

RecoverFx user guide

Release 3.0.0

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1) RecoverFx

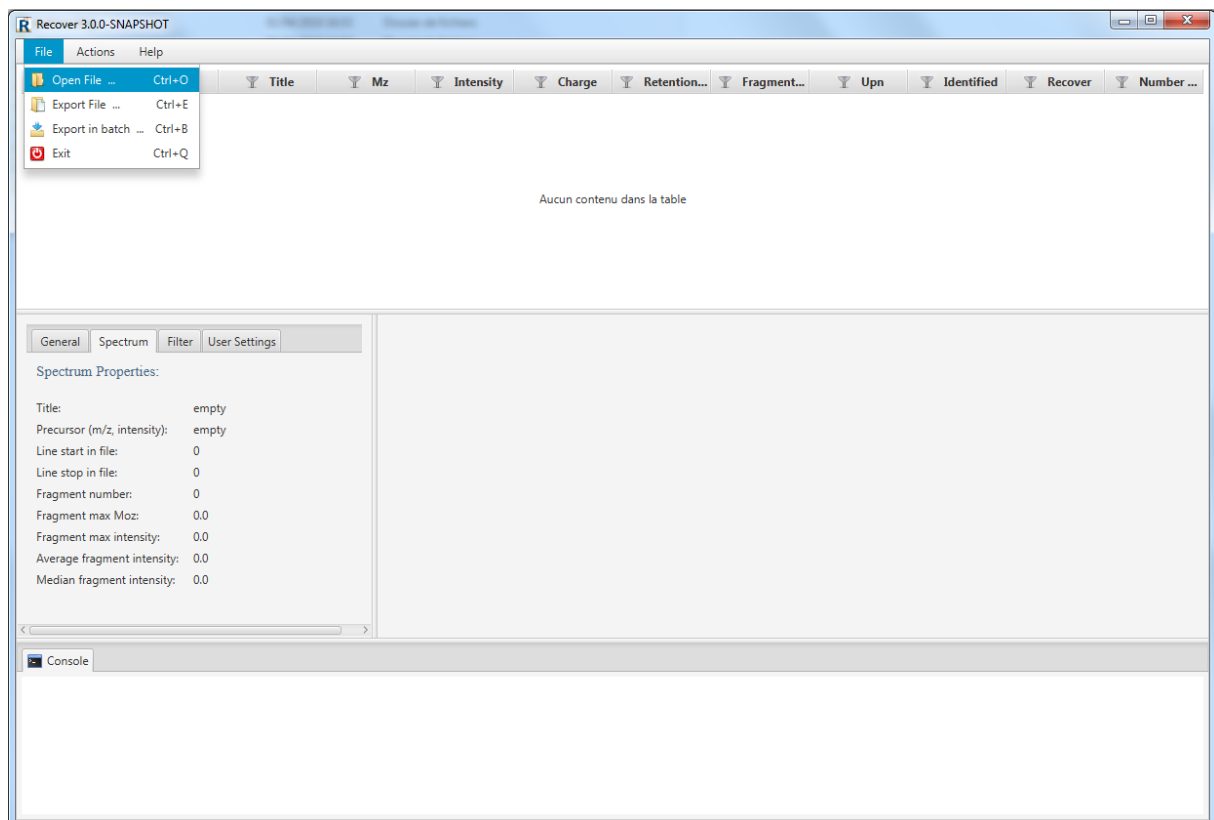
RecoverFx is the future version of Recover, the MS/MS spectra viewer/extractor designed to extract "high quality" spectra from peaklist files.

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

2) Load Peak list

The user must select a valid MGF file via the menu "Open file" or via the keyboard shortcut "Ctrl+ O".

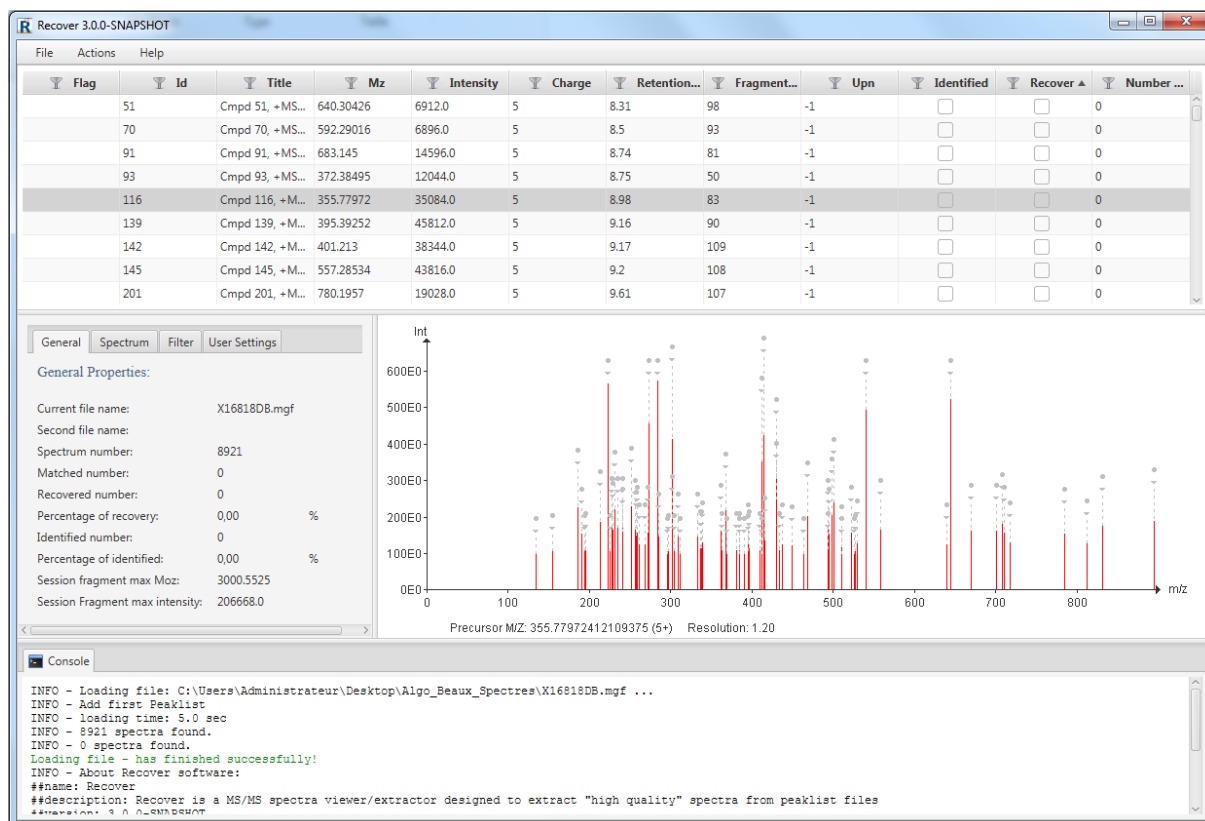
This action could take a while; it depends on MGF file size.



3) Graphical user interface:

a. Information pane

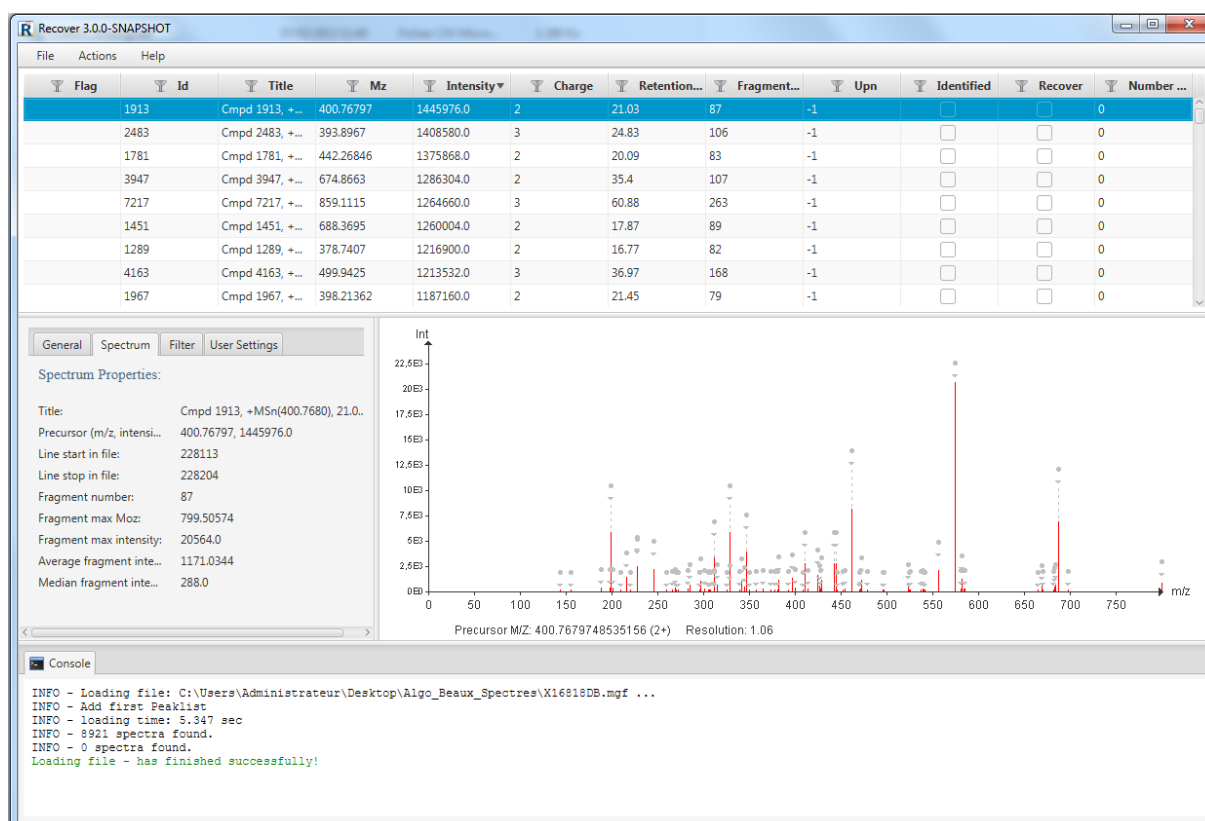
General properties:



This tab pane contains general information:

- The current file name: the loaded file name.
- The spectrum number: The number of spectrum found in the loaded file.
- Recovered number: The number of the spectrum that recovered.
- Percentage of recovery.
- Identified number: The number of the spectrum that identified.
- Percentage of identified.
- Session fragment max moz: The maximum fragment moz found in the current file.
- Session fragment max intensity: The maximum fragment intensity found in the current file.

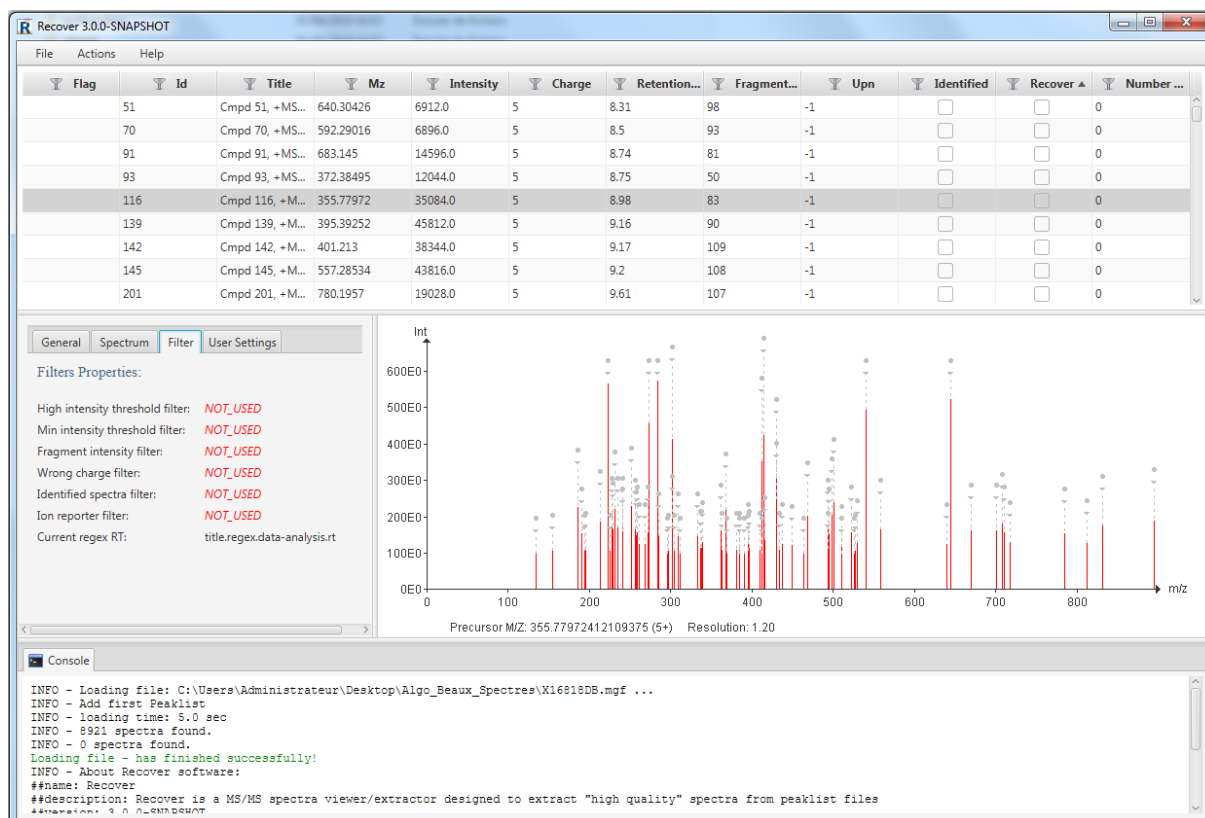
Spectrum properties:



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

- Title: The title of the spectrum.
- Precursor (m/z, intensity).
- Line start in the file: the line number where spectrum starts in the file.
- Line stop in the file: the line number where spectrum stop in the file.
- Fragment: 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 fragment intensity found in the current spectrum.
- Average fragment intensity: The average fragment intensity computed in the current spectrum.
- Median fragment intensity: The median fragment intensity computed in the current spectrum.

Filters:



This tab pane contains information about the filters:

High intensity threshold filter, low intensity threshold filter, fragment intensity filter, wrong charge filter, identified spectra filter and ion reporter filter.

The filters could be:

- Not used
- True: applied on the selected spectrum.
- False: not applied on the applied spectrum.

This tab pane contains information about the used regex to retrieve retention time as well.

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.
- Parsing rules: The parsing rules.
- Comparison: The user comparison.

b. Spectrum pane

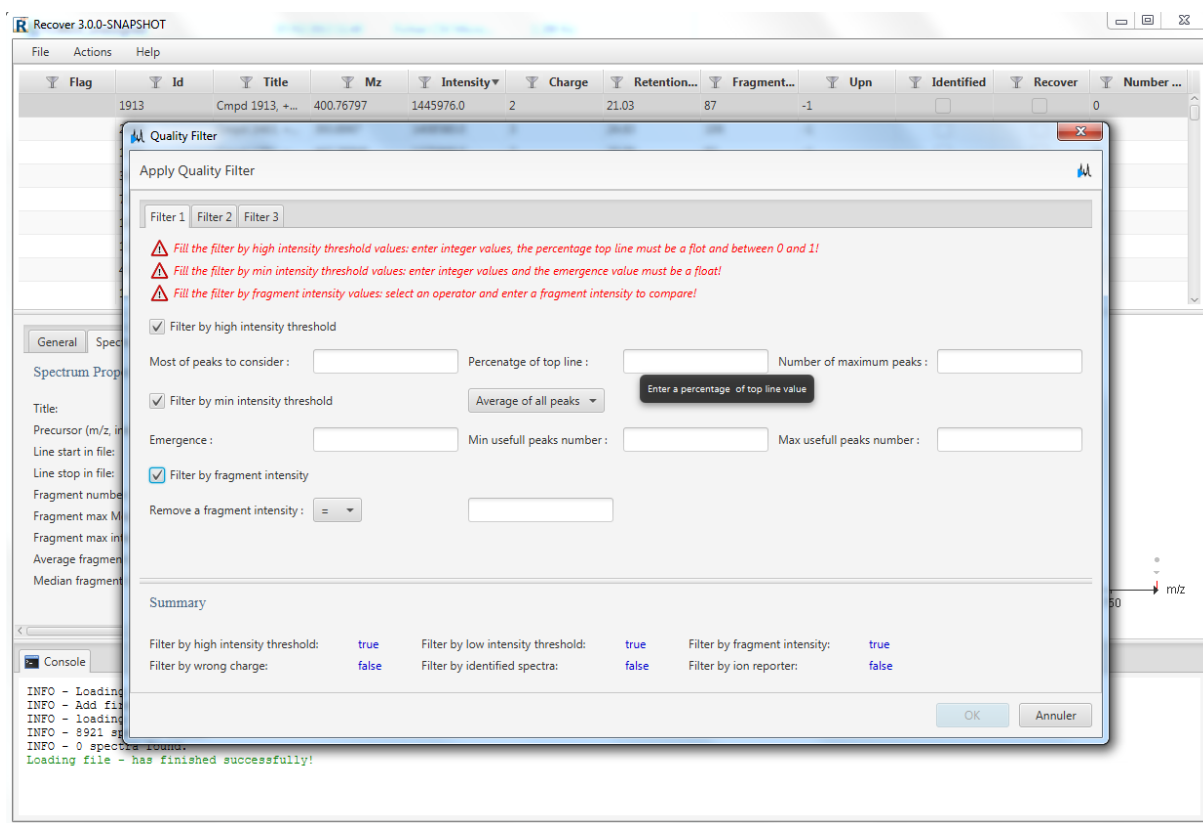
It represents a graph of the selected spectrum. There some actions to view the graph:

- Zoom: Select from the right to the left.
- Cancel zoom: left click.

- Show difference between 2 fragments: Select a fragment and select the others fragments.
- Cancel the comparison: Ctrl+right click.

4) Actions:

a. Apply quality filter



This dialog let the user to select the filters that he wants to apply.

- High intensity threshold filter:

The user must enter a number of the most intense peaks of the spectrum to consider computing the top line, a percentage of top line value and a number of maximum peaks of the spectrum above the threshold to keep it.

- Low intensity threshold filter:

The user must enter an emergence value, min usefull peaks number and max usefull peaks number.

- Fragment intensity filter:

This filter will remove some fragments via their intensity; the user must select a comparator and the value to compare.

- Wrong charge filter.
- Identified spectra filter:

The user must choose between identified spectra and non-identified spectra.

- Ion reporter filter:

The user should insert data, the values of m/z , tolerance and name.

The button clear data clear the data in the input fields to add a new row in the table view.

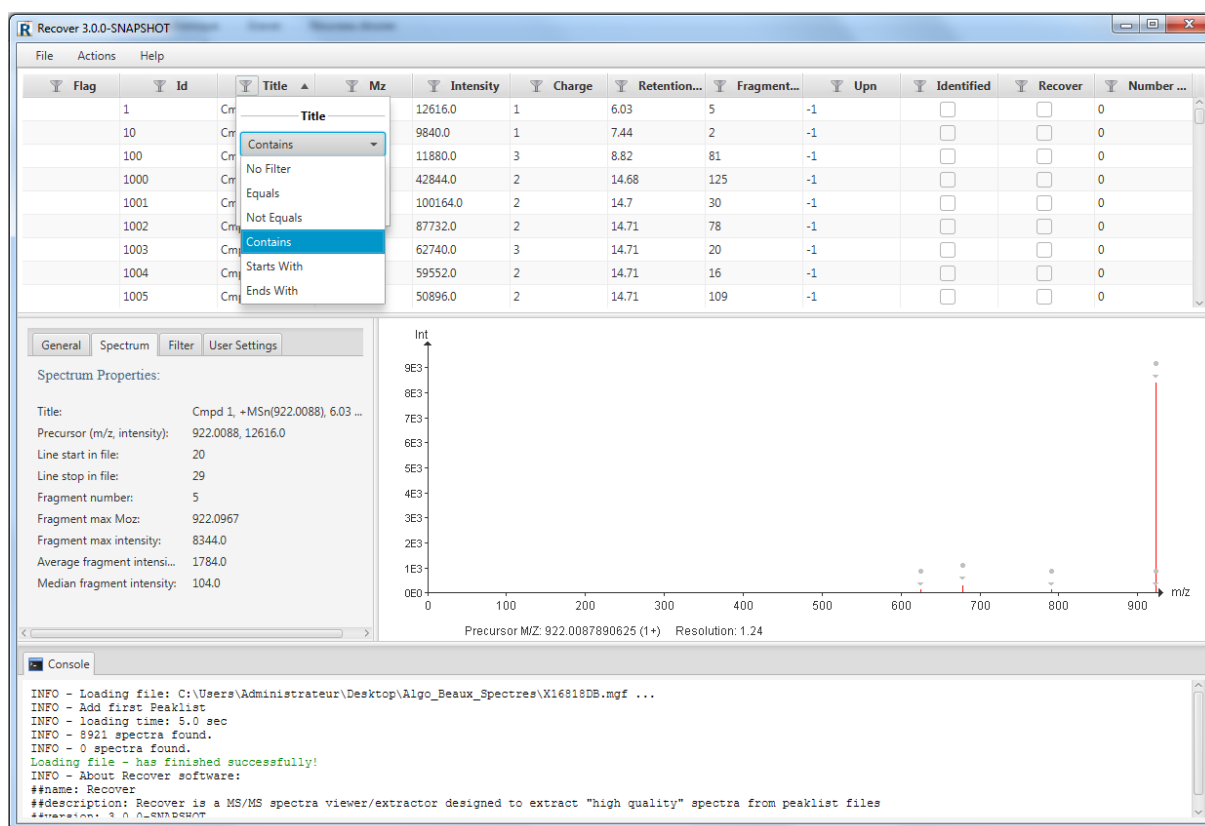
Note:

- Some fields accept only numeric values.
- The summary pane helps the user to see the selected filters when he navigates.
- The “ok” button will be enabled only when the filters are validated.

b. Customized filters

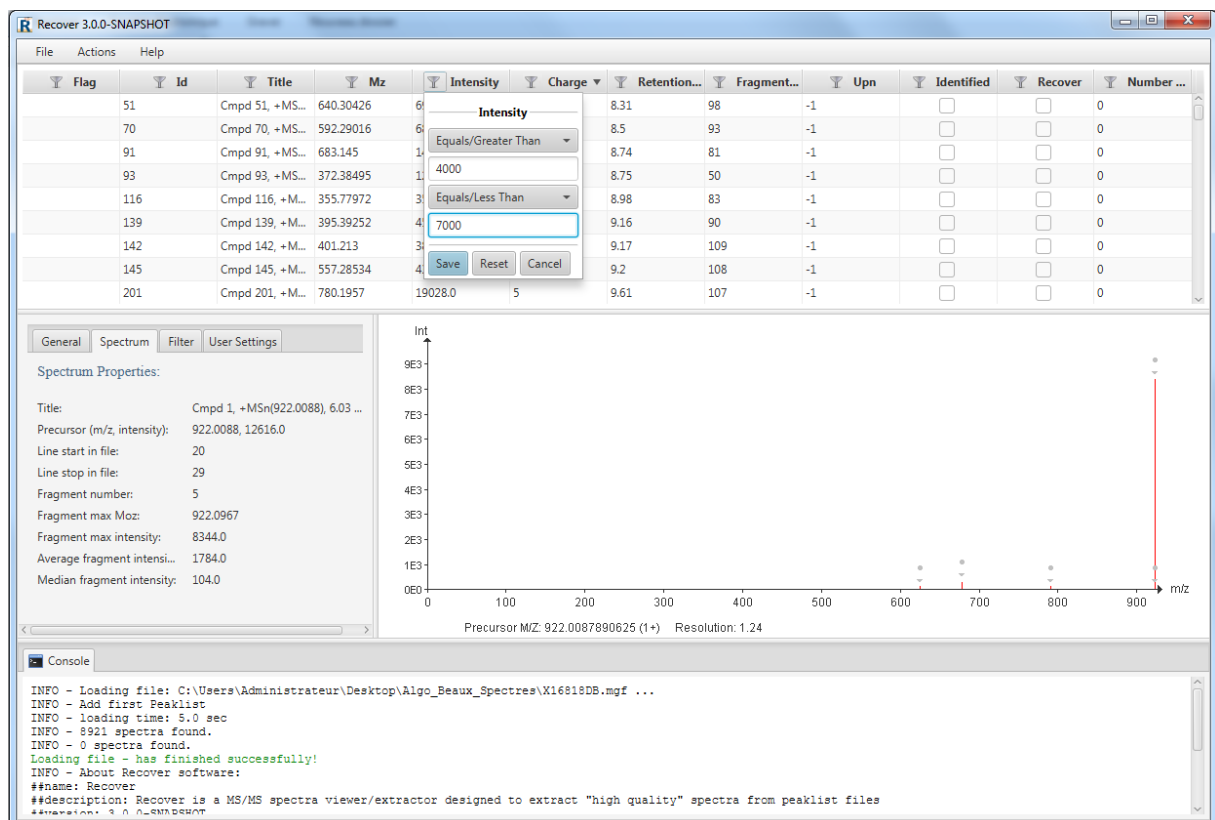
The user could apply filters on the table view to keep or remove some spectrum using some criteria.

- Filters on Strings: contains, equals, not equals, contains, starts with and ends with.

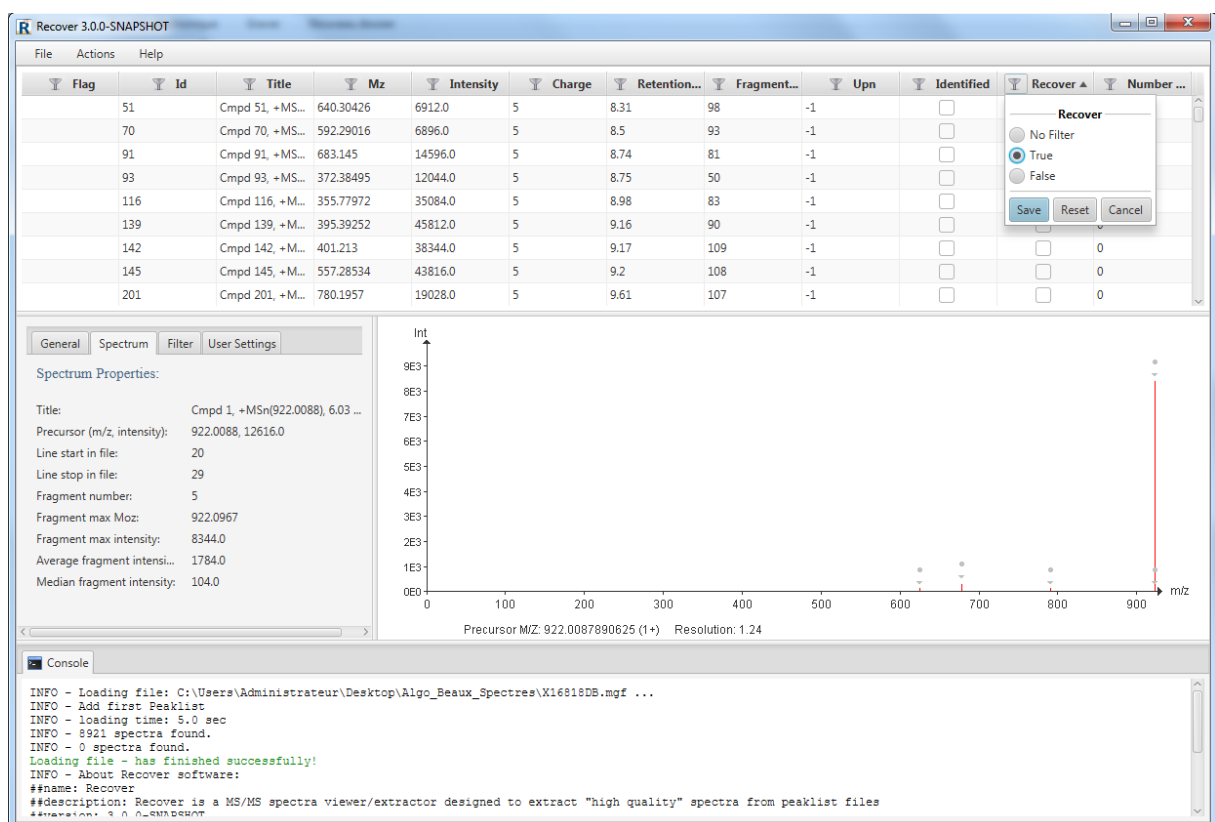


- Filters on numeric values: equals, not equals, greater than, equals/greater than, less and equals/less than.

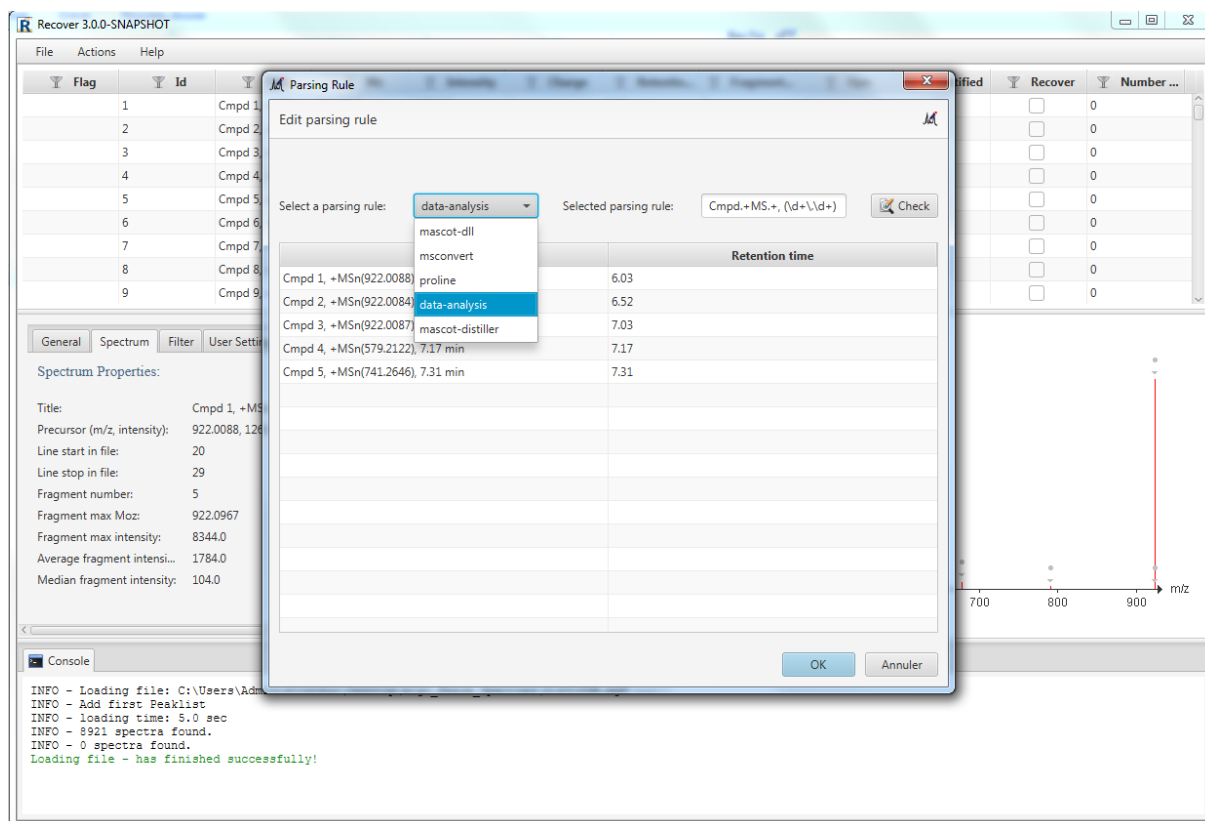
The second filter is used to select a range.



- Filters on Boolean: true or false.



c. Edit Parsing rules



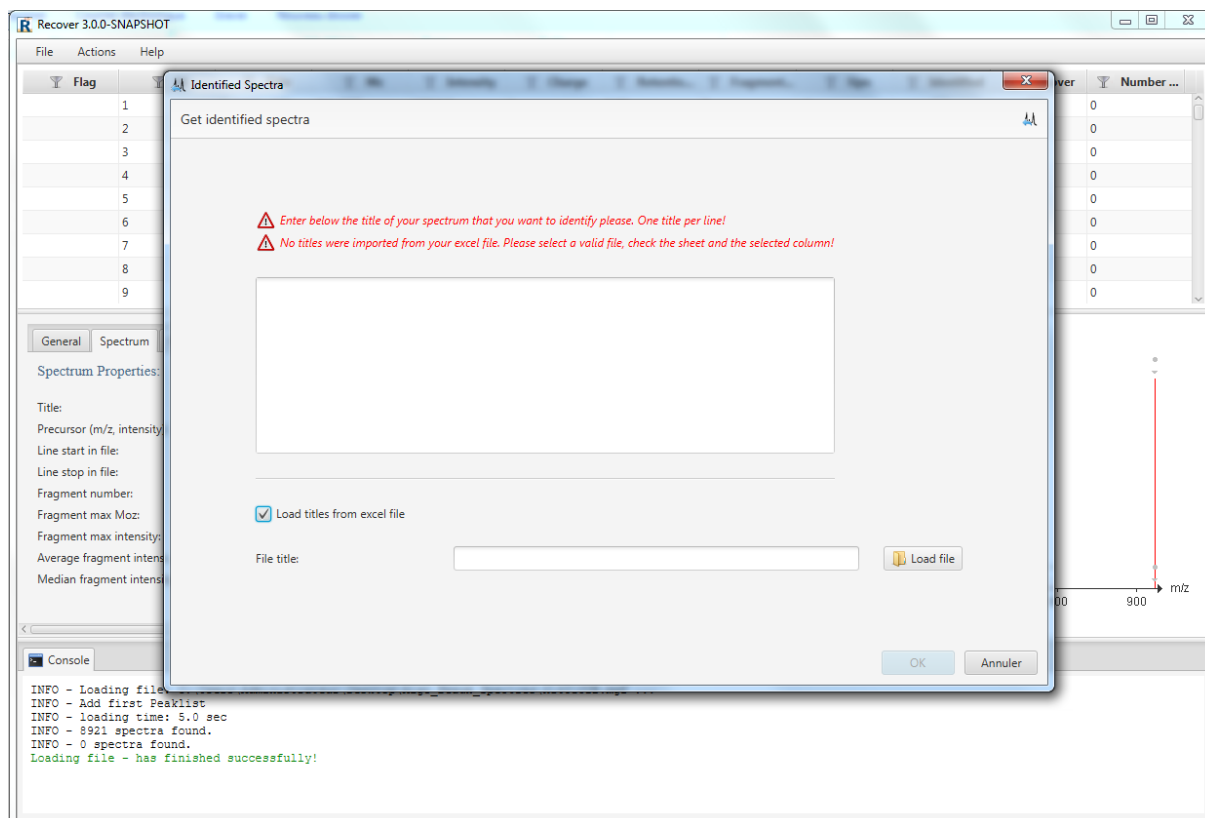
This action help the user to change the parsing rule used to retrieve the retention time from a title. Per default, there are some parsing rules: mascot-dll, data-analysis, msconvert, proline and mascot-distiller.

Whenever you changed the parsing rule, RecoverFx will try to retrieve the retention time via the selected parsing rules from the list of titles in the table view.

Note:

- If the selected parsing rule does not match the retention time will be set to 0.0.
- Ok will apply the selected parsing rule to retrieve the retention time from the title.

d. Identified Spectra:



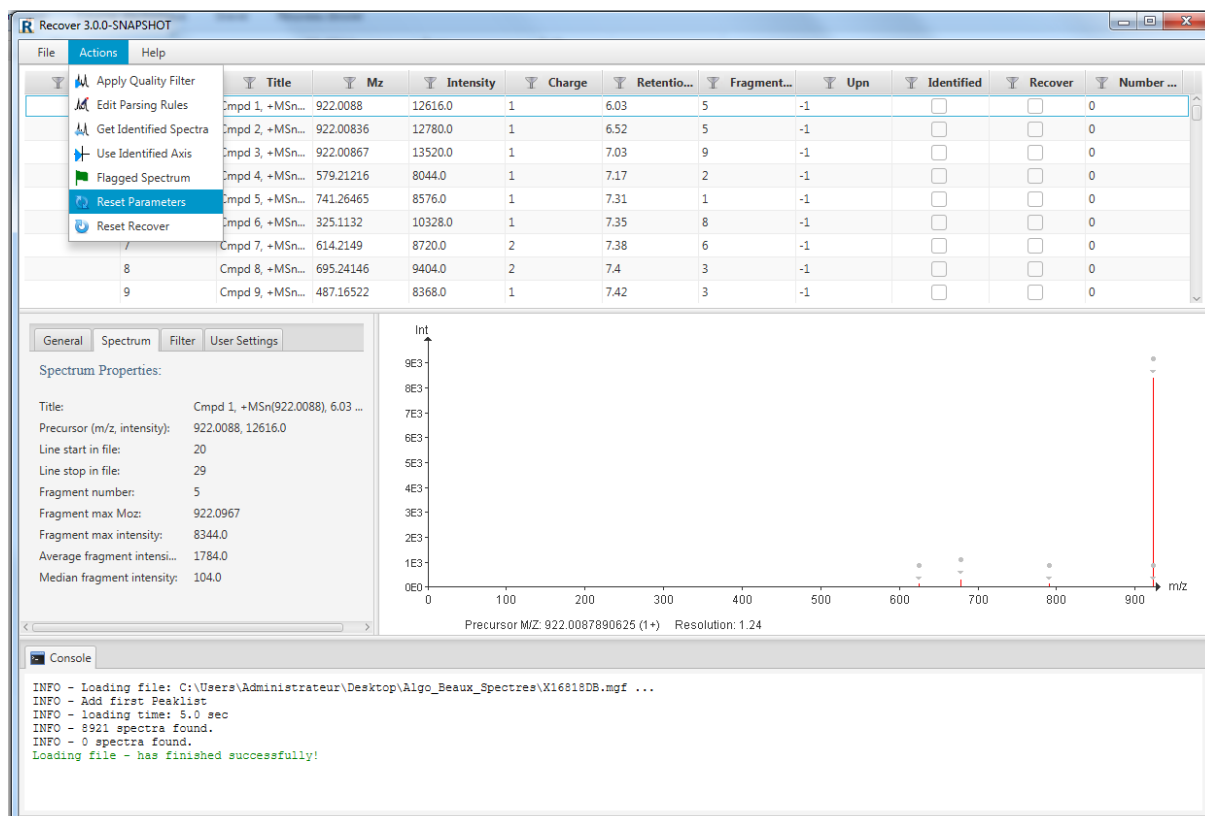
This action will let the user to enter a list of titles or to load a list of titles from an excel file to identify.

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

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

The identified spectrum will be checked in the table view.

e. Reset Parameters



This action will reset all the recovered parameters: reset the applied filters, reset recovered the spectrum, reset the applied parsing rules to retrieve the retention time and reset the identified spectrum.

f. Reset Recover

This action will reset all the parameters: reset the applied filters, reset recovered the spectrum, reset the applied parsing rules to retrieve the retention time, reset the identified spectrum and delete the loaded file as well.

