



msXpertSuite

the expert massist's
software suite

Simulating and analyzing
ionized flying species

Suite version 5.1.1

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mineXpert User Manual

This User Manual is distributed at
<http://www.msxpertsuite.org>

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***mineXpert* User Manual**

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<http://www.msxpertsuite.org>

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Revision History

- * **march 2018** Update the document to include new m/z integration features and scripting capabilities.
- * **december 2017** Major rewriting of the document to incorporate all the new features. Large chapter on the scripting of *mineXpert*.
- * **may 2017** Refactored document. First version documenting almost all the of current features of the software program.
- * **november 2016** Resume writing, with new program name: *mineXpert*.
- * **september 2016** Start of writing.

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1

Preface

This manual is about the *msXpertSuite* mass spectrometric software suite, a software environment that aims at:

- * Letting users predict/analyze mass spectrometric data on (bio)polymers (*massXpert* module);
- * Letting user load, view, analyse and mine mass spectrometric data (*mineXpert* module).

As such, this manual is intended for people willing to learn how to use the comprehensive *msXpertSuite* software package.

Mass spectrometry has gained popularity across the past twenty years or so. Indeed, developments in polymer mass spectrometry have made this technique appropriate to accurately measure masses of polymers as heavy as many hundreds of kDa, and of any chemical type.

There are a number of utilities—sold by mass spectrometer constructors with their machines, usually as a marketing “plus”—that allow predicting/analyzing mass spectrometric data obtained on polymers. These programs are usually different from a constructor to another. Also, there are as many mass spectrometric data prediction/analysis computer programs as there are different polymer types. You will get a program for oligonucleotides, another one for proteins, maybe there is one program for saccharides, and so on. Thus, the biochemist/massist, for example, who happens to work on different biopolymer types will have to learn to use several different software packages. Also, if the software user does not own a mass spectrometer, chances are he will need to buy all these software packages.

The *msXpertSuite* mass spectrometric software is designed to provide *free* solutions to all these problems by providing the following features:

* *massXpert*:

- ◆ Model *ex nihilo* polymer chemistry definitions (in the *XpertDef* module that is part of the *massXpert* program);
- ◆ Perform simple yet powerful mass computations to be made in a mass desktop calculator that is both polymer chemistry definition-aware and fully programmable (that's the *XpertCalc* module also part of the *massXpert* program);
- ◆ Edit polymer sequences on a polymer chemistry definition-specific basis, along with chemical reaction simulations, finely configured mass spectrometric computations. . . (all taking place in the *XpertEdit* module that is the main module of the *massXpert* program);
- ◆ Customize the way each monomer will show up graphically during the program operation (in the *XpertEdit* module);
- ◆ Edit polymer sequences with immediate visualization of the mass changes elicited by the editing activity (in the *XpertEdit* module);
- ◆ Open an unlimited number of polymer sequences at any given time and of any given polymer chemistry definition type (in the *XpertEdit* module).

* *mineXpert*:

- ◆ Load mass spectrometry data files of the main known open formats (*mzML*, *mzXML*, *txt*, *xy*, thanks to the excellent *libpwiz* library of ProteoWizard¹ fame);
- ◆ Display the data in powerful ways in a unified graphical user interface. The interface was designed to integrate all the most useful characteristics of the various proprietary environments known by the author (thanks to the excellent *libqcustomplot* library²);
- ◆ Configure the way mass spectrometry data integrations are performed and optionally configure and apply a Savitzky-Golay smoothing;
- ◆ Perform data mining by performing data integrations in various ways;
- ◆ Ion mobility mass spectrometry data are handled with an automatic $m/z = f(dt)$ color map plot calculation;
- ◆ Data integration allows easy quantitation of spectral data at any level (TIC chromatogram, mass spectrum, drift spectrum);
- ◆ Innovative data analysis recording allows to store the features mined during the data mining sessions in flexible ways that allow further data processing, like injection in databases;
- ◆ Convert data from *mzML* to the private (albeit open) database file format that allows to load data much faster. *mineXpert* can slice big data files into smaller chunks retaining all the data selected by the user in the most flexible ways.

¹<http://proteowizard.sourceforge.net/>

²<http://qcustomplot.com/>.

PROJECT HISTORY

This is a brief history of *msXpertSuite*.

- * **1998–2000** The name *massXpert* comes from a project I started while I was a post-doctoral fellow at the École Polytechnique (Institut Européen de Chimie et Biologie, Université Bordeaux 1, Pessac, France).

The *massXpert* program was published in *Bioinformatics* (Rusconi, F. and Belghazi, M. *Desktop prediction/analysis of mass spectrometric data in proteomic projects by using massXpert* · *Bioinformatics*, 2002, 644–655).

At that time, *MS-Windows* was at the *Windows NT 4.0* version and the next big release was going to be “you’ll see what you’ll see” : *MS-Windows 2000*.

When I tried *massXpert* on that new version (one colleague had it with a new machine), I discovered that my software would not run normally (the editor was broken). The Microsoft technical staff’ would advise to “buy a new version of the compiler environment and rebuild”. This was a no-go: I did not want to continue paying for using something I had produced.

- * **2001–2006**

During fall 1999, I decided that I would stop using Microsoft products for my development. At the beginning of 2000 I started as a CNRS research staff in a new laboratory and decided to start fresh: I switched to GNU/Linux (I never looked back). After some months of learning, I felt mature to start a new development project that would eventually become an official GNU package: GNU polyxmass.

The GNU polyxmass software, much more powerful than what the initial *massXpert* software used to be, was published in *BMC Bioinformatics* in 2006 (Rusconi, F., *GNU polyxmass: a software framework for mass spectrometric simulations of linear (bio-)polymeric analytes*. *BMC Bioinformatics*, 2006,226).

Following that publication I got a lot of feedback (very positive, in a way) along the lines: —“*Hey, your software looks very interesting; only it’s a pity we cannot use it because it runs on GNU/Linux, and we only use MS-Windows and MacOSX!*”

- * **2007–2016**

In december 2006, I decided to make a full rewrite of GNU polyxmass. The software of which you are reading the user manual is the result of that rewrite. I decided to “recycle” the *massXpert* name because this software is written in C++, as was the first *massXpert* software. Also, because the first *MS-Windows*-based *massXpert* project is not developped anymore, taking that name was kind of a “revival” which I enjoyed. However, the toolkit I used this time is not the Microsoft Foundation Classes (first *massXpert* version) but the Trolltech Qt framework (see the “About Qt” help menu in *massXpert*).

Coding with Qt libraries has one big advantage: it allows the developer to code once and to compile on the three main platforms available today: *GNU/Linux*, *MacOSX*, *MS-Windows*. Another advantage is that

Qt libraries are wonderful software, technically and philosophically (Free Software).

*** 2016–**

In 2016, I started a new project about visualization of mass spectrometric data. The project developed pretty quickly, as we needed at the mass spectrometry facility a software that would allow to cope efficiently with ion mobility mass spectrometric experimental data. *mineXpert* was thus started.

To bundle both *massXpert* and *mineXpert* in a single software suite, I bought the *msXpertSuite* website <http://msxpertsuite.org> and created that new name.

TYPGRAPHICAL CONVENTIONS

Throughout the book the following typographical conventions are used:

- * *emphasized text* is used each time a new term or concept is introduced
- * **shell-prompt \$** shows the prompt at which a command should be entered as non-root
- * **shell-prompt #** shows the prompt at which a command should be entered as root
- * **this typography** applies to commands that the user enters at the shell prompt along with eventual options
- * ↵ symbolizes pressing the Enter key
- * **this typography** applies to an output resulting from entering a command at the shell prompt
- * **emacs** or **libQtCore** names of a program or of a library
- * **KDE**, **The Gimp** is the name of a generic software (not a specific executable file)
- * **/usr/local/share/massxpert**, **/usr/bin/massxpert** are names of a directory or of a file
- * <http://www.gnu.org> is an URL (Uniform Resource Locator)

PROGRAM AVAILABILITY, TECHNICALITIES

The ancestor of *massXpert*, GNU polyxmass, was initially developed on a *GNU/Linux* system (RedHat distribution versions successively 6.0, 7.0, 7.2, 7.3, 8.0, 9.0) using software from the Free Software Foundation (FSF³). The main

³For an in-depth coverage of the philosophy behind the FSF, specifically creating a *free operating system*, you might desire to visit <http://www.gnu.org>.

libraries used were `libglib`, `libgobject`, `libxml2` and `libgtk+`. Since mid-2002, the development was performed on a *Debian GNU/Linux* system (<http://www.debian.org>), which I find to be the ultimate highly-configurable easy-to-use distribution. *massXpert* is still developed using the *Debian GNU/Linux* system, using Free Software libraries that allow cross-platform computer program development with unprecedented ease (Qt libraries⁴). Developing for *GNU/Linux* has been utterly exciting and extremely efficient.

msXpertSuite' LICENSING

The front matter of this manual contains a Copyright statement. I retain the copyright to *msXpertSuite* and all related writings (source and configuration files, programmer's documentation, user manual. . .) I encourage others to make copies of the work, to distribute it freely, to modify the work and redistribute that derivative work according to the GNU General Public License version 3. The aim of this licensing is to favor spread of knowledge to the widest public possible. Also, it encourages interested hackers⁵ to change the code, to improve it and to send patches to the author so that their improvements get into the program to the benefit of the widest public possible. For an in-depth study of the FREE SOFTWARE philosophy I kindly urge the reader to visit <http://www.gnu.org/philosophy>.

⁴Originally from the Trolltech company (<http://www.trolltech.com>); now The Qt Company Ltd (doc.qt.io).

⁵*Hacker* is a specialized term to design the programmer who codes programs; this term should *not* be mistaken with *cracker* who is a person who uses computer science knowledge to break information systems' security barriers.

CONTACTING THE AUTHOR

msXpertSuite is the fruit of years of work on my part.⁶ While I've put a lot of energy into making this program as stable and reliable a piece of software as possible, *msXpertSuite* comes with no warranty of any kind.

The public home page is at <http://www.msxpertsuite.org>.

The Git code repository is at <https://salsa.debian.org/lopippo/msXpertSuite>

Discussion of the *msXpertSuite* project happens at
<https://groupes.renater.fr/sympa/info/msxpertsuite-discussion>

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⁶As said earlier, *msXpertSuite* is the successor to the *massXpert* project of which it inherits all the original features, while still integrating new interesting developments.

2

mineXpert Generalities

In this chapter, I wish to introduce some general concepts around the *mineXpert* program and the way data elements are called in this manual and in the program.

A mass spectrometry experiment generally involves monitoring the m/z value of analytes injected in the mass spectrometer along a certain time duration. The m/z value of each detected analyte is recorded along with the corresponding signal intensity (i), so that a mass spectrum is nothing but a series of (mz, i) pairs recorded along the acquisition duration. All along the acquisition, the precise moment at which a given analyte is detected (and its (mz, i) pair is recorded), is called the retention time of that analyte. This retention time is not to be misunderstood as the drift time of that analyte in an ion mobility mass spectrometry experiment.

GENERAL CONCEPTS AND TERMINOLOGIES

Most generally, the mass spectrometer acquires an important number of spectra in, say, one second. But all these spectra are *combined* together, and, on the surface, the massist only sees a “slow” acquisition of 1 spectrum per second. This apparent slow acquisition rate is configurable. At the time of writing, generally 1 spectrum per second is recorded on disk. So, say we record mass spectra for 5 minutes, we would have recorded $(5*60)$ spectra.

ACQUIRING MASS DATA ALONG TIME: TO PROFILE OR NOT TO PROFILE?

As a mass spectrometry user, the reader of this manual certainly has used mass spectrometers where mass spectra are acquired and stored in different ways:

- * Mass spectra are acquired and summed—the next to the previous—in such a manner that one is left, at the end of the acquisition, with a single spectrum of which the various peak intensities have been increasing all along the acquisition. Indeed, in this mode, each new spectrum is actually “*combined*” to the previously acquired ones. The resulting mass spectrum that is displayed on screen and that gets ultimately stored on disk is called a *combined spectrum*. This is typically the way MALDI-TOF mass spectrometers are used when acquiring data from samples deposited onto sample plates. We refer to this kind of acquisition as an “*accumulation*” mode acquisition;
- * Mass spectra are acquired and stored on disk as a single file containing all the spectra, appended one after the other. There is no combination of the spectra: each time a new spectrum is displayed on screen, that spectrum is appended to the file¹. This is typically the case when mass spectra are acquired all along a chromatography run and is generally called a “*profile*” mode acquisition.

MASS DATA VISUALISATION: TO COMBINE OR NOT TO COMBINE?

In the previous section, we mentioned *spectrum combination* a number of times. What does that mean, that spectra are “*combined*” together into a single “*combined spectrum*”? Say we have 200 spectra that need to be combined together into a *single* spectrum that summatively represents the data of these 200 spectra.

First, a new spectrum would be allocated (*result spectrum*), entirely empty at first. Then, the very first spectrum of the 200 spectra is literally copied into that result spectrum. At this point the combination occurs, according to an iterative process that has the following steps:

- * Pick the next spectrum of the 200-spectra dataset;
 1. Pick the first (m/z , i) pair of the currently iterated spectrum;
 2. Look up in the *result spectrum* if a m/z value identical to the m/z value of the current (m/z , i) pair is already present;
 3. If the m/z value is found, increment its intensity by the intensity of the (m/z , i) pair;

¹Although there certainly *is* spectrum combination going on in the guts of the software, because the system actually acquires much more spectra than is visible on screen and each newly displayed spectrum is actually the combination of many spectra acquired under the surface.

4. Else, if the m/z value is not found, add the current $(m/z, i)$ pair to the result spectrum;
 5. Iterate over all the remaining $(m/z, i)$ pairs of the current spectrum and redo these steps.
- * Iterate over all the 198 remaining spectra of the dataset and do the steps above for each single iterated spectrum.

At the end of the two nested loops above, the combined spectrum is still a single spectrum that represents—summatively—all the 200 spectra. This whole process is very computing-intensive, in particular if:

- * The m/z range is large: there are lots of points in each spectrum, which means that for each new $(m/z, i)$ pair we need to iterate in the long list of m/z values that make the result spectrum;
- * The resolving power of the mass spectrometer is high: there are many points per m/z range unit.

When a profile mode acquisition is performed, the user gets an innumerable number of distinct spectra, all appended to a single file. These unitary spectra are virtually unusable if an initial processing is not performed. This initial processing of the spectra is called *“total ion current chromatogram calculation”*. What is it? Let’s say that the user has performed a profile mode mass spectrometry acquisition on the eluate of a chromatography column. Now, imagine that the spectrometer stores the mass data at a rate of one spectrum per second and that the chromatography gradient develops over 45 min: there would be a total of $(45 * 60)$ spectra in that file. The question is: *“How can we provide the user with a data representation that might be both meaningful and useful to start mining the data?”* The conventional way of doing so is to load all the mass spectra and compute the *“total ion current chromatogram”* (the TIC chromatogram). The analogy with chromatography is evident: the TIC chromatogram is the same as the UV chromatogram unless optical density is not the physical property that is measured over time; instead, the amount of ions that are detected in the mass spectrometer is measured over time. That amount is actually the sum of the intensities of all the $(m/z, i)$ pairs detected in each spectrum. When mass data are acquired during a chromatography run, often, the total ion current chromatogram mirrors (mimicks) the UV chromatogram². For each retention time (RT) a TIC value is computed by summing the intensities of all the $(m/z, i)$ pairs detected at that specific RT.

How is this total ion current chromatogram computed? This is an iterative process: from the first spectrum (retention time 0 s), to the second spectrum (retention time 1 s) up to the last spectrum (retention time 45 min), the program computes the sum of the intensities of all the spectrum’s $(m/z, i)$ pairs. That computation ends up with a map that relates each RT value with the corresponding TIC value. The TIC chromatogram is nothing but a plot of the TIC values as a function of RT values. In that sense, it is indeed a chromatogram.

mineXpert works exactly in this way. When mass spectrometry data are loaded from a file, the TIC chromatogram is computed and displayed. This TIC

²Unless eluted analytes *do* absorb UV light but *do not* either desorb/desolvate or ionize, or both.

chromatogram serves as the basis for the mass data mining, as described in this manual. The TIC chromatogram serves as the basis for spectral combinations that can be performed in various ways, and not all formally *combinations*, which is why I prefer the term “*integrations*”. Some of these integrations are described below:

- * Integrating data from the TIC chromatogram to a single mass spectrum;
- * Integrating data from the TIC chromatogram to a single drift spectrum;

Note that the reverse actions are possible (and indeed necessary for a thorough data mining): selecting a region of a mass spectrum and asking that the TIC chromatogram be reconstituted from there; or selecting a region of a drift spectrum and asking that the TIC chromatogram be reconstituted from there also. Finally, integrations may, of course, be performed from a mass spectrum to a drift spectrum, and reverse.

EXAMPLES OF VARIOUS INTEGRATIONS

In the sections below, the inner workings of *mineXpert* are described for some exemplary mass data integrations. For example, when doing ion mobility mass spectrometry data mining, it is essential to be able to characterize most finely the drift time of each and any analyte. Since each analyte is actually defined as one or more (mz,i) pairs, it is essential to be able to ask questions like the following:

- * What is the drift time of the ions below this mass peak³?
- * What are all the drift times of all the analytes going through the mobility cell for a given retention time range?
- * What are all the ions that are responsible for this shoulder in the drift spectrum?

TIC→MZ INTEGRATION

What computation does actually *mineXpert* do when a mass spectrum is computed starting from a TIC chromatogram region, say between retention time RT minute 7 and RT minute 8.5?

1. List all the mass spectra that were acquired between RT 7 and RT 8.5. In this *spectral set*, there might be many hundreds of spectra that match this criterion, if we think that in ion mobility mass spectrometry ≈ 200 spectra are acquired and stored individually every second (I mean it, every 1 s time lapse);
2. Allocate a new empty spectrum—the “*combined spectrum*”—and copy into it without modification the first spectrum of the spectral set;

³Be that mass peak an isotopic cluster or the average envelope of a large analyte at a given charge.

3. Go to the next spectrum of the spectral set and iterate into each (mz, i) pair:
 - * Check if the m/z value of the iterated pair is already present in the combined spectrum. If so, increment the combined spectrum's (mz, i) pair's intensity value by the intensity of the iterated (mz, i) pair. If not, simply copy the iterated (mz, i) pair in the combined spectrum;
 - * Iterate over all the remaining (mz, i) pairs and perform the same action.
4. Iterate over all the remaining spectra of the spectral set and perform step number 3.

mineXpert then displays the combined spectrum.

TIC→DT INTEGRATION

What computation does *mineXpert* actually do when a drift spectrum is computed starting from a given TIC chromatogram region, say between retention time RT minute 7 and RT minute 8.5?

What is a drift spectrum? A drift spectrum (mobilogram) is a plot where the cumulated ion current of the detected ions is plotted against the drift time at which they were detected. Let's see how that computation is handled in *mineXpert*.

1. Create a map to store all the (drift time, intensity) pairs that are to be computed below, the (dt, i) map;
2. List all the mass spectra that were acquired between RT 7 and RT 8.5. The obtained list of mass spectra is called the "*spectral set*";
3. Go to the first spectrum of the spectral set and compute its TIC value (sum of all the intensities of all the (mz, i) pairs of that spectrum). Get the drift time value at which this mass spectrum was acquired. We thus have a value pair: (dt, i) , that is, for drift time dt , the intensity of the total ion current is i ;

At this point, we need to do a short digression: we saw earlier that, at the time of this writing, one of the commercial instruments on which the author of these lines does his experiments stores 200 spectra each second. These 200 spectra actually correspond to the way the drift cycle is divided into 200 bin (time bins). That means that in the retention time range [7–8.5], there are (1.5×60) complete drift cycles. And thus there are (1.5×60) spectra with drift time x , the same amount of spectra with drift time y , and so on for the remaining 198 time bins. Of course, a large number of these spectra might be almost empty, but these spectra are there and we need to cope with them.

The paragraph above must thus lead to one interrogation about the current (dt, i) pair: –“*Has the current dt value be seen before, during the previous iterations in this loop?*” If no, create the (dt, i) pair and add it to the (dt, i) map; if yes, get the dt element in the map and increment its intensity value by the TIC value computed above;

4. Iterate over all the remaining spectra of the spectral set and perform step number [3](#).

At the end of the loop above, we get a map in which each item relates a given drift time with a TIC value. This can be understood this way: –*“For each drift time value, what is the accumulated ion current of all the ions having that specific drift time?”*.

At this point, *mineXpert* displays the drift spectrum (mobilogram).

3

mineXpert: A Powerful Mass Spectrum Viewer

Data mining, in mass spectrometry, entails, for a large part, the relentless scrutinization of the mass spectra by an expert eye. Without a powerful mass spectrum viewer, capable of numerous data display modes, the expert eye remains powerless.

After having completed this chapter you will be able to perform mass spectrum visualization and analysis, optionally reporting all the analysed peaks to a file on disk.

OPENING MASS SPECTRUM FILES

To start a *mineXpert* session, open one or more mass spectra using the menu *File*→*Open full mass spectrum file(s)*. The following file formats are understood by *mineXpert*, partly thanks to the `libpwiz` library from the *ProteoWizard* project¹:

- * *mzML*, *mzXml*, *MS1*, *MS2*, *MGF* files (`libpwiz`);
- * *txt*, *asc* files where *m/z* and *i* values are separated by any character that is neither a newline nor a dot nor a digit (loading is handled by a private parser);
- * *xy* files from Bruker (private parser);
- * *SQLite3*, a private open/documented database format (private parser).

There are two variants of the mass spectrometry file opening menu, one for which *all* the mass data are read from file and stored in memory and one for which the mass data are read from file in streamed mode, used to compute the TIC chromatogram and discarded. The latter mode is useful when the mass data are so large that they cannot fit in memory. The TIC chromatogram that is computed in streamed mode is then used to access the mass data in the file according to criteria set by the user (retention time range, for example).

THE WINDOW LAYOUT

The graphical interface of *mineXpert* comprises a number of windows where data and informations are displayed. These windows are described below (see Figure 3.1 on page 16):

- * *mineXpert* main program window: this is an unintrusive window sporting the main menu and a status bar where messages are displayed;
- * The Loaded mass spectrum files window, that lists all the mass spectrometry data files that are currently loaded in the program;
- * The TIC chromatogram window² where the various TIC chromatograms are displayed for the various mass spectrometry data files that have been loaded. There is, by definition, a single TIC chromatogram per data file currently loaded in the program. However, this window will also display TIC chromatograms that are computed as an integration step from the other windows, like from the Mass spectrum window or from the Drift spectrum window. In this case, the chromatogram is an extracted ion current chromatogram (XIC chromatogram);
- * The Mass spectrum window, where the various mass spectra are displayed. A given mass spectrum may originate from a TIC chromatogram or from

¹Please, see <http://proteowizard.sourceforge.net/>

²TIC stands for “total ion current”.

a drift spectrum, or even from a color map. A given originating chromatogram or drift spectrum or color map may be the origin of more than one derived mass spectrum;

- * The **Drift spectrum** window, where the various drift spectra are displayed. Drift spectra can originate from the TIC chromatograms, from the mass spectra or from the color map;
- * The **Color map** window, that contains a single color map for each loaded mass data file. At the time of this writing, there is no way to produce a color map from any other window;
- * The **m/z integration parameters** window, where the parameters governing the mass data integrations to a mass spectrum are set;
- * The **XIC extraction parameters** window, where the parameters governing the XIC extractions to a XIC chromatogram are set;
- * The **Console** window, where the various messages or analysis data elements are displayed for the user to select, copy and paste in an electronic lab-book;

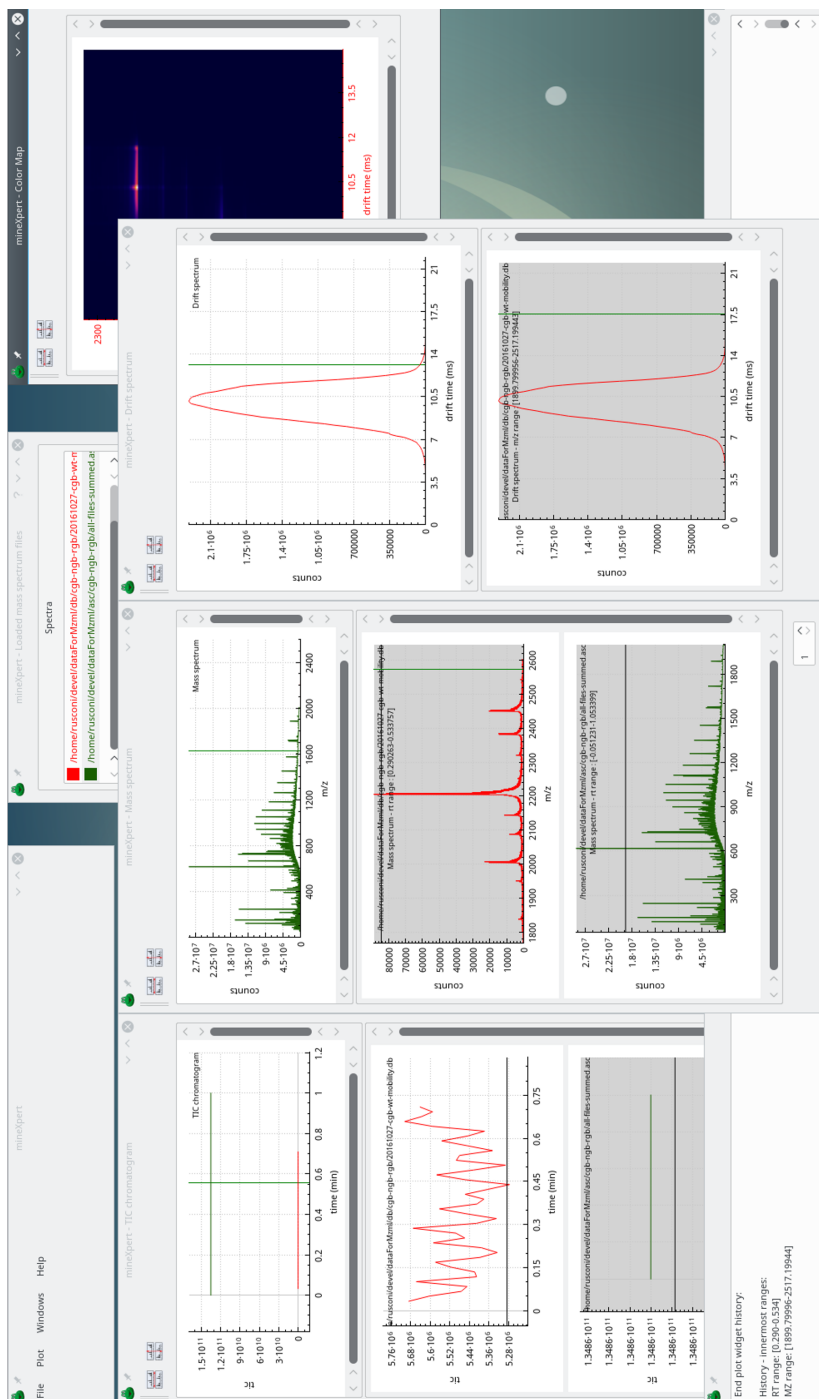


Figure 3.1: General view of the graphical user interface

THE MAIN PROGRAM WINDOW MENU

The menu bar in the main program window displays a number of menu items, reviewed below:

* *File*

- ◆ *File*→*Open full mass spectrum file(s)* Choose the mass spectrum file(s) to load. Note that the “full” descriptor indicates that the user wants to actually load the full data set in memory. This means that she explicitly knows that the system’s memory will cope with all the data in the file;
- ◆ *File*→*Open streamed mass spectrum file(s)* Choose the mass spectrum file(s) to load. Note that the “streamed” descriptor indicates that the user wants *not* to actually load the full data set in memory. This is typically the case when the data file is so large that its data cannot fit in memory. The program then only “looks” at the data in the file and crafts, piecemeal, the TIC chromatogram and the color map. In this context, any other data integration will be performed by looking into the same mass data file since no data are available in memory;
- ◆ *File*→*Mass spectrum from clipboard* creates a mass spectrum from a textual representation of (mz, i) pairs in the same format as described above for the *txt,asc* file format;
- ◆ *File*→*Analysis preferences* Define the analysis preferences. The analysis preferences govern how the data about scrutinized mass peaks are recorded to the console, to the clipboard, to a selected file, or any combination of the three.

* *Plot*

- ◆ *Plot*→*Clear plots* Clears all the plots currently displayed in the program. The plot items in the **Loaded mass spectrum files** window are all removed. Note that this releases all the memory that was used by the data. This menu is equivalent to “closing all files”;
- ◆ *Windows*
The menus are self-explanatory, as they explicitly explain which window is to be shown. The *Save workspace* menu records on disk the position and size of all the windows, so that upon reopening the program, the windows all position themselves at the recorded position and size;
- ◆ *Help*
This menu’s items show help about the program itself and also about the Qt libraries that were used to build it. These informations are essential in case the user wants to make a bug report.

THE MAIN DATA WINDOWS

This section will succinctly describe the main data windows of *mineXpert*. Each window will be described in greater detail when the features of the program will be described.

THE TIC CHROMATOGRAM WINDOW

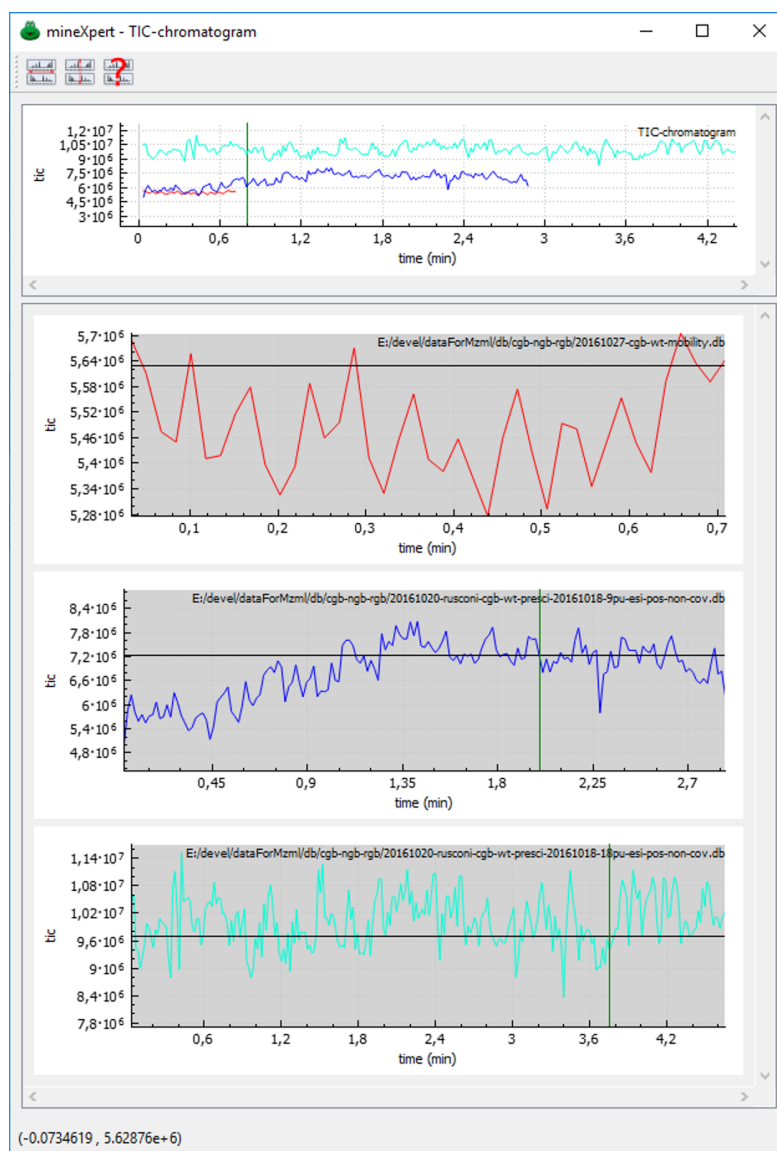


Figure 3.2: **The TIC chromatogram window** This TIC chromatogram window shows multiple chromatograms. Each plot has its own set of markers.

Each time a new mass spectrum file is loaded, its corresponding TIC chromatogram is computed and then displayed in a new plot widget in the TIC chromatogram window (Figure 3.2 on the preceding page). Each new TIC chromatogram plot generated as a result of the loading of a mass spectrometry data file is plotted using a new color. That color encodes the filiation of the whole set of plots that are generated starting from that initial TIC chromatogram plot. For example, a red TIC chromatogram plot that serves as the starting point for a mass spectrum integration will trigger the creation of a mass spectrum plot widget that will have a red graph in it. Same is true for the color map widget that has its axis and tick labels of the same color as that of the TIC chromatogram plot.

The attention of the reader is drawn on the specific situation corresponding to the loading of mass spectrometric data from a non-profile acquisition data file. For example, when a mass spectrum is opened from a `txt,asc,xy` text-based format file where the data correspond to a single spectrum, not a sequence of spectra. In this case, the TIC chromatogram really has a single (rt,i) pair denoting the TIC intensity at the single retention time of that very unique spectrum. The TIC chromatogram window thus artificially created and displayed like shown in Figure 3.3 on the following page. See the caption of that figure for the explanation.

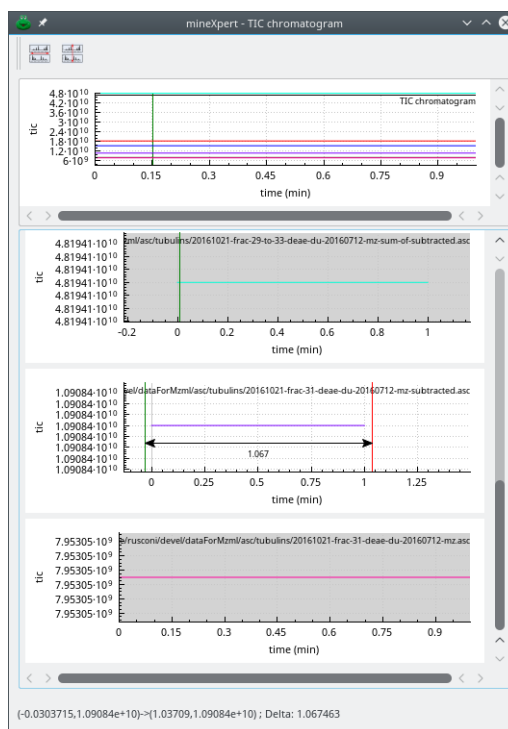


Figure 3.3: **The TIC chromatogram window** This TIC chromatogram window shows the peculiar situation of non-profile acquisitions, for which there is no real TIC chromatogram. The graph is thus artificially created. To perform an integration to a mass spectrum, unzoom the graph and enclose it fully in the integration range as shown for the integration process going on in the middle graph (the two extreme points of the graph need to be enclosed in the selection).

THE MASS SPECTRUM WINDOW

The mass spectrum window contains all the plot widgets that display mass spectra that originated in other windows. For example, the user might select a region in a TIC chromatogram and then ask that a mass spectrum integration be computed. In this case, the resulting mass spectrum is displayed in a new plot widget that is located in the mass spectrum window (Figure 3.4 on the next page).

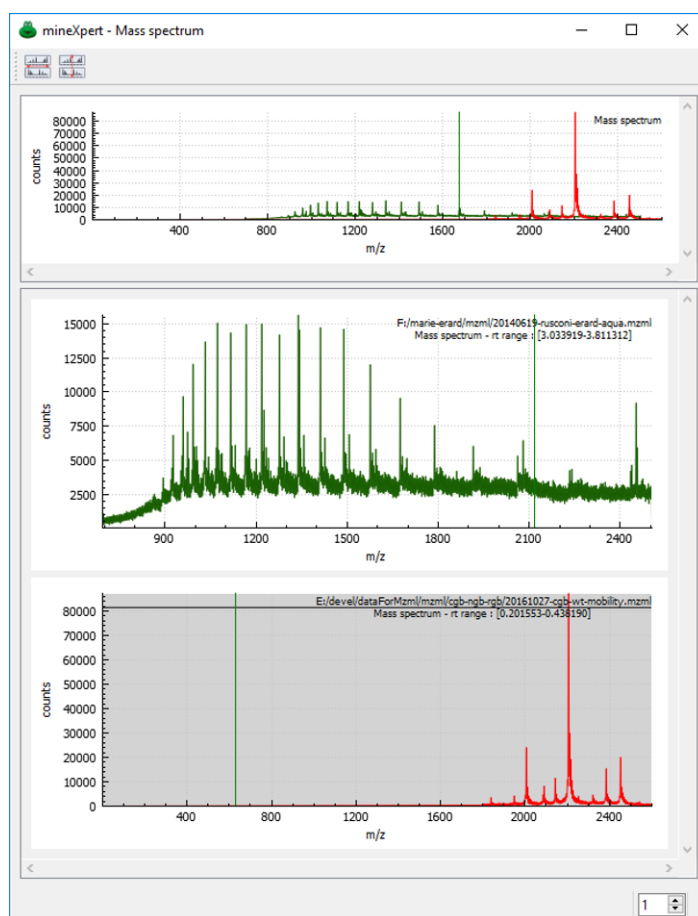


Figure 3.4: **The mass spectrum window** This mass spectrum window shows multiple mass spectra.

THE DRIFT SPECTRUM WINDOW

As described for the mass spectrum window, the drift spectrum window contains all the plot widgets that display drift spectra (Figure 3.5 on the following page).

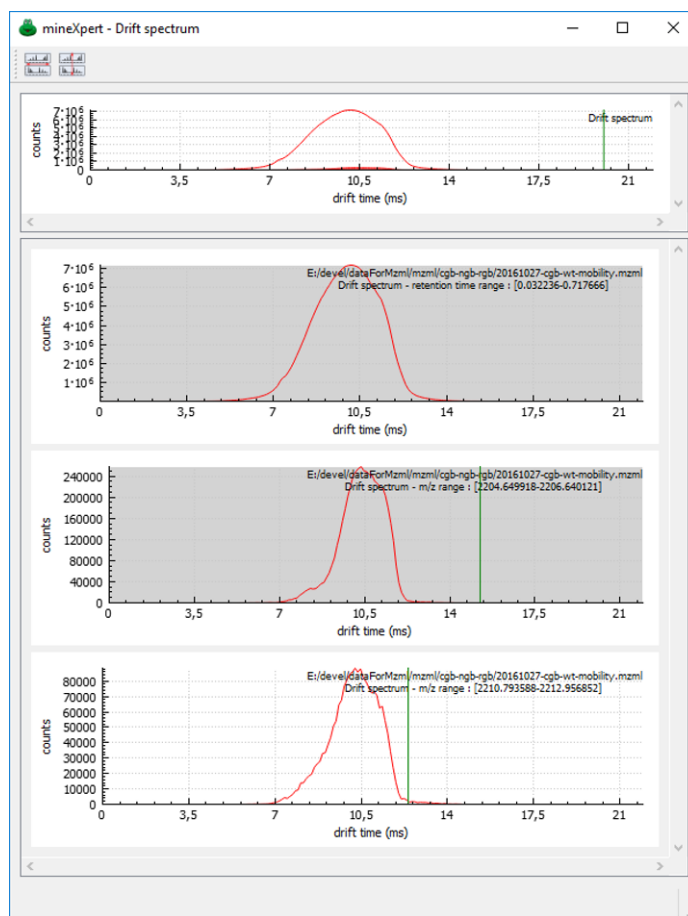


Figure 3.5: **The drift spectrum window** This drift spectrum window shows multiple mass spectra.

THE COLOR MAP WINDOW

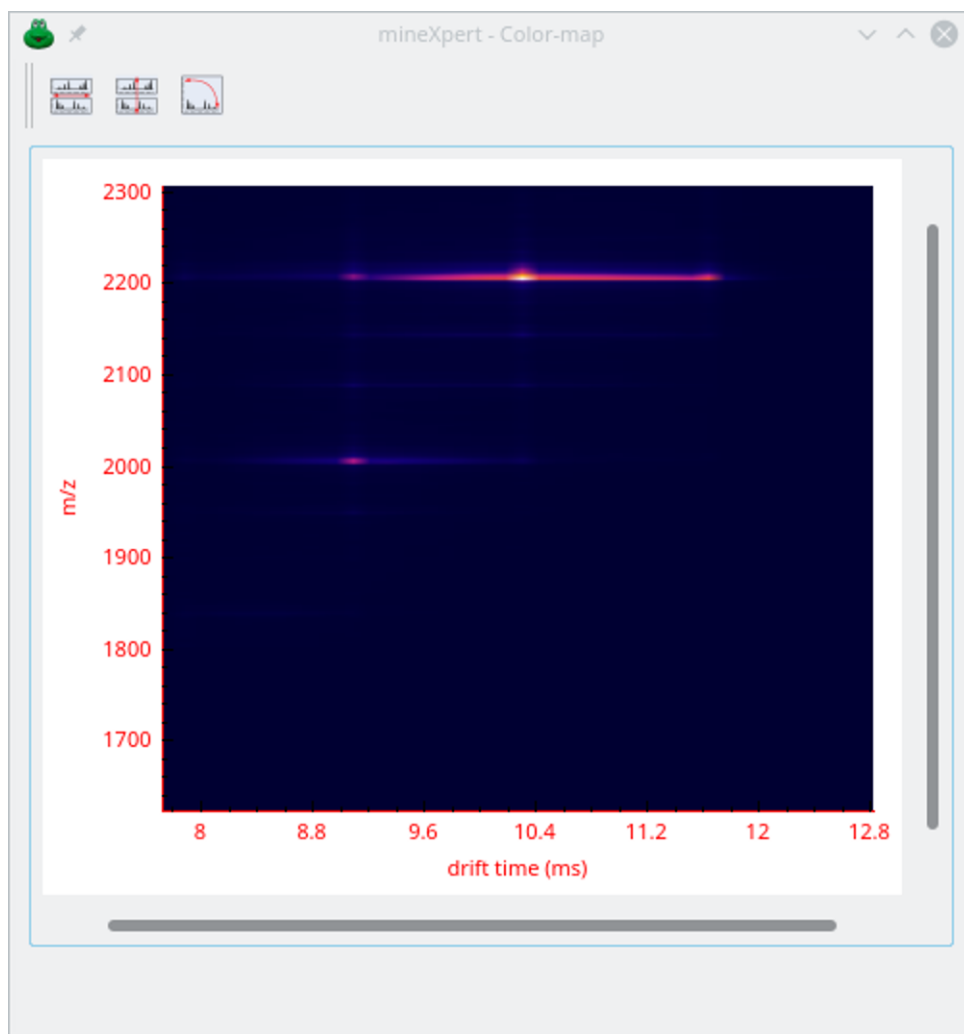


Figure 3.6: **The color map window** The color map window relates mass spectra to drift times.

The color map window displays a color map view of the drift data in the form of m/z vs drift time (dt). The intensity of the m/z values is coded in colour. The axes can be switched, such that either the m/z vs dt or the dt vs m/z representation can be obtained (see toolbar button on Figure 3.6).

GENERAL STRUCTURE OF THE WINDOWS CONTAINING PLOT WIDGETS




The TIC chromatogram, mass spectrum and drift spectrum windows are all structured in a similar way. The window is divided vertically in two compartments. The bottom compartment will host all the plot widgets stacked vertically. The top compartment hosts a single plot widget where all the graphs that are displayed unitarily in the lower compartment are shown superimposed.

The plot widget that is packed in the top compartment of the window is called the “multi-graph” plot widget because it can hold more than one graph. The plot widget(s) that is(are) packed in the bottom compartment of the windows is(are) called “single-graph” plot widget(s) because each plot contains only one graph.



The two vertical compartments of the window are resizable by dragging the sliding horizontal bar that separates them. It is possible to totally occlude one of the compartments by dragging that sliding bar all the way up (or down) to the window side.

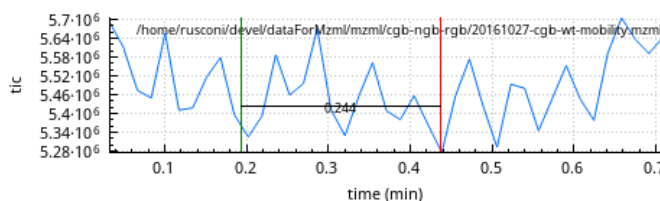
The behaviour described above does not apply to the Color map window that has no upper compartment with all the color maps superimposed.

GENERAL WORKING OF THE WIDGETS DISPLAYING DATA

The TIC chromatogram, color map, mass spectrum and drift spectrum windows all contain plot widgets (or color map widgets) that have a general working scheme as to how the data can be visualized. The main visualization operations are succinctly described below. The following convention will be used to describe the mouse buttons : : left mouse button, : middle mouse button and : right mouse button.

* Zooming in and zooming out:

- ◆ Zoom in: -click-drag to draw a selection rectangle. When the mouse button is released, the new plot view contains the data contained in the selection rectangle;
- ◆ Zoom in: -click-drag along the X-axis over the region to zoom and release the mouse button. The new zoomed view does not automatically scale to full scale in the Y-axis direction. To ensure that the new view automatically scales on the Y-axis, press Shift while releasing the mouse button;



As seen in the figure above, the region defined by the ⌨ -click-dragging operation is delimited by green and red markers, respectively at the start and at the end of the selection. The distance between the start and end points is updated along the mouse move operation.

- ◆ Zoom in/out: ⌨ -click-drag on the X- or Y-axis to interactively zoom in or out along the selected axis. In this mode, the zoom operates by contracting/expanding the data in such a manner that the left/bottom part of the graph (the origin of the graph) is anchored and does not move. When the drag occurs towards larger values on the clicked axis, the view is zoomed in along that axis. Conversely, it is possible to zoom out by dragging the mouse towards lower axis values. When the number of points in the plot is so large that the zoom operation is sluggish, pressing ⌘ will fluidify the zoom operation;
- ◆ Zoom in/out: The ⌨ -wheel-rotation can be used to zoom in or out the whole plot on both the X- and Y-axis simultaneously. Note that the position of the mouse cursor when the wheel is rolled defines the new view of the plot. Practising a bit allows to make that zooming in/out mode very powerful.
- ◆ Zoom out: To reset the zoom along one axis, ⌨ -double-click that axis. In this case, only the clicked axis will be full-scale, the other axis remains unchanged. To reset the zoom such that the full scale is calculated on the data set displayed after the zoom, maintain the ⇧ key pressed when double-clicking. To reset the zoom on both axes in one go, ⌨ -double-click one of the axes maintaining the ⌘ key pressed;

* Panning:

- ◆ ⌨ -click-drag on one of the axes to pan the plot view along that axis;


* History:

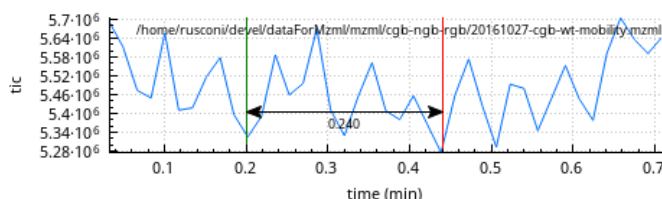
- ◆ Each time a new zoomed in/out view of the plot is triggered, a history element is stored in the plot widget. To back-replay the various steps of the zoom in/out operations in sequence, from pre-last to first, hit the ⌫ key. The exceptions to this mechanics is when the plot view is panned or when the mouse wheel is used.


The tool bar located at the top of the windows described above contains two buttons that allow to lock the x axis (the button icon has the horizontal red line) and/or the y axis (red line is vertical) range throughout all the graphs displayed in the window. This is of great use when the user wants to compare a number of graphs that have been obtained on comparable samples. The movements and zooming-in or zooming-out operations in one graph are then synchronized to all the other graphs. The third button performs a transpose operation. When the color map is initially created, the horizontal axis (the keys of the map) is the drift time axis and the vertical axis (the values of the map) is the m/z axis. The transpose operation switches the representation of the map such that the axes are inverted.


DATA INTEGRATIONS FEATURED BY *mineXpert*

Analyzing mass spectrometric data (with or without drift data) usually involves performing various data integrations in sequence. We saw earlier that the first data that are plotted upon loading a mass spectrometry data file are the TIC chromatograms along with (if applicable) the m/z vs dt color maps. These two graphed data sets are the starting points for the mass spectrometric data mining, that may involve the following integration operations:

- * **TIC chromatogram to mass spectrum** This kind of operation is triggered upon -click-dragging the mouse over the region of interest and maintaining the **[S]** key pressed. *mineXpert* integrates all the spectra that have been acquired at all the retention times between the start and the end of the selected region. A new mass spectrum is then plotted in a new plot widget in the mass spectrum window;



As seen on the figure above, the region defined by the -click-dragging operation is delimited by arrows, a green marker at the start and a red marker at the end.

- * **TIC chromatogram to drift spectrum** This kind of operation is similar to the one described above, unless the **[d]** key must be pressed. As above, a new drift spectrum is appended to the drift spectrum window.
- * **Color map to mass spectrum** This operation involves -selecting a rectangular region of interest on the color map and by maintaining the **[S]**

key pressed. A new mass spectrum is then plotted in a new plot widget in the mass spectrum window. Note that, due to a bug in the plotting library, the rectangle is not currently drawn on top of the color map.

- * **Color map to drift spectrum** Same as above, but with the **[s]** key pressed. As above, a new drift spectrum is appended to the drift spectrum window. Same remark as above.
- * The same mechanics is at work in the other plot widget windows. For example, to trigger the integration of a mass spectrum starting from a drift spectrum, simply drag the mouse over the drift spectrum and maintain the **[s]** key pressed. Rule of thumb: when a mass spectrum is to be generated, use the **[s]** key, when a drift spectrum is to be generated, use the **[d]** key and, finally, when a TIC chromatogram is to be generated, use the **[t]** key.
- * One of the most interesting features for detailed mass data mining is the integration to a TIC intensity. That integration can be triggered from any of the data window (any plot widget in any of these windows, that is). Not plot is created, the data are simply displayed in the status bar of the window. This integration will be discussed later.

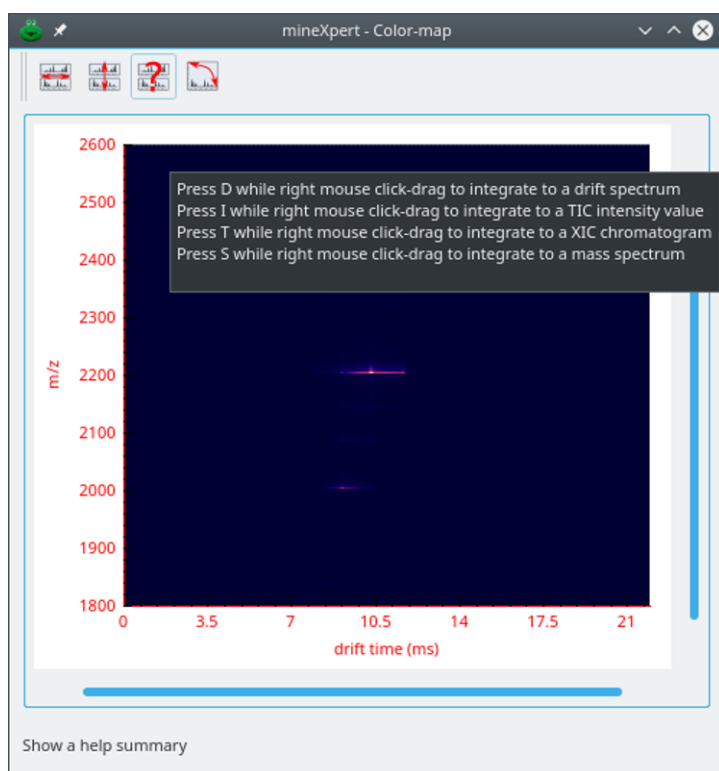



Figure 3.7: **The tool bar and its buttons** The '?' button shows a tool tip helping the user to select the proper keyboard/mouse combination to perform a given integration task.

Figure 3.7 on the preceding page shows the various buttons of the characteristic plot window. The button with the ‘?’ character will show a tool tip describing the various keyboard/mouse combinations to use to trigger the various data combinations described above.

The “filiation” of the plots is maintained using identifying colors. However, color is not enough to unambiguously identify the “filiation” of any given plot. Indeed, the same TIC chromatogram or Color map plot can be used multiple times to perform integrations. The newly created plots will have the same color as the originating plot, but it will not be possible to distinguish between all the “child” plots. This is why the plots maintain a “history” of the way they have derived from the initial TIC chromatogram/Color map plot. This history is shown in a small widget that shows up when the  key is pressed while the mouse cursor hovers over the widget at hand. One example of plot “history” is shown in Figure 3.8 on the next page.

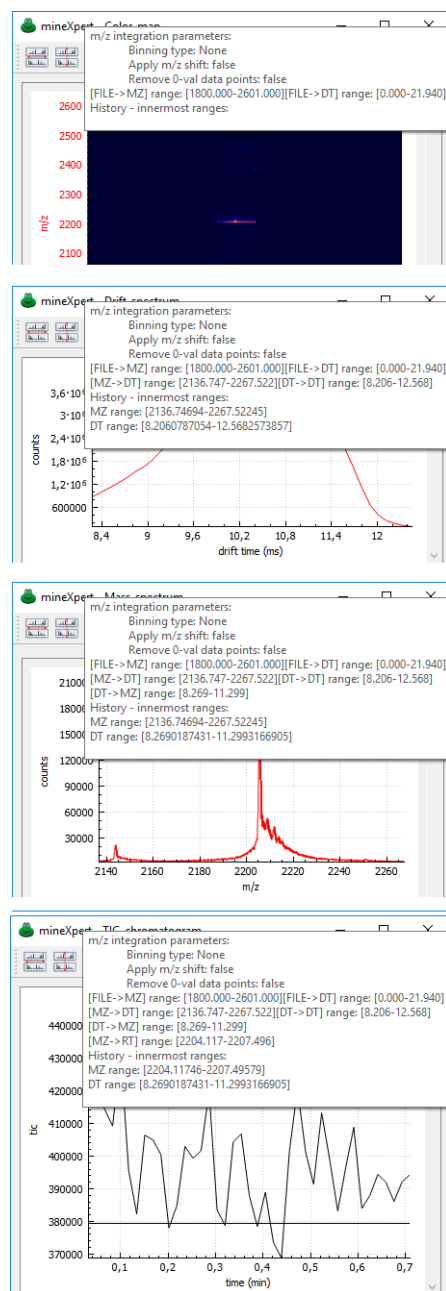


Figure 3.8: **The plot filiation history widget** Each plot has a filiation history that can be displayed by keying **[O]**.

This figure shows the filiation history of plots. By necessity, the first history item, because the first integration started from the $dt = f(m/z)$ color map is the [File→MZ][File→DT] item that indicates that the graph originates from loading a file and computing the color map.

Below, the drift time was computed by integrating from the color map according to both indications: [MZ→DT] and [DT→DT]. The concerned ranges are displayed.

The, the drift spectrum is used as a starting point for an integration to a mass spectrum according to the history item: [DT→MZ], and the range indicated that the user dragged the integration range from 8.2 to 11.3 ms (rounded values).

Finally, the user performed an integration from the drift spectrum to a XIC chromatogram, as evidenced by the last history item [MZ→RT] with the m/z 2204.117→m/z 2207.49 range.

As can be seen in the various filiation history items of Figure 3.8 on the preceding page, there is always a **History - innermost ranges** section that lists the three ranges for RT, MZ and DT. What is that “innermost range” concept? The idea is that, at any given time, the user might desire to know what it the smallest range that a given plot is originating from. For example, imagine:

1. an [RT→MZ] integration starting from a TIC chromatogram;
2. the m/z range obtained is [500-2500]. From that mass spectrum, the user integrates to a drift spectrum [MZ→DT];
3. then, from the drift spectrum, a peak seems interesting and the user back-integrates to a mass spectrum [DT→MZ];
4. in the mass spectrum, a mass peak is of interest and the user want to see at which retention times the m/z value elutes: she does an integration [MZ→RT].

The innermost m/z range in the XIC chromatogram obtained will be the last range selected, at step 4, not the range at step 2.

DETAILED DESCRIPTION OF THE INTEGRATION CALCULATIONS

Depending on the integration that is triggered in the various data plot/map widgets, the computations vary significantly. This section will describe the general computation algorithms in such a manner that the *mineXpert* user can grasp what is actually going on in the guts of the software.

INTEGRATIONS TO A MASS SPECTRUM

This integration occurs when the user \mathbb{Q} -selects a range in a given plot while pressing the $\boxed{\text{S}}$ key. Integrations to a mass spectrum can be elicited from a TIC chromatogram plot, a color map plot or a drift spectrum plot. In all these cases, the integration computation (that is, a mass spectral combination) needs to be aware of the kind of data at hand.

In order to clarify what integration means in the context of the creation of a mass spectrum, that is the summative integration (also known as “combination”) of any number of mass spectra, the following describes a combination in detail.

In this example, the user has loaded a mass data file obtained after an acquisition of mass data in profile mode. *mineXpert* calculates the TIC chromatogram right after having loaded the mass data. The user performs an integration for a given retention time range in the TIC chromatogram. If we consider an integration range [0–15] min, this is what would occur in the guts of *mineXpert*. In this example, we omit any step corresponding to any binning.

- * First of all, create a new mass spectrum (let's call it newMs, also known as the “combination spectrum”, that is, the result spectrum);
- * Extract from the mass spectrometry data all the spectra that have their internal rt value (retention time) contained in the [0–15] min interval. The list of extracted mass spectra (let's call that list msL) is then processed as follows:
 - * Iterate in msL and for each iterated mass spectrum (ms):
 - ♦ Iterate in all the (mz,i) pairs of ms and for each one check if the m/z value was already found in any of the previous mass spectra, that is, if a (mz,i) pair in newMs has that m/z value. If:
 - ★ the m/z was not found, copy the (mz,i) pair in newMs;
 - ★ else if the m/z value was already encountered in previously iterated mass spectra, increment the intensity of the corresponding (mz,i) pair of newMs by the value of the iterated (mz,i) pair. This is where the summative combination of mass spectra is at work.

At the end of this process, newMs will correspond to the summation of all the spectra contained in the msL list. The newMs mass spectrum is then plotted in the mass spectrum window as a new plot. The color of the newMs plot is the same as the color of the initial TIC chromatogram plot.

The process described above can only work in very limited circumstances, with data files generated with particular instruments. In general, this process does not lead to a usable mass spectrum, as described in Figure 3.9. In this combination mass spectrum computed from Lumos Orbitrap-originating data, the plot shows what should have been a high resolution monoisotopic peak (the m/z delta of the whole signal is 0.009). As can be seen, the signal in this mass spectrum is totally useless and the integration to a mass spectrum requires binning to overcome the presence of so many peaks in that 0.009 m/z interval.

mineXpert provides a number of ways to configure mass spectral combinations such that the obtained mass spectrum is usable. The m/z integration parameters that might be set are described in the following sections.

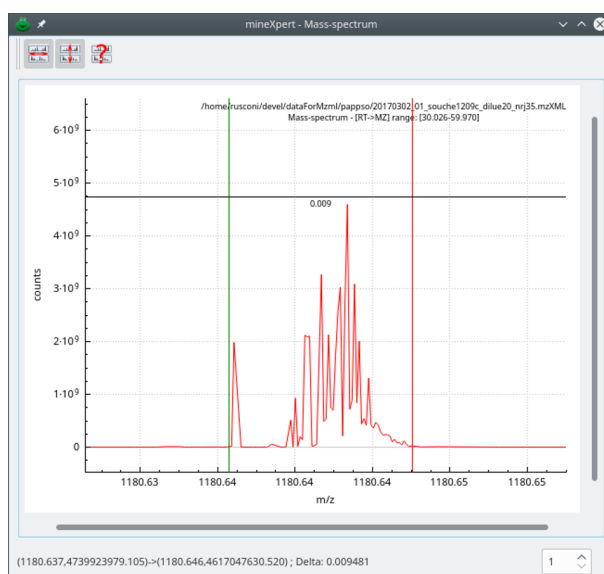


Figure 3.9: **Unusable combination spectrum without binning** The mass data used to compute this combination spectrum originate from a Lumos Orbitrap analyzer. The visible signal should have been a single high-resolution monoisotopic peak. The width of signal is 0.009.

CONSIDERATIONS ON THE DIVERSITY OF MASS DATA CONTENTS

Loading data from mass data files in *mzML* format does not guarantee that the data will be of the same kind if they come from different mass spectrometers. For example, data from Orbitrap mass spectrometers have the following characteristics:

- * all spectra do not start at the same m/z value;
- * all spectra do not have the same number of data points (they do not have the same size);
- * a large number of data points might have 0 values (intensity at a given m/z value is 0);
- * the m/z delta between two consecutive m/z values is not constant, and this is the major difficulty for data integration to a mass spectrum.

This is the output of the statistical analysis of the data loaded from a Lumos Orbitrap-originating file:

```
Spectral data set statistics:
Total number of spectra: 6203
Average of spectrum size: 391.311946
```

```

StdDev of spectrum size: 168.062934
Minimum m/z value: 400.007111
Average of first m/z value: 401.448935
StdDev of first m/z value: 1.590049
Maximum m/z value: 1999.928589
Average of last m/z value: 1901.852315
StdDev of last m/z value: 45.864131
Minimum m/z shift: -0.344452
Maximum m/z shift: 0.000000
Average of m/z shift: 1.097372
StdDev of m/z shift: 1.590049
Smallest Delta of m/z (step): 0.006195
Average of smallest Delta of m/z (step): 0.023757
StdDev of smallest Delta of m/z (step): 0.013179
Greatest Delta of m/z (step): 405.356934
Average of greatest Delta of m/z (step): 163.112057
StdDev of greatest Delta of m/z (step): 75.947334

```

As mentioned earlier, the most interesting bit of information is in the line reproduced below:

```
Smallest Delta of m/z (step): 0.006195
```

That 0.0062 value somehow gives an indication of the “definition” of the spectrum, that is, the smallest distance possible between two consecutive m/z values. We derive from this observation that the spectral combination may require setting up bins of a size at most of m/z 0.0062.

In general, the fact that the spectra of an acquisition do not all have the same m/z vector as the m/z axis is a great difficulty for mass spectral integration because it requires setting up binning prior to performing the mass spectral combination. That binning is nothing else than crafting a m/z value vector able to receive the intensities of all the m/z data points in the spectra to be combined. These concepts are developed in the following paragraphs.

STATISTICAL ANALYSIS OF MASS DATA

At the end of the data file loading, *mineXpert* performs a rudimentary statistical analysis of the data. The main datum of interest is the smallest m/z step that is observed in the whole set of mass data loaded from disk (the mass spectrum list, that can hold mass spectra in the thousands). For each mass spectrum in the list, the smallest m/z delta between any two consecutive data points is recorded. Then, the smallest ever m/z delta value is sought amidst all the recorded values. Intuitively, that smallest m/z delta value provides an idea of the resolution power of the instrument that generated the mass spectra. It is the value that is suggested by default to arbitrarily construct the bins during an integration to a mass spectrum, as described in Figure 3.10. In this example, the smallest m/z delta encountered in all the spectra loaded from file is used to fill-in the Arbitrary binning numerical value with bin size unit *MZ*.

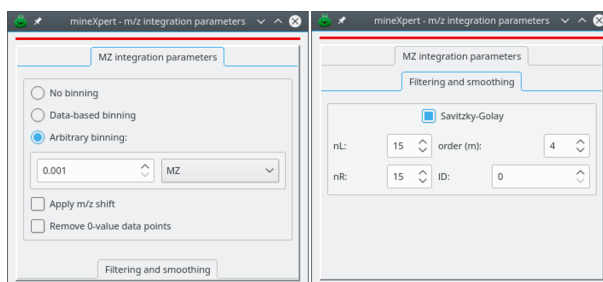


Figure 3.10: **The m/z integration parameters window** Any integration to a mass spectrum can be configured to ensure the best result depending on the kind of mass data (typically, data from different vendors behave in distinct ways upon integration).

The bin size units, when using **Arbitrary binning**, might be *MZ*, *PPM* or *RES*. In the two latter cases, the bin size changes along the m/z axis. It increases along with increasing m/z values. For example, if the bin size unit is *PPM* and the size unit is *10*, then at m/z 300, the bin size would be m/z 0.003, while at m/z 2000, the bin size would be m/z 0.02. If the bin size unit is *RES* and the bin size is *10000*, then at m/z 300, the bin size would be m/z 0.003, while at m/z 2000, the bin size would be m/z 0.02.

Once the **Arbitrary binning** is selected in the m/z integration parameters window, the bin size and bins size unit have been set, the program creates the bins in the combination mass spectrum according to these settings. The first bin and the last bin are simply the smallest and greatest m/z values found in all the spectra to be combined. The program fills in the void in between these two values in steps matching the bin size with or without PPM/RES ponderation: In case the bin size unit is *MZ*, there is no specific calculation; if the bin size unit is either *PPM* or *RES*, then the bins are calculated accordingly, as shown in the examples above. Once the bins have been set up in the combination spectrum, the actual combination of all the mass spectra can take place.

EFFECTS OF THE M/Z INTEGRATION PARAMETERS

This section provides some examples of how the integration parameters might impact the mass spectrum resulting from combination of mass spectra. Also, this section details the general guidelines for ensuring the best combination calculation.

When *Data-based binning* is recommended Data-based binning means that the bins in the combination spectrum are nothing but the m/z values of the first spectrum of the mass spectral set to be combined. This is the simplest integration mechanism and is recommended when the mass data are perfectly coherent, that is, when all the mass spectra are rooted in the (roughly) same m/z value and the vector of m/z values along the m/z axis is reproduced over all the mass spectra of the combination set. This situation is exemplified in [Figure 3.11 on the next page](#).

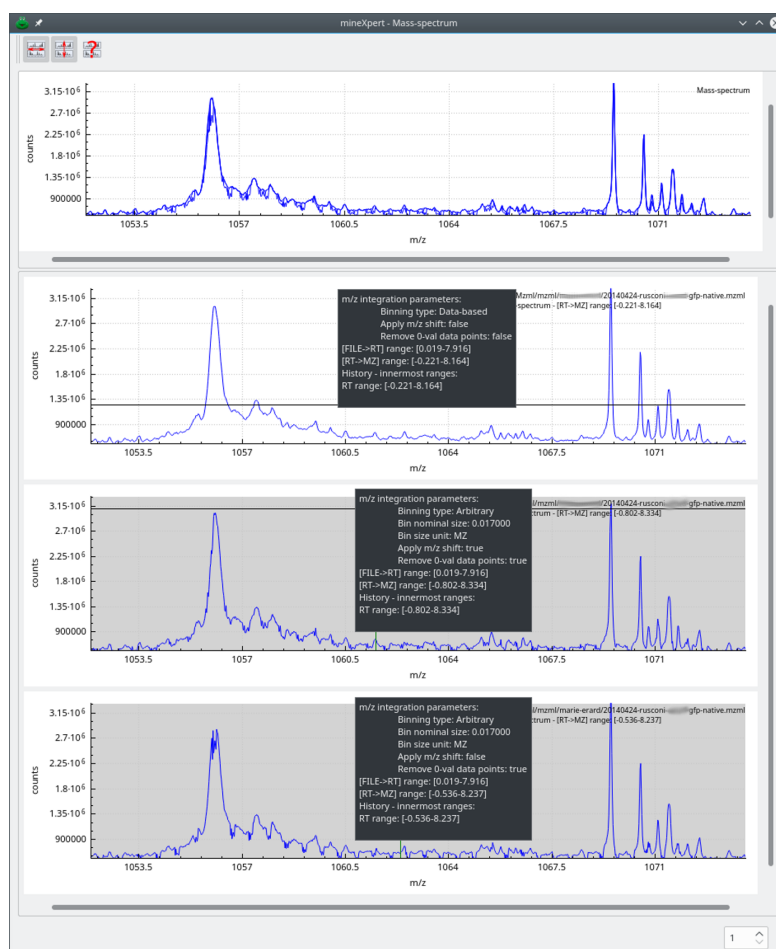


Figure 3.11: **Bruker microQToF acquisition of a protein mass data** In this example, the various m/z integration settings produce acceptable results for the combination mass spectrum. Note that the best results are for *Data-based binning* and that in the case of *Arbitrary binning*, applying the m/z shift is beneficial.

These combination spectra were obtained by performing a mass spectral integration of mass data acquired for a protein in a microQToF Bruker instrument. The mass acquisition settings were characteristic of a protein analysis in the 25–35 kDa range. The third spectrum from bottom was obtained by performing an integration with data-based binning, without applying any m/z shift and without removing m/z data points that have a 0-intensity value. The spectrum is perfect. The statistical analysis of the mass data calculated after loading of the mass data had shown that the smallest m/z delta value was of 0.017. The second spectrum from bottom was obtained after an integration with an arbitrary binning of size 0.017 and with bin size unit MZ (constant bin size throughout the m/z vector). In this case m/z shift was applied so as to realign slightly m/z axis-misaligned spectra. The result is pretty similar to

the one obtained earlier. There is a slight noise appearing on the lowest intensity peaks, denoting that the spectra, although pretty well m/z axis-aligned were not *perfectly* aligned. To check for that hypothesis, the same integration was performed but without performing the spectrum alignment (not m/z shift is applied in this case). The obtained spectrum is indeed more noisy, and the noise also appears on the highest intensity peaks. This unequivocally demonstrates that the spectra acquired by the instrument were not *precisely* aligned.

When removing 0-intensity m/z data points is useful The setting up of bins ultimately consists in creating a mass spectrum out of preexisting data (the first mass spectrum of the set in the case of **Data-based binning**) or out of arbitrary values (the smallest and greatest m/z values of the spectral set, the bin size and finally the bin size unit). In the latter case, the data points making the newly created mass spectrum have their m/z value calculated and their intensity set to 0. Because the m/z value is calculated starting from an arbitrary bin size value, it might be possible that not a single data point in the whole set of mass spectra has a m/z value matching that bin m/z value. In that case, the m/z data point still has a 0-intensity value at the end of the mass spectral combination. This is illustrated in Figure 3.12. When the 0-intensity data points are not removed (upper spectrum), the signal is deteriorated by these inverted spikes. Removal of the 0-intensity data points, cleans the trace perfectly.

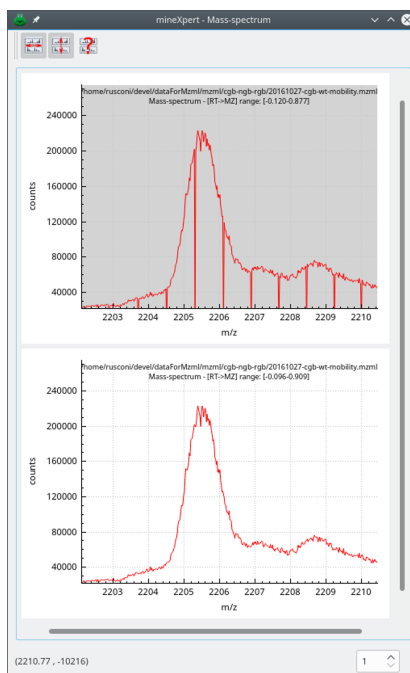


Figure 3.12: **Removing 0-intensity data points** When arbitrary binning is performed, residual 0-intensity data points might survive in the combination spectrum, which deteriorates the resulting mass spectrum. Removing these data points from the combined mass spectrum cleans the trace.



Savitzky-Golay filtering of the data might be useful The Savitzky-Golay filtering method is widely known for its effectiveness in removing noise from mass spectral data. It is possible to apply that filter at the end of a mass spectral combination. The m/z integration parameters window allows setting the Savitzky-Golay parameters:

- * nL: specifies the number of data points to the left of the point being filtered;
- * nR: specifies the number of data points to the right of the point being filtered;

The total number of points in the window that is considered for the regression is thus $nL + nR + 1$

- * m: specifies the order of the polynomial to use in the regression analysis leading to the Savitzky-Golay coefficients (typically between 2 and 6);
- * ID: specifies the order of the derivative to extract from the Savitzky-Golay smoothing algorithm (for regular smoothing, use 0);



INTEGRATIONS TO A DRIFT SPECTRUM

This integration occurs when the user  selects a range in a given plot while pressing the  key. The integration occurs for a given retention time range in the TIC chromatogram. If we consider an integration range [0–15] min, this is what would occur in the guts of *mineXpert*:

- * First of all, create a <dt,tic> map to store all the drift time values encountered below, along with the cumulated total ion current intensity value of the spectra acquired at the corresponding dt drift time.
- * Extract from the mass spectrometry data all the spectra that have their internal rt value (retention time) contained in the [0–15] min interval. The list of extracted mass spectra (msL) is then processed as follows:
- * Iterate in msL and for each iterated mass spectrum (ms):
 - ◆ Get the dt at which ms was acquired;
 - ◆ Calculate the total ion current (tic) for ms;
 - ◆ In the <dt,tic> map, check if the dt value was already found. If:
 - ★ the dt was not already found, create one (dt,tic) pair and insert it in the map;
 - ★ else if the dt was already encountered in previously iterated mass spectra, increment the tic value of the corresponding (dt,tic) pair in the map by the tic value calculated above for ms.

At the end of this process, the <dt,tic> map will correspond to the drift spectrum. That spectrum is then plotted in the drift spectrum window as a new plot with the same color as that of the initial TIC chromatogram plot.

INTEGRATIONS TO A TIC INTENSITY VALUE

This integration occurs when the user -selects a range in the TIC chromatogram plot while pressing the  key. The integration is performed by looking into the mass data for (m/z, i) pairs that match the current integration history of the current data plot and sums all the intensities to yield a final TIC intensity value. This value is printed in the status bar of the window.

Worthy of note is the fact that this kind of integration can be performed in the exact same way in the various data plots (TIC chromatogram, mass spectrum, drift spectrum, $m/z=f(dt)$ color map).

INTEGRATIONS TO A XIC CHROMATOGRAM

When a given ion of interest is researched in a mass spectral data set, usually the user asks the following question: “When is the ion at m/z xxx.yyy eluting from the chromatography column”? To extract the total ion current for a given m/z value as a function of the retention time, the XIC extraction parameters window can be filled-in as shown in Figure 3.13. In this process, the whole data set is searched for the requested ion.

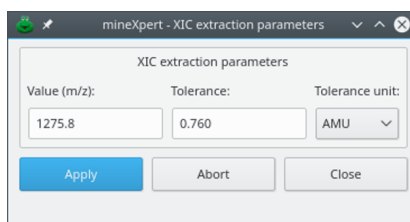


Figure 3.13: **Extraction of an ion current** It is possible to extract from a mass spectra data set the total ion current for that m/z value. The result is a TIC chromatogram for that m/z value: a XIC chromatogram.

The extracted ion current chromatogram is displayed in the TIC chromatogram window.

CHAINED INTEGRATIONS

The user, in the process of mining the data, will inevitably chain integrations to pinpoint a specific feature of interest. For example, let's say that the user performs the following chained integrations (see Figure 3.14 on page 40):

1. From a TIC chromatogram that spans [0–1] min, integrate to a mass spectrum the [0.3–0.6] range;
2. From the mass spectrum, that spans a m/z range of [500–5000], integrate to a drift spectrum the [2202.4–2204.4] range;

3. From the drift spectrum that spans [0–22] ms, where two unresolved peaks are visible, integrate back to a mass spectrum the drift region spanning [10.29–12] ms and then the drift region spanning [12–14] ms.

What happens during all these integrations? In the first integration, the whole m/z range of the mass spectrometric data is considered and the data filtering is only based on the retention time of the spectra that were acquired. Only those spectra, acquired at retention times between 0.3 and 0.6 min are considered for the combination that will lead to the production of a mass spectrum. In the second integration, two elements are to be taken into account for the filtering of the mass data: the fact that we only care of spectra acquired in the [0.3–0.6] retention time range *and* the fact that we are only interested in the mobility of ions whose m/z value is contained in the [2202.4–2204.4] range. The mobility spectrum shows a broad peak with a poorly resolved shoulder. The user wants to get the m/z values that are responsible for these unresolved peaks. She integrates to a mass spectrum the drift region [10.29–12] ms. In this integration the initial mass spectrometric data are filtered according to all the criteria mentioned above: retention time range *and* m/z range *and* drift time range. The same applies for the other drift spectrum to mass spectrum integration starting from drift time range [12–14] ms. As shown in the last two mass spectra, the data is indeed contained in the m/z [2202–2204] range. Incidentally, it appears from the analysis that the same ions have different drift times, since both drift spectrum shoulders back-integrate to very similar mass spectral patterns.

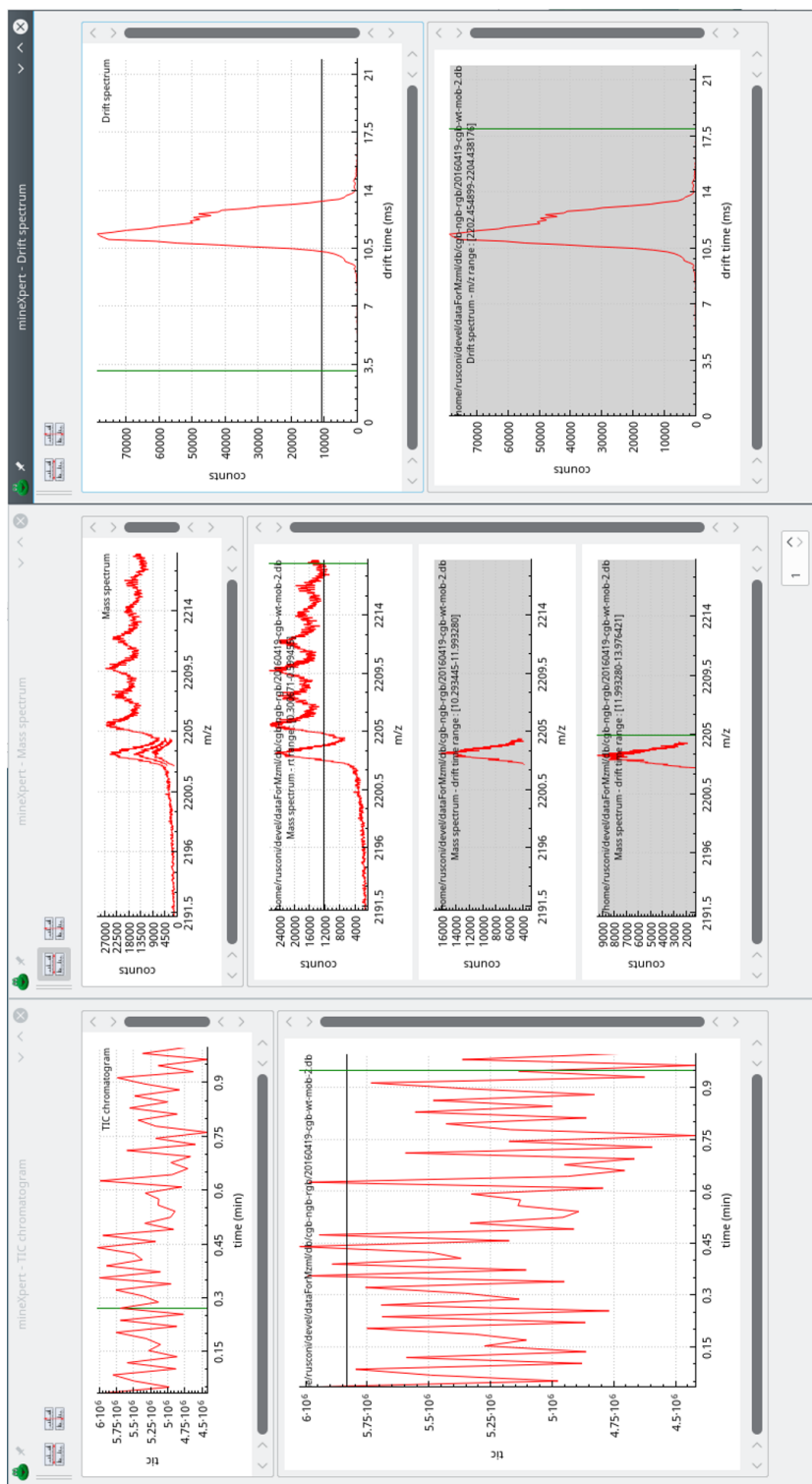


Figure 3.14: Example of chained integrations

MASS SPECTRAL FEATURE ANALYSIS

When analysing a mass spectrum, two major deconvolutions are performed to get back to the mass of the analyte while reading m/z values: the charge state family-based deconvolution and the monoisotopic cluster-based deconvolution. In the following sections, both deconvolutions are described.

MASS SPECTRAL DECONVOLUTION BASED ON CHARGE STATE ENVELOPE MASS PEAKS

In this kind of deconvolution, at the present time, the software assumes that the ionization agent is the proton and that the ionization is positive.

The deconvolution is based on the determination of the distance between consecutive (or not) peaks of a given charge state envelope. When the user click-drag the cursor from one peak to another, the program tries to calculate if the distance between two peaks matches a charge difference of 1 (or less). If so, it computes the molecular (Mr) mass of the analyte whose mass peak is located under the cursor. Figure 3.15 shows that precise state for two *consecutive* peaks of a charge state envelope.

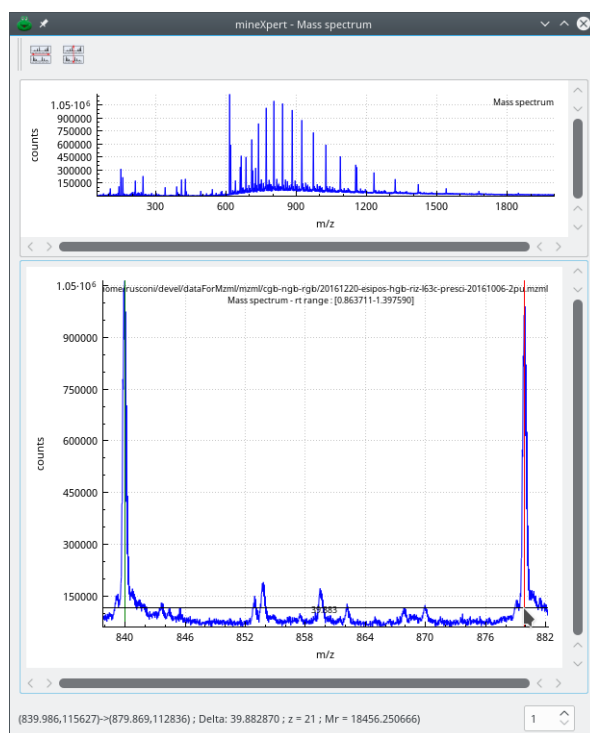




Figure 3.15: **Charge state envelope-based mass deconvolution** Approach using two *consecutive* mass peaks.

The status bar of the window documents the current inter-peak distance

measurement operation that is performed by -click-drag of the cursor starting at the left peak towards the right peak. The start peak is marked with a green marker and the end peak is marked with a red marker. Start and end positions are documented in the form (m/z start, i)→(m/z end, i). Then, the delta, that is, the distance between both positions is provided. When the end position matches a theoretically expected distance corresponding to a charge difference of 1, then the charge z of the peak under the cursor is provided and the molecular mass (Mr) is provided for the analyte whose peak is under the cursor.

It might happen that two *consecutive* peaks of the charge state envelope are not of a good shape enough to point and click precisely in the center of the peaks. In that case, the software allows indicating the number of intervals that run between two -click-drag-connected peaks. This is illustrated in Figure 3.16. The user knew that she had to measure the distance between two peaks that were separated by two intervals. She thus incremented the interval value in the status bar to 2 and performed the measurement. The Mr value that is displayed is different than the previous one because without enlarging the window, it is more difficult to click right at the center of the gaussian shape of each peak. Theoretically, the Mr values should be identical, and actually are when the measurements are performed cleanly in widely-laid mass spectra.

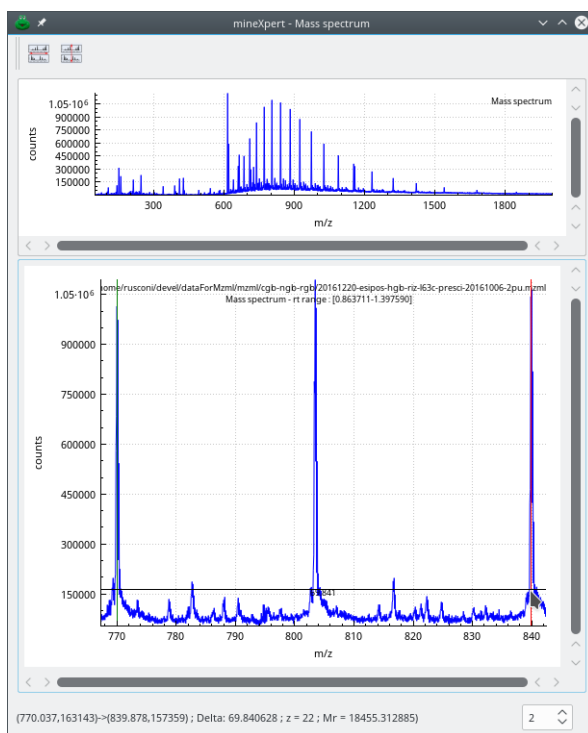




Figure 3.16: **Charge state envelope-based mass deconvolution** Approach using two *non*-consecutive mass peaks. Note the 2 interval value in the status bar of the window.

Note that the -click-dragging direction (left→right or right→left) has an impact on the value of the charge (z) that is obtained, since that charge value

is relative to the peak *under* the cursor at the moment of the deconvolution. Conversely, the mouse-dragging direction has no effect on the Mr (molecular mass) of the analyte obtained as a result of the deconvolution process.

MASS SPECTRAL DECONVOLUTION BASED ON ISOTOPIC CLUSTER PEAKS

In this kind of deconvolution, the user  click-drags the cursor between the first two peaks (when possible) of the isotopic cluster. The charge state of the ion is $\frac{1}{\Delta m/z}$, with $\Delta m/z$ the distance between the two consecutive peaks. Figure 3.17 shows that deconvolution process at work.

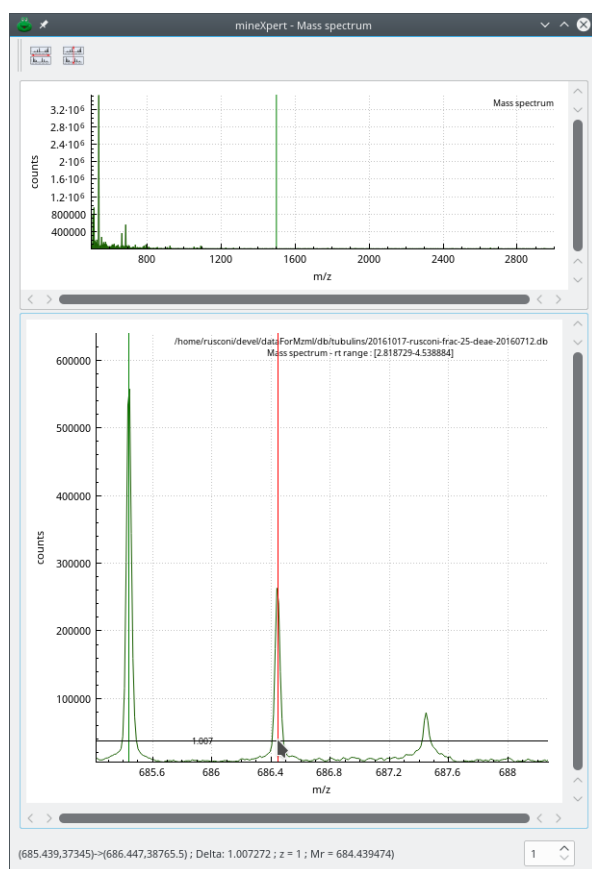



Figure 3.17: Isotopic cluster-based mass deconvolution

Note that the direction of  click-dragging (left→right or right→left) does not have any effect on the Mr value that is obtained as a result of the deconvolution process.

RECORDING THE DATA MINING WORK

When doing mass analysis work it is often desirable to store the painstakingly manually picked m/z or Mr values for later use. *mineXpert* provides a number of solutions to record the data mining work.

SIMPLEST DATA RECORD: IN-CONSOLE FEATURE LABELING

The simplest way to record any graph feature is to point that feature with the mouse and press the `[1]` ('el') key. That key shortcut prints to the console window the coordinates of the current mouse cursor location. To be able to trace back the graph source of that (x,y) pair, the text is printed in the console using the same color as the graph whence the labelling action came. The console is actually a rich text format editor in which it is possible to edit the text contents so as to copy/paste them in the lab-book or an email to a colleague, for example. This is shown in Figure 3.18. The label operation described here does not require any previous integration operation. This is in contrast to the requirements of the mass spectral data analysis recording described below.

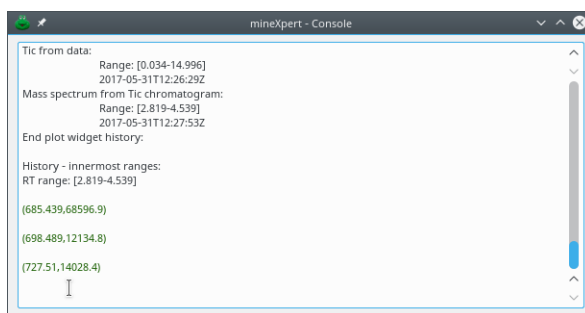


Figure 3.18: **Recording the peak feature coordinates to the console** The text color helps to identify the graph being analyzed.

*The label recording process works without ambiguity when the cursor is located in the single-graph plot widgets. However, when the cursor is located in the multi-graph plot widget (top part of the window displaying TIC chromatograms, mass spectra or drift spectra) then, only the graph(s) currently selected in the **Loaded mass spectrum files** window is(are) concerned by the label operation.*

CONSOLE-/CLIPBOARD-/FILE-BASED DATA ANALYSIS RECORDING

In order to record the innumerable analysis steps that make a data mining session, the *File*→*Analysis preferences* might be called to display the window shown in Figure 3.19. In that window, the user can select the destination of the data

analysis recording system: console, clipboard, file or any combination of the three. When selecting file recording, the user might specify if the recording should overwrite any preexisting file or, instead, append to that file. Depending on the kind of graph where data mining occurs, the format of the data to be recorded will change. For example, it makes no sense to record the charge z when mining data in the **Drift spectrum** window. This is why the text format of the data export might be defined for the three kinds of graphs: TIC chromatogram, mass spectrum or drift spectrum.

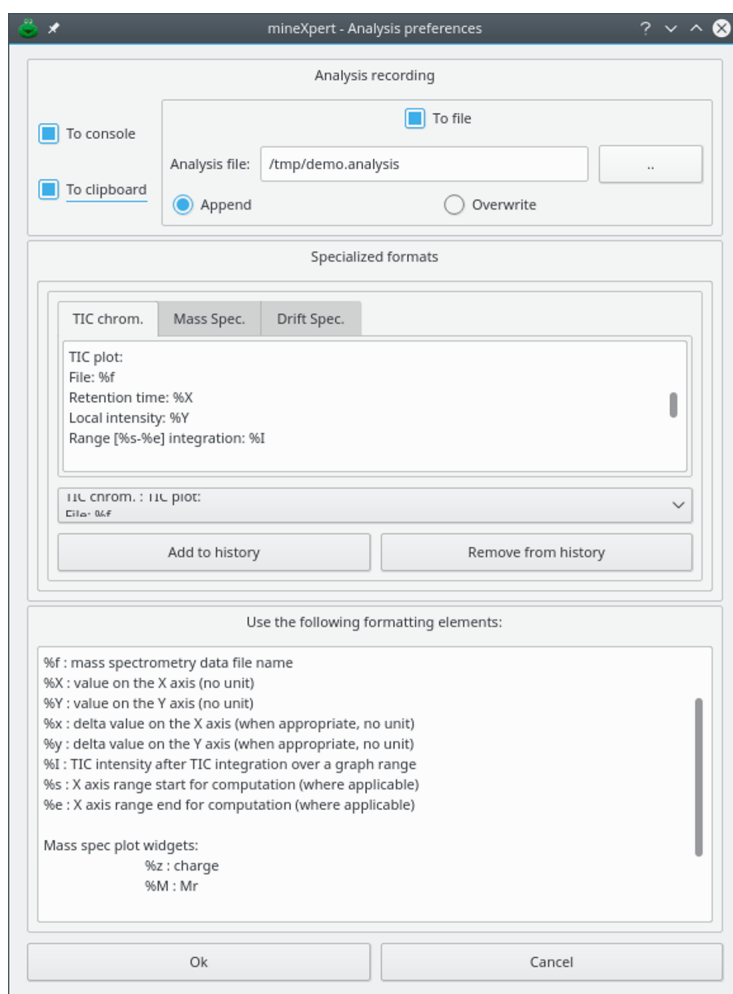


Figure 3.19: Setting-up of the recording of the data analysis It is possible to configure the recording system to record to either the console, the clipboard, a file (in append mode or in overwrite mode) or any combination of the three. The format of the string is defined using special characters (see text) and might be defined specifically for the three main graphs: TIC chromatogram, mass spectrum and drift spectrum.

The format used to define the text string to be stored on console and/or in

file can contain particular tokens as described below:

- * %f : mass spectrometry data file name
- * %X : value on the X axis of the graph (no unit)
- * %Y : value on the Y axis of the graph (no unit)
- * %x : delta value on the X axis (when appropriate, no unit)
- * %y : delta value on the Y axis (when appropriate, no unit)
- * %I : TIC intensity after TIC integration over a graph range
- * %s : X axis range start for computation (where applicable)
- * %e : X axis range end for computation (where applicable)

For mass spec plot widgets:

- * %z : charge
- * %M : Mr

It is important to keep in mind that the %z and %M format strings can only work if the user is actually analyzing a mass spectrum and if the user has effectively performed a deconvolution operation that has allowed computing these two values. If the values are not available, the program shows nan (“not a number”) in the textual output when the space bar is hit (see below).

In the drift spectrum window, the data recording processes data matching the cursor position at the last \leftarrow -single-click. The program tries to define the intensity by looking at the graph ordinate (y axis) matching the nearest abscissa point (x axis) to the last \leftarrow -clicked location.

*Also, as stated above for the simple labelling of cursor location points, the recording of data analysis steps work both in the multi-graph plot widgets (those at the top of the plot windows) and in the single-graph plot widgets (those at the bottom of the windows). When doing data analysis in the top multi-graph widget, it is necessary to select the traces to be analyzed in the **Loaded mass spectrum files** window, otherwise no data will be recorded. This is of course not necessary when working in bottom plot widgets because in that case there is no ambiguity on what data to record.*

It is possible to store the format strings in a drop down box for later reuse. Simply click onto the **Add to history** button while having the format text displayed in the text editor and it will be appended to the drop-down list. The list gets stored when the dialog window is closed and will be filled-up again when the program is restarted.

As an example, if the user defined the following format string for a mass spectrum graph:

```

Mass spec. :
mz = (%X, %Y) z = %z
filename = %f
date = 20161021
session = 20161021
mslevel = 1 msion = esi msanal = tof
chrom = DEAE fraction = 25
seq = pos =      oxlevel = 0 pos =
intensity =
comment =

```

then, a resulting data mining stanza that would be recorded will look like this:

```

Mass Spec. :
mz = (1051.8, 50863) z = 1
filename = 20161017-rusconi-frac-25-deae-20160712.db
date = 20161021
session = 20161021
mslevel = 1 msion = esi msanal = tof
chrom = DEAE fraction = 25
seq = pos =      oxlevel = 0 pos =
intensity =
comment =


```

Interestingly, the user can define any kind of format, leaving fields available for later filling-in. This feature is of immense value when the analysis file is used later to fill-in a database for easy storage and interrogation of the mining findings.

At this point, it would be useful to have the file opened in an editor and at each new stanza edit the **comment** field if something needs to be commented, like the shape/intensity of a mass peak, for example.

Note that the program closes the file each time a new stanza has been written. This makes it possible to edit that file safely in between each stanza record. Remember to force the editor to reload the file from disk after each stanza recording.

When the recording involves sending the analysis data to the console, the data are sent to it as text colored the same as the spectrum that was under scrutiny.

When the mouse cursor has been placed at the proper location (with or without -click-dragging, depending on the situation) on the graph, the user hits the space bar and the data analysis stanza is recorded to the selected destination(s): console, clipboard, file.

SPLITTING VERY LARGE FILES INTO SMALLER CHUNKS

Mass spectrometry data acquisitions performed in line with a chromatography setup generally yields massive data files holding mass data acquired all along a

chromatographic development. Depending on the application, the data in the obtained file might not be of interest throughout all the acquisition duration. For example, a size exclusion chromatography might have resolved the molecular species of interest only in a very short retention time range. In this case, it might be useful to extract the data corresponding to that retention time range of interest from the initial very large file and store them in another file that will be sufficiently light to be loaded and analyzed quickly and easily.

mineXpert can export data according to various modes, as illustrated in Figure 3.20.

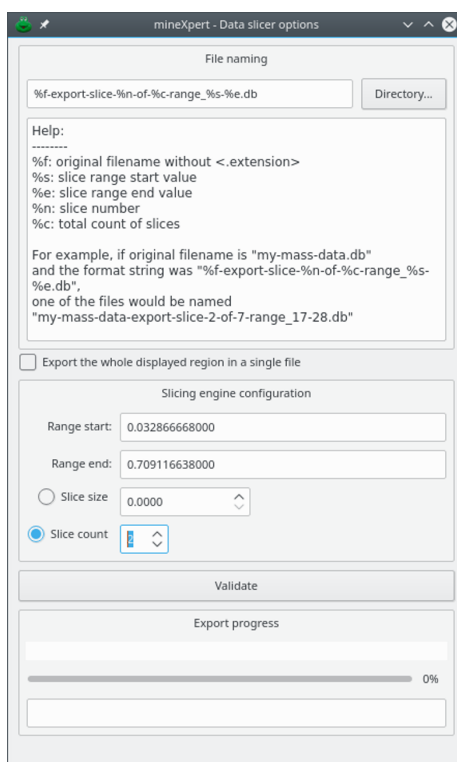


Figure 3.20: **Setting-up of the data export** It is possible to split very large files into smaller chunk files. In this example, the number of slices to be created is 2. The program computes automatically the size of the chunks by looking at the `rangeStart` and `rangeEnd` values.

Depending on the “slicing” configuration, the program will calculate the missing data to perform the required action. If the user specifies the number of slices, the size of the slices is automatically calculated. Conversely, if the user specifies the size of the slices, the number of slices is deduced. Note that the **Range start** and **Range end** values correspond to the limits of the data range currently displayed in the plot widget from which the data export was triggered using the *Export*→*data* context menu (right-click the mouse when the cursor is over the plot widget of interest). If the **Export the whole region in a single file** is checked, the data relating to the range displayed in the plot widget is exported to a single

file. For this operation to be meaningful, either zoom-in the data to the desired data range in the plot widget and start the configuration of the slicing process, or set manually the **Range start** and **Range end** values.

The file naming pattern used for the various data files generated in the process of the data export is governed by the format string displayed at the top of the window. By default, the generated files are located in the same directory as the source data file. If a new directory is to be used, it can be selected by pressing the **Directory...** push button.

Once the configuration is done, the **Validate** push button needs to be pressed so that the user can review the various file names that have been chosen for the various data slices to be written to (Figure 3.21). If the configuration is correct, the user clicks the **Confirm and start data export** button.

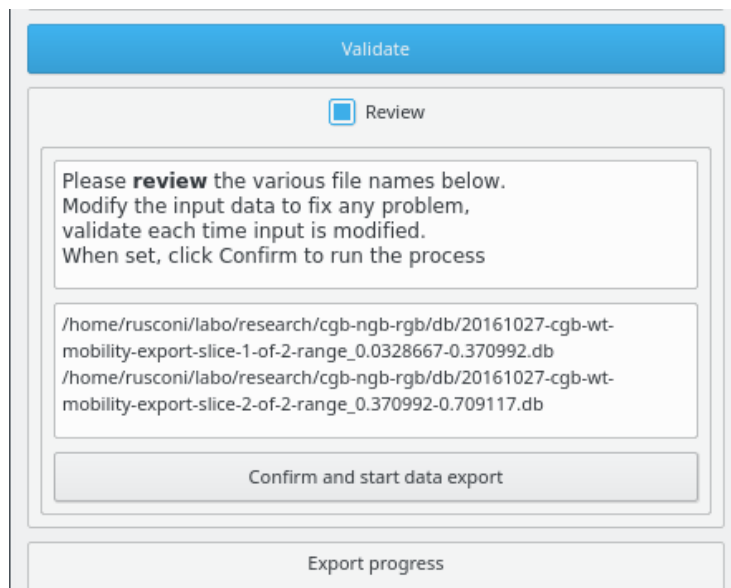


Figure 3.21: Setting-up of the data export - validation Once the configuration has been done, the user clicks the **Validate** push button and the program checks the consistency of all the parameters, then designs the slices and crafts file names for these various slices. The user has the opportunity to check that the file names match her desire. If so, clicking the **Confirm and start data export** button starts the data export process.

Note that the data export feature can only be used with the following two data ranges:

- * Retention time ranges: the data export configuration window must be activated from one of the TIC chromatogram plot widgets;
- * Ion mobility drift time ranges: the data export must be triggered from one of the Drift spectrum plot widgets;

This is because it does not make sense to split up a given data file into smaller files on the basis of m/z data ranges.

4

Converting *mzML* to *SQLite3*

The *mzML* format is very verbose and parsing it causes a notable delay during loading of mass spectrometry files. *mineXpert* allows one to convert *mzML* files to a private open file format based on the *SQLite3* database software.

Using the *SQLite3* format also allows to slice very large data files into smaller files on the basis of user-selected criteria (see *mineXpert* manual).

minexpert can be used in a console without needing to open any window. To show a detailed help, type the following:

```
minexpert --help
```

Use the following parameters (or flags) to perform a data file conversion:

```
minexpert -x -o <db file name> <mzML file name>
```

For example, to convert file `test-file.mzML` into `test-file.db`, the command line would be:

```
minexpert -x -o test-file.db test-file.mzml
```

Alternatively, the `-o` flag can specify a directory, in which case the new file name is crafted from the *mzML* file and written into that directory. In that case, the extension of the *mzML* file needs to be either *mzML* or *mzml* for the automatic renaming to occur.

Note that *in batch* conversion is possible using this kind of command line:

```
minexpert -x -o /tmp /home/<user>/lab/mzml/*.mzml
```

In this case, automatic file renaming happens and the new *db* files are all stored in the `/tmp` directory.

5

mineXpert JavaScript- based Scripting

When mining data, often, the user finds herself repeating tasks time and time again. Scripting allows to craft text files in which commands are run by the software program one after the other.

mineXpert makes a scripting environment available to the user. That environment is materialized by a window, shown on [Figure 5.1 on the next page](#).

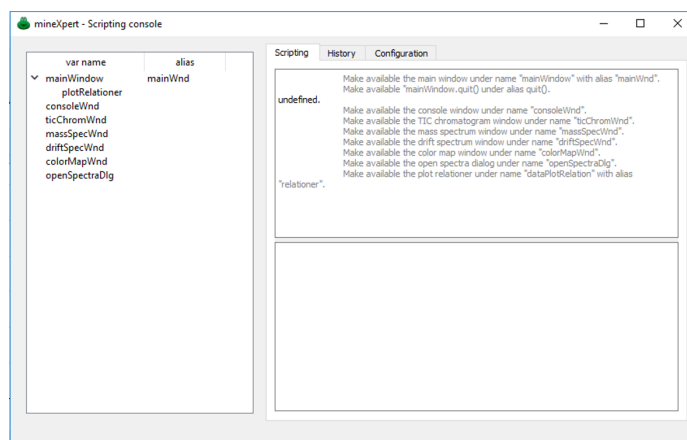


Figure 5.1: Scripting console, scripting tab

The left panel is a tree view listing all the objects or function names that are made available to the scripter. The right panel has three tabs. The **Scripting** tab has two sections; the upper section is where the scripting engine output is recorded; the lower section is the actual console where the user enters the script text.

USING THE SCRIPTING CONSOLE

The scripting console is a multiline text edit widget. The user may enter multiple lines in that widget, using the carriage `Return` key. Once all the lines have been entered to make one or more complete JavaScript statements, the whole set of lines is executed by pressing the `Ctrl+Return` key combination.

Upon execution of the script statements, any output is recorded in the upper section. When the output obtained from the engine evaluates to true, it is recorded in green color, if it evaluates to undefined, its color is black, and if it evaluates to error, it is colored in red.

Looking at the script engine output section, it is possible to read indented text, colored in grey (Figure 5.2).

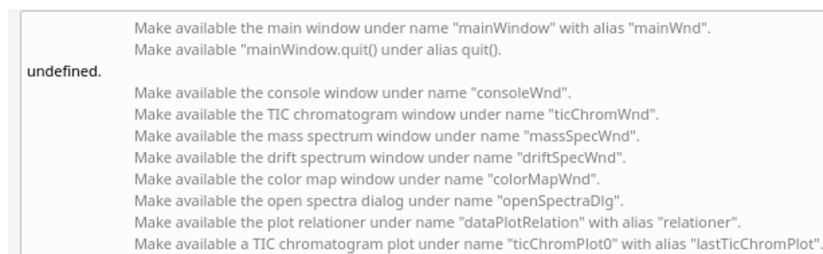


Figure 5.2: Informative comments to the user

These are comments that *mineXpert* provides when it runs script statements itself as part of making available to the user globally accessible objects. For

example *Make available the console window under name “consoleWnd”* is an explanatory text for the script statement (that the user does neither enter or see anywhere in the interface because it is run in the guts of *mineXpert*) that creates a globally accessible object for the scripter to use if necessary. The *consoleWnd* object that is created is listed in the tree view in the left panel of the window.

THE AVAILABLE OBJECTS LIST

The left panel of the scripting window lists objects that are made available by *mineXpert* to the scripter. The main objects that *mineXpert* makes available are shown in [Figure 5.1 on the facing page](#)

- * *mainWindow*: the window of the program, where the *File* menu resides;
- * *consoleWnd*: the console window where the various feedback messages to the user are displayed;
- * *ticChromWnd*: the window where all the total ion current chromatograms are shown;
- * *massSpecWnd*: the window displaying all the mass spectra;
- * *driftSpecWnd*: the window displaying all the drift spectra;
- * *colorMapWnd*: the window showing all the $m/z=f(dt)$ color maps;
- * *xicExtractionWnd*: the window displaying the XIC integration parameters;
- * *mzIntegrationParamsWnd*: the window displaying the m/z integration parameters;
- * *sqlMassDataSlicerWnd*: the window displaying the mass data file slicer configuration;
- * *openSpectraDlg*: the window listing all the currently opened mass spectrometry data files;
- * *scriptingWnd*: the where all the scripting occurs.

All the items listed above are systematically made available upon launching of the application. For some, they are of no use until a new mass spectrometry file is loaded. Upon opening of a mass spectrometric data file, new objects are created that are made available and listed in this same treeview. For example, upon loading of a mass spectrometry data file, a total ion current chromatogram is computed by *mineXpert* and displayed in a *TicChromPlotWidget* object that is made available under the *ticChromWnd* object in the tree view. If the data file were for ion mobility mass spectrometry, a $m/z = f(dt)$ color map would be computed also and made available as a new plot widget object under the *colorMapWnd* object in the tree view.

When a given object is used for scripting, a shortcut to writing its name in the scripting editor is to simply double-click its item in the treeview and the name will be copied into the scripting editor.

THE SCRIPTING HISTORY LIST

Each time a JavaScript statement (single- or multi-line) is executed, that statement gets stored in the History tab that contains a list, as shown in Figure 5.3.

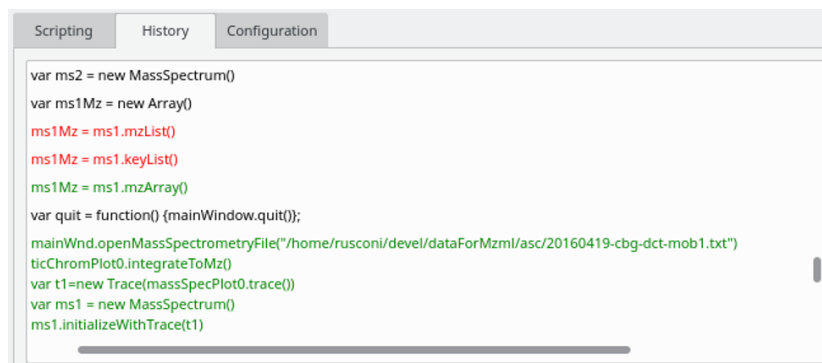


Figure 5.3: Scripting console, history tab

The items in the history list are reusable by double-clicking on them (or selecting them and hitting **Return**). By doing so, the selected items are copied to the **Scripting** tab, in the script input widget. It is then only required to hit **Ctrl**+**Return** to execute the script line(s).

Note that the history list might become very long, and the user might want to filter the entries of the list. By typing a regular expression in the edit widget below the list and pressing **Return**, the user can select history items matching that expression.

EXPLORING THE AVAILABLE OBJECTS' FEATURES

There are three kinds of objects that are available to the scripting environment:

- * High-level graphical user interface objects that are semi-automatically made available to the JavaScript environment by the Qt libraries. These objects are not fully scriptable and comprise the highest-level windows that are automatically made available upon running the program as top level branches of the tree view in the left panel of the scripting window;
- * Middle-level graphical user interface objects that are created “on demand”, like the various plot widgets that are created to display data. These objects have a useful range of features, typically listed in the upper pane of the scripting window by double-clicking their item in the tree view (see below);
- * Low-level C++ classes that are mapped to first-class JavaScript objects (with support for the `new` constructor operator, for example) such that they expose their full functionality to the scripting environment. The methods of these classes are described in detail in the JavaScript reference section number 5.

The functional capabilities of the various objects listed in the tree view can be explored by double-clicking the item of interest while maintaining the **Ctrl** key pressed. The list of functional capabilities is printed in the script output widget, as shown in Figure 5.4.

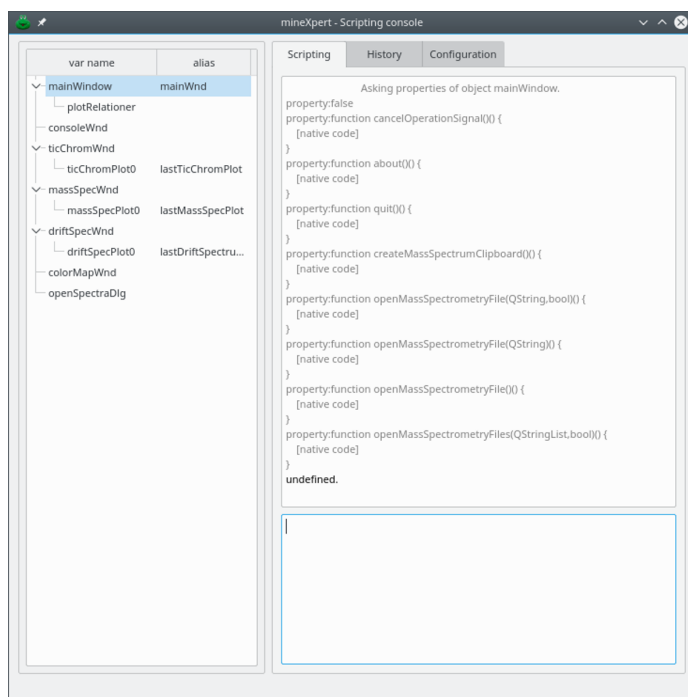


Figure 5.4: Scripting console, checking object methods

As shown in the figure, the `mainWindow` has a number of member functions that can be called according to the conventional `<object>.<function>` notation. For example, entering `mainWindow.quit()` in the script input text widget will trigger the `quit()` function of the `mainWindow` object, effectively quitting the application (the `mainWindow` is actually the main *mineXpert* window).

Calling `mainWindow.createMassSpectrumFromClipboard()`, for example, will create a new mass spectrum on the basis of data presently in the clipboard, if the data are in the conventional `x<sep>y` format, with `x` the `m/z`, `y` the intensity and `<sep>` any character that is neither a cipher or a dot (decimal separator).

It is essential to understand that not all functions are of use in the scripting context. This is because the listing of the functional capabilities of the objects also comprise functions that are not aimed at the scripting environment but are for internal Qt or mineXpert use.

This is more specifically the case of the plot objects, like `ticChromPlotWidget0`, `massSpecPlotWidget0` or `driftSpecPlotWidget0`, all listed in the tree view in [Figure 5.4 on the previous page](#). The creation of these plot objects is discussed in the section below.

Another way to iterate in the JavaScript properties of the objects made available in the JavaScript environment is by using this JavaScript code (using `massSpecPlotWidget0` as an example object):

```
for (var prop in massSpecPlotWidget0)
{
    print("prop: " + prop)
}
```

This is particularly useful to explore the various functions that are available for any given C++ object that is “exported” to the JavaScript environment (the `GlobalObject`, really).

THE JAVASCRIPT REFERENCE

The JavaScript reference material related to all the classes available in the JavaScript environment is located in the form of formatted plain text in the JS reference tab of the scripting window ([Figure 5.5 on the facing page](#)).

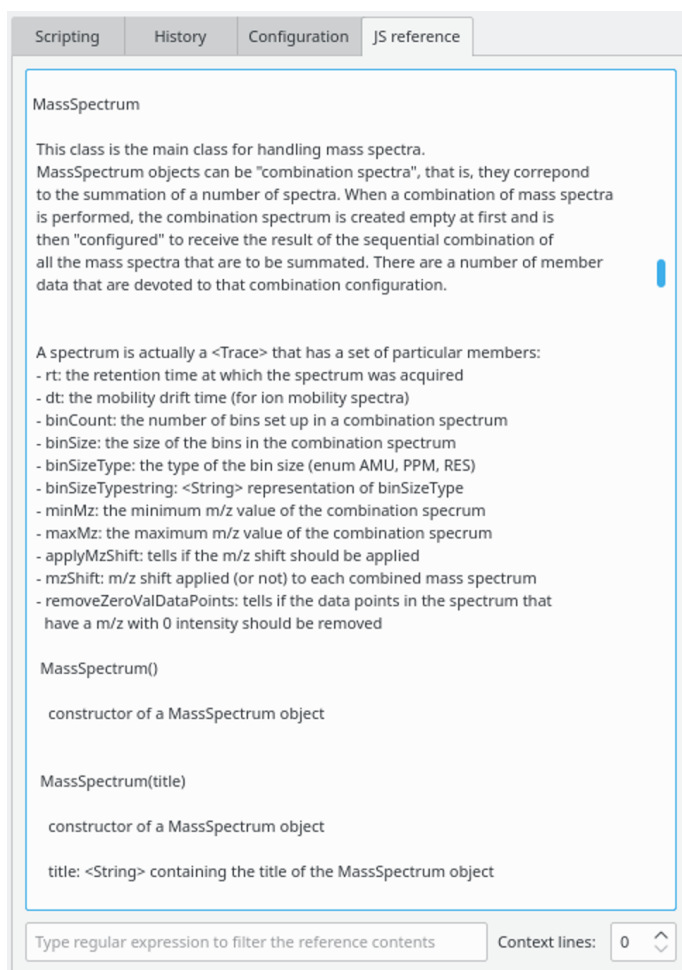


Figure 5.5: **Scripting console, JavaScript reference tab** The reference tab displays all the JavaScript-related documentation extracted from the source code. This documentation describes all the JavaScript classes available to the scripting environment. The description details the members and the methods of the class.

The line edit widget at the bottom of the tab provides an easy means to filter the documentation such that only the matching lines are displayed in the text widget. To filter the documentation, enter a regular expression (or a simple text) and press the **Return** key. To display the original contents anew, remove the regular expression and press the **Return** key.

Sometimes, some context around the matching lines might be desirable. The number of lines upstream and downstream of the matching lines that need to be output can be defined with the **Context lines** spin box. A value of 0 indicates that only the matching lines are output. A value of 5 indicates that five lines above the matching line and below that matching line are output.

That JavaScript reference is also available in identical form in the JavaScript reference section 5 on page 66 below.

CREATION OF THE PLOT OBJECTS AS A RESULT OF DATA MINING

When new plots are created as a result of the user making data mining operations, new JavaScript objects are created. The JavaScript objects mirror the C++ objects that live in the guts of *mineXpert*. The convention is to name the plot objects made available to the scripting environment using an index, like in *ticChromPlotWidget0*, *ticChromPlotWidget1*... For example, when a new mass spectrometry data file is loaded, *mineXpert* automatically computes the TIC chromatogram and makes it available to the scripting environment under object name *ticChromPlotWidget0*. That name is listed as a child of the *ticChromWnd* object in the tree view of the available objects. This object will remain available as long as the plot lives in the *ticChromWnd*. Note that simultaneously, the *lastTicChromPlotWidget* alias is provided to the scripter to capture that newly created object. The scripter willing to store the name of a newly created plot can thus make an assignment like in the following code:

```
mainWindow.openMassSpectrometryFile('massSpecFile1.mzml');

// The last TIC chromatogram plot is made available under the
// temporary name lastTicChromPlotWidget, take advantage to store it
// under a meaningful name for later use

msFile1TicPlot = lastTicChromPlotWidget

// Open a new file so that comparisons can be made
// against the previous one

mainWindow.openMassSpectrometryFile('massSpecFile2.mzml');

// The lastTicChromPlotWidget is made available, take advantage to store
// it under a meaningful name for later use

msFile2TicPlot = lastTicChromPlotWidget

// Now it is possible to reference the two TIC chromatograms
// with their new names:

msFile1TicPlot.integrateToMz(4.5, 7);
msFile2TicPlot.integrateToMz(4.5, 7);
```

JAVASCRIPT-ORIENTED CLASSES

At the time of writing, there are a number of C++ classes that have a full JavaScript counterpart: `DataPoint`, `Trace`, `MassSpectrum`, `MzIntegrationParams`, `SavGolFilter`, for example. In the following sections, a number of use cases are detailed to give the reader a flavor of what is scriptable in *mineXpert*. Note that the classes are detailed in the scripting reference section [5 on page 66](#).

CREATING A DATAPOINT OBJECT

The C++ class `DataPoint` has two member data: `m_key` and `m_val`. Both are high precision double values. The JavaScript counter part is also named `DataPoint` and can be initialized in two ways:

```
// create a new DataPoint object, initialized using double values
var dp1 = new DataPoint(123.321,456.654);

// check that this worked fine:
dp1.key;
// --> returns 123.321 (same as dp1["key"])
dp1.val;
// --> returns 456.654 (same as dp1["val"])

dp1.isValid();
// --> returns true

// create a new DataPoint object, initialized using an xy-formatted string
var dp2 = new DataPoint("147.741 258.852");

// check that this worked fine:
dp2.key;
// --> returns 147.741
dp2.val;
// --> returns 258.852

dp2.isValid();
// --> returns true

// create an empty DataPoint object
var dp3 = new DataPoint()

// an empty DataPoint object is invalid
dp3.isValid();
// --> returns false

// a DataPoint can be initialized a posteriori
dp1.initialize(159.951, 357.753)

// or using a string
dp2.initialize("258.852 741.147");
```

The `DataPoint` class is the main building block `Trace` objects are made of. A `Trace` object is nothing but a list of `DataPoint` instances.

CREATING TRACE OBJECTS

A JavaScript `Trace` object is nothing but an array of `DataPoint` objects. One useful application of scripting is to perform a variety of calculations on a given `Trace` or on a set of `Trace`s.

A JavaScript `Trace` object can be created and initialized in a number of ways.

CREATING AN EMPTY TRACE AND INITIALIZING IT

```
// create a new Trace using an xy-formatted string
var t1 = new Trace("This is the title of the trace object");
t1.title
// --> returns "This is the title of the trace object"

t1.initialize("123.321 456.654\n789.987 147.741\n258.852 369.963");
// --> returns 3 // the number of created DataPoint objects

// check that the trace has effectively 3 items:
t1.length
// --> returns 3

// check that the initialization was ok
print("(" + t1[0].key + "," + t1[0].val + ")")
// --> returns (123.321,456.654)

// create a new Trace using two arrays of numbers (key list and value list)
var t2 = new Trace();
t2.initialize([123.321,456.654,789.987],[147.741,258.852,369.963])
// --> returns 3 (the number of created DataPoint objects)

// check actual length
t2.length
// --> returns 3

// check that the initialization went fine
t2[0].key
// --> returns 123.321
t2[0].val
// --> returns 147.741

// get the key and value lists
t2.keyArray()
// --> returns 123.321,456.654,789.987
t2.valArray()
// --> returns 147.741,258.852,369.963

// once a Trace has been initialized, it can undergo interesting actions:

// calculate the sum of all the values:
t2.valSum()
// --> returns 776.556

// a Trace object can combine into itself another Trace object
t2.combine(t1)

// now check if the t2 values have increased accordingly
t2.valArray()
// --> returns 604.395,369.963,258.852,517.704 // correct combination

// now subtract t2 from t2:
t2.subtract(t2)

// now check that subtraction worked fine
t2.valArray()
// --> returns 0,0,0

// it is possible to initialize a trace with limitation to a given key range
var t3 = new Trace()
t3.initializeRange([123.321,456.654,789.987],[147.741,258.852,369.963], 200, 500);

// there should be only one DataPoint in t3
t3.length
// --> returns 1
t3.keyArray();
// --> returns 456.654
```

CREATING A TRACE OBJECT STARTING FROM A PLOT

A Trace object can be easily created by using data already obtained from using *mineXpert*. For example, a Trace object can be made so that it reproduces a plot displayed in the graphical user interface. The process is shown below:

```
// load mobility data file
mainWnd.openMassSpectrometryFile('mobility.mzml')

// integrate over the full TIC chromatogram range
// creates the massSpecPlotWidget0 object

ticChromPlotWidget0.integrateToMz()

// create a new Trace JavaScript object
var t0 = new Trace()

// now initialize t0 with the plot data of ticChromPlotWidget0
t0.initialize(massSpecPlotWidget0.keys(),massSpecPlotWidget0.values());

// check that the initialization actually worked
t0.length // should return the number of DataPoint objects in that Trace

// load a blank data file that acts as a baseline data file
mainWnd.openMassSpectrometryFile('mobility-blank.mzml')

// integrate over the full TIC chromatogram range
// creates the massSpecPlotWidget1 object

ticChromPlotWidget1.integrateToMz()

// create Trace JavaScript object
var t1 = new Trace()

// now initialize t1 with the plot data of ticChromPlotWidget1
t1.initialize(massSpecPlotWidget1.keys(),massSpecPlotWidget1.values());

// check that the initialization actually worked
t1.length // should return the number of DataPoint objects in that Trace

// finally perform some useful task: subtract noise from t0
t0.subtract(trace1)

// Trace object t0 now has the baseline removed.
```

EXPORTING A TRACE OBJECT TO A FILE

It is possible at each moment to export a given Trace object (or plot) to a file.

This is possible either at the JavaScript Trace object level:

```
mainWnd.openMassSpectrometryFile("mobility.mzml")
ticChromPlotWidget0.integrateToMz()
var t0 = new Trace()
t0.initialize(massSpecPlotWidget0.keys(),massSpecPlotWidget0.values());
t0.exportToFile("/home/rusconi/demo.xy");
```

Or, at the plot level:

```
mainWnd.openMassSpectrometryFile("mobility.mzml")
ticChromPlotWidget0.integrateToMz()

// note how the export function name has 'Plot' in it.
massSpecPlotWidget0.exportPlotToFile("/home/rusconi/demobis.xy");
```

At this point both files `demo.xy` and `demobis.xy` are bit-by-bit identical.

PLOTTING A JAVASCRIPT TRACE OBJECT TO A PLOT WIDGET WINDOW

It is necessary for the data miner to be able to look at her data graphically. Nobody wants to scrutinize data in ASCII files.

Anytime the scripter has a Trace object, she can plot it in the window that makes sense for the data. For example, if a plot derives from mass spectral data, then logically, the new plot should derive for these mass spectral data, as exemplified below:

```
mainWnd.openMassSpectrometryFile("mobility.mzml");
ticChromPlotWidget0.integrateToMz();

var t1 = new Trace();
t1.initialize(massSpecPlotWidget0.keys(), massSpecPlotWidget0.values());

// and now plot that Trace object as a descendant of massSpecPlotWidget0.
// if massSpecPlotWidget0 is removed, then the descendant will be removed also
massSpecPlotWidget0.newPlot(t1);
```

Displaying a new plot using the `<existingPlot Object>.newPlot(<Trace>)` call occurs in the window that matches the type of `<existingPlot>`. If `<existingPlot>` is a mass spectrum, then the descendant plot will be displayed in the Mass Spectrum Window.

Any of the plot widget windows can receive a new plot according to the mechanics described above.

PRINTING A JAVASCRIPT TRACE OBJECT TO THE CONSOLE

It is possible to have a look at the numerical data of a Trace object like so:

```
mainWnd.openMassSpectrometryFile("mobility.mzml");
ticChromPlotWidget0.integrateToMz();

var t1 = new Trace();
t1.initialize(massSpecPlotWidget0.keys(), massSpecPlotWidget0.values());

// print the data to the console
t1.asText()

// outputs a series of xy-formatted lines like so:
// 2504.3185084749 1262.0000000000
// 2504.3503266026 1277.0000000000
// ...

// doing this is also possible at the plot widget level
// note the function name change
massSpecPlotWidget0.asXyText()
```

RUNNING A JAVASCRIPT SCRIPT FROM FILE

It is possible to run a script directly from file by using either the following flag to the *mineXpert* command line:


```
minexpert -j <scriptFile>
```

or by using the *File*→*Run a JavaScript from file* menu of the scripting window. In that case the script is immediately run and the results are printed in the upper part of the **Scripting** tab of the scripting window.

JAVASCRIPT REFERENCE

DataPoint

The `DataPoint` class describes a data point. Its members are:

- `key`: the X-axis coordinate
- `val`: the Y-axis coordinate

`DataPoint()`

Constructor of a `DataPoint` object

Ex:

```
var dp = new DataPoint;
dp.key; // --> NaN
dp.val; // --> NaN
dp.isValid(); // --> false
```

`DataPoint(xyLine)`

Constructor of a `DataPoint` object initialized using the xy-formatted line.

`xyLine`: `<String>` holding the key,val pair in the format `key<sep>val`, with `<sep>` being any character not a cipher nor a decimal point.

Ex:

```
var dp = new DataPoint("123.321,456.654");
dp.key; // --> 123.321
dp.val; // --> 456.654
dp.isValid(); // --> true
```

`DataPoint(dataPoint)`

Constructor of a `DataPoint` object initialized with another `DataPoint` object

`dataPoint`: `<DataPoint>` object used to initialize this object.

Ex:

```
var dp1 = new DataPoint(dp);
```

`DataPoint(key, val)`

Constructor of a `DataPoint` object initialized with the numerical parameters.

`key`: key (X-value)
`val`: value (Y-value)

Ex:

```
var dp = DataPoint(123.321, 456.654);
```

`<DataPoint>.key`

Return the key `<Number>` property.

Ex:

```
var dp = new DataPoint(123.321, 456.654);
var mz = dp.key;
```

```
mz // --> 123.321
```

```
<DataPoint>.val
```

Return the val <Number> property.

```
Ex:
var dp = new DataPoint(123.321, 456.654);
var i = dp.val;
i // --> 456.654
```

```
DataPoint.initialize(other)
```

Initialize this DataPoint object with a <DataPoint> object

other: <DataPoint> object

```
Ex:
var newDp = new DataPoint(123.321,456.654);
var otherDp = new DataPoint();
otherDp.initialize(newDp);
otherDp.key; // --> 123.321
otherDp.val; // --> 456.654
otherDp.isValid(); // --> true
```

```
DataPoint.initialize(key, val)
```

Initialize this DataPoint object with two <Number> entities

key: <Number> holding the key of this DataPoint
val: <Number> holding the value of this DataPoint

```
Ex:
var dp = new DataPoint();
dp.initialize(123.321,456.654);
dp.key; // --> 123.321
dp.val; // --> 456.654
dp.isValid(); // --> true
```

```
DataPoint.isValid()
```

Return if this <DataPoint> object is valid.

```
Ex:
var dp = new DataPoint();
dp.initialize(123.321,456.654);
dp.key; // --> 123.321
dp.val; // --> 456.654
dp.isValid(); // --> true
```

Trace

The Trace class is fundamentally an <Array> of DataPoint objects.

```
Trace()
```

Constructor of a Trace object

Ex:
 var t = new Trace;
 t.length; // --> 0

Trace(title)

Constructor of a Trace object

title: <String> containing the title of the Trace object

Ex:
 var t = new Trace("Trace title");
 t.title; // --> Trace title

Trace(other)

Constructor of a Trace object

other: <Trace> object to be used to initialize this object

Ex:
 var t2 = new Trace();
 t2.initialize("123.3321 456.654\n147.741 258.852\n");
 t2[0].key; // --> 123.3321
 t2[0].val; // --> 456.654
 t2[1].key; // --> 147.741
 t2[1].val; // --> 258.852
 var t3 = new Trace(t2);
 t3[0].key; // --> 123.3321
 t3[0].val; // --> 456.654
 t3[1].key; // --> 147.741
 t3[1].val; // --> 258.852

Trace[index]

Return the <DataPoint> object at index.

Ex:
 var t1 = new Trace();
 t1.initialize([123.321,456.654,789.987],[147.741, 258.852, 369.963]);
 t1.asText();

 123.3210000000 147.7410000000
 456.6540000000 258.8520000000
 789.9870000000 369.9630000000

 var dp0 = t1[0];
 dp0.key; // --> 123.321
 dp0.val; // --> 147.741

 t1[0].key; // --> 123.321
 t1[0].val; // --> 147.741

Trace.initialize(xyFormatString)

Initialize this Trace object with a <String> object representing the

mass data in the xy text format:

```
"<key><sep><val>\n<key><sep><val>\n..."
```

xyFormatString: <String> object representing the <DataPoint> data points of the <Trace> in the format <key> <value>, with one such key-value pair per line. The separator between <key> and <value> might be anything non-numerical and not a dot (decimal separator).

Ex:

```
var t2 = new Trace();
t2.initialize("123.3321 456.654\n147.741 258.852\n");
t2[0].key; // --> 123.3321
t2[0].val; // --> 456.654
t2[1].key; // --> 147.741
t2[1].val; // --> 258.852
```

Trace.initialize(other)

Initialize this Trace object with a <Trace> object

other: <Trace> object

Ex:

```
var t1 = new Trace();
t2.initialize("123.3321 456.654\n147.741 258.852\n");
var t2 = new Trace();
t2.initialize(t1);
t1[0].key; // --> 123.3321
t1[0].val; // --> 456.654
t1[1].key; // --> 147.741
t1[1].val; // --> 258.852
```

Trace.initialize(keyArray, valArray)

Initialize this Trace object with two numerical <Array> entities

keyArray: the <Array> object containing all the keys of the <Trace>

valArray: the <Array> object containing all the values of the <Trace>

Ex:

```
var t1 = new Trace();
t1.initialize([123.321,456.654,789.987],[147.741, 258.852, 369.963]);
t1.length; // --> 3
var dp0 = t1[0];
dp0.key; // --> 123.321
dp0.val; // --> 147.741
```

Trace.initialize(keyArray, valArray, keyStart, keyEnd)

Initialize this Trace object with two numerical <Array> entities and two <Number> entities

keyArray: the <Array> object containing all the keys of the <Trace>

valArray: the <Array> object containing all the values of the <Trace>

keyStart: the <Number> value defining the beginning of the acceptable key range

keyEnd: the <Number> value defining the end of the acceptable key range

Ex:

```
var t1 = new Trace;
t1.initialize([123.321,456.654,789.987],[147.741, 258.852, 369.963], 124, 450);
t1.length; // --> 3
var dp0 = t1[0];
dp0.key; // --> 123.321
dp0.val; // --> 147.741
```

Trace.keyArray()

Return an <Array> of <Number> entities corresponding to all the keys of this Trace object

Ex:

```
var t7 = new Trace;
t7.initialize([123.321,456.654,789.987],[147.741, 258.852, 369.963]);
t7.keyArray(); // --> 123.321,456.654,789.987
```

Trace.valArray()

Return an <Array> of <Number> entities corresponding to all the values of this Trace object

Ex:

```
var t7 = new Trace;
t7.initialize([123.321,456.654,789.987],[147.741, 258.852, 369.963]);
t7.valArray(); // --> 147.741,258.852,369.963
```

Trace.asText()

Return the <DataPoint> data points of this Trace object as a <String> formatted according to this schema: <key> <value>, with one such pair per line

Ex:

```
var t7 = new Trace;
t7.initialize([123.321,456.654,789.987],[147.741, 258.852, 369.963]);
t7.asText(); // --> output is:
123.3210000000 147.7410000000
456.6540000000 258.8520000000
789.9870000000 369.9630000000
```

Trace.exportToFile(fileName)

Export the <DataPoint> contents of this Trace object to a file. The format is according to this schema: <key> <value>, with one such pair per line

fileName: <String> containing the path to the file in which to store the data

Ex:

```
var t7 = new Trace;
t7.initialize([123.321,456.654,789.987],[147.741, 258.852, 369.963]);
t7.exportToFile("/tmp/trial.txt"); // --> file contains:
123.3210000000 147.7410000000
456.6540000000 258.8520000000
789.9870000000 369.9630000000
```

Trace.valSum()

Return the <Number> value corresponding to the sum of all the values of all the <DataPoint> object in this Trace object

Ex:

```
var t7 = new Trace;
t7.initialize([123.321,456.654,789.987],[147.741, 258.852, 369.963]);
t7.valSum; // --> 776.556
```

Trace.combine(dataPoint)

Combine into this Trace object the <DataPoint> object

dataPoint: <DataPoint> object to combine into this MassSpectrum

Ex:

```
var t7 = new Trace;
t7.initialize([123.321,456.654,789.987],[147.741, 258.852, 369.963]);

t7.asText(); // --> output is:

123.3210000000 147.7410000000
456.6540000000 258.8520000000
789.9870000000 369.9630000000

t7.combine(new DataPoint(200.002,1000)); // --> 1, the number of added DataPoint objects

t7.asText(); // --> output is:

123.3210000000 147.7410000000
200.0020000000 1000.0000000000
456.6540000000 258.8520000000
789.9870000000 369.9630000000

t7.combine(new DataPoint(200.002,1000)); // --> 0, no added DataPoint, only increment the value

t7.asText(); // --> output is:

123.3210000000 147.7410000000
200.0020000000 2000.0000000000 // value increment by the same original amount.
456.6540000000 258.8520000000
789.9870000000 369.9630000000
```

Trace.combine(trace)

Combine into this Trace object the <Trace> object

trace: <Trace> object to combine into this Trace

Ex:

```
var t1 = new Trace;
t1.initialize([123.321,456.654,789.987],[147.741, 258.852,369.963]);
var t2 = new Trace(t1);
t2.length; // --> 3
t2.asText(); // --> output is:

123.3210000000 147.7410000000
456.6540000000 258.8520000000
```

```
789.9870000000 369.9630000000
```

```
t2.asText(); // --> output is:
```

```
123.3210000000 147.7410000000
```

```
456.6540000000 258.8520000000
```

```
789.9870000000 369.9630000000
```

```
t2.combine(t1); // --> 3: 3 DataPoint objects were combined
```

```
t2.asText(); // --> output is:
```

```
123.3210000000 295.4820000000
```

```
456.6540000000 517.7040000000
```

```
789.9870000000 739.9260000000
```

```
Trace.combine(key, val)
```

Combine into this Trace object a data point in the form of two <Number> entities, key and val

Ex:

```
var t1 = new Trace;
```

```
t1.initialize([123.321,456.654,789.987],[147.741, 258.852,369.963]);
```

```
t1.length; // --> 3
```

```
t1.asText(); // --> output is:
```

```
123.3210000000 147.7410000000
```

```
456.6540000000 258.8520000000
```

```
789.9870000000 369.9630000000
```

```
t1.combine(456.654, 1000);
```

```
t1.asText(); // --> output is:
```

```
123.3210000000 147.7410000000
```

```
456.6540000000 1258.8520000000
```

```
789.9870000000 369.9630000000
```

```
t1.combine(800, 2000);
```

```
t1.asText(); // --> output is:
```

```
123.3210000000 147.7410000000
```

```
456.6540000000 1258.8520000000
```

```
789.9870000000 369.9630000000
```

```
800.0000000000 2000.0000000000
```

```
Trace.subtract(dataPoint)
```

Subtract from this Trace object the <DataPoint> object

dataPoint: <DataPoint> object to subtract from this MassSpectrum

```
Trace.subtract(trace)
```

Subtract from this Trace object the <Trace> object

trace: <Trace> object to subtract from this Trace

```
Trace.subtract(mz, i)
```

Subtract from this Trace object a data point in the form of two <Number> values, key and value

MassSpectrum

This class is the main class for handling mass spectra. MassSpectrum objects can be "combination spectra", that is, they correspond to the summation of a number of spectra. When a combination of mass spectra is performed, the combination spectrum is created empty at first and is then "configured" to receive the result of the sequential combination of all the mass spectra that are to be summated. There are a number of member data that are devoted to that combination configuration.

A spectrum is actually a <Trace> that has a set of particular members:

- rt: the retention time at which the spectrum was acquired
- dt: the mobility drift time (for ion mobility spectra)
- binCount: the number of bins set up in a combination spectrum
- binSize: the size of the bins in the combination spectrum
- binSizeType: the type of the bin size (enum AMU, PPM, RES)
- binSizeTypestring: <String> representation of binSizeType
- minMz: the minimum m/z value of the combination spectrum
- maxMz: the maximum m/z value of the combination spectrum
- applyMzShift: tells if the m/z shift should be applied
- mzShift: m/z shift applied (or not) to each combined mass spectrum
- removeZeroValDataPoints: tells if the data points in the spectrum that have a m/z with 0 intensity should be removed

MassSpectrum()

Constructor of a MassSpectrum object

Ex:

```
var ms1 = new MassSpectrum();
```

MassSpectrum(title)

Constructor of a MassSpectrum object

title: <String> containing the title of the MassSpectrum object

Ex:

```
var ms1 = new MassSpectrum("spectrum title");
ms1.title; // --> spectrum title
```

MassSpectrum(other)

Constructor of a MassSpectrum object

other: <Trace> object to be used to initialize this object

Ex:

```
var t1 = new Trace;
t1.initialize([123.321,456.654,789.987],[147.741, 258.852, 369.963]);
t1.asText();
```

```
123.3210000000 147.7410000000
456.6540000000 258.8520000000
789.9870000000 369.9630000000
```

```
var ms1 = new MassSpectrum(t1);
ms1.asText();
```

```
123.3210000000 147.7410000000
456.6540000000 258.8520000000
789.9870000000 369.9630000000
```

MassSpectrum(other)

Constructor of a MassSpectrum object

other: <MassSpectrum> object to be used to initialize this object

Ex:

```
var ms1 = new MassSpectrum();
ms1.initialize([123.321,456.654,789.987],[147.741, 258.852, 369.963]);
ms1.asText();
```

```
123.3210000000 147.7410000000
456.6540000000 258.8520000000
789.9870000000 369.9630000000
```

```
ms1.rt = 1.2;
ms1.dt = 0.00325698;
```

```
var ms2 = new MassSpectrum(ms1);
ms2.asText();
```

```
123.3210000000 147.7410000000
456.6540000000 258.8520000000
789.9870000000 369.9630000000
```

```
ms2.rt; // --> 1.2
ms2.dt; // --> 0.00325698
```

MassSpectrum.title

Return the title <String> property.

Ex:

```
var ms1 = new MassSpectrum("spectrum title");
ms1.title; // --> spectrum title
```

MassSpectrum.length

Return the length <Number> property (number of <DataPoint> objects).

Ex:

```
var ms1 = new MassSpectrum();
ms1.initialize([123.321,456.654,789.987],[147.741, 258.852, 369.963]);
ms1.asText();
```

```
123.3210000000 147.7410000000
456.6540000000 258.8520000000
```

```
789.9870000000 369.9630000000
```

```
ms1.length; // --> 3
```

MassSpectrum.rt

Return the rt <Number> property (retention time at which this mass spectrum was acquired).

Ex:

```
var ms1 = new MassSpectrum();  
ms1.rt = 1.2;
```

```
ms1.rt; // --> 1.2
```

MassSpectrum.dt

Return the dt <Number> property (ion mobility drift time at which this mass spectrum was acquired).

Ex:

```
var ms1 = new MassSpectrum();  
ms1.dt = 0.00325698;
```

```
ms1.dt; // --> 0.00325698
```

MassSpectrum.binCount

Return the bin count <Number> property (number of bins in this mass spectrum).

MassSpectrum.binSize

Return the bin size <Number> property (size of the bins in this mass spectrum).

MassSpectrum.binSizeType

Return the bin size type property as a <Number>.

Ex:

```
var ms1 = new MassSpectrum();  
ms1.binSizeType = 2;  
ms1.binSizeType; // --> 2  
ms1.binSizeTypeString = "RES";  
ms1.binSizeType; // --> 4
```

MassSpectrum.binSizeTypeString

Return the bin size type property as a <String>.

Ex:

```
var ms1 = new MassSpectrum();  
ms1.binSizeType = 2;  
ms1.binSizeTypeString; // -> MZ;
```

`MassSpectrum.minMz`

Return the <Number> minimum m/z value to be used to craft the bins.

`MassSpectrum.maxMz`

Return the <Number> maximum m/z value to be used to craft the bins.

`MassSpectrum.applyMzShift`

Return the <Boolean> value telling if the m/z shift should be applied.

`MassSpectrum.mzShift`

Return the <Number> m/z shift value to apply when combining spectra.

`MassSpectrum.removeZeroValDataPoints`

Return the <Boolean> value telling if the <DataPoint> objects having m/z keys of a 0-intensity value should be removed from the spectrum.

`MassSpectrum[index]`

Return the <DataPoint> object at index.

Ex:

```
var ms1 = new MassSpectrum();
ms1.initialize([123.321,456.654,789.987],[147.741, 258.852, 369.963]);
ms1.asText();
```

```
123.3210000000 147.7410000000
456.6540000000 258.8520000000
789.9870000000 369.9630000000
```

```
var dp0 = ms1[0];
dp0.key; // --> 123.321
dp0.val; // --> 147.741
```

```
ms1[0].key; // --> 123.321
ms1[0].val; // --> 147.741
```

`MassSpectrum.initialize(other)`

Initialize this `MassSpectrum` object with a <Trace> object

`other`: <Trace> object

Ex:

```
var t1 = new Trace;
t1.initialize([123.321,456.654,789.987],[147.741, 258.852, 369.963]);
t1.asText();
```

```
123.3210000000 147.7410000000
456.6540000000 258.8520000000
```

```
789.9870000000 369.9630000000
```

```
var ms1 = new MassSpectrum();
ms1.initialize(t1);
ms1.asText();
```

```
123.3210000000 147.7410000000
456.6540000000 258.8520000000
789.9870000000 369.9630000000
```

`MassSpectrum.initialize(other)`

Initialize this `MassSpectrum` object with a `<MassSpectrum>` object

other: `<MassSpectrum>` object

Ex:

```
var ms1 = new MassSpectrum();
ms1.initialize([123.321,456.654,789.987],[147.741, 258.852, 369.963]);
ms1.asText();
```

```
123.3210000000 147.7410000000
456.6540000000 258.8520000000
789.9870000000 369.9630000000
```

```
var ms2 = new MassSpectrum();
ms2.initialize(ms1);
ms2.asText();
```

```
123.3210000000 147.7410000000
456.6540000000 258.8520000000
789.9870000000 369.9630000000
```

`MassSpectrum.initialize(mzArray, iArray)`

Initialize this `MassSpectrum` object with two `<Array>` of numerical values

mzArray: `<Array>` object containing the m/z values of the spectrum

iArray: `<Array>` object containing the intensity values of the spectrum

Ex:

```
var ms1 = new MassSpectrum;

var mzArray = [123.321,456.654,789.987];
var iArray = [147.741, 258.852, 369.963];
```

```
ms1.initialize(mzArray, iArray);
```

```
ms1.asText(); // --> output is:
```

```
123.3210000000 147.7410000000
456.6540000000 258.8520000000
789.9870000000 369.9630000000
```

`MassSpectrum.initialize(mzArray, iArray, mzStart, mzEnd)`

Initialize this `MassSpectrum` object with two `<Array>` of numerical

values and two <Number> entities delimiting a range of acceptable m/z values.

mzArray: <Array> object containing the m/z values of the spectrum
 iArray: <Array> object containing the intensity values of the spectrum
 mzStart: m/z value used to filter the data points to be used for the initialization (the start of the acceptable m/z range)
 mzEnd: m/z value used to filter the data points to be crafted for the initialization (the end of the acceptable m/z range)

Ex:

```
var ms1 = new MassSpectrum;

var mzArray = [123.321,456.654,789.987];
var iArray = [147.741, 258.852, 369.963];

ms1.initialize(mzArray, iArray, 122.231, 789.986); // range: [122.231-789.986]

ms1.asText(); // --> output is:

123.3210000000 147.7410000000
456.6540000000 258.8520000000
```

MassSpectrum.mzArray()

Return a list of <Number> entities corresponding to all the m/z values of the spectrum

Ex:

```
var ms1 = new MassSpectrum;

var mzArray = [123.321,456.654,789.987];
var iArray = [147.741, 258.852, 369.963];

ms1.initialize(mzArray, iArray, 122.231, 789.986); // range: [122.231-789.986]

ms1.asText(); // --> output is:

123.3210000000 147.7410000000
456.6540000000 258.8520000000

ms1.mzArray; --> output is:
123.321,456.654
```

MassSpectrum.iArray()

Return a list of <Number> entities corresponding to all the intensity values of the spectrum

Ex:

```
var ms1 = new MassSpectrum;

var mzArray = [123.321,456.654,789.987];
var iArray = [147.741, 258.852, 369.963];

ms1.initialize(mzArray, iArray, 122.231, 789.986); // range: [122.231-789.986]

ms1.asText(); // --> output is:

123.3210000000 147.7410000000
```

```
456.6540000000 258.8520000000
```

```
ms1.iArray; --> output is:
147.741,258.852
```

`MassSpectrum.asText()`

Return the data points of the spectrum in `<String>` object. The format of the string is of the kind `<m/z>,<intensity>`, one data point per line.

Ex:

```
var ms1 = new MassSpectrum;

var mzArray = [123.321,456.654,789.987];
var iArray = [147.741, 258.852, 369.963];

ms1.initialize(mzArray, iArray, 122.231, 789.986); // range: [122.231-789.986]

ms1.asText(); // --> output is:

123.3210000000 147.7410000000
456.6540000000 258.8520000000
```

`MassSpectrum.tic()`

Return the total ion current calculated for this `MassSpectrum` object

Ex:

```
var ms1 = new MassSpectrum;
ms1.initialize([123.321, 456.654, 789.987], [147.741, 258.852, 369.963]);
ms1.asText();
ms1.tic(); // --> 776.556
```

`MassSpectrum.combine(dataPoint)`

Combine into this `MassSpectrum` object the `<DataPoint>` object

`dataPoint`: `<DataPoint>` object to combine into this `MassSpectrum`

Ex:

```
var ms1 = new MassSpectrum;
ms1.initialize([123.321, 456.654, 789.987], [147.741, 258.852,369.963]);
ms1.asText(); // --> output is:

123.3210000000 147.7410000000
456.6540000000 258.8520000000
789.9870000000 369.9630000000

ms1.tic(); // -> 776.556

var dp1 = new DataPoint(123.321, 456.654);
ms1.combine(dp1);
ms1.asText(); // --> output is:

123.3210000000 604.3950000000 // value incremented
456.6540000000 258.8520000000
789.9870000000 369.9630000000

dp1.key = 800;
```

```

dp1.val = 1000;
ms1.combine(dp1);
ms1.asText(); // --> output is:

123.3210000000 604.3950000000
456.6540000000 258.8520000000
789.9870000000 369.9630000000
800.0000000000 1000.0000000000 // creation of new data point

```

`MassSpectrum.combine(trace)`

Combine into this `MassSpectrum` object the `<Trace>` object

`trace`: `<Trace>` object to combine into this `MassSpectrum`

Ex:

```

var ms1 = new MassSpectrum;
ms1.initialize([123.321, 456.654, 789.987], [147.741, 258.852, 369.963]);
ms1.asText(); // --> output is:

123.3210000000 147.7410000000
456.6540000000 258.8520000000
789.9870000000 369.9630000000

ms1.tic(); // --> 776.556
var t1 = new Trace;
t1.initialize([123.321, 600.000, 789.987], [147.741, 300.000, 369.963]);
t1.asText(); // --> output is:

123.3210000000 147.7410000000
600.0000000000 300.0000000000
789.9870000000 369.9630000000

t1.valSum(); // --> 817.704
ms1.combine(t1);
ms1.asText(); // --> output is:

123.3210000000 295.4820000000
456.6540000000 258.8520000000
600.0000000000 300.0000000000
789.9870000000 739.9260000000

ms1.tic(); // --> 1594.26

```

`MassSpectrum.combine(massSpectrum)`

Combine into this `MassSpectrum` object the `<MassSpectrum>` object

`massSpectrum`: `<MassSpectrum>` object to combine into this `MassSpectrum`

Ex:

```

var ms1 = new MassSpectrum;
ms1.initialize([123.321, 456.654, 789.987], [147.741, 258.852, 369.963]);

ms1.asText(); // --> output is:

123.3210000000 147.7410000000
456.6540000000 258.8520000000

```



```

789.9870000000 369.9630000000

ms1.tic(); // --> 776.556

var ms2 = new MassSpectrum(ms1);
ms2.combine(1500, 1000);
ms2.asText(); // --> output is:

123.3210000000 147.7410000000
456.6540000000 258.8520000000
789.9870000000 369.9630000000
1500.0000000000 1000.0000000000

ms2.combine(ms1);
ms2.asText(); // --> output is:

123.3210000000 295.4820000000
456.6540000000 517.7040000000
789.9870000000 739.9260000000
1500.0000000000 1000.0000000000

ms2.tic(); // --> 2553.112

MassSpectrum.combine(mz, i)

Combine into this MassSpectrum object a data point in the form of
two <Number> values, m/z and intensity

Ex:
var ms1 = new MassSpectrum;
ms1.initialize([123.321, 456.654, 789.987], [147.741, 258.852, 369.963]);
ms1.asText(); // --> output is:

123.3210000000 147.7410000000
456.6540000000 258.8520000000
789.9870000000 369.9630000000

ms1.tic(); // --> 776.556
var mz1 = 123.321;
var i1 = 300.000
ms1.combine(mz1, i1);
ms1.asText(); // --> output is:

123.3210000000 447.7410000000 // value incremented
456.6540000000 258.8520000000
789.9870000000 369.9630000000

ms1.combine(800, 1000);
ms1.asText(); // --> output is:

123.3210000000 447.7410000000
456.6540000000 258.8520000000
789.9870000000 369.9630000000
800.0000000000 1000.0000000000 // new data point created

MassSpectrum.subtract(dataPoint)

Subtract from this MassSpectrum object the <DataPoint> object

dataPoint: <DataPoint> object to subtract from this MassSpectrum

```

```
MassSpectrum.subtract(trace)
```

Subtract from this MassSpectrum object the <Trace> object

trace: <Trace> object to subtract from this MassSpectrum

```
MassSpectrum.subtract(massSpectrum)
```

Subtract from this MassSpectrum object the <MassSpectrum> object

massSpectrum: <MassSpectrum> object to subtract from this MassSpectrum

Ex:

```
var ms1 = new MassSpectrum;
ms1.initialize([123.321, 456.654, 789.987], [147.741, 258.852, 369.963]);
ms1.asText(); // --> output is:
123.3210000000 147.7410000000
456.6540000000 258.8520000000
789.9870000000 369.9630000000
```

```
var ms2 = new MassSpectrum(ms1);
ms2.subtract(ms1);
ms2.asText(); // --> output is:
```

```
123.3210000000 0.0000000000
456.6540000000 0.0000000000
789.9870000000 0.0000000000
```

```
MassSpectrum.subtract(mz, i)
```

Subtract from this MassSpectrum object a data point in the form of two <Number> values, m/z and intensity

Ex:

```
var ms1 = new MassSpectrum;
ms1.initialize([123.321, 456.654, 789.987], [147.741, 258.852, 369.963]);
ms1.asText(); // --> output is:
```

```
123.3210000000 147.7410000000
456.6540000000 258.8520000000
789.9870000000 369.9630000000
```

```
ms1.subtract(123.321,100);
ms1.asText(); // --> output is:
```

```
123.3210000000 47.7410000000
456.6540000000 258.8520000000
789.9870000000 369.9630000000
```

```
SavGolFilter
```

```
SavGolFilter()
```

Constructor of a SavGolFilter object

```
SavGolFilter(savGolParams)
```

Constructor of a SavGolFilter object initialized using a <SavGolParams> object

savGolParams: <SavGolParams> object to be used to initialize this object's SavGolParams

SavGolFilter(nL, nR, m, lD, convolveWithNr)

Constructor of a SavGolFilter object initialized using parameters that initialize the SavGolParams member object

nL: number of data points on the left of the point being filtered

nR: number of data points on the right of the point being filtered

m: order of the polynomial to use in the regression analysis leading to the Savitzky-Golay coefficients (typicall [2-6])

lD: order of the derivative to extract from the Savitzky-Golay smoothing algorithm (for regular smoothing, use 0);

convolveWithNr: set to false for best results

SavGolFilter(savGolFilter)

Constructor of a SavGolFilter object

savGolFilter: <SavGolFilter> object to be used to initialize this object

SavGolFilter.initialize(other)

Initialize this SavGolFilter object with another <SavGolFilter> object

other: <SavGolFilter> object used to initialize this object

SavGolFilter.initialize(nL, nR, m, lD, convolveWithNr)

Initialize this SavGolFilter object with parameters to configure the SavGolParams member object

nL: number of data points on the left of the point being filtered

nR: number of data points on the right of the point being filtered

m: order of the polynomial to use in the regression analysis leading to the Savitzky-Golay coefficients (typicall [2-6])

lD: order of the derivative to extract from the Savitzky-Golay smoothing algorithm (for regular smoothing, use 0);

convolveWithNr: set to false for best results

SavGolFilter.asText()

Return a <String> object containing a textual representation of all the member data of this SavGolFilter object.

MzIntegrationParams

The `MzIntegrationParams` class provides an interface to all the parameters that are required to configure all the integrations of mass spectral data that combine into a `MassSpectrum` object.

When combining multiple mass spectra into a single one, the process might involve the creation of bins according to specific parameters measured on the whole set of the spectra to be combined into the combination spectrum. These parameters are configured using a `MzIntegrationParams` object. Its members are:

- `binningType`: <Number> type of the binning. The type of binning specifies if binning is arbitrary or data-based (refer to `msXpS::BinningType` for details). It might also specify that no binning is required.
- `binSize`: <Number> size of the bins. A typical bin size would be 0.005 for a high resolution mass spectrometer with unit m/z .
- `binSizeType`: <Number> type of the bin size. The bin size type specifies if the `binSize` value is to be considered a m/z value or a atomic mass unit value or a resolution value or a part-per-million value (refer to `msXpS::MassToleranceType` for details)
- `binSizeTypeString`: <String> type of the bin size. This member datum hold a textual representation of the `binSizeType` member datum, like "PPM" or "RES" or "AMU" or "MZ".
- `applyMzShift`: <Boolean> value that tells if the m/z shift correction should be applied.
- `removeZeroValDataPoints`: <Boolean> that tells if the 0-val m/z data points should be removed from the combination spectrum once all the source mass spectra have been effectively combined into the combination spectrum.
- `applySavGolFilter`: <Boolean> that tells if a Savitzky-Golay filtering is to be applied to the combination spectrum after all the source mass spectra have been combined to the combination spectrum.
- `savGolParams`: <SavGolParams> object holding the configuration of a Savitzky-Golay filtering process.

`MzIntegrationParams()`

Constructor of a `MzIntegrationParams` instance

`MzIntegrationParams(binningType, binSize, binSizeType, applyMzShift, removeZeroValDataPoints)`

Constructor of a `MzIntegrationParams` instance

`binningType`: <Number> type of the binning (refer to `msXpS::BinningType` for details)
`binSize`: <Number> size of the bins
`binSizeType`: <Number> type of the bin size (refer to `msXpS::MassToleranceType` for details)
`applyMzShift`: <Boolean> tells if the m/z shift correction should be applied
`removeZeroValDataPoints`: <Boolean> tells if the 0-val m/z data points should be removed

`MzIntegrationParams(mzIntegrationParams)`

Constructor of a `MzIntegrationParams` object

`mzIntegrationParams`: <MzIntegrationParams> to be used to initialize this object

`MzIntegrationParams(savGolParams)`

Constructor of a `MzIntegrationParams` object

`savGolParams`: `<SavGolParams>` object to be used to initialize this object's `SavGolParams`

`<MzintegrationParams>.binningType`

Return the binning type property as a `<Number>`.

`<MzintegrationParams>.binningTypeString`

Return the binning type property as a `<String>`.

`<MzIntegrationParams>.binSize`

Return the bin size `<Number>` property (size of the bins in the mass spectrum).

`<MzintegrationParams>.binSizeType`

Return the bin size type property as a `<Number>`.

`<MzintegrationParams>.binSizeTypeString`

Return the bin size type property as a `<String>`.

`<MzIntegrationParams>.applyMzShift`

Return the `<Boolean>` value telling if the `m/z` shift should be applied.

`<MzIntegrationParams>.removeZeroValDataPoints`

Return the `<Boolean>` value telling if the `<DataPoint>` objects having `m/z` keys of a 0-intensity value should be removed from the `<MassSpectrum>` object.

`<MzIntegrationParams>.applySavGolFilter`

Return the `<Boolean>` value telling if the Savitzky-Golay filter should be applied to the `<MassSpectrum>` object.

`<MzIntegrationParams>.savGolParams`

Return the `<SavGolParams>` object from this `<MzIntegrationParams>` object.

`MzIntegrationParams.initialize(other)`

Initialize this MzIntegrationParams object with a <SavGolParams> object

other: <SavGolParams> object

MzIntegrationParams.initialize(other)

Initialize this MzIntegrationParams object with a
<MzIntegrationParams> object

other: <MzIntegrationParams> object

MzIntegrationParams.initialize(nL, nR, m, lD, convolveWithNr)

Initialize this MzIntegrationParams object with the individual <SavGolParams> parameters

nL: number of data points on the left of the point being filtered

nR: number of data points on the right of the point being filtered

m: order of the polynomial to use in the regression analysis
leading to the Savitzky-Golay coefficients (typical [2-6])

lD: order of the derivative to extract from the Savitzky-Golay
smoothing algorithm (for regular smoothing, use 0);

convolveWithNr: set to false for best results

MzIntegrationParams.asText()

Return a <String> object containing a textual representation of all the
member data of this MzIntegrationParams object.

AbstractPlotWidget

This class is not exported to the JavaScript environment, but it serves as the base class for all the plot widget subclasses. Its methods are thus available to all the objects of the various subclasses, like MassSpecPlotWidget, DriftSpecPlotWidget, ColorMapPlotWidget and TicChromPlotWidget, collectively referred to as <PlotWidget> below.

When using objects of the various classes above, the object name will thus be, for example, ticChromPlotWidget0 or driftSpecPlotWidget1. These objects are made available to the scripting environment in the tree view on the left part of the scripting window. See the user manual for details.

<PlotWidget>.showHistory()

Shows a tooltip with the History of this plot widget.

<PlotWidget>.historyAsText()

Return a textual representation of the history of this plot widget.

<PlotWidget>.showHelpSummary()

Show a tooltip with a help string summarizing the various keyboard key combinations.

`<PlotWidget>.shouldDestroyPlotWidget()`

Start the destruction of this plot widget.

`<PlotWidget>.toggleMultiGraph()`

If the multi-graph plot corresponding to this plot widget is visible, make it invisible. And vice versa.

`<PlotWidget>.showMultiGraph()`

Make the multi-graph plot corresponding to this plot widget visible.

`<PlotWidget>.hideMultiGraph()`

Make the multi-graph plot corresponding to this plot widget invisible.

`<PlotWidget>.exportData()`

Open the data export configuration window. Exporting data allows exporting only a subset of the whole data set. It can only be performed if the original data were read from a SQLite3 database-formatted mass data file.

`<PlotWidget>.asXyText()`

Return a textual representation of \c this plot widget data.

Only the data range currently displayed is processed.

`<PlotWidget>.exportPlot()`

Open a file selection dialog window to select a file in which to export this plot widget's data.

Unlike the `exportData()` function, this function only exports the currently displayed graph data to a comma-separated value text file.

`<PlotWidget>.exportPlotToFile(fileName, rangeStart, rangeEnd)`

Export plot data to a text file as a simple plot. Limit the data range to export using the numerical parameters.

fileName: <String> holding the file name

rangeStart: <Number> holding the beginning of the range to be exported

rangeEnd <Number> holding the end of the range to be exported

`<PlotWidget>.savePlotToGraphicsFile()`

Open the graphics export configuration dialog window.

```
<PlotWidget>.saveToPdfFile(fileName, noCosmeticPen, width, height, pdfCreator, title)
```

Save this plot widget as a PDF file graphics.

```
fileName: <String> holding the file name
noCosmeticPen: <Boolean> that tells if pen optimizations should be performed
width: <Number> holding the size of the graphics file in pixels
height: <Number> holding the size of the graphics file in pixels
pdfCreator: <String> holding the name of the creator of the PDF file
title: <String> holding the title of the graphics file
```

```
<PlotWidget>.keys()
```

Return an <Array> of <Number> values representing the keys of the data plotted.

```
<PlotWidget>.values()
```

Return an <Array> of <Number> values representing the values of the data plotted.

```
<PlotWidget>.lastTicIntensity()
```

Return the last TIC intensity value that was computed.

```
<PlotWidget>.trace()
```

Return a Trace object initialized with the data in this plot widget.

```
<PlotWidget>.replotWithAxisRangeX(lower, upper)
```

Replot this plot widget with new key (X-axis) data range.

```
lower: <Number> holding the start value of the range
upper: <Number> holding the end value of the range
```

```
<PlotWidget>.replotWithAxisRangeY(lower, upper)
```

Replot this plot widget with new value (Y-axis) data range.

```
lower: <Number> holding the start value of the range
upper: <Number> holding the end value of the range
```

```
<PlotWidget>.getYatX(x)
```

get the value at key x.

```
x: <Number> holding the X-axis key for which the value is returned.
```

ColorMapPlotWidget

This class cannot be instantiated with the new operator. Objects of this class are made available to the scripting environment under the form of object variable names `colorMapPlotWidget[index]`, with `[index]` being 0 for the first object created and being incremented each time a new

ColorMapPlotWidget is created.

ColorMapPlotWidget.integrateToRt(dtRangeStart, dtRangeEnd, mzRangeStart, mzRangeEnd)

Starts an integration of mass spectra data to a XIC chromatogram limiting the data ranges specified with the numerical arguments.

dtRange(Start | End) drift time range values

mzRange(Start | End) m/z range values

This function creates a new plot widget to display the obtained results.

ColorMapPlotWidget.integrateToMz(dtRangeStart, dtRangeEnd, mzRangeStart, mzRangeEnd)

Starts an integration of mass spectra data to a mass spectrum limiting the data ranges specified with the numerical arguments.

dtRange(Start | End) drift time range values

mzRange(Start | End) m/z range values

This function creates a new plot widget to display the obtained results.

ColorMapPlotWidget.integrateToDt(dtRangeStart, dtRangeEnd, mzRangeStart, mzRangeEnd)

Starts an integration of mass spectra data to a drift spectrum limiting the data ranges specified with the numerical arguments.

dtRange(Start | End) drift time range values

mzRange(Start | End) m/z range values

This function creates a new plot widget to display the obtained results.

ColorMapPlotWidget.integrateToTicIntensity(dtRangeStart, dtRangeEnd, mzRangeStart, mzRangeEnd)

Starts an integration of mass spectra data to a TIC intensity single value limiting the data ranges specified with the numerical arguments.

dtRange(Start | End) drift time range values

mzRange(Start | End) m/z range values

The TIC intensity value is returned

ColorMapPlotWidget.transposeAxes()

Transpose the axes of this color map plot widget

ColorMapPlotWidget.jsSetMzIntegrationParams(mzIntegrationParams)

Set the MzIntegrationParams object passed as parameter to this color map plot widget.

These parameters are taken into account for the integrations to a mass spectrum.

ColorMapPlotWidget.jsMzIntegrationParams()

Return the `MzIntegrationParams` object currently set for this color map plot widget.

These parameters are taken into account for the integrations to a mass spectrum.

`TicChromPlotWidget`

This class cannot be instantiated with the `new` operator. Objects of this class are made available to the scripting environment under the form of object variable names `ticChromPlotWidget[index]`, with `[index]` being 0 for the first object created and being incremented each time a new `TicChromPlotWidget` is created.

`TicChromPlotWidget.integrateToMz(lower, upper)`

Starts an integration of mass spectra data to a mass spectrum limiting the data range specified with the numerical arguments.

`lower, upper`: retention time values limiting the integration. If no values are provided, there is no limitation to the integration.

This function creates a new plot widget to display the obtained results.

`TicChromPlotWidget.integrateToDt(lower, upper)`

Starts an integration of mass spectra data to a drift spectrum limiting the data range specified with the numerical arguments.

`lower, upper`: retention time values limiting the integration. If no values are provided, there is no limitation to the integration.

This function creates a new plot widget to display the obtained results.

`TicChromPlotWidget.integrateToTicIntensity(lower, upper)`

Starts an integration of mass spectra data to a TIC intensity single value limiting the data range specified with the numerical arguments.

`lower, upper`: retention time values limiting the integration. If no values are provided, there is no limitation to the integration.

The TIC intensity value is returned

`TicChromPlotWidget.newPlot(trace)`

Create a new `TicChromPlotWidget` using `<Trace>` trace for the initialization of the data.

This function creates a new plot widget to display the `<Trace>` data.

`MassSpecPlotWidget`

This class cannot be instantiated with the `new` operator. Objects of this class are made available to the scripting environment under the form of object variable names `massSpecPlotWidget[index]`, with `[index]` being 0 for the first object created and being incremented each time a new

MassSpecPlotWidget is created.

`MassSpecPlotWidget.integrateToDt(lower, upper)`

Starts an integration of mass spectra data to a drift spectrum limiting the data range specified with the numerical arguments.

lower, upper: retention time values limiting the integration. If no values are provided, there is no limitation to the integration.

This function creates a new plot widget to display the obtained results.

`MassSpecPlotWidget.integrateToRt(lower, upper)`

Starts an integration of mass spectra data to a XIC chromatogram limiting the data range specified with the numerical arguments.

lower, upper: retention time values limiting the integration. If no values are provided, there is no limitation to the integration.

This function creates a new plot widget to display the obtained results.

`MassSpecPlotWidget.integrateToTicIntensity(lower, upper)`

Starts an integration of mass spectra data to a TIC intensity single value limiting the data range specified with the numerical arguments.

lower, upper: retention time values limiting the integration. If no values are provided, there is no limitation to the integration.

The TIC intensity value is returned

`MassSpecPlotWidget.newPlot(trace)`

Create a new MassSpecPlotWidget using <Trace> trace for the initialization of the data.

This function creates a new plot widget to display the <Trace> data.

DriftSpecPlotWidget

This class cannot be instantiated with the new operator. Objects of this class are made available to the scripting environment under the form of object variable names `driftSpecPlotWidget[index]`, with [index] being 0 for the first object created and being incremented each time a new DriftSpecPlotWidget is created.

`DriftSpecPlotWidget.integrateToMz(lower, upper)`

Starts an integration of mass spectra data to a mass spectrum limiting the data range specified with the numerical arguments.

lower, upper: retention time values limiting the integration. If no values are provided, there is no limitation to the integration.

This function creates a new plot widget to display the obtained results.

```
DriftSpecPlotWidget.integrateToRt(lower, upper)
```

Starts an integration of mass spectra data to a XIC chromatogram limiting the data range specified with the numerical arguments.

lower, upper: retention time values limiting the integration. If no values are provided, there is no limitation to the integration.

This function creates a new plot widget to display the obtained results.

```
DriftSpecPlotWidget.integrateToTicIntensity(lower, upper)
```

Starts an integration of mass spectra data to a TIC intensity single value limiting the data range specified with the numerical arguments.

lower, upper: retention time values limiting the integration. If no values are provided, there is no limitation to the integration.

The TIC intensity value is returned

```
DriftSpecPlotWidget.newPlot(trace)
```

Create a new DriftSpecPlotWidget using <Trace> trace for the initialization of the data.

This function creates a new plot widget to display the <Trace> data.

MainWindow

This is the main mineXpert program window. It is not instantiable through the JavaScript environment. Some functionalities are available to allow highlevel tasks to be automated. The MainWindow single instance of the minexpert software program is made available to the JavaScript environment under the object name mainWinwod, with an alias mainWnd.

```
MainWindow.quit()
```

Quit the application.

```
MainWindow.clearPlots()
```

Clear all plots and give back all memory associated to the mass data.

```
MainWindow.createMassSpectrumFromClipboard()
```

Create a new mass spectrum from data in the clipboard. The data in the clipboard need to be under the format of <number><separator><number>, <separator> being any non-numerical and non-'.' character. The first <number> is the m/z and the second <number> is the intensity.

Upon completing the parsing of the textual data in the clipboard, a pseudo TIC chromatogram is created that needs to be integrated to a mass spectrum using:

```
lastTicChromPlotWidget.integrateToMz();
```

Ex:
`mainWindow.createMassSpectrumFromClipboard();`
`lastTicChromPlotWidget.integrateToMz();`

`MainWindow.openMassSpectrometryFile(fileName, streamed)`

Load mass spectrometry data from fileName.

fileName: <String> holding the mass spectrometry data file name
 streamed: <Boolean> telling if the loading should be in streamed mode.

Ex:
`mainWindow.openMassSpectrometryFile("/tmp/20161027-cgb-wt-mobility.db", true);`

reads the data in the file in streamed mode.

`mainWindow.openMassSpectrometryFile("/tmp/20161027-cgb-wt-mobility.db", false);`

reads the data in the file in full mode.

`MainWindow.openMassSpectrometryFiles(fileNameList, streamed)`

Load mass spectrometry data from all the files in the fileNameList.

fileNameList: <Array> of <String> objects holding the mass spectrometry data file names
 streamed: <Boolean> telling if the loading should be in streamed mode.

`MainWindow.about()`

Open an About dialog window.

Ex:
`mainWindow.about();`

SqlMassDataSlicerWnd

This class cannot be instantiated with the new operator. The only object of this class that is published to the scripting environment is named 'sqlMassDataSlicerWnd'.

This class can only be used safely if it is first activated by using the `exportData()` function of the <PlotWidget> classes (see <PlotWidget>). Indeed, the `<PlotWidget>.exportData()` activates this `sqlMassDataSlicerWnd` object and initializes it with the current data range displayed in the widget.

The following describes the various methods that can be used to automate fully the slicing of very large mass spectrometry data files in a set of smaller files. There are three ways to create new files of a reduced size with respect to the initial mass data file:

- export data from the original file in a single file but with a smaller set of data. For example, export only part of a TIC chromatogram or export only the mass data corresponding to a given drift time range.
- export data from the original file in multiple smaller files (either the whole initial data range or a smaller range). Two possibilities are offered:

- define the number of slices (their size is dynamically computed);
- define the size of the slices (their number is dynamically computed);

This window is available for any <PlotWidget> displaying TIC/XIC chromatogram data or drift spectrum data. It is therefore essential to start a data export process from that specific plot widget of interest by calling <PlotWidget>.exportData(). This call will initialize all the widget-specific data into this data export configuration window.

Ex:

```
mainWnd.openMassSpectrometryFile("/path/to/file/20161027-cgb-wt-mobility.db", false);
// The TIC chromatogram window displays the TIC chromatogram in ticChromPlotWidget0

// Activate and initialize the SqlMassDataSlicerWnd (its object name is sqlMassDataSlicerWnd)
ticChromPlotWidget0.exportData();

// Set the number of slices to 2
sqlMassDataSlicerWnd.setSliceCount(2);

// Set the start of the range of interest (retention time)
sqlMassDataSlicerWnd.rangeStart(0.2);

// Set the end of the range of interest (retention time)
sqlMassDataSlicerWnd.rangeEnd(12.7);

// Set the format string to use to craft the file names
sqlMassDataSlicerWnd.setFormatString("%f-export-slice-%n-of-%c-range_%s-%e.db");

// Validate the configuration settings (crafts the file names according to
the configuration of the data export and according to the format string)

sqlMassDataSlicerWnd.validate(false);

// Take a peek at the various file names that have been crafted.
sqlMassDataSlicerWnd.reviewFileNames();

// If the file names have no error, then start the data export process.
sqlMassDataSlicerWnd.confirm();
```

Note that the calls to validate() and reviewFileNames() and confirm() can be shortened to a single call to run() if it is expected that no error will occur upon validation of the data export parameters (typically when the script has been thoroughly tested). In that case, the script runs perfectly unattended.

```
sqlMassDataSlicerWnd.setSrcFileName(fileName)
```

Set the source SQLite3 db mass data file name. Only use this function if you know the range of the data you are willing to export. Usually this function is not used, because when starting the data export process using the <PlotWidget>.exportData() function, that source file name is set automatically. Thus we recommend you use this function only if you know what you are doing.

fileName : <String> that holds the name of the source mass spectrometry data file in the SQLite3 database format.

```
sqlMassDataSlicerWnd.setDestDirectory(dir)
```

Set the directory (create it if it does not exist) where all the slice

files are to be written to. If this function is not called before calling the `validate()` or `run()` functions, the destination directory will be the directory where the source file is residing.

`dir`: <String> holding the name of the directory in which to write all the slice files.

`sqlMassDataSlicerWnd.setFormatString(format)`

Set the string that configures the naming of the slice files. The following format specification is available:

%f: original filename without <.extension>
 %s: slice range start value
 %e: slice range end value
 %n: slice number
 %c: total count of slices

For example, if the original (source) filename were "my-mass-data.db" and the format string were "%f-export-slice-%n-of-%c-range_%s-%e.db", the first file would be named
 "my-mass-data-export-slice-1-of-7-range_17-28.db"
 the second file
 "my-mass-data-export-slice-2-of-7-range_29-40.db"
 and so on for another 5 files since the total count of slices is 7.

`sqlMassDataSlicerWnd.setRangeStart(start)`

Set the start value of the data range to be exported. For example, if the data export process was started in a TIC chromatogram plot widget, and the whole acquisition run spanned [0-35] minutes, then the user might want to only export a fraction of that span: [17-28]. In that case, the range start value would be 17.

`start`: <Number> setting the start value of the range to be exported.

`sqlMassDataSlicerWnd.rangeStart()`

Return the start value of the data range to be exported. For example, if the data export process was started in a TIC chromatogram plot widget, and the whole acquisition run spanned [0-35] minutes, then the user might want to only export a fraction of that span: [17-28]. In that case, the range start value would be 17.

`sqlMassDataSlicerWnd.setRangeEnd(end)`

Set the end value of the data range to be exported. For example, if the data export process was started in a TIC chromatogram plot widget, and the whole acquisition run spanned [0-35] minutes, then the user might want to only export a fraction of that span: [17-28]. In that case, the range end value would be 28.

`end`: <Number> setting the end value of the range to be exported.

`sqlMassDataSlicerWnd.rangeEnd()`

Return the end value of the data range to be exported. For example, if the

data export process was started in a TIC chromatogram plot widget, and the whole acquisition run spanned [0-35] minutes, then the user might want to only export a fraction of that span: [17-28]. In that case, the range end value would be 28.

```
sqlMassDataSlicerWnd.setRange(start, end)
```

Set the data range to be exported. For example, if the data export process was started in a TIC chromatogram plot widget, and the whole acquisition run spanned [0-35] minutes, then the user might want to only export a fraction of that span: [17-28]. In that case, the range start and end values would be 17 and 28 respectively.

start: <Number> setting the start value of the range to be exported.
end: <Number> setting the end value of the range to be exported.

```
sqlMassDataSlicerWnd.setSliceCount(count)
```

Set the number of slices to be created out of the initial data set.

count: <Number> indicating the number of slices.

```
sqlMassDataSlicerWnd.setSliceSize(size)
```

Set the size of the slices to be created out of the initial data set.

size: <Number> indicating the size of the slices.

```
sqlMassDataSlicerWnd.setExportToOneFile()
```

Tells that the initial mass data set must be exported into a single file. Any [rangeStart-rangeEnd] export range that might have been set is taken into account. Not limiting the range of the exported data makes the data export operation equivalent to copying the file into another file virtually identical to the initial one.

```
sqlMassDataSlicerWnd.fileNames()
```

Print the names of the files that will be written during the data export process. For the list of file names to be created and be available, first set the various data export options (format string, number or size of slices...) and call `sqlMassDataSlicerWnd.validate()`.

```
sqlMassDataSlicerWnd.reviewFileNames()
```

Print the names of the files that will be written during the data export process. For the list of file names to be created and available, first set the various data export options (format string, number or size of slices...) and call `sqlMassDataSlicerWnd.validate()`. In this function, the graphical user interface is modified to allow the user to review the file names and makes available a push button to start the export process.

```
sqlMassDataSlicerWnd.validate(noconfirm)
```

Verify the configuration settings for the data export operation. Upon this

validation, the file names of the files that will be written during the data export are crafted according to the file format string (see `setFormatString()`). This function needs to be called prior to calling `reviewFileNames()` or `fileNames()`. After reviewing the file names, a call to the function `confirm()` starts the data export process.

`noconfirm`: <Boolean> value telling if the data export process can proceed automatically. If true, no call to `confirm()` needs to be done for the data export to start immediately if there is no error during the validation step.

`sqlMassDataSlicerWnd.confirm()`

Confirm that the data export process can start. This function must be called after the validation has been performed (see `validate()`) and the user has checked that the file names have been correctly crafted upon validation according to the format string.

`sqlMassDataSlicerWnd.run()`

After having set the range, the number (or size) of the slices, let the program compute the size (or number, respectively) of the slices and run the data export. This function calls `validate()` with `noconfirm` set to True (see `validate()`). This way, if no error is encountered during the validation, then the data export process is started right way, which is expected for a script to run unattended.

6

Appendices

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Version 3, 29 June 2007

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