

# RecoverFx user guide

Release 3.0.0

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## **1) RecoverFx**

RecoverFx is the future version of Recover, the MS/MS spectra viewer/extractor designed to extract "high quality" spectra from peak list files.

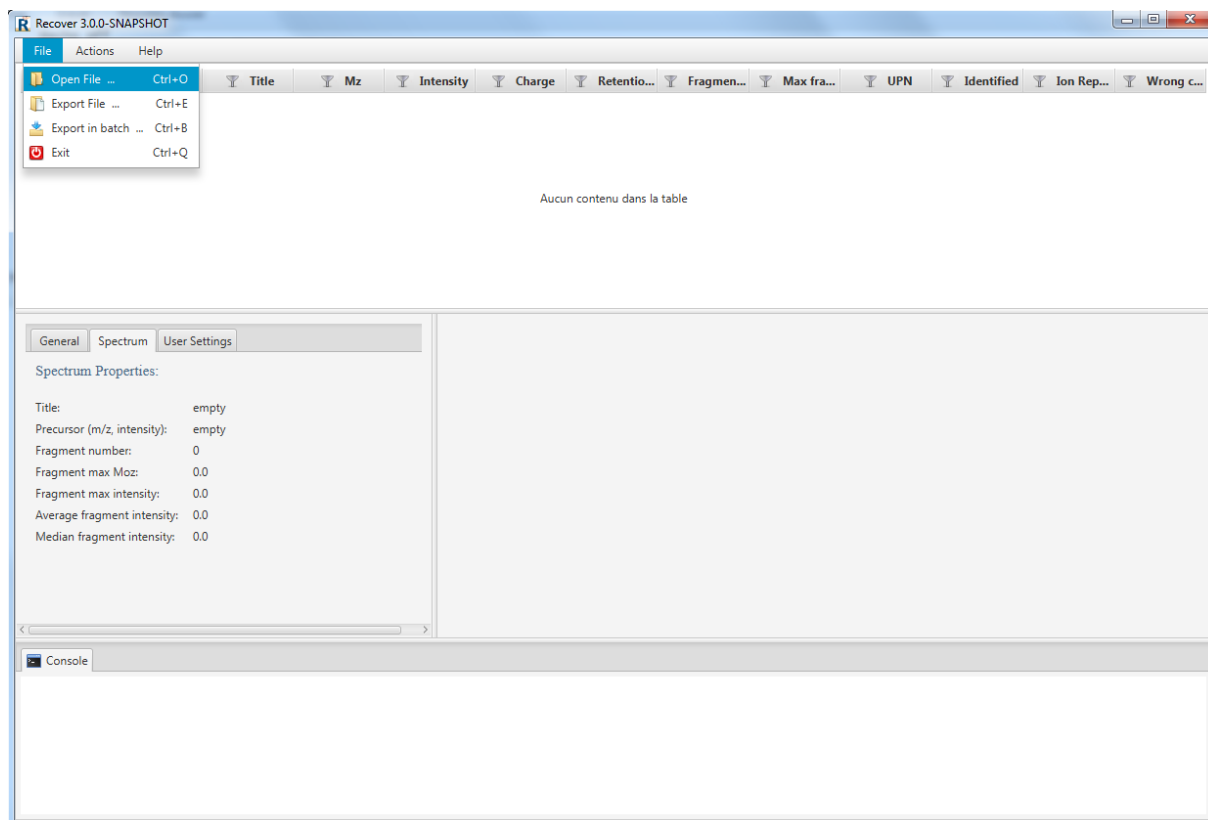
Recover has been developed to filter out high quality spectra from peaklists based on the user-adjustable variables.

## **2) File:**

### **a. Open file**

The user must select a valid peaklist file (with extension .mgf or .pkl) via the menu "Open file" or via the keyboard shortcut "Ctrl+ O".

It will read the peaklist file and extract the spectra. This action could take a while; it depends on peaklist file size.



### b. Export file:

This action will export the spectrum that contains in the table view after applying the filters.

The spectra that's does not exist in the graphical interface (in the table view) will be removed from the peaklist file. In the head of the new peaklist file, there are the number of recovered spectra and the identified spectra.

**Note:** the number of the recovered spectra is the number of spectra in the table view after applying filters.

### c. Export in batch:

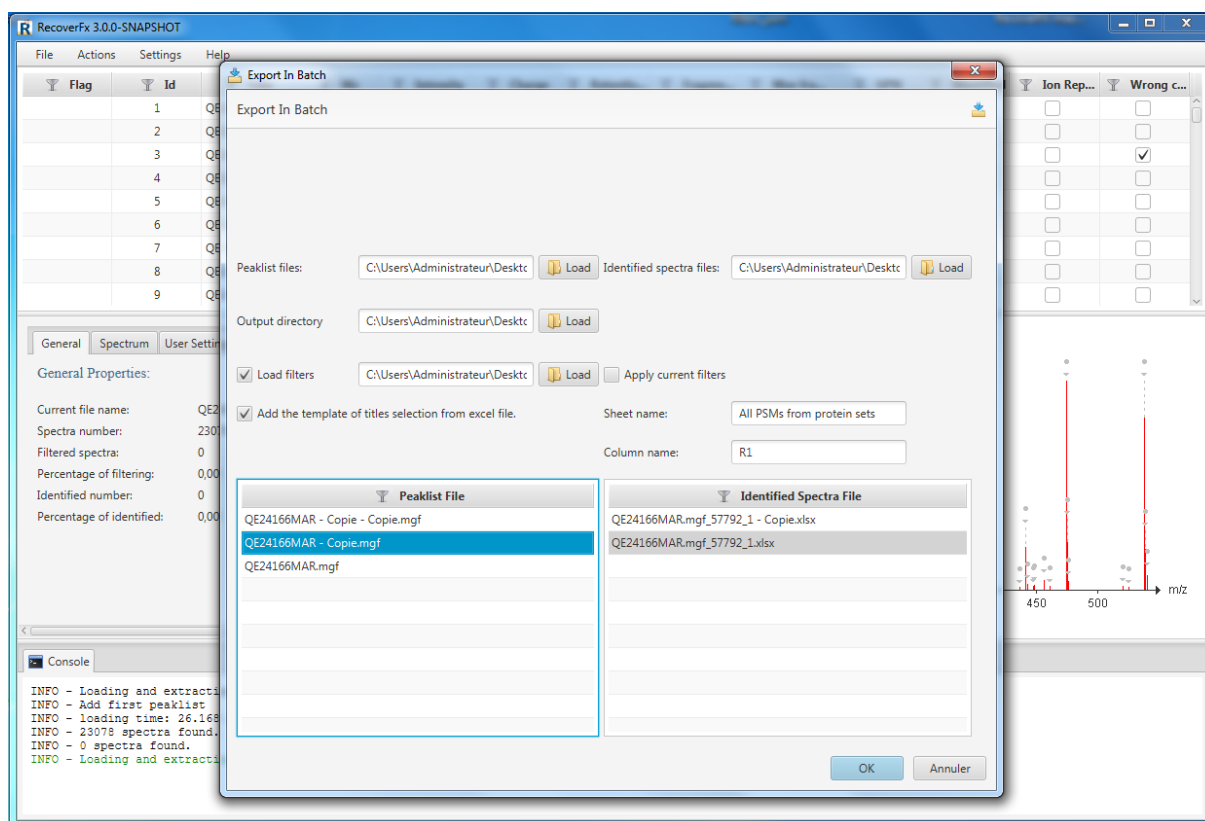
This action will let the user to apply a list of filters to a list of peak list files and to filter out the identified spectra. The filters could be loaded from a JSON file or from the current session filters.

If you have specified an identified spectra files, you must enter the title template from an excel file.

- The sheet name of identified spectra
- The column name of identified spectra for example (A1 or R1 ...)

The output directory: the folder where the files will be exported. The exported files will be renamed as : date\_original\_file\_name.

Note: To link each peak list file and its identified spectra file you must reorganize the order of columns via drag and drop.



#### d. Exit:

This action will close the RecoverFx correctly.

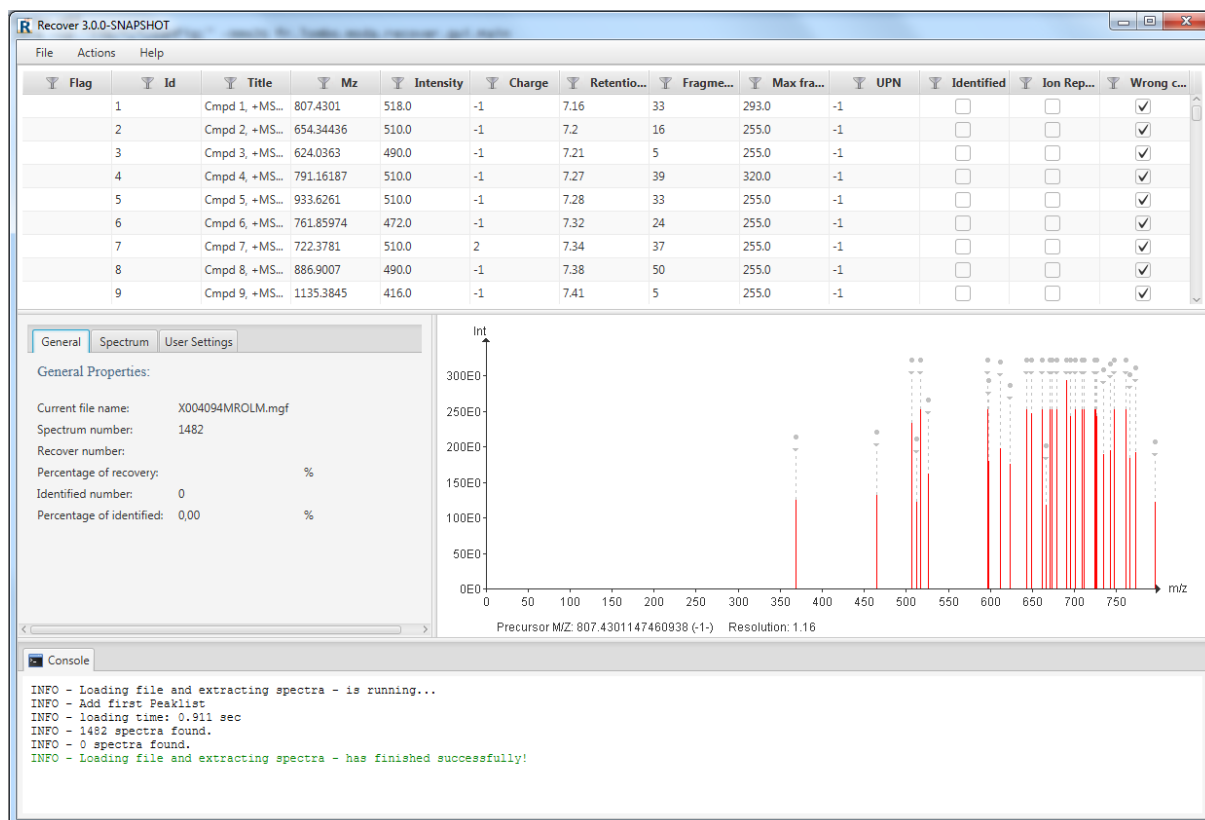
#### Warning:

This action will remove all spectra from the table view. And reset all filters.

### 3) Graphical user interface:

#### a. Information pane

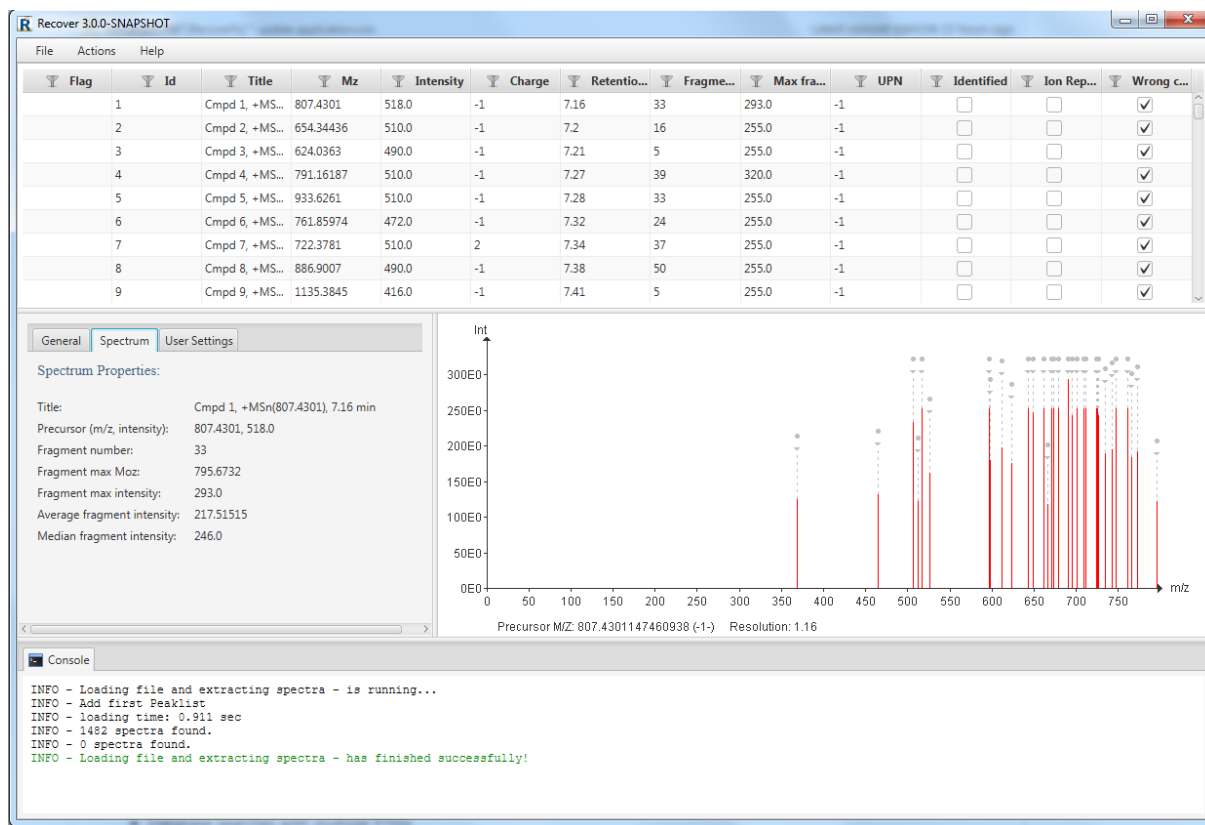
General properties:



This tab pane contains general information:

- Current file name: the loaded file name.
- The spectrum number: The number of spectrum extracted from the loaded file.
- Filtered spectra: The number of the spectrum that's filtered. The filtered number is the number of the spectra that remained in the table view.
- Percentage of filtering.
- Identified number: The number of the spectrum that identified. This property is updated whenever the "get identified spectra" is applied.
- Percentage of identified.

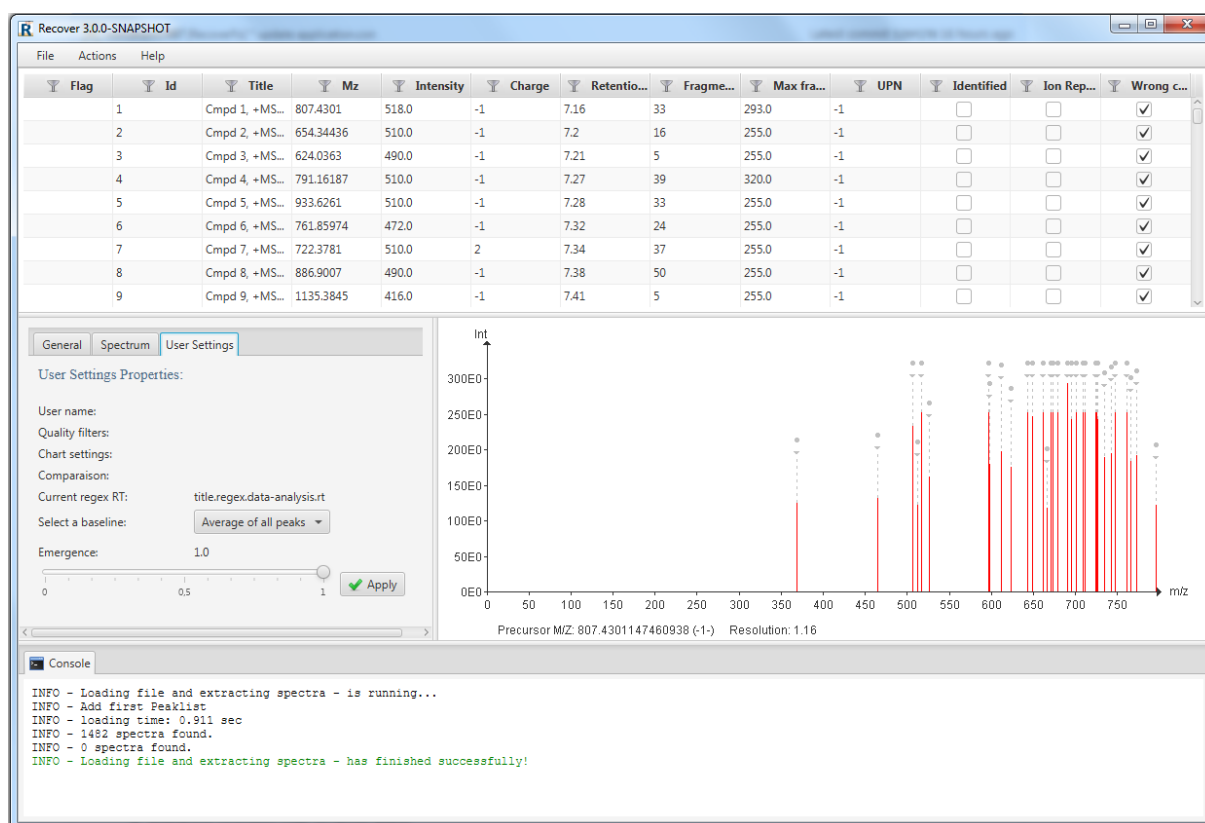
Spectrum properties:



This tab pane contains the information about the selected spectrum in the table view.

- Title: The title of the spectrum.
- Precursor (m/z, intensity).
- Fragment number: the fragment number found in the selected spectrum.
- Fragment max moz: The maximum fragment moz found in the selected spectrum.
- Fragment max intensity: The maximum of fragment intensity found in the selected spectrum.
- Average fragment intensity: The average of fragment intensity computed in the current spectrum.
- Median fragment intensity: The median fragment intensity computed in the selected spectrum.

User's settings:



This tab pane contains the information about the user settings; the user settings could be loaded or exported from/to a JSON file.

- User name: The user name.
- Quality filters: The user filters.
- Char settings: The user char settings.
- Current regex RT: The current parsing rule used to retrieve retention time from the title.
- Baseline :
  - Average of all peaks
  - Median of all peaks
- Emergence: The Emergence (E) is a multiplication factor applied to the noise level (computed with an appropriate algorithm for each spectrum) allowing to define "Useful Peaks" with intensities higher than  $E \times \text{noise level}$ .  
On apply button click will compute the useful peaks number.

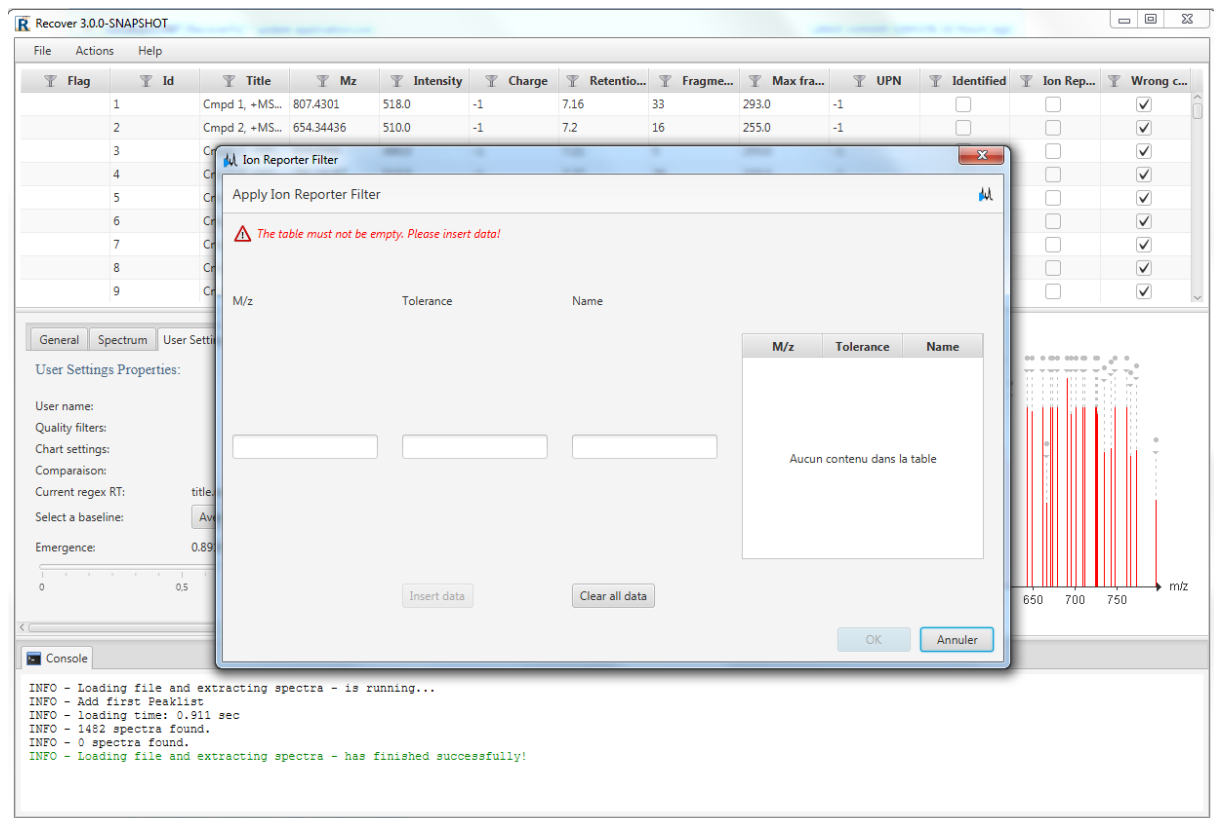
## b. Spectrum pane

It represents a graph of the selected spectrum. There some actions to view the graph:

- Zoom: Select an area.
- Cancel zoom: left click.
- Show a sequence of AA: Select a fragment and select the others fragments.
- Cancel the comparison: Ctrl+right click.

## 4) Actions:

### a. Add ion reporter



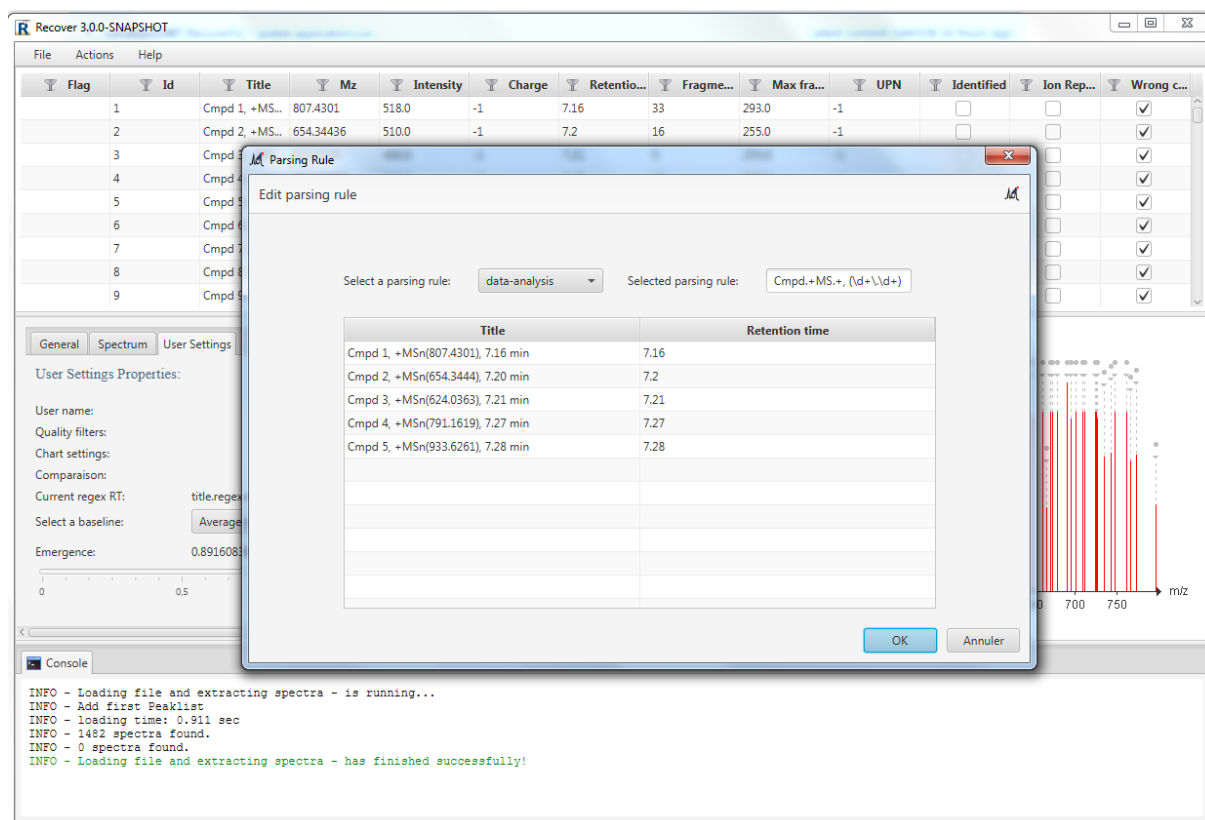
This dialog let the user add a list of ion reporter:

- M/z: the value of M/z, accept numeric values only.
- Tolerance accepts numeric values only.
- Name: the name of the ion reporter.

The user enters a list of ion reporters. The result will be show within the column ion reporter in the table view; whenever a spectrum is covered it will be checked (set to true).

## b. Edit parsing rules



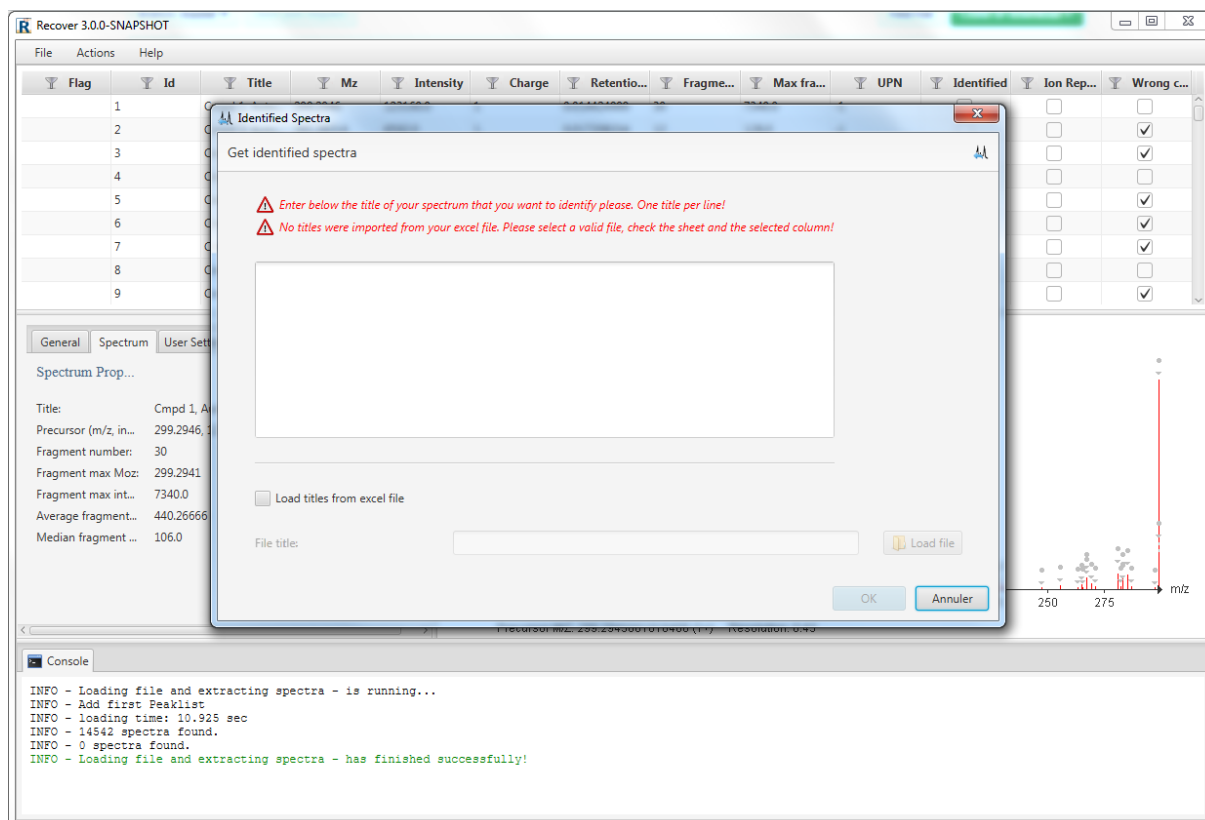


This action let the user to edit the parsing rules used to retrieve retention time from the title of spectrum. The defined parsing rules are:

- data-analysis: *Cmpd.+MS.+ (\d+\. \d+) min*
- mascot-dll: *Elution: (.+?) to .+? min | Elution: (.+?) min*
- Proline: *first\_time: (\d+);*
- msconvert: *RTmin: "(\d+\. \d+)"*
- mascot-distiller: *in range \d+ \(rt=(\d+\. \d+)\) /\(rt=(\d+\. \d+)\)*

To check the result within the parsing rule, Recover extracts the top five spectrums and shows the result. On apply button the selected parsing will be used among all the spectra.

### c. Get identified spectra



This action will let the user to filter out the identified spectra previously from an excel file.

The user can import from an excel file, he must select the sheet and enter the column name of titles.

For example: Select sheet 1 and column A3. All the titles in the column A3 will be compared to the titles.

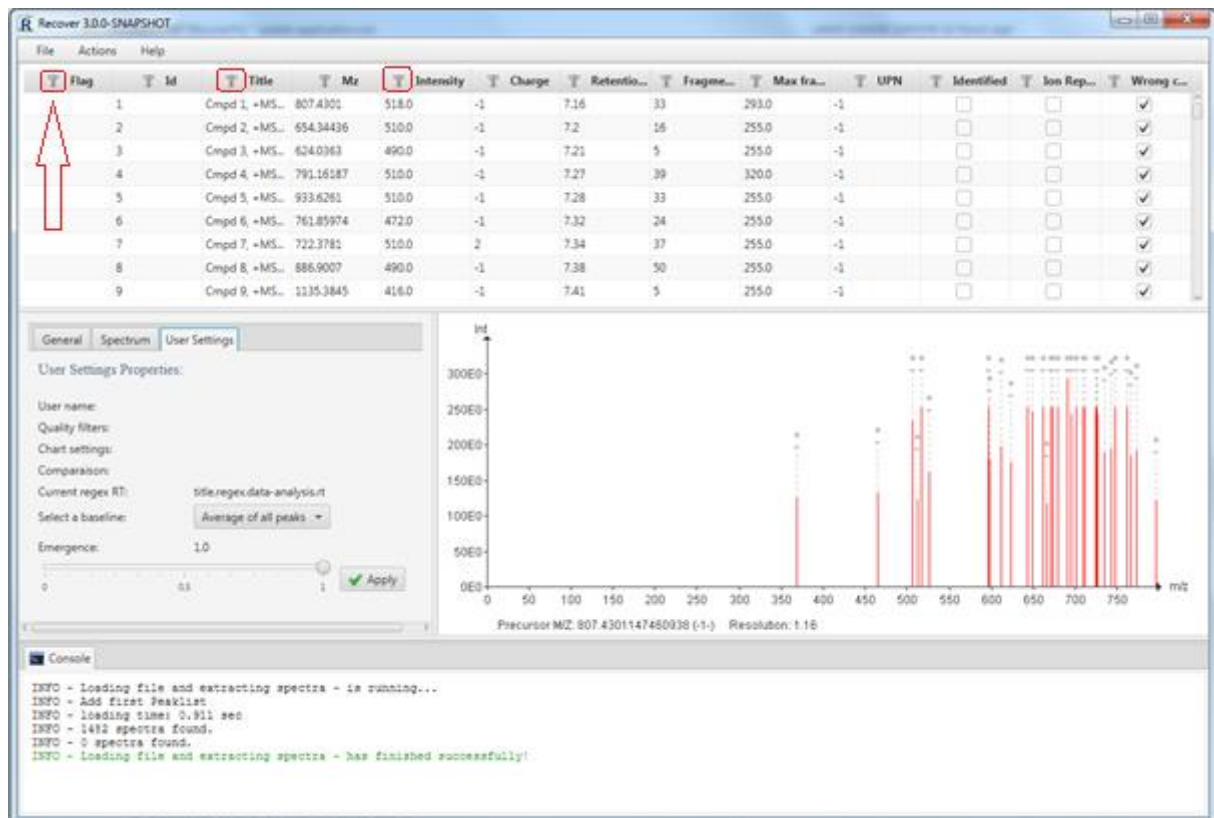
On apply button all the identified spectrum via their titles will be checked in the table view.

#### d. Reset Flagged spectrum

This action will reset all flagged spectrum.

#### e. Customized filters

The user of RecoverFx can retrieve list of spectra via column filters. The user can mix lot of filters to get the result in the table view.



The filters that the user can retrieve are:

- Boolean: Applied on columns: Flag, the identified spectra, ion reporter spectra and the wrong charge.

The values of the filter could be: True, false or not applied.

- Numeric: Applied on columns: Mz, intensity, charge retention time, Max fragment and useful peaks number.

The values of filters could be: equals, not equals, greater than, greater than or equals, less than or equals or less than.

**Note:** the user can search by a range [GREATER THAN, LESS THAN] or ] EQUALS GREATER THAN, LESS THAN OR EQUALS] ...

- String (Sequence of characters): Applied on columns: title.

The values of filters could be:

-Equals: equals the entered value.

-Not equals: different from the entered value.

-Contains: will search on column all the values that contains the entered value.

-Starts with: will search on column all the values that starts with the entered value.

-Ends with: will search on column all the values that ends with the entered value.

**Note:**

The users may mix the filters. It will be applied as: filter1 AND filter2 AND filterN...

The final result it's Boolean of filter1 AND filter2 AND filterN...

## **5) Help**

This menu will open a dialog of about the software and the user guide file.