Description:

OpenMS-Simulator is a tool with a graphics user interface (GUI) that allows the user to predict the theoretical spectra of peptides with the new approach, called MS-Simulator, which focuses on the accurate prediction of the relative intensity ratio of two adjacent y-ions. The software allows the user to re-score the results of the other packages by input the raw data files and the output files of other software, such as SEQUEST or Tandem. The correlation between the experiment spectrum and the theoretical spectrum produced by the peptide sequence can be calculated. It also has the application of labeling the spectrum with the frequent ions, such as a, b, c, x, y, z, dehydration ions, deamination ions, and their isotopic ions.

The detailed description of this tool is as follows:

Download:

The package of this tool is a property of http://www.bioinfo.org.cn/OpenMS-Simulator .

It can download at http://www.bioinfo.org.cn/OpenMS-Simulator.

Required Software:

This tool runs on the JAVA SE Development Kit (JDK). The JDK 5 Update 16 (version 1.5.0_16) or newer must be installed on your system before you use this tool. If you have not installed the JDK, you can download the download the latest JDK version at http://java.sun.com/javase/downloads.

Installation:

MS-Simulator is a green software which does not need to be installed or uninstalled. The user can download the executable file, called OpenMS-Simulator.jar, to use it directly. It is a lighter program take less system resource and has quite enough features.

OpenMS-Simulator is system-independent. On any platforms, you can run the OpenMS-Simulator.jar to start the software without any other special setting.

Usage Instructions:

1. The Main UI

The main UI of OpenMS-Simulator is display as Figure 1. On the top of the Interface labeled “File”, “Help”. The main body divided into two parts, the left part is the logo of this software and the right one is the applications operation. Four applications are display as buttons on the right part.

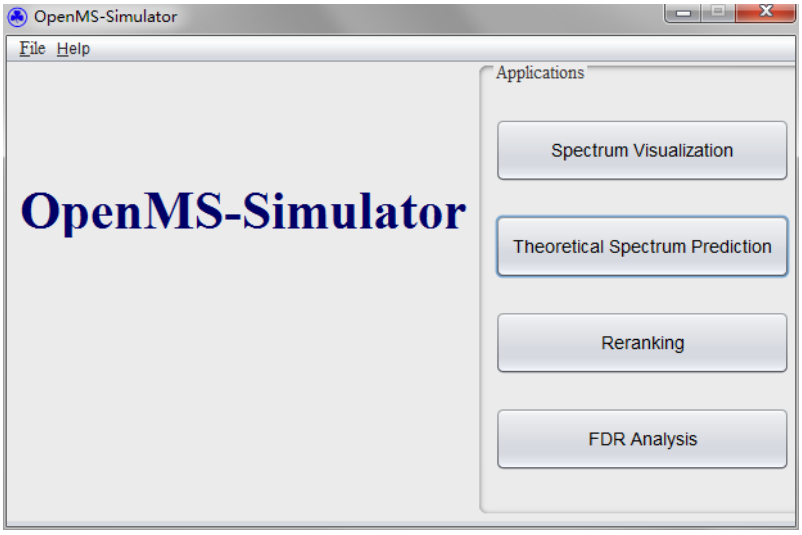

Figure 1 the main UI of MS-Simulator

2. How to label the spectrum

Applications-> Spectrum Visualization: first, you should click the "Spectrum Visualization" on the main UI, a frame displaying, called "Spectrum Visualization". On the top of this frame labeled "File", "View", "Correlation", "Help", see Figure 2.

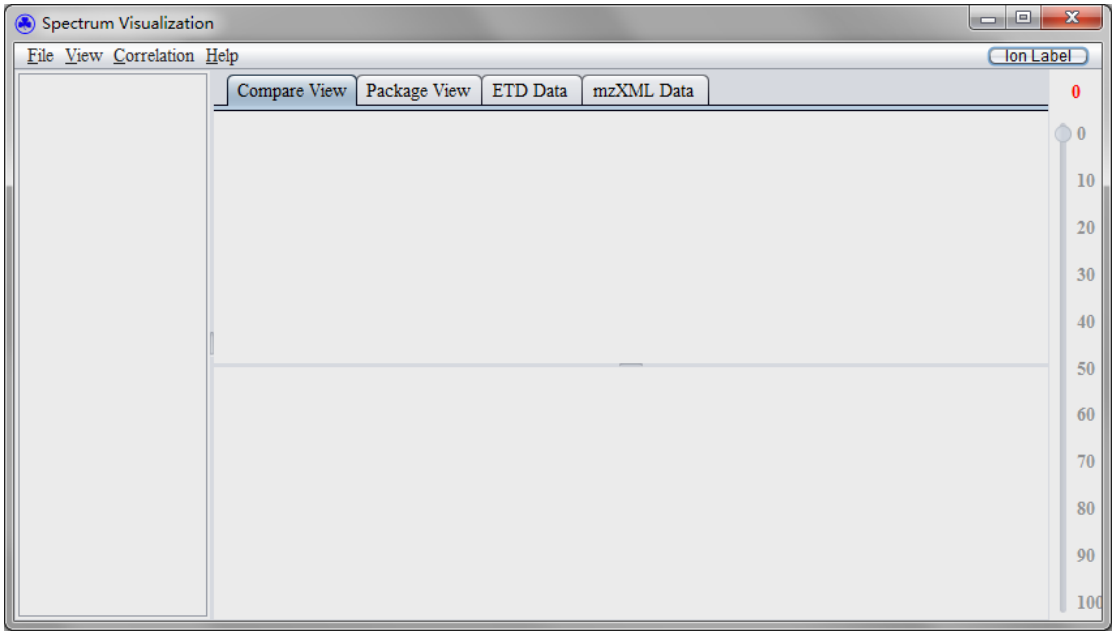

Figure 2 Spectrum Visualization Frame

File->New Project/Open Project: first, you should click "File", and then click "New Project" or "Open Project" (if a project is already existed.) in the pull-down menu, See Figure 3. A new project is built.

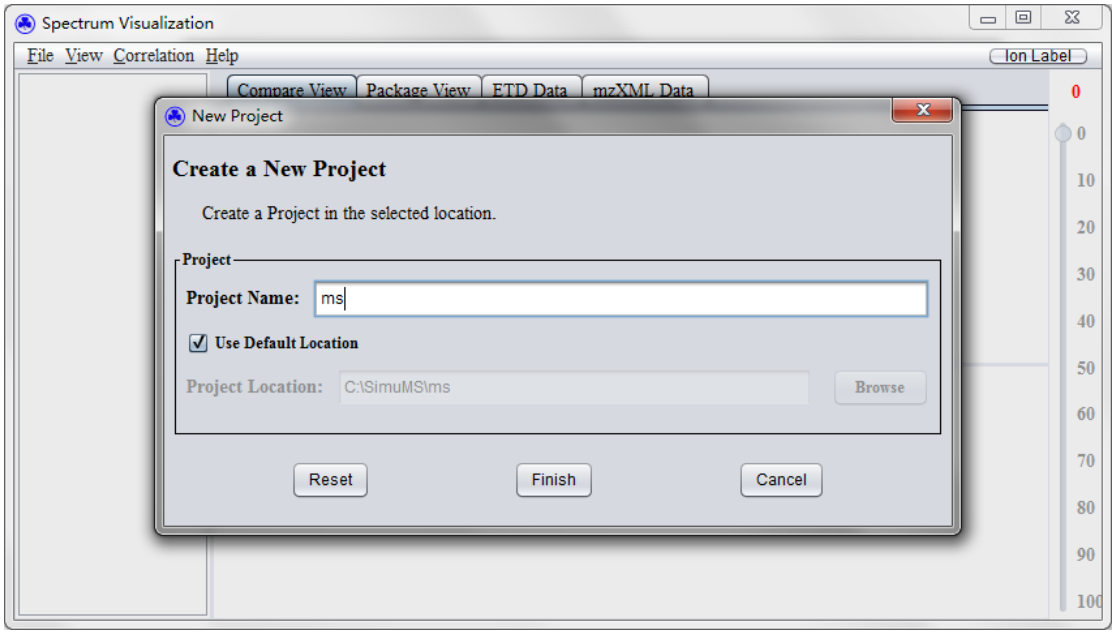

Figure 3 A new project, called 'ms', is built.

Second, when a project has been created, you can open a spectrum data file by right clicking the project name. There are four file formats: DTA file, MGF file, MZXML file and OUT file. According

the file type, you should select a destination folder, and the Figure 4 will show when the “DTA file” selected.

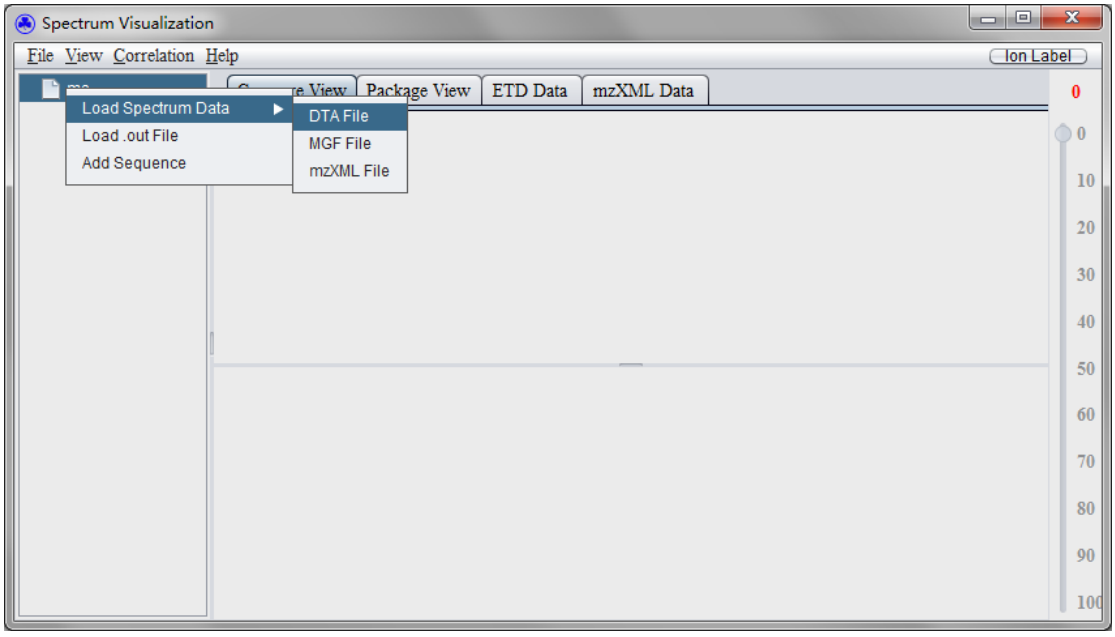

Figure 4 choose a type of spectra dataset to add.

Third, you can choose the objective .dta file and click the button of “Open”. You will see the interface as Figure 5.

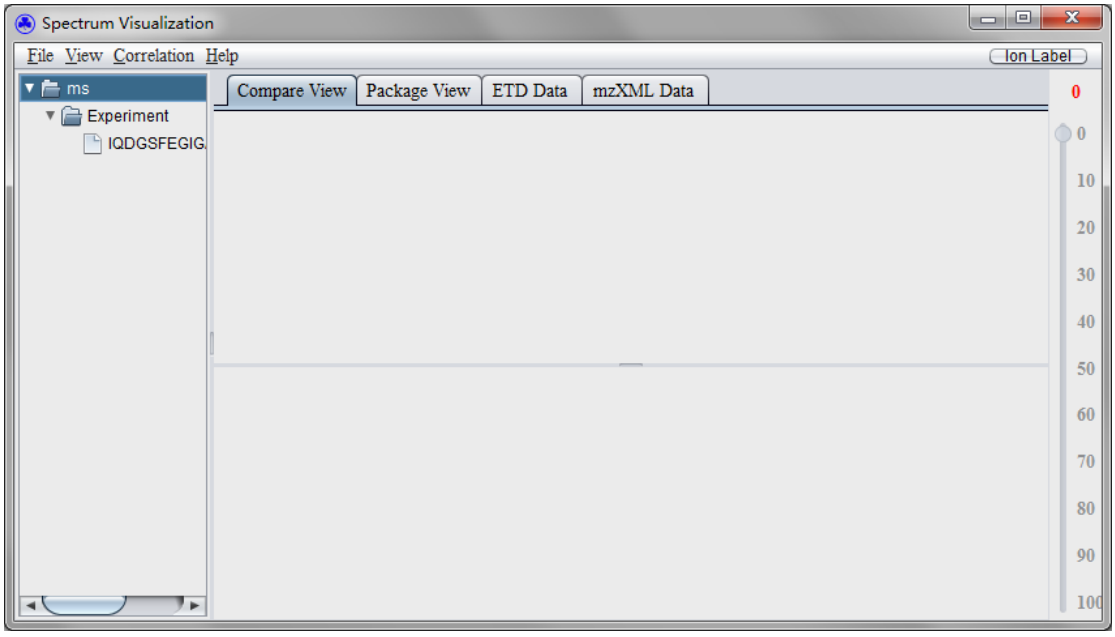

Figure 5 open a spectrum format (.dta) file.

Fourth, in order to label the spectrum, you should click the “Ion Label” on the top of the frame. You can input or copy the sequence of the target peptide in the box of “InputSEQ”, and choose the types of ions that need to be labeled on the spectrum, simultaneously, show as Figure 6.

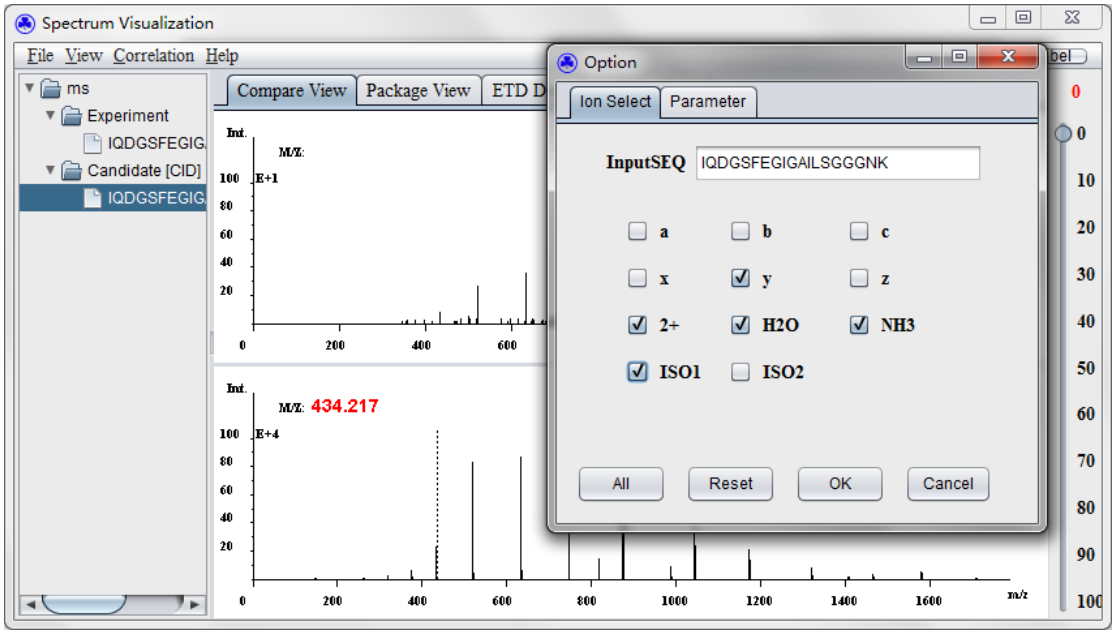

Figure 6 input a sequence for labeling and select the ion types.

Final, after clicking the button of “OK”, the labeled spectrum shows in the frame as Figure 7, you can observe and compare spectra intuitively.

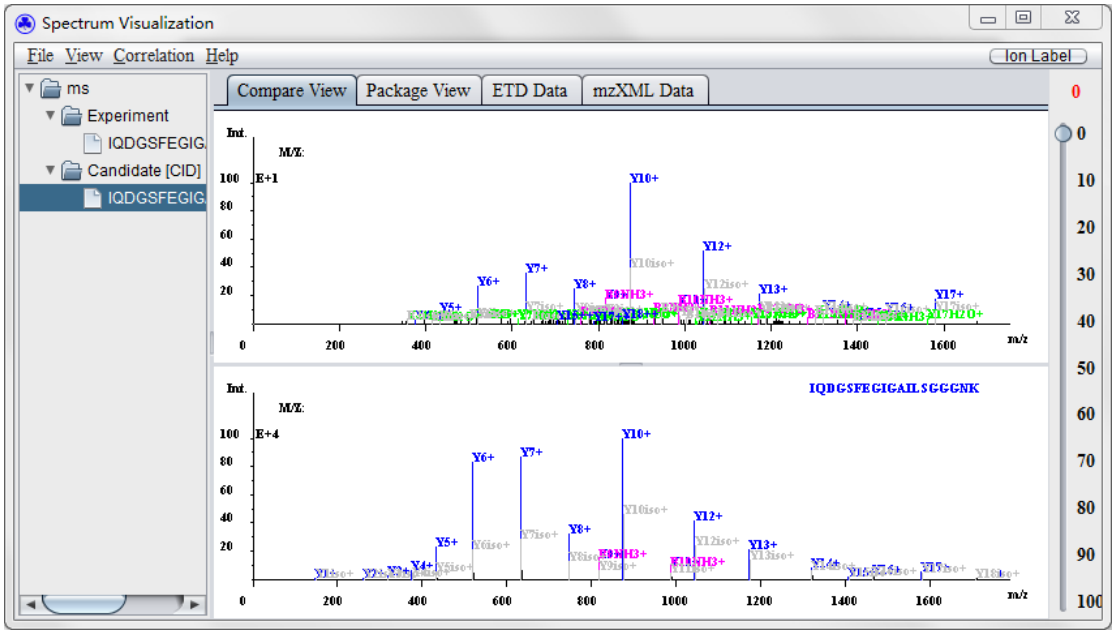

Figure 7 the label result on the visual frame.

3. How to calculate the correlation

Correlation: first, you should open an experiment spectrum and a theoretical spectrum generated by sequence of peptide. The Figure 8 indicates the display of the two spectra. Also, you can compare the two spectra together by double clicking the left key of the mouse on the theoretical spectrum, just as the Figure 9 showed.

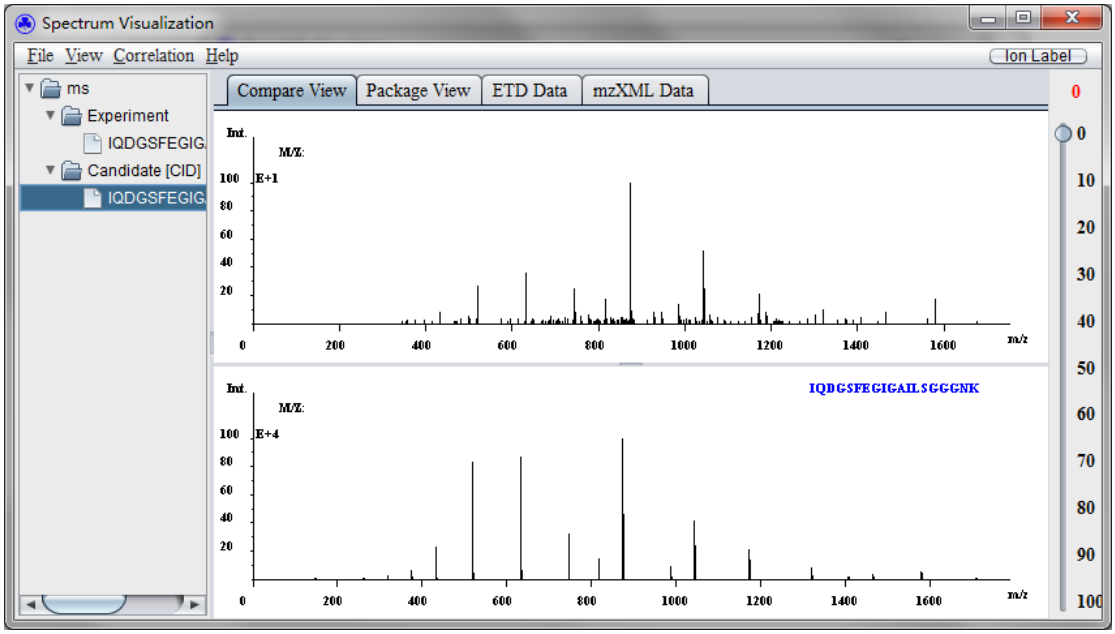

Figure 8 open an experiment spectrum and a theoretical spectrum.

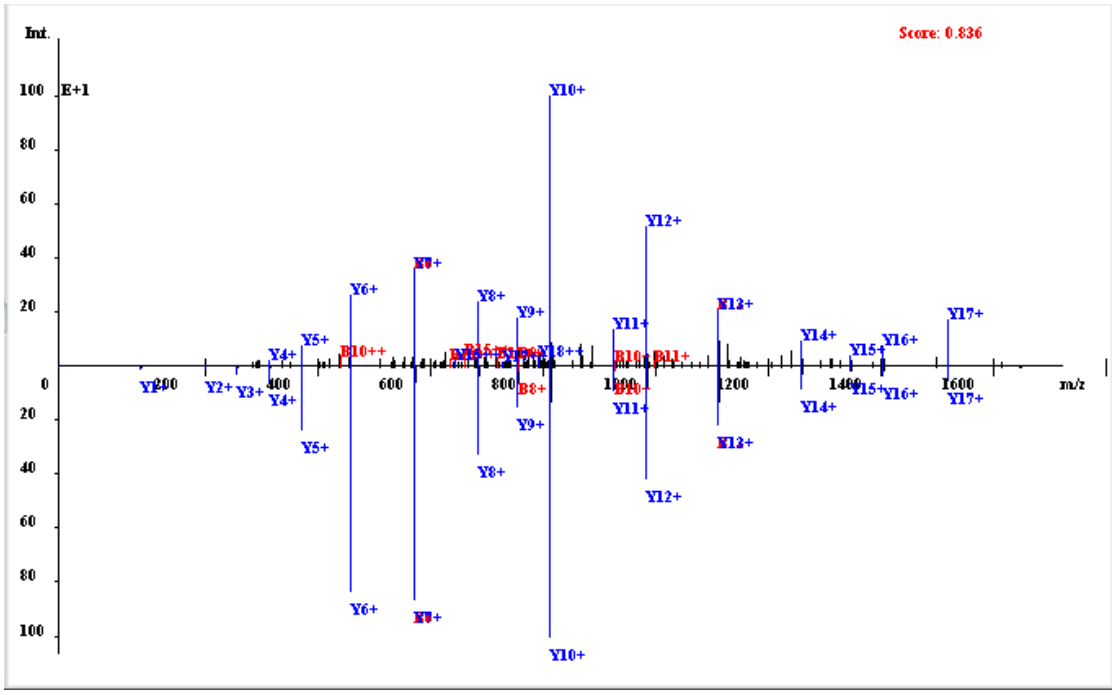

Figure 9 compare the two spectra (the correlation of this two spectra is 0.836).

Second, you should click “Correlation” on the top of the frame. You will see the interface as Figure 10. Then you will select the “Score Type”—“Corr” or “Dot” (“Corr” is utilized to calculate the correlation of the two spectra, “Dot” is used to calculate the dot product of the two spectra). Then you can set the “Tolerate” when calculate the correlation. After the “OK” button clicked, the result of the correlation will be show on the theoretical spectrum.

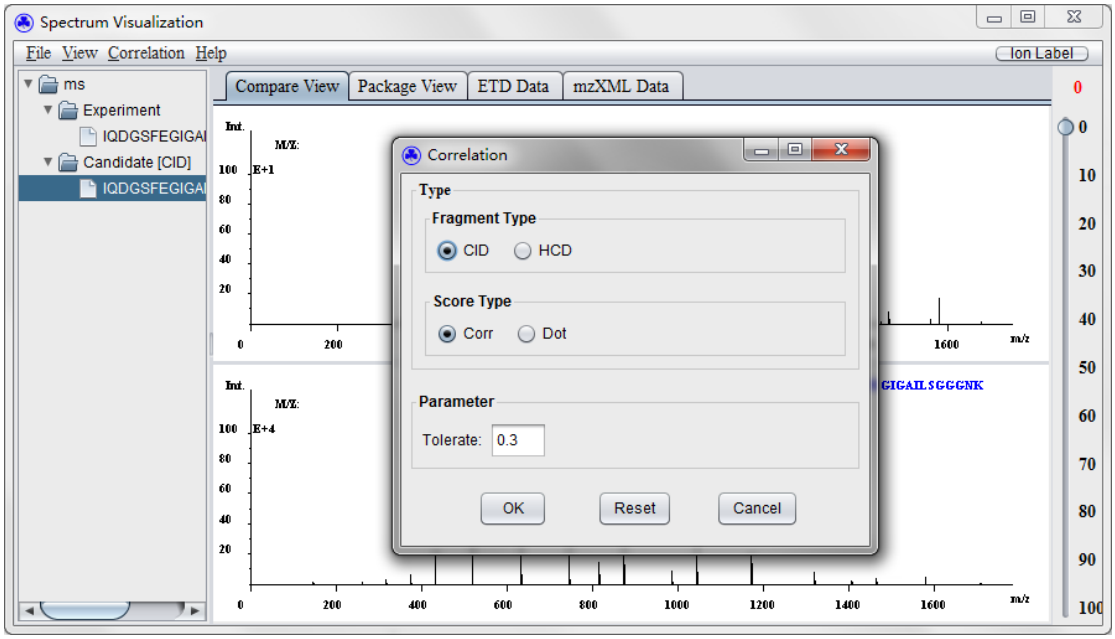

Figure 10 the frame of correlation, several parameters should be selected by user.

4. How to predict the theoretical spectrum of the sequence.

Applications->Theoretical Spectrum Prediction: you should click the "Theoretical Spectrum Prediction" button, and an interface as Figure 11 will be showed. In order to predict the sequence of peptide, you should set the parameters on the interface (This tool only realized prediction when the charge=2+). After you setting the parameters, you should input a file, which only contains the sequences of peptide and location of the output file. Then you can click the "Run" button to predict the sequences, a MGF file will be created in the selected path.

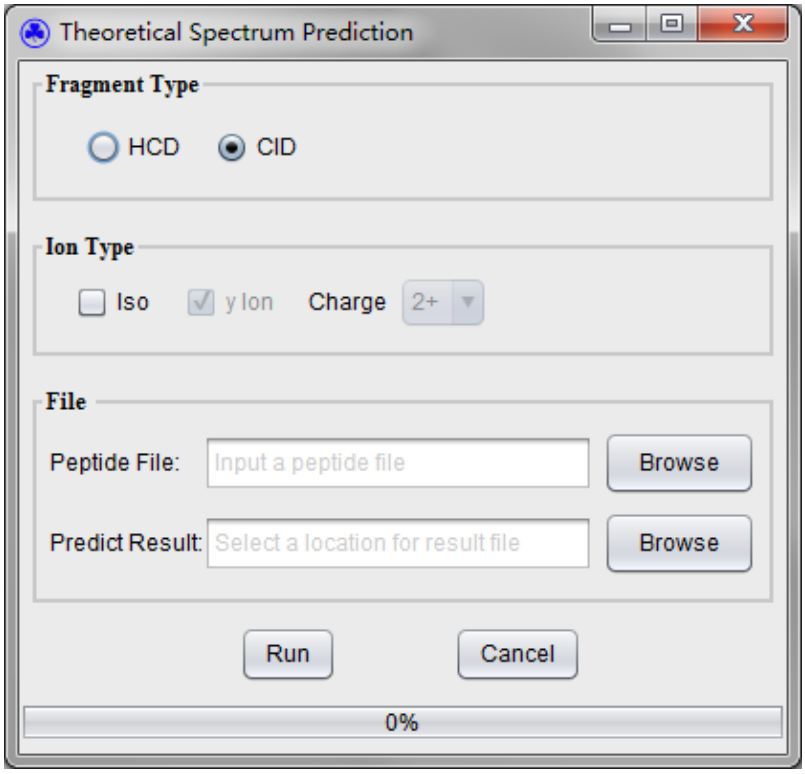

Figure 11 the frame for peptides prediction

5. How to re-score the SEQUEST result

Applications->Reranking: you should click “Reranking”, you will see the interface as Figure 12. Then, you will choose the original software and model, and input the destination spectrum format (.dta) files folder and corresponding output format (.out) files folder if you choose SEQUEST as the software. You can default or change “Parameter Setting” according to the practical situation. Do not forget inputting the location of the result file, as well as their names, in the box of “Result Location”. Finally, you only click the button of “Run”, and wait for the result.

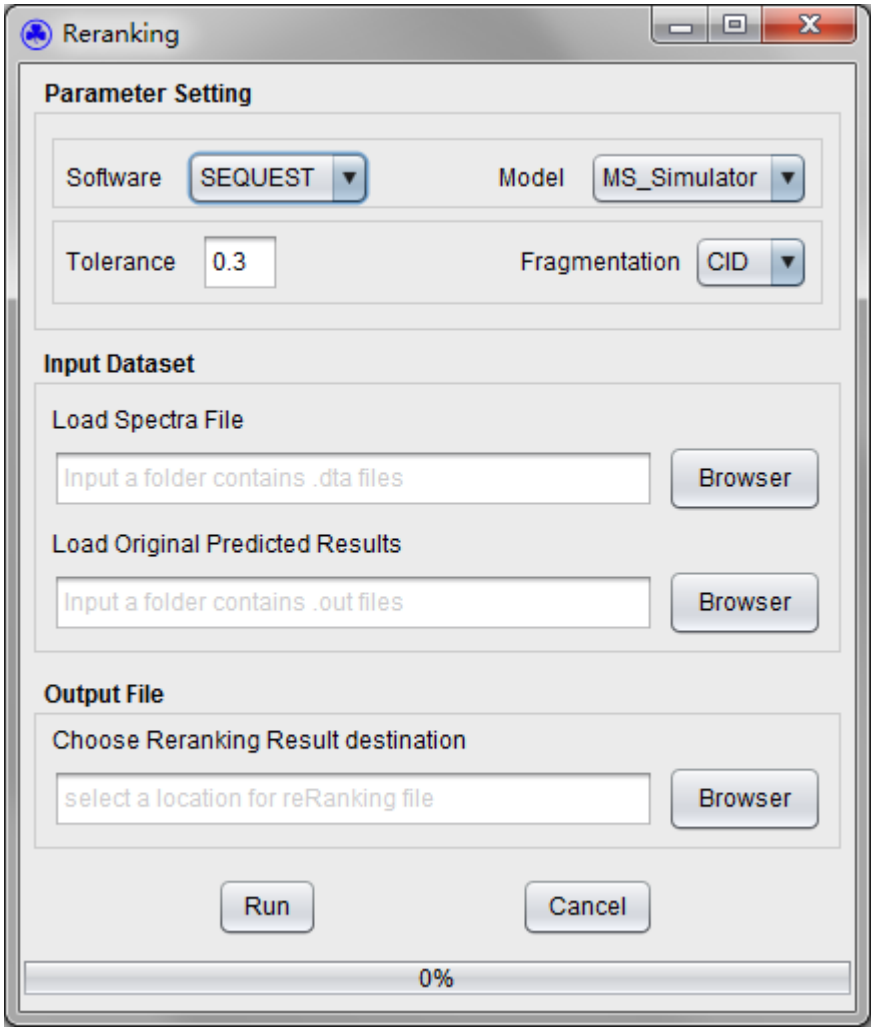

Figure 12 the frame for the result of SEQUEST re-scoring

6. How to analysis the FDR of the rescore

Applications->FDR Analysis: you should click “FDR Analysis” on the main UI, the interface of Figure 13 will display on your screen. Then, you select a result file, and input the decoy mark in the box of “Decoy Mark”. Ultimately, click the button of “Execute”, and the result of validation is shown as Figure 14.

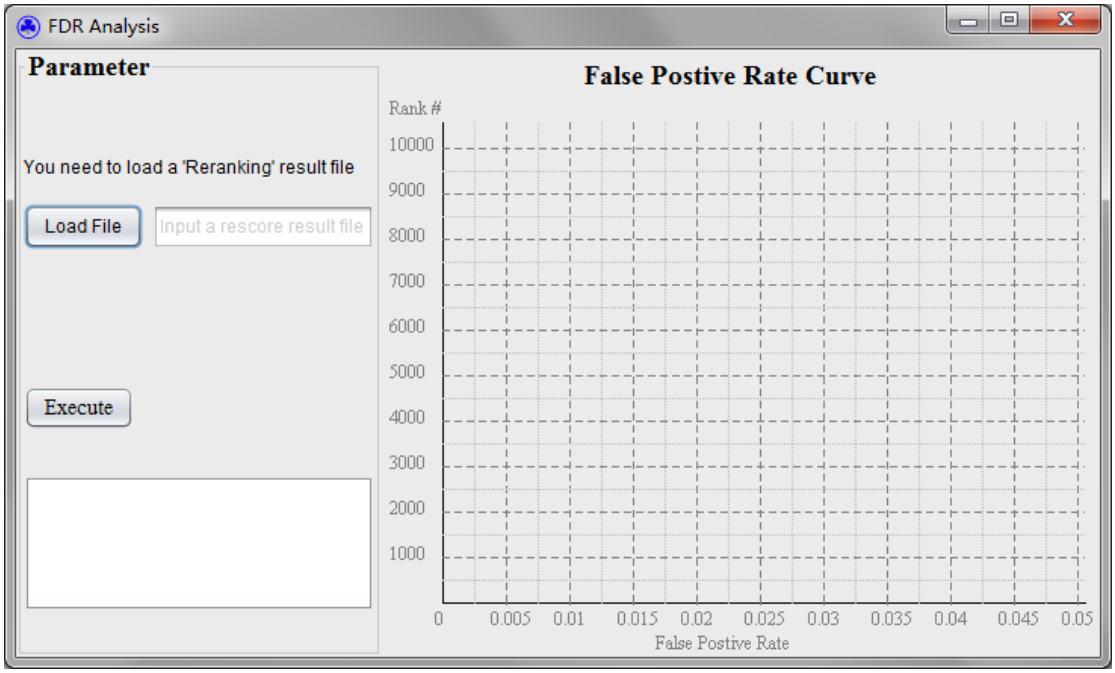

Figure 13 the main frame of FDR analysis

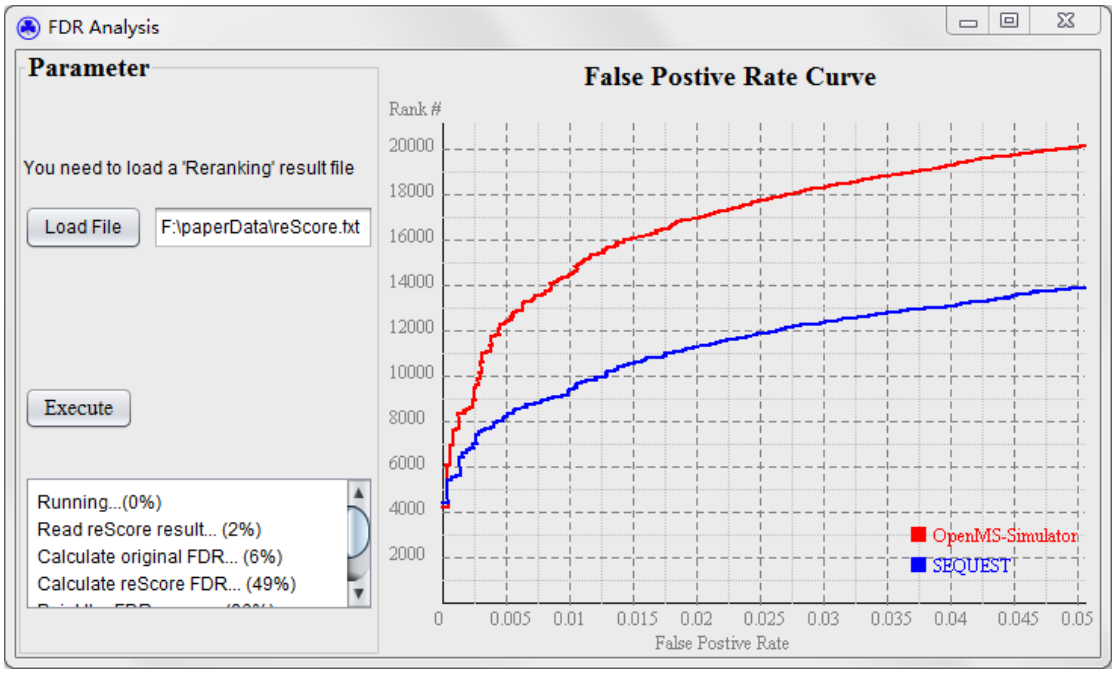

Figure 14 two curves drawn when a rescore file input
(The red line (OpenMS-Simulator) improve the blue line(SEQUEST) significantly)