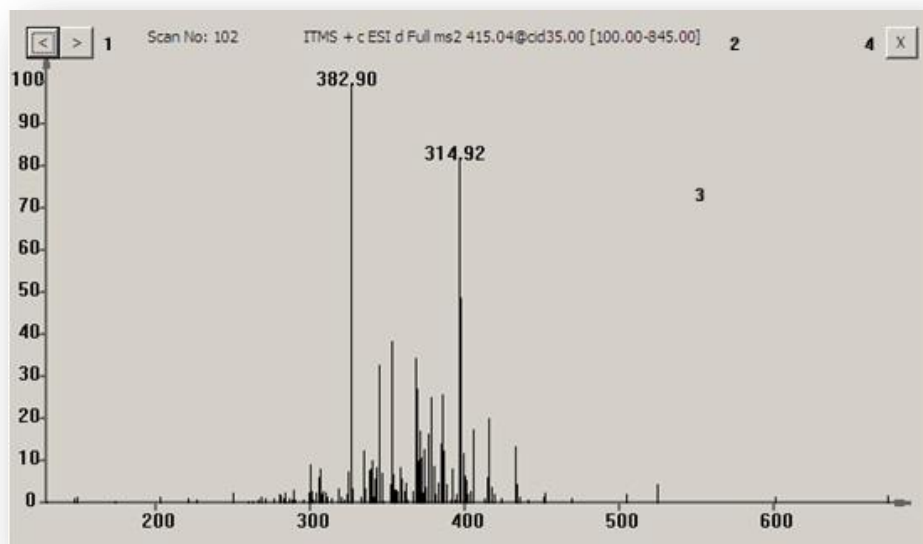
Save the data currently being viewed

After the spectrum information has been shown in 1-7 and 1-8, click the button 1-11, and

input the name in the save dialog and choose the save button. The spectrum data will be saved into a DTA file.



View the figure of the spectrum



After the spectrum information has been shown in 1-7 and 1-8, click the button 1-10, the spectra view dialog will appear. 3-2 is used to show the basic information of the spectrum. 3-3 reveals the figure. 3-1 can be used to view the previous or the next spectrum. To quit the spectra view dialog, please click 3-4.

Create DTA, MGF or MS2 input files from the raw file

- 1 Click the button 1-1, choose the raw file.
- 2 Click the button 1-9, the Convert File dialog pop-outs. After setting parameters, click the button 2-7 to start the conversion.



How to set the parameters when exporting the raw data

Choose or input the path at 2-1 where the DTA, MGF or MS2 files will be created. The default path is the same as that of the raw file. Select 2-2 to centralize the data. Select 2-3 to convert the raw file into different folders for different activation types.

Choose the file type at 2-4. Currently MSn, DTA and MGF are supported. 2-5 is used to input or choose the precision of the exported data. 2-6 only works for the MSn file.

After setting the parameters or just using the default setting, click the button 2-7 to start the exporting. There will be an icon in the taskbar to notify you that how much has been done. You can deal with your other work while the program is working, and a dialog will call your attention after the exporting is finished.

Change program languages

Click the button 1-6 to switch the language. Right click on the main interface can also work.
Currently English and Chinese are supported.

Contact Information

If you have any problem, please email to fanshengbo@ict.ac.cn for help.