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pFind Studio

pLabel User Guide

Version 2.4.0.5

Released time: 2017.12.22

pFind Group

2017.12

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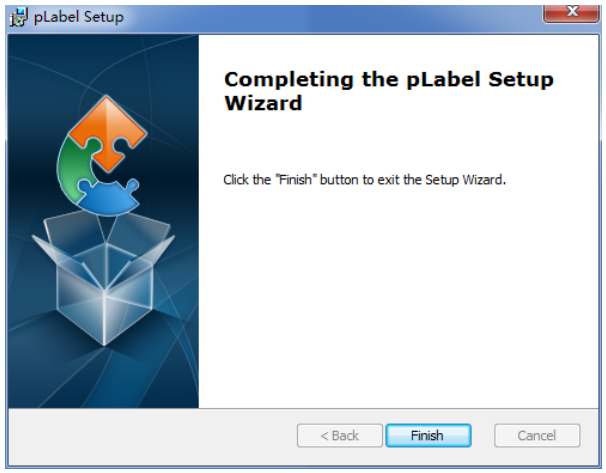
- Labeling a spectrum
- Saving pictures

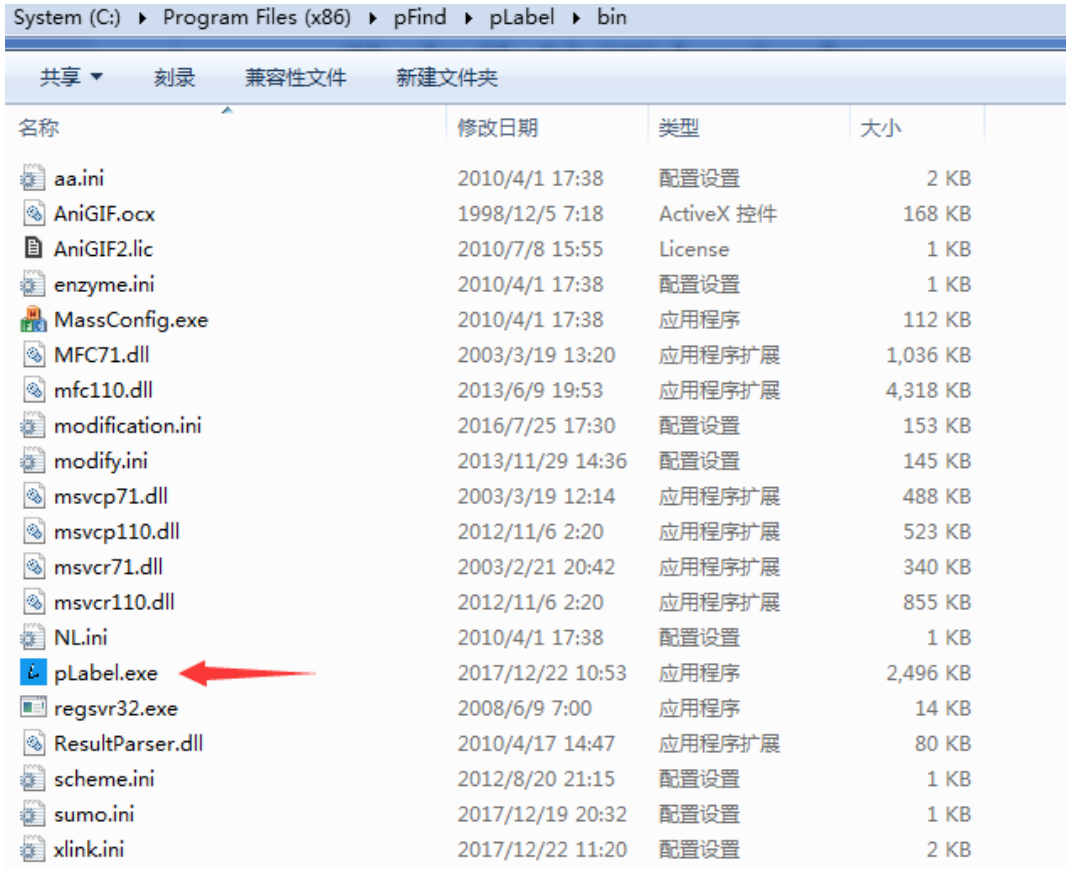
Software installation

- pLabel is written by C++.
- Microsoft Visual C++ environment is required.
- pLabel runs on windows operating systems.
- Latest setup file download link:
  - http://pfind.ict.ac.cn/software/pLabel/index.html

Installation completed

❖Click “pLabel.exe” to run pLabel.



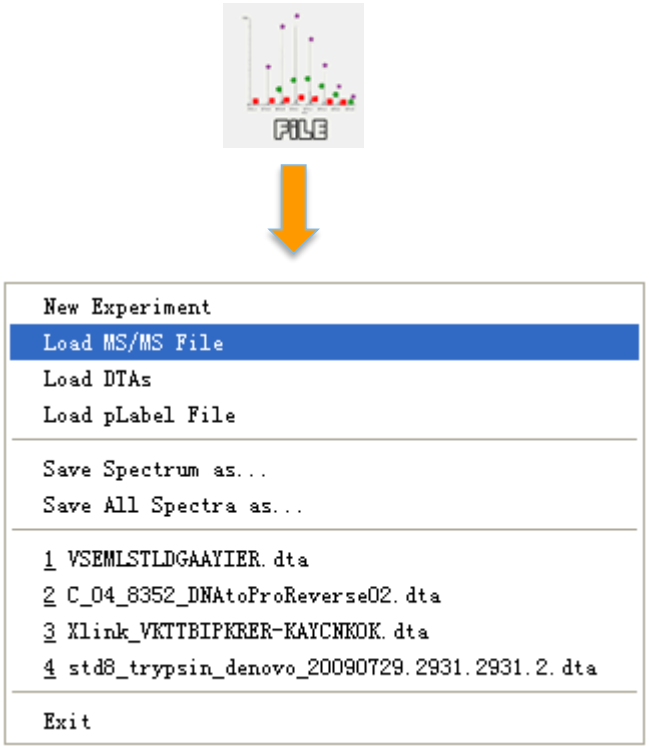


Opening a spectrum file

- Clicking “Load MS/MS File” in File menu.

- pLabel 2.4 supports DTA file (.dta), MS2 file (.ms2), Mascot Generic Format (.mgf).

- To avoid a huge number of DTA files, clicking Load DTAs would be a better choice.



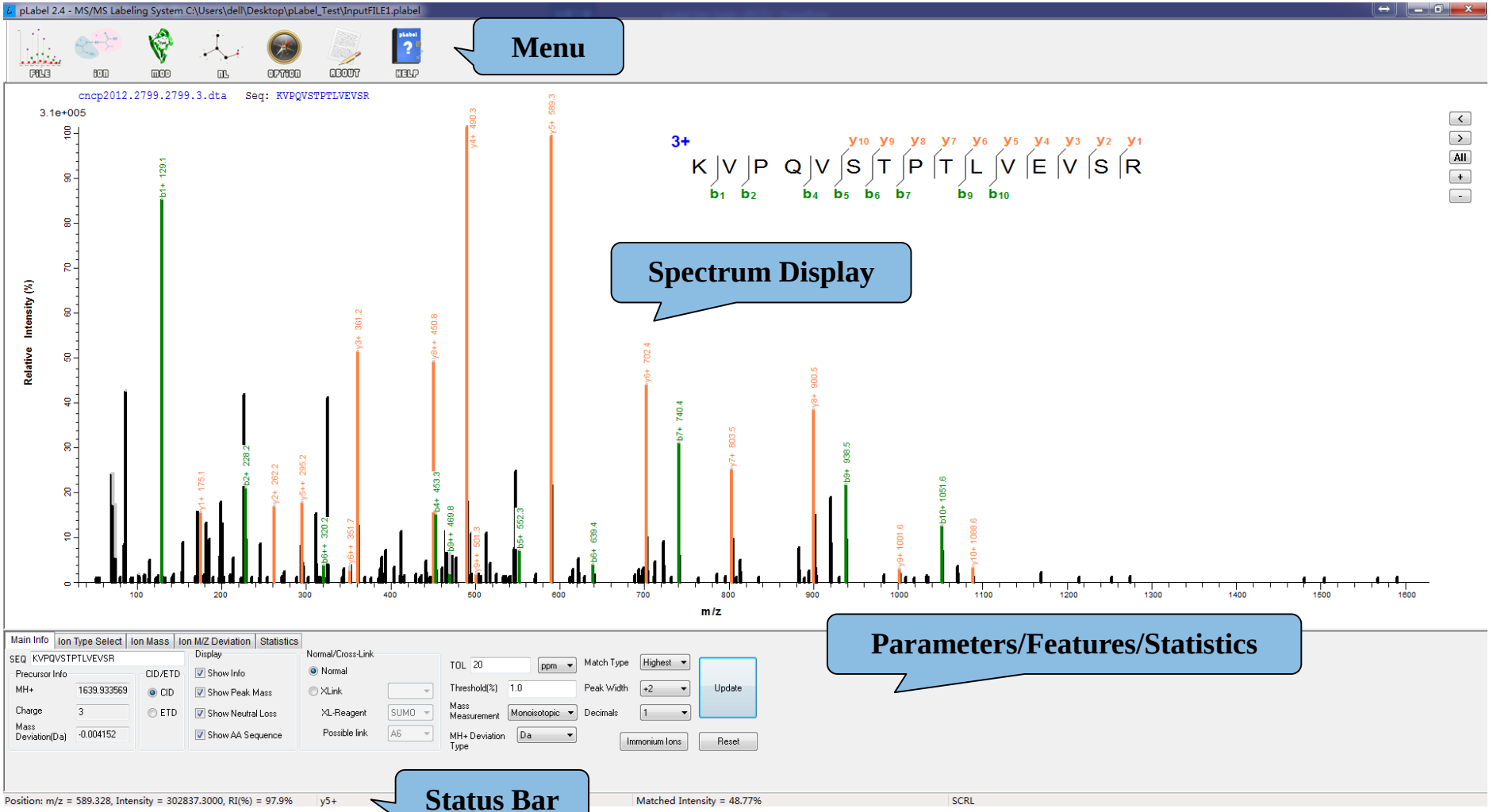
pLabel file format

- **pLabel file (.plabel) is our own file format for labeling spectra with amino acid sequences given by search engines, which is generated by pBuild.**

- **A sample pLabel file may begin like this:**

```
[FilePath]
File_Path=G:\testdata\data\n2-090721-etd-ltq-rep1-01.ms2
[Modification]
1=Oxidation_M
2=Carbamidomethyl_C
[Total]
total=5204
[Spectrum1]
name=N2-090721-ETD-LTQ-REP1-01.13.13.2.DTA
pep1=0 EDKAFCK 0.32
[Spectrum2]
```

Graphic user interface



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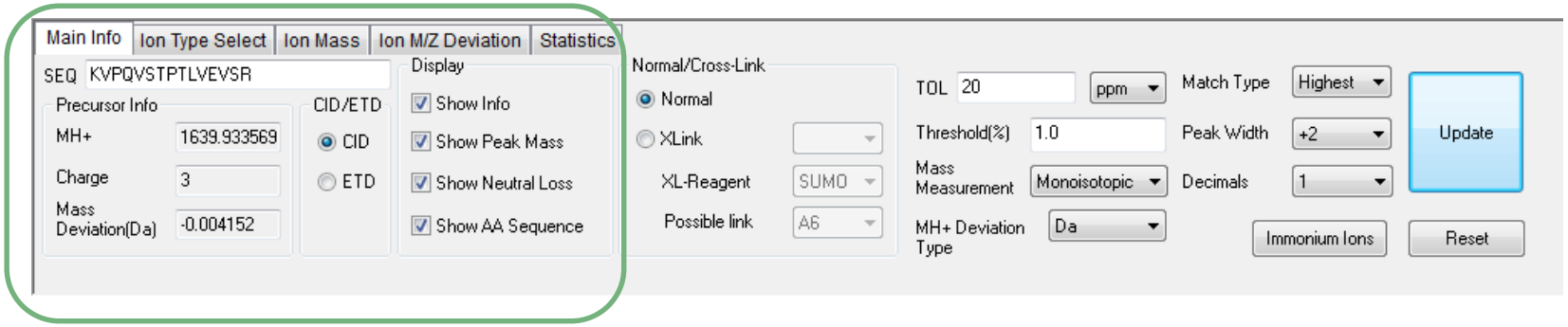
Labeling a spectrum

❖ Setting Parameters-1:



SEQ: Peptide sequence, only characters ‘A’- ‘Z’, a’- ‘z’, ‘-’ are allowed.

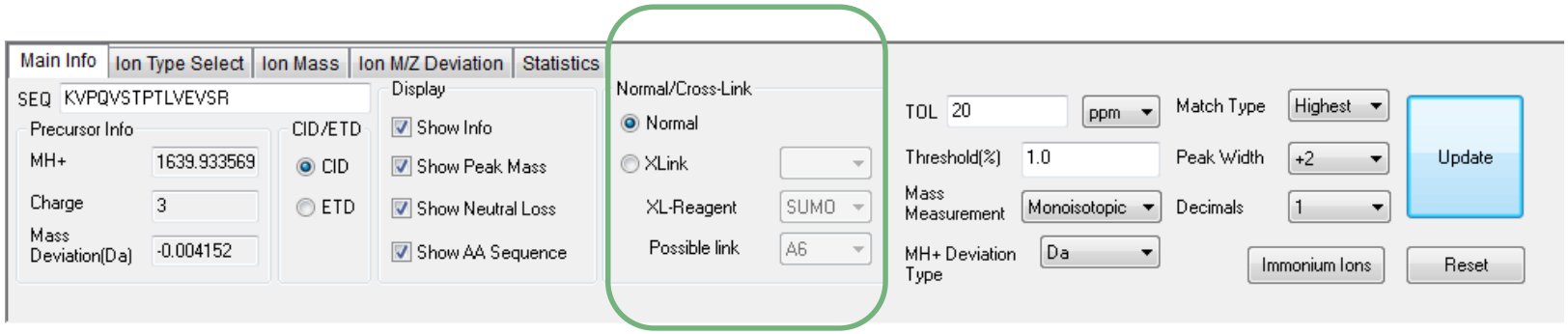
Precursor Info: Precursor charge, precursor mass(MH+) and precursor mass deviation are listed here, they can not be edited.

CID/ETD: Activation type.

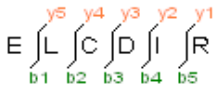
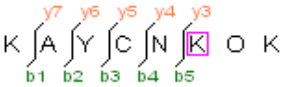
Display: Spectrum number, AA Sequence and other information.

Labeling a spectrum

❖ Setting Parameters-2:

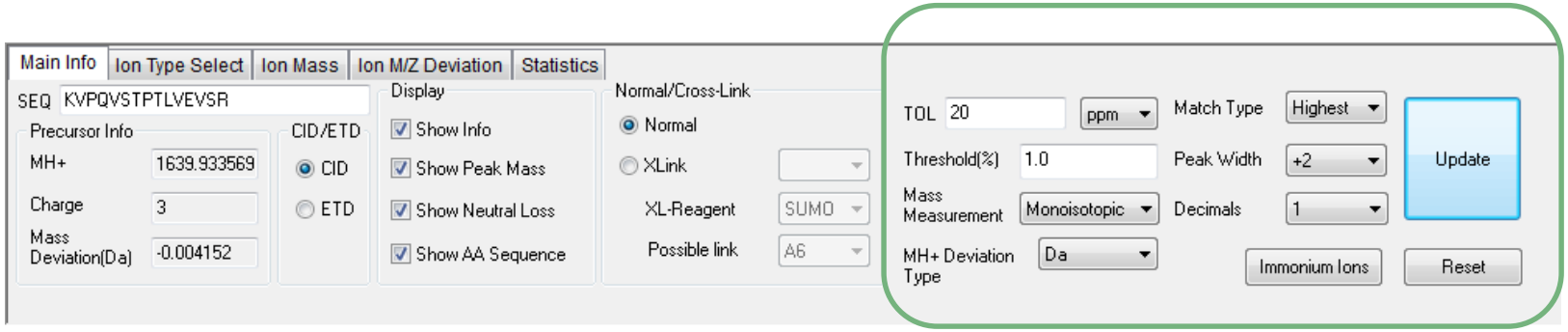


Normal/Cross-Link:

Normal		
Cross-link	Xlink	
	Mono	
	Loop	

Labeling a spectrum

❖ Setting Parameters-3:



TOL: The peaks within which will be taken into account. Click the button on the right to change between Da/ppm mode.

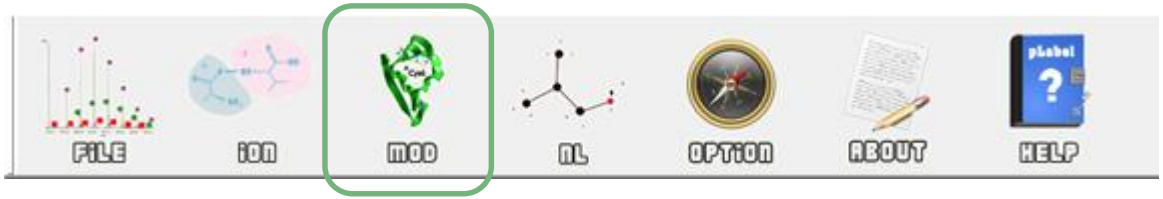
Threshold: Peaks under this threshold will not be matched.

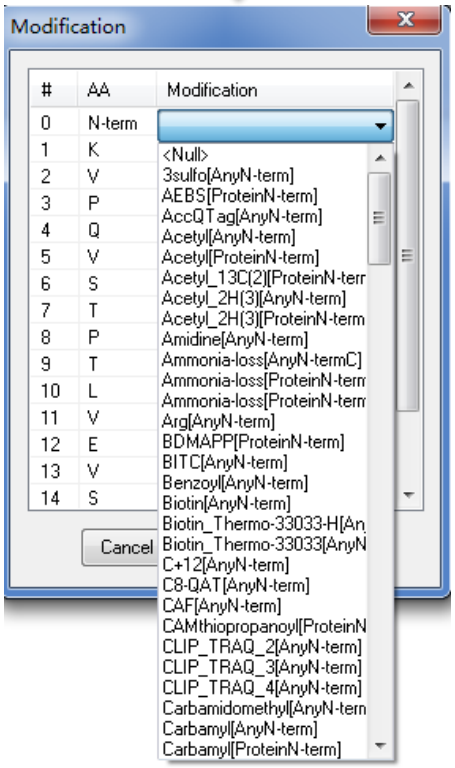
Mass Measurement: mono/average.

Match Type: In the highest mode, the most intensive peak in the tolerance window of a theoretical peak is selected as a matched peak. While in the nearest mode, the peak which is nearest to the theoretical peak is selected.

Labeling a spectrum

❖ Choosing Modifications:

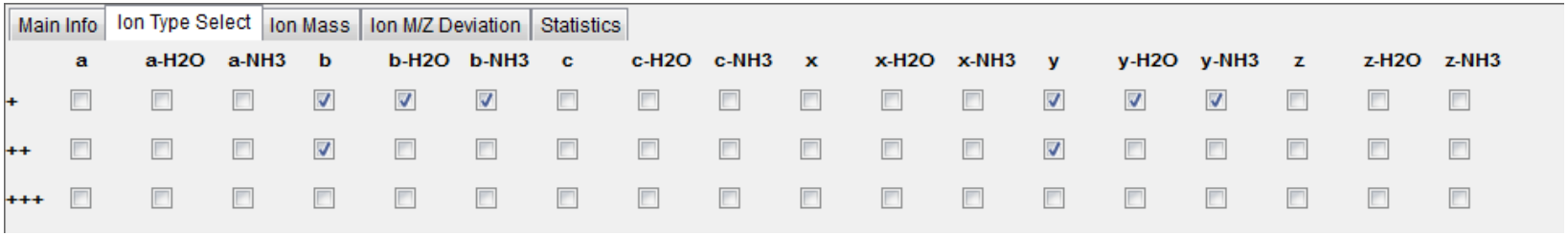




Labeling a spectrum

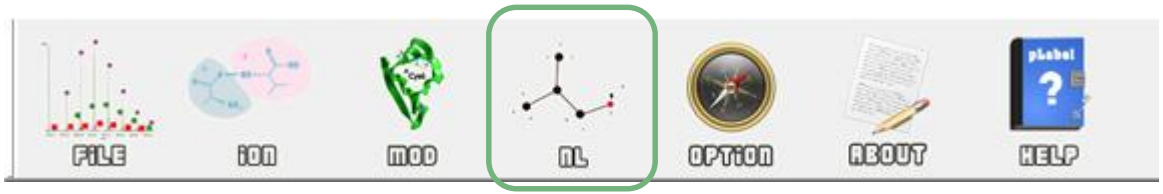
- **Choosing fragment ion types:**

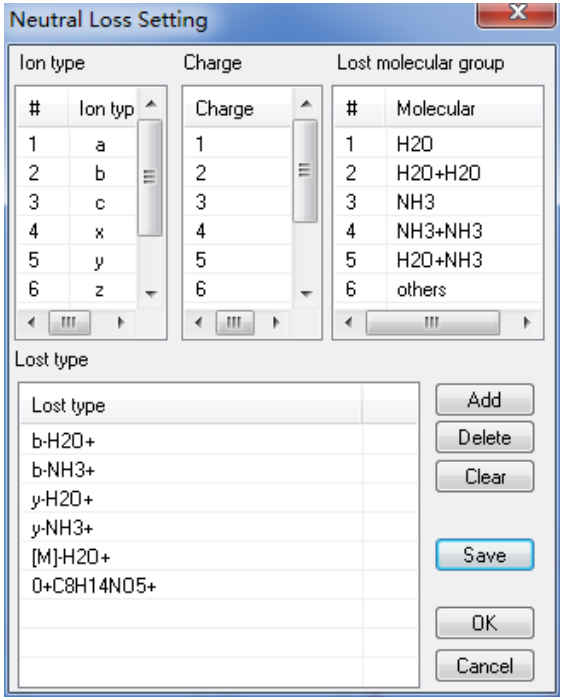
- **pLabel will use the specified ion types to label peaks in the spectrum display area.**



Labeling a spectrum

❖ Adding new neutral lost:





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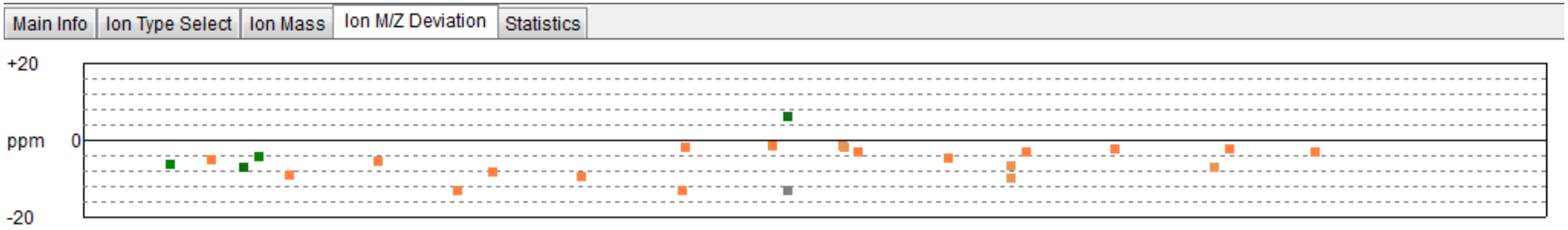
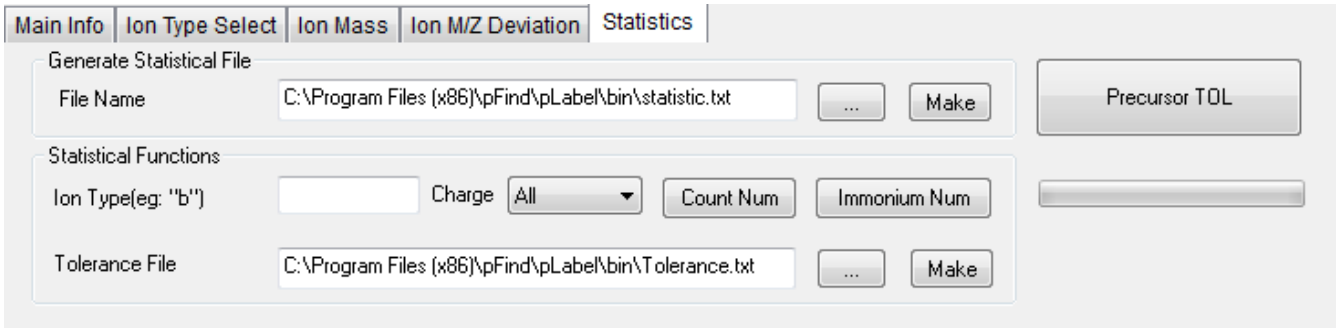
Viewing deviations

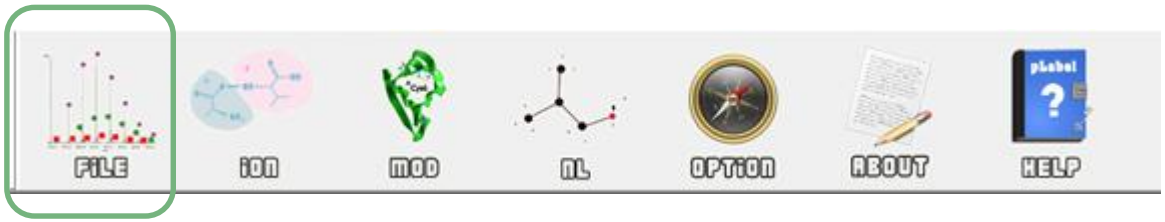
❖ **All matched peaks' deviations:**

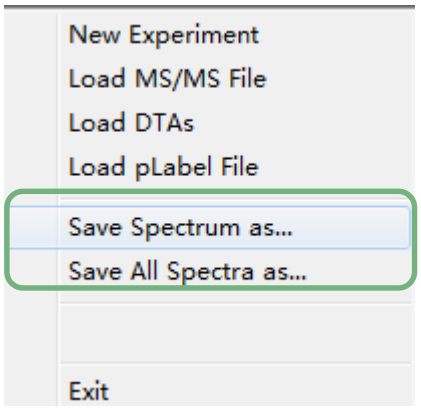


❖ **Get all ion deviations:**

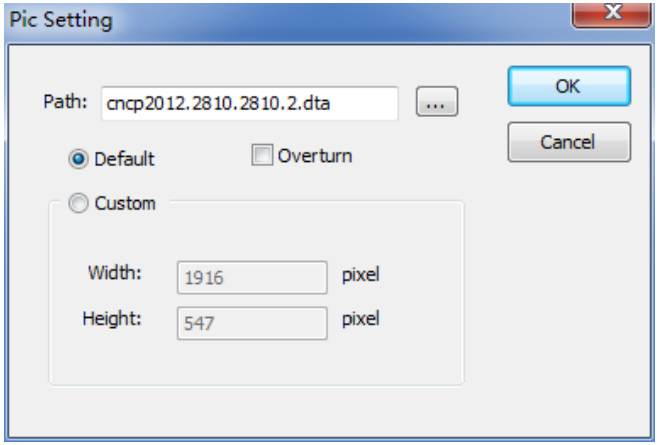


Saving Pictures

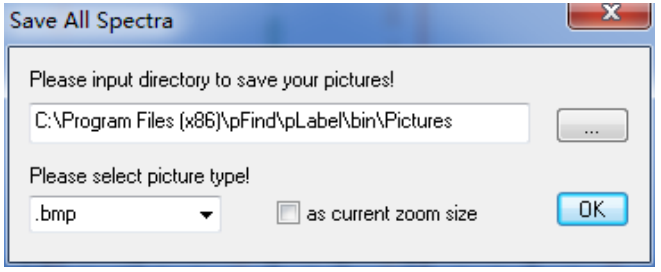




Saving one spectrum



Saving all spectra



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- **Thank you for using pLabel.**

- **If you have any questions, please contact pfind@ict.ac.cn.**