

#### Description:

PI (Peptide Identification) is a tool with a graphical user interface (GUI) that allows the user to validate the result of database searching methods by direct input of the raw data output file of other packages, such as SEQUEST or Mascot. This software utilizes accurate intensity information and the neutral losses property of the spectrum to predict more reasonable theoretical spectrum. It also has the function of labeling the spectrum with frequent ions, such as b, y, a, dehydration ions, deamination ions, and their isotopic ions.

This tool is described in detail in the following:

#### Download:

The package PI is a property of ..... It can download at .....

#### Required Software:

PI will run on the Java SE Development Kit (JDK). Before you install the package PI, the JDK 5 Update 16 (version 1.5.0\_16) or newer (including JDK 6 Update 11) must be installed on your system. If you do not have an installation of JDK, you cannot proceed with the installation. You can download the latest JDK version at <http://java.sun.com/javase/downloads>.

#### Installation: (?)

PI is green software which needs not to be installed or uninstalled. You can extract the compressed package to a destination folder to use it directly. It's a lighter program takes less system resource and have quite enough features, easy to use.

PI is system-independent. On any platforms, you can run PI.jar to start the application. No any other special settings are needed.

#### Usage Instruction:

##### 1 The Main UI of PI

The main UI of PI is displayed as Fig.1. On the top of the interface labeled "File, View, Processing, Analysis, Tools, and Windows".

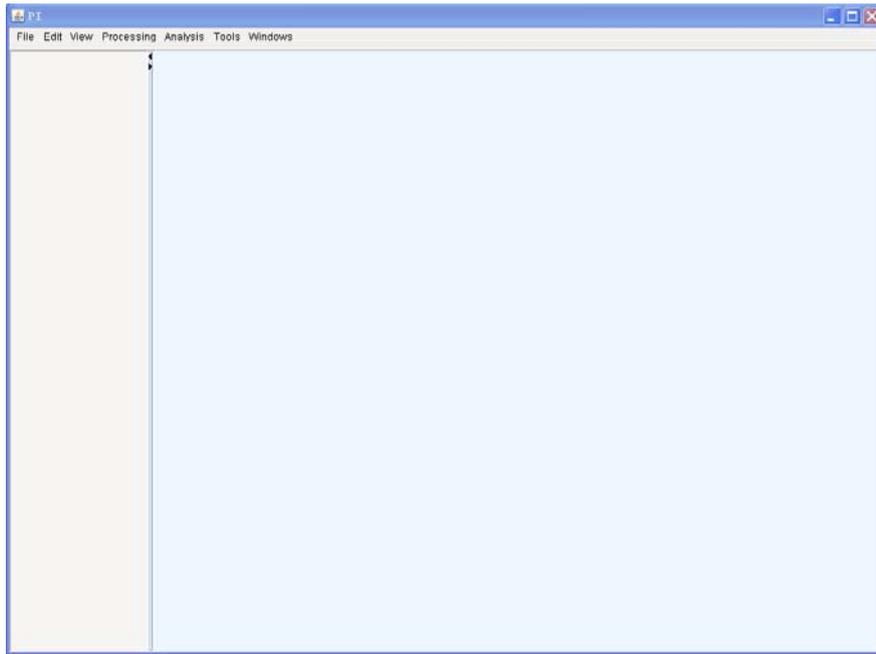


Fig. 1 the main UI of PI

## 2. How to label the spectrum

**File->open:** first, you should click "File", and then click "open" in the pull-down menu. Second, according to the interface, you should select a destination folder, and the Fig.2 will show in the main UI.

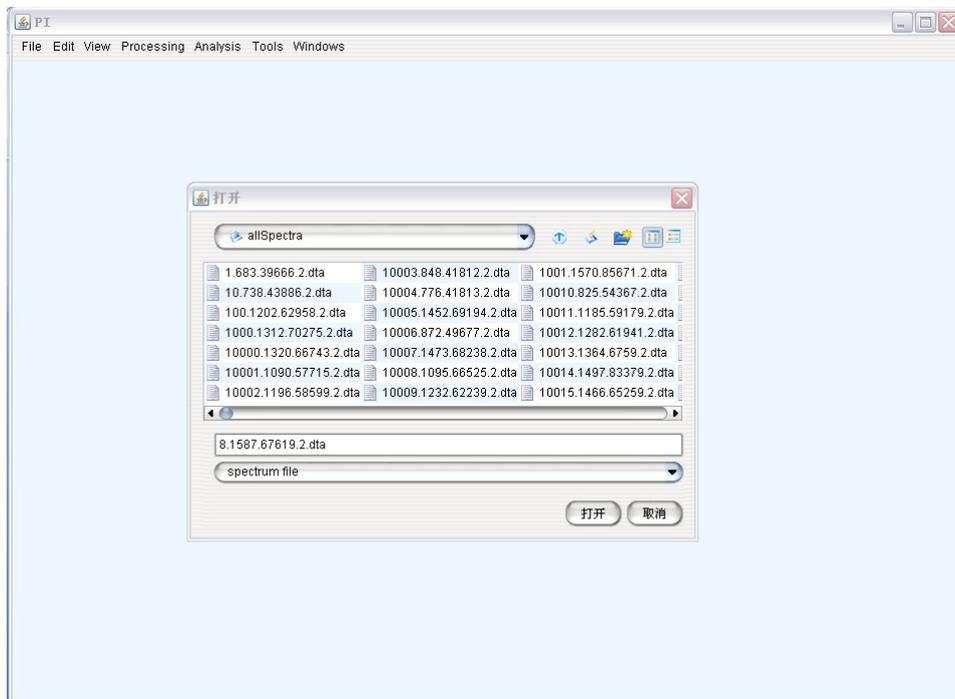


Fig. 2

You then choose the objective .dta file and click the button of "Open". You will see the interface as Fig.3.

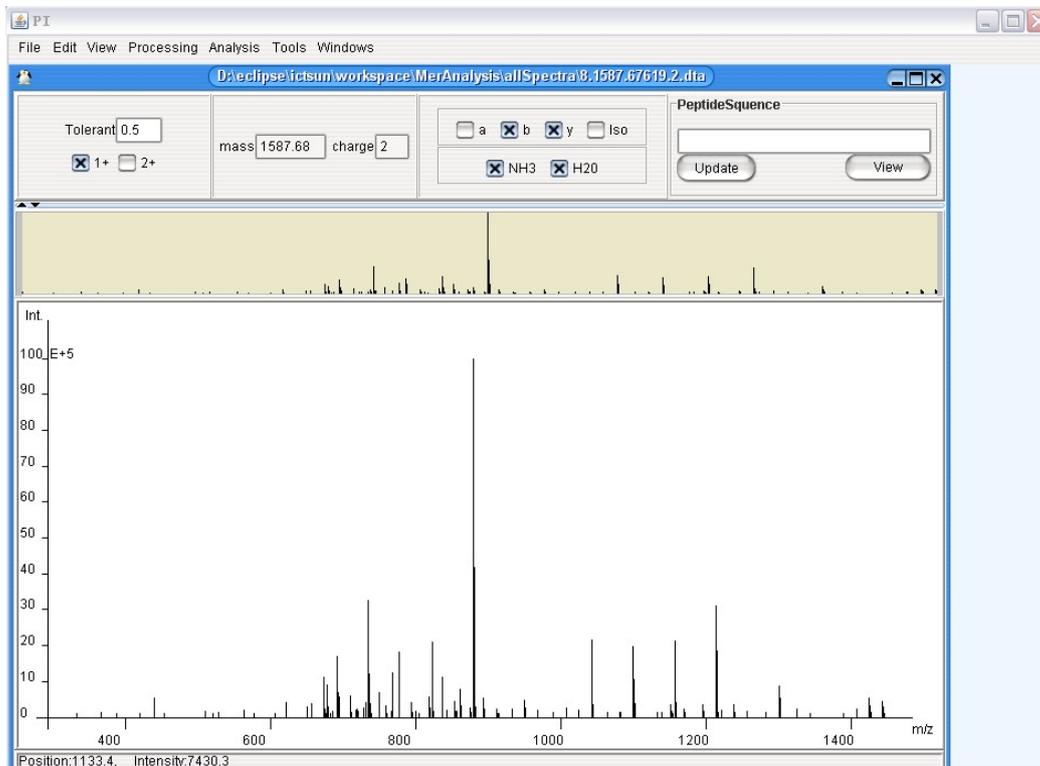


Fig 3

In order to label the spectrum, you can input or copy the sequence of the target peptide in the box of "Peptide Sequence", and choose the types of ions that need to be labeled on the spectrum, simultaneously. Finally, click the button of "Update". With the interface shown as Fig.4, you can observe and compare spectra intuitively.

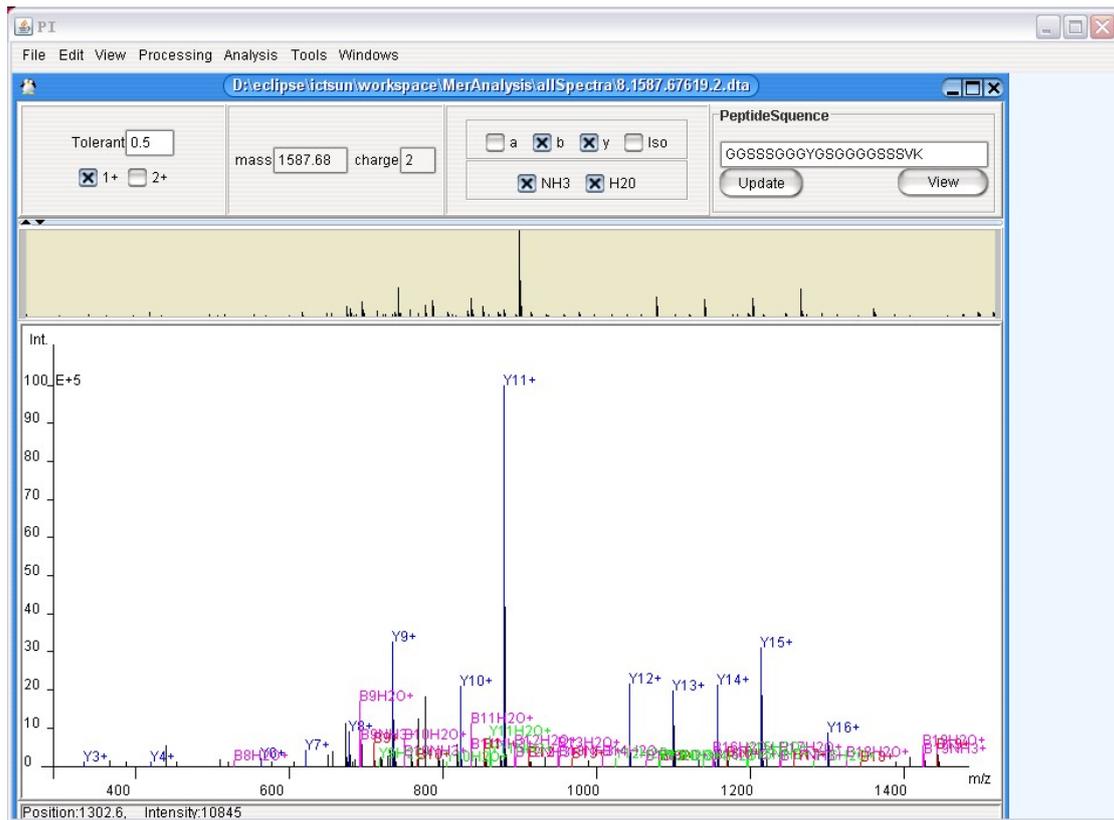


Fig 4

## 2. How to validate the result of other packages

**Processing->rerank:** first, you should click "Processing", and then click "rerank". You will see the interface as Fig 5. Then, you will choose the types of the output and model, and input the destination .out files. If the corresponding .dta files and .out files are under the same directory, you need to select ".dta attached" directly. Otherwise, you should input the corresponding .dta files in the box of "spectral pool" one by one. You can default or change "Parameter Setting" according to the practical situation. Don't forget inputting the location of the result files, as well as their names, in the box of "result location". Finally, you only click the button of "Run", and wait for the result.

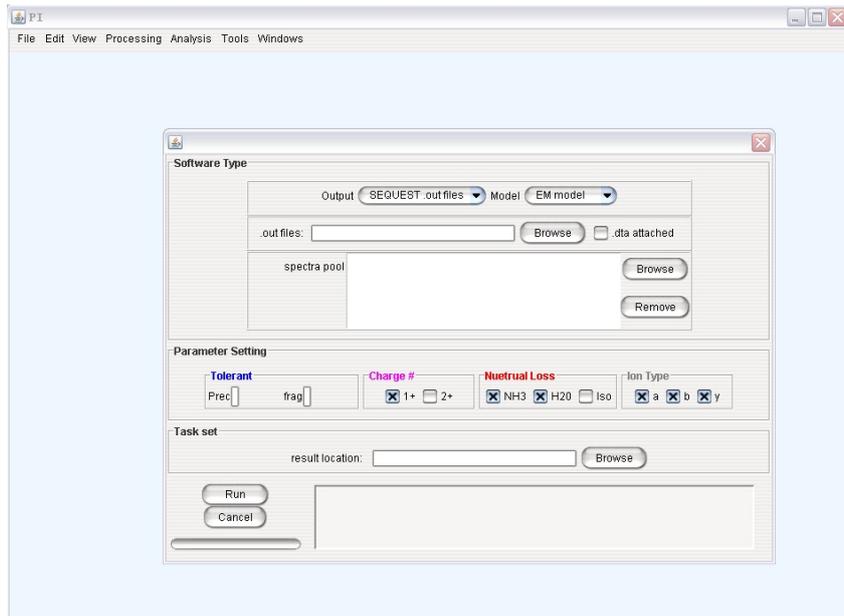


Fig 5

**Analysis->rerank:** you should click "Analysis", and then click "rerank". The interface of Fig. 6 will display on your screen.

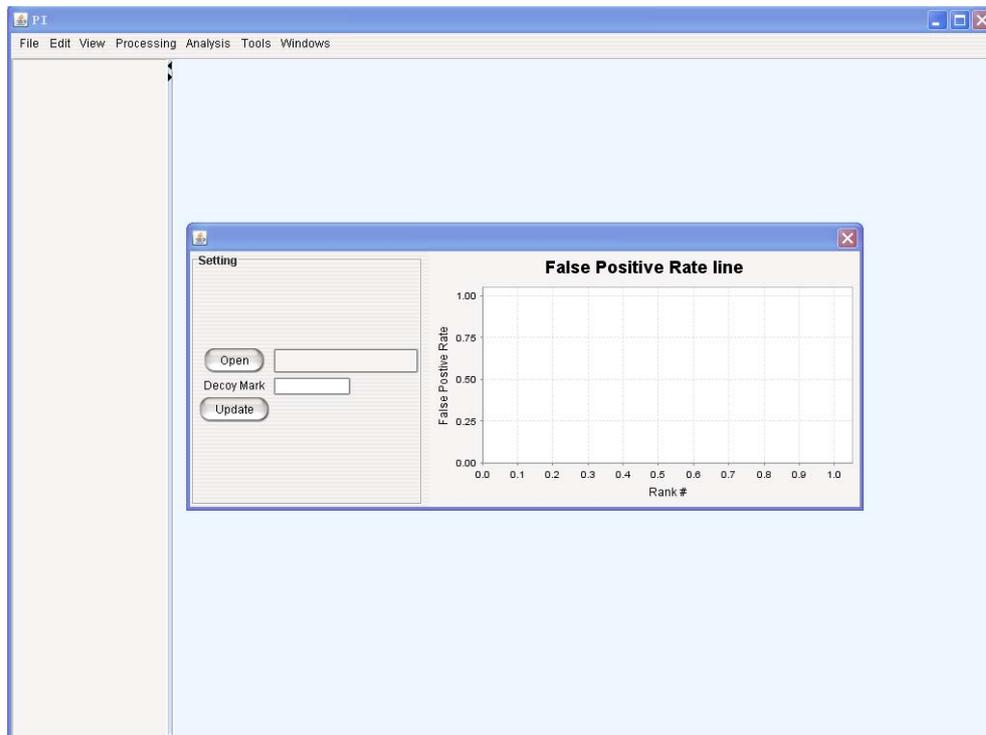


Fig. 6

Then, you open the result file, and input "DECOY" in the box of "Decoy Mark". Ultimately, click the button of "Update", and the result of validation is shown as Fig.7

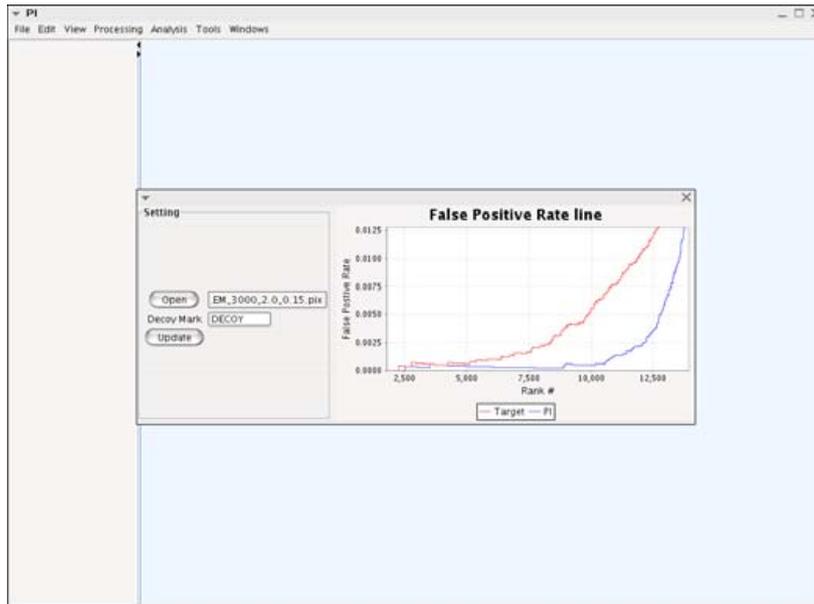


Fig.7