mMass 3.9 User's Guide

written by **Martin Strohalm**

Contents

1. Preface

1.1. Motivation

While tools for the automated analysis of MS and LC-MS/ MS data are continuously improving, it is still often the case that at the end of an experiment, the mass spectrometrists will spend time carefully examining individual spectra. Current software support is mostly provided only by the instrument vendors, and the available software tools are often instrument-dependent. Such software can only be used to analyze data from a specific instrument, and this causes serious problems for laboratories that use more than one instrument. This tight software-instrument relationship also causes problems for laboratories that do not possess their own instruments, and have to obtain mass spectra from other, collaborating, laboratories. To provide a solution to these limitations I have started to develop *mMass* - open source multi-platform tool for precise mass spectrometric data analysis and interpretation.

1.2. Authors

mMass is the fruit of years of study and development. While I've put a lot of energy into making this program as stable and reliable as possible, *mMass* comes with no warranty of any kind. You are however welcome to read the code, modify it and send me any suggestions or patches. *mMass* development still continues, so any ideas, function requests or bug reports are more than welcome. Feel free to contact me through the *mMass's* web page http://www.mmass.org or join the forum at http://forum.mmass.org.

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http://www.mmass.org

I wish to express my thanks to all the people involved in the excellent *Python* language, *wxPython* and *NumPy* libraries, and namely to the people helping me to make *mMass* still better:

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Institute of Microbiology, Prague
Academy of Sciences of the Czech Republic
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Sebastian Gibb: OpenSUSE packages
Universität Leipzig, Germany

Filippo Rusconi, PhD: Debian packages
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Petr Man, PhD:
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Petr Pompach, PhD: Mass spectrometry consultations
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1.3. Publications to Cite

- Strohalm M, Kavan D, Novák P, Volný M, Havlíček V: mMass 3: A Cross-Platform Software Environment for Precise Analysis of Mass Spectrometric Data. *Anal Chem* **82** (11), 4648-51 (2010). DOI:10.1021/ac100818g

- Strohalm M, Hassman M, Košata B, Kodíček M: mMass data miner: an open source alternative for mass spectrometric data analysis. *Rapid Commun Mass Spec* **22** (6), 905-908 (2008). DOI:10.1002/rcm.3444

1.4. Technicalities

At the very beginning *mMass* started as a simple *PHP*-based tool to compare peak differences within mass spectrum. Fortunately, *PHP* wasn't powerful enough for calculations and I stated to learn *Python*...

Current version of *mMass* is written completely in *Python* programing language (http://www.python.org) and uses *wxPython* libraries (http://www.wxpython.org) for graphical user interface (GUI). In addition, *NumPy* module (http://www.numpy.org) is used for faster computing of mathematical tasks.

Since resolution of modern mass spectrometers grows up, resulting data sets become very large. Even *Python* is not powerful enough for some calculations, therefore a piece of code written in *C* has been added into *mMass* to speed-up a spectrum drawing.

1.5. Typographical Conventions

Following typographical conventions are used throughout this document:

Names of mMass's components and modules, names of dialog values etc.

Menu items and buttons.

```
Terminal commands, scripts and other pieces of code.
```

Advanced tips and hints.

Important notes and warnings.

2. Version History

Version 3.9.0 (released Dec 15, 2010)

- **New:** *Compare Peak Lists* tool to compare peak lists between multiple documents.
- **New:** Simple math functions are now available to add, subtract and multiply spectra.
- **New:** Peptides, fragments or compounds lists can be filtered to show matched/unmatched items only.
- **New:** Sequences from digest list, fragments list or peptide search list can be copied into clipboard.
- **New:** Duplicate copy of selected document can be make via pop-up menu in *Documents Panel*.
- **New:** Distance measurement tool shows current distance in both *m/z* and *ppm* (in bottom bar only).
- **Improved:** Multiple documents can be opened at once using Open dialog.
- **Fixed:** Correct drawing of spectra with no continuous baseline (typically for SIM experiments).
- **Fixed:** FWHM and resolution columns in a peak list can now be copied into clipboard as well.
- **Fixed:** Option to enable/disable notation marks now works correctly.

Version 3.8.0 (released Aug 20, 2010)

- **New:** TIC and BPC chromatograms are now available in scan selection dialog.
- **New:** Support for *mzML* data format.
- **New:** Spectrum intensity offset (visual only) can now be set either manually or using new mouse tool.
- **New:** Intensity bar is now available in *Spectrum Panel*.
- **New:** Height of position bar and intensity bar can now be set in *Canvas Properties*.
- **New:** New view option to show/hide spectrum data points.
- **Improved:** Peak width is assigned automatically when overlaying theoretical isotopic patterns.
- **Fixed:** Incorrect charge calculation in *Deisotoping* module.
- **Fixed:** Incorrect file extension for files converted by *CompassXport*.

Version 3.7.0 (released Jul 19, 2010)

- **New:** Simplified interface for *Protein Prospector* tools *MS-Fit* and *MS-Tag*.
- **New:** FWHM and resolution is now calculated for each peak and shown in *Peaklist Panel*.
- **New:** Global modifications can now be stored as presets.
- **New:** Spectrum polarity can now be set in *Document Info* panel.
- **Fixed:** Application crashed when "None" document was sent into *Calibration Panel*.
- **Fixed:** Some of the potential peaks were skipped in *Shoulder Peaks Removal* algorithm.
- **Fixed:** Data matching for negative spectra was not possible with *Ignore charge* option unchecked.

Version 3.6.0 (released Jul 5, 2010)

- **New:** *Match Summary* is now available for each data matching.
- **New:** *Remove shoulder peaks* option is now available for FTMS data peak-picking.
- **New:** All annotations and sequence matches can now be removed at once from *Document panel*.
- **New:** Compounds and calibration masses can now be imported using corresponding library editor.
- **Improved:** Faster peak-picking, especially when *Adaptive threshold* option is used.
- **Improved:** Spectrum flipping is now accessible from the *View* menu.
- **Fixed:** Loading of some *mzXML* files with parameter *"compressionType=none"* was not possible.
- **Fixed:** Application crashed on a single right-click in *Isotopic pattern* panel.

Version 3.5.0 (released Jun 4, 2010)

- **New:** Possibility to vertically flip spectra in *Spectrum Viewer*.
- **New:** -H_2O can now be searched in *Compounds Search* tool.
- **Fixed:** Normalized view did not worked for non-profile spectra.

Version 3.4.0 (released May 12, 2010)

- **New:** Radical ions can now be calculated in *Mass Calculator* and *Compounds Search* tools.

- **New:** Single-point linear calibration has been enabled.
- **New:** Calibration curve is now shown in the calibration error plot.
- **New:** Current peak list is now shown as a background in error plots (calibration, data matching).
- **New:** New view option to enable/disable normalized view of opened documents.
- **New:** New view option to enable/disable notation marks.
- **New:** All annotations and matches can now be highlighted by selecting a document root.
- **New:** Theoretical and matched sequence coverage is now shown in *Protein Digest* tool.
- **New:** Final composition of ion is validated in ion series calculations.
- **New:** Automatic checking for available updates has been added.
- **New:** Application preferences for updates and *compassXport* utility has been added.
- **Fixed:** *Mass Calculator* - calculation of ions with negative agent charge.
- **Fixed:** *Mass Calculator* - pattern modeling with complex charging agent.
- **Fixed:** Normalization now includes baseline shift.

Version 3.3.0 (released Apr 9, 2010)

- **New:** *Periodic Table* of the elements has been added.
- **New:** Bruker's raw data are imported using *CompassXport* tool (MSW only).
- **Fixed:** Small fixes in manual peak picking.
- **Fixed:** Dragging documents to *mMass* caused the source window to freeze until data were not loaded.
- **Fixed:** *Mass Search* tool - Enzyme endings selection did not worked.
- **Fixed:** *Mass Search* tool - *Max charge* has been replaced by *Charge.*
- **Improved:** *Mass Search* tool - better filtering.

Version 3.2.0 (released Mar 14, 2010)

- **New:** *Isotopic Pattern* panel is now collapsable.
- **New:** Hidden modifications can now be enabled in *Mascot Search* interface.
- **New:** Modified documents are marked by asterisk.
- **Improved:** Relative intensity for annotations and matches is now calculated on-the-fly.

Version 3.1.0 (released Mar 3, 2010)

- **New:** Lipid database (by *LIPID MAPS Consortium*) has been added to *Compounds Search* tool.
- **New:** *ProFound Search* interface has been implemented.
- **New:** Sequences can now be imported form *mMass's* and *FASTA* files.
- **New:** Manually labeled peak can now be automatically set as monoisotopic.
- **New:** Specific cursor images for spectrum tools has been added.
- **New:** Scan list buffer is now used to speed-up loading of multi-scan documents.
- **Fixed:** Multiple fixes in *Mascot Search* interface.
- **Improved:** Peak-picking algorithm has been improved.
- **Improved:** More "Pythonic" syntax in the *mspy* module.
- **Improved:** Spectrum tools are now accessible from the main menu as well.

Version 3.0.0 (released Feb 1, 2010)

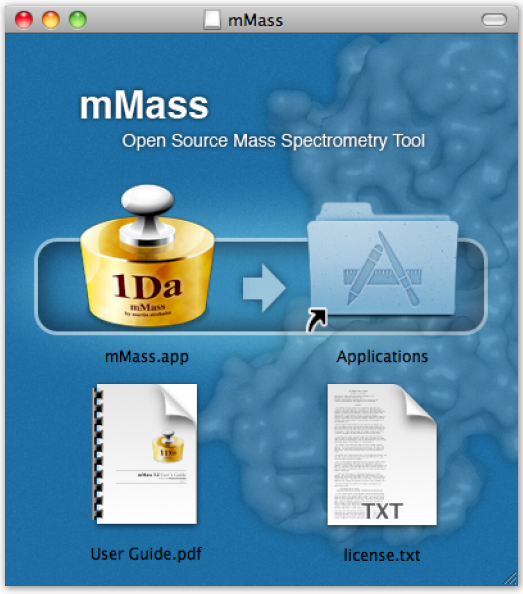
- Complete *mMass* redesign - new user interface, new features and new source code architecture.

3. License

4. Installation

4.1. Mac OS X

As usually, there is no special installation procedure for Mac OS X. *mMass* is available as a regular disk image containing the *"mMass.app"* application. This is a standalone package containing all the necessary modules and libraries. To install *mMass* just open the disk image and drag the *mMass.app* to your application folder. After first run *mMass* creates the specific folder *"~/Library/Application Support/mMass/"* to store all your presets and objects libraries. Current version of *mMass* was successfully tested on the Intel based computers with Mac OS X 10.5 and 10.6.



mMass's installation disk image for Mac OS X.

4.2. MS Windows

In most cases, installation on MS Windows is very easy. *mMass* is available as regular ZIP archive containing the *"mMass"* application folder. There are no installation steps needed to run *mMass* under MS Windows. This means that you can run the program directly after unpacking downloaded archive. Simply run the *"mmass.exe"*. Current version of *mMass* was successfully tested on XP SP3, Vista and Windows7.

⚠ *Please note that you must have the privileges for writing to the "mMass" folder, otherwise you will not be able to store any program presets such as startup defaults, modifications etc..*

⚠ *Do not try to associate any file type with mMass on MS Windows since it does not work properly. Instead of adding document to the running instance of mMass, every document will be opened within a new instance of the program.*

For older versions of MS Windows, *mMass* sometimes doesn't want to start up showing the following message instead: ***The application failed to start because the application configuration is incorrect. Reinstalling the application may fix this problem.*** In such a case you'll need to download and install the runtime components of Visual C++ Libraries from Microsoft's website.

http://www.microsoft.com/downloads/details.aspx?familyid=9B2DA534-3E03-4391-8A4D-074B9F2BC1BF&displaylang=en

4.3. Linux

I have to say that I'm not very familiar with Linux platform and therefore there is no special build of *mMass* available for Linux. Nevertheless, I am always testing and debugging *mMass* on my virtual version of *Debian* distribution to make it work properly and to retain application native look. If you want to run *mMass* on Linux see the following chapter to run it from the source code.

4.4. Running from Source

mMass belongs to the wide family of open source software so why not to modify it? All you need to do is download and unpack the *mMass's* source ZIP archive and then do what you can. There are some additional modules and libraries needed to run *mMass*, however, all of them are available for free and easy to install.

Dependencies

Python (http://www.python.org) *"Python is a programming language that lets you work more quickly and integrate your systems more effectively. You can learn to use Python and see almost immediate gains in productivity and lower maintenance costs."*

wxPython (http://www.wxpython.org) *"wxPython is a GUI toolkit for the Python programming language. It allows Python programmers to create programs with a robust, highly functional graphical user interface, simply and easily. It is implemented as a Python extension module (native code) that wraps the popular wxWidgets cross platform GUI library, which is written in C++."*

NumPy (http://www.numpy.org) *"NumPy is the fundamental package needed for scientific computing with Python. It contains among other things: a powerful N-dimensional array object, sophisticated (broadcasting) functions, tools for integrating C/C++ and Fortran code, useful linear algebra, Fourier transform, and random number capabilities."*

⚠ *Please note that current version of mMass was developed and tested using Python 2.6, wxPython 2.8.10.1 and NumPy 1.4. I cannot guarantee that mMass will work with different version of particular libraries.*

Compiling C-code

In addition to installing all of the above libraries and modules you'll need to compile a piece of *C* code used to speed up spectrum drawing. It can be done very easily with the *"setup.py"* script located in *"mspy/plot/"* folder.

On Mac OS X go to the *"mspy/plot/"* folder and run compilation command in *Terminal*, then locate resulted *"calculations.so"* file in the build folder and move it to *"mspy/plot/"*. The compilation command should be like:

```
python setup.py build
```

On MS Windows go to the *"mspy/plot/"* folder and run compilation command in *Command Prompt*, then locate resulted *"calculations.pyd"* file in the build folder and move it to *"mspy/plot/"*. If you are using *MinGW* (http://www.mingw.org) the compilation command should be like:

```
python setup.py build --compiler=mingw32
```

On Linux go to the *"mspy/plot/"* folder and run compilation command in *Terminal*, then locate resulted *"calculations.so"* file in the build folder and move it to *"mspy/plot/"*. The compilation command should be like this:

```
python setup.py build
```

Running Application

To start up *mMass* go to *mMass's* main folder and simply run the following command:

```
python mmass.py
```

Making Application Bundle

If you want to make your own application bundle for Mac OS X or MS Windows you need to have *py2app* (http://pypi.python.org/pypi/py2app) or *py2exe* (http://pypi.python.org/pypi/py2exe) respectively. After installing the corresponding utility you can make the bundle simply by using *"setup.py"* script located in *mMass's* main folder. Just go to the folder and run the following command:

On Mac OS X

```
python setup.py py2app
```

On MS Windows

```
python setup.py py2exe
```

5. User Interface

5.1. Application Layout

Beside the standard elements, like toolbar etc., *mMass's* user interface is divided into three main parts: *Documents Panel, Spectrum Viewer* and *Peaklist Panel*. All the processing and analyzing modules and tools are available as floating panels to enable direct validation of results with acquired data.

mMass's user interface.

5.2. Main Menu

File

New - creates a blank document with no data.

Open - opens document.

Open Recent - opens one of the recent documents.

Close - closes selected document.

Close All - closes all opened documents.

Save - saves selected document into *mMass's* native format.

Save As - saves selected document as a new file.

Export - exports current spectrum image, spectrum points or peak list.

Print Spectrum - prints current spectrum view.

Analysis Report - generates analysis report for selected document.

Preferences - shows application preferences dialog. (Moved to mMass menu on Mac OS X.)

Document Info - shows document information panel for selected document.

View

Show/Hide Gridlines - shows or hides gridlines in spectrum viewer.

Show/Hide Legend - shows or hides legend in spectrum viewer.

Show/Hide Position Bar - shows or hides position bar in spectrum viewer.

Show/Hide Intensity Bar - shows or hides intensity bar in spectrum viewer.

Show/Hide Gel - shows or hides gel-view in spectrum viewer.

Show/Hide Gel Legend - shows or hides legend in gel-view.

Show/Hide Cursor Tracker - shows or hides cursor tracker in spectrum viewer.

Show/Hide Data Points - shows or hides spectrum data points on detailed zoom.

Show/Hide Labels - shows or hides peak labels in spectrum viewer.

Show/Hide Labels Ticks - shows or hides ticks for peak labels.

Show/Hide Labels Charge - shows or hides charge value for peak labels.

Show/Hide Labels Background - shows or hides a solid white background for peak labels.

Show/Hide Notation Marks - shows or hides marks for annotated or matched peaks.

Horizontal/Vertical Labels - shows peak labels horizontally or vertically.

Overlapping/Non-Overlapping Labels - enables or disables automatic managing of labels overlaps.

Labels in All Documents - shows or hides peak labels in all visible spectra.

Autoscale Intensity - enables or disables automatic scaling of intensity axis.

Normalize Intensity - enables or disables normalization of intensity axis for all spectra.

Flip Spectrum - flips selected spectrum vertically.

Offset Spectrum - specifies intensity offset for current spectrum.

Clear Offsets - clears intensity offsets for all spectra.

Canvas Properties - additional options for spectrum canvas (gel height, mass precision, font sizes etc.).

Processing

Undo - reverts back last operation. Most of the operations in *mMass* can be undone such as all processing functions or editing of labels, matches and annotations. One step back is currently available.

Peak Picking - automatically finds and labels peaks in selected document.

Deisotoping - automatically assigns charges and deletes isotopes in current peak list.

Correct Baseline - corrects baseline in selected spectrum.

Smooth Spectrum - smooths selected spectrum.

Crop - crops spectrum points and peak list in selected document.

Math Operations - add, subtract or multiply selected spectrum.

Calibration - calibrates data in selected document using internal, external or statistical calibration.

Normalize Data - normalizes data in selected document to 0 - 100% intensity range.

Swap Data - swaps data between spectrum and peak list in selected document.

Sequence

New - creates new sequence object in selected document.

Import - imports sequence object from a file into selected document.

Edit Sequence - shows sequence editor with selected sequence.

Edit Modifications - shows sequence modifications editor with selected sequence.

Digest Protein - generates digestion peptides from selected sequence.

Fragment Peptide - generates fragments from selected sequence.

Mass Search - searches for peptide corresponding to given m/z value within selected sequence.

Calibrate by Matches - uses current sequence matches as reference masses for data re-calibration.

Delete Matches - deletes all the matches for selected sequence.

Delete Sequence - deletes selected sequence object.

Sort By Titles - sorts all sequences in selected document by titles.

Tools

Label Peak - sets mouse tool to label peaks in selected spectrum.

Label Point - sets mouse tool to label exact points in selected spectrum.

Delete Label - sets mouse tool to delete labels in selected spectrum.

Measure Distances - sets mouse tool to measure distances between two peaks in a spectrum.

Offset Spectrum - sets mouse tool to offset spectrum intensity.

Periodic Table - shows periodic table of elements.

Mass Calculator - calculates ion series and isotopic pattern for specified molecular formula.

Compounds Search - searches for specified compounds and adducts within selected document.

Peak Differences - generates table of peak differences to searches for amino acids or any m/z difference.

Compare Peak Lists - compare multiple peak lists.

Mascot Peptide Mass Fingerprint - sends selected peak list to Mascot's Peptide Mass Fingerprint tool.

Mascot MS/MS Ion Search - sends selected peak list to Mascot's MS/MS Ion Search tool.

Mascot Sequence Query - sends selected peak list to Mascot's Sequence Query tool.

ProFound Search - sends selected peak list to ProFound Search tool.

Protein Prospector MS-Fit - sends selected peak list to Protein Prospector MS-Fit Search tool.

Protein Prospector MS-Tag - sends selected peak list to Protein Prospector MS-Tag Search tool.

Libraries

Modifications - shows modifications library editor.

Enzymes - shows shows enzymes library editor.

Compounds - shows compounds library editor.

Calibration Masses - shows calibration masses library editor.

Mascot Servers - shows Mascot servers library editor.

Presets - shows presets library editor.

Help

Homepage - opens *mMass's* website in a default web browser.

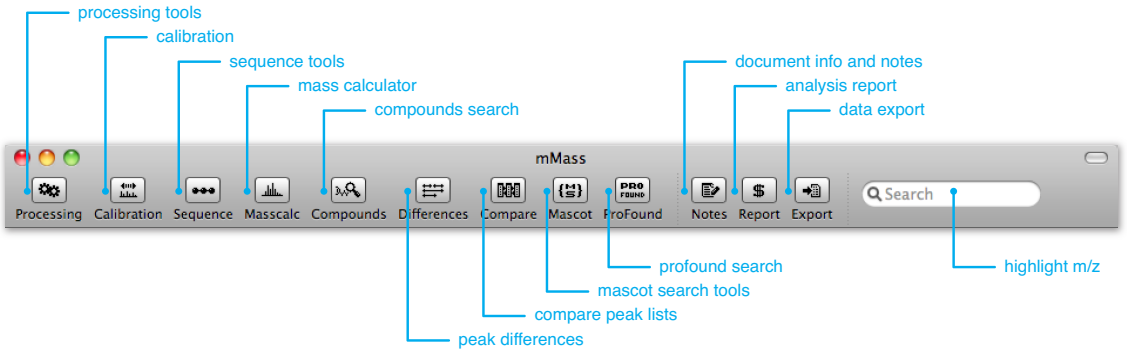
Check for updates - checks for available updates.

Paper to Cite - shows related papers in a default web browser.

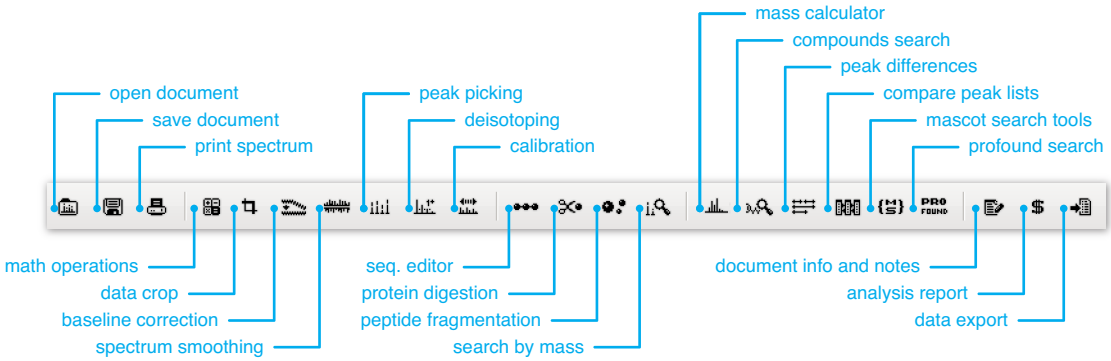
Donate - shows donation website in a default web browser.

5.3. Toolbar

To retain platform conventions and user experience there are two slightly different toolbars. In contrast to Linux and MS Windows, on Mac OS X there are no individual buttons for common document operations such as *Open, Save, Print* etc. and all related tools are grouped into a single button such as *Processing* or *Sequence*. The *Search* filed is available on Mac OS X to highlight selected m/z value in a spectrum.



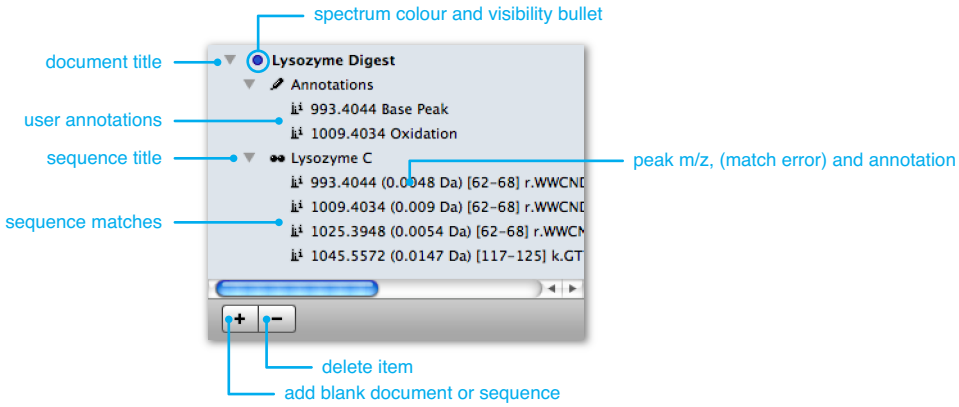
Main application toolbar on Mac OS X platform.



Main application toolbar on MS Windows and Linux platforms.

5.4. Documents Panel

The main purpose of *Documents Panel* is to provide a structured view of loaded documents with all its sub-elements. In this panel, each element of selected document can be edited by double-clicking or processed via specific command or context menu. Most of the sequence related functions are also available via the main menu Sequence.



Documents Panel.

Document

➡ **To add blank document:**
Press + button from the bottom toolbar and select New Document, or choose File → New from the main menu.

➡ **To select document for analysis:**
Click on any sub-element of the document you want to select. Regardless of a document color, when document is selected all labels ticks are shown in red. Selected document is marked by a bold title.

➡ **To make a document copy:**
Right-click on the document title and choose Duplicate Document.

➡ **To temporarily hide document in spectrum viewer:**
Click on a color bullet next to document title.

➡ **To change document title, information or notes:**
Double-click on the document title, or choose File → Document Info from the main menu to show up *Document Info* panel. See *Document Information* chapter for more details.

➡ **To vertically flip document in spectrum viewer:**
Right-click on the document title and choose Flip Spectrum, or choose View → Flip Spectrum from the main menu.

➡ **To offset spectrum intensity in spectrum viewer:**
Right-click on the document title and choose Offset Spectrum, or choose View → Offset Spectrum from the main menu to show up offset dialog. Set *Intensity offset* and press Offset button.

➡ **To clear spectrum offset:**
Right-click on the document title and choose Clear Offset. Choose View → Clear Offsets from the main menu to clear offset for all documents.

➡ **To change document color:**
Right-click on the document title and choose Change Colour.

➡ **To delete all annotations and sequence matches:**
Right-click on the document title and choose Delete All Notations.

➡ **To close document:**
Right-click on the document title and select Close Document, press [-] button from the bottom toolbar and choose Close Document, or choose File → Close from the main menu.

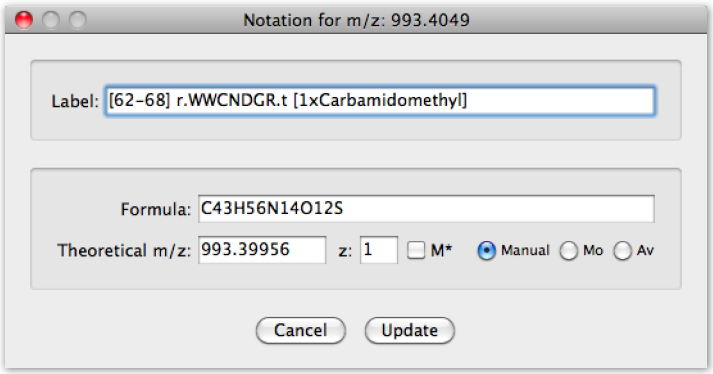
➡ **To close all documents:**
Press [-] button from the bottom toolbar and choose Close All Documents, or choose File → Close All from the main menu.

⚠ *Please note that spectrum offset is applied only if normalization is disabled.*

⚠ *Please note that normalization and spectrum offset do not modify any document data. These are just visualization tools.*

User Annotations

It is possible to add user annotations to any peak in a peak list. You can specify annotation *Label*, which is then shown in *Documents Panel*, and assign molecular *Formula* and *Theoretical m/z* value. All the annotations with theoretical m/z value can be used as calibration standards to re-calibrate your data. If the molecular formula is specified you can generate its isotopic pattern to see the difference between theoretical and measured peak.



Annotation dialog.

➡ **To add user annotation:**
Double-click on the peak in *Peaklist Panel* or press [✎] button from the bottom toolbar of *Peaklist Panel* to show up annotation dialog and type your annotation.

➡ **To edit user annotation:**
Double-click on the annotation to show up annotation dialog and edit the annotation.

➡ **To delete user annotation:**
Right-click on any annotation and select Delete Annotation, or press [-] button from the bottom toolbar and choose Delete Annotation.

➡ **To delete all user annotations:**
Right-click on any annotation or the annotations root and select Delete All Annotations, or press [-] button from the bottom toolbar and choose Delete All Annotations.

➡ **To highlight user annotation in spectrum viewer:**
Click on the annotation and spectrum moves to the m/z value. Small red arrow shows up on m/z axis of the spectrum.

➡ **To show isotopic pattern of user annotation:**
Right-click on the annotation and select Show Isotopic Pattern. *Mass Calculator* panel shows up with the annotation formula and corresponding peak charge. This function is available only if molecular formula and charge is specified in annotation dialog. See *Mass Calculator* chapter for more information.

➡ **To re-calibrate data by user annotations:**
Right-click on any single annotation or annotations root and select Calibrate by Annotations. All the user annotations will be send to *Calibration* panel. Only those annotations with specified theoretical m/z value can be used for data calibration. See *Calibration* chapter for more information.

Sequence

In order to use some *mMass's* tools such as *Protein Digest* or *Peptide Fragmentation,* specific sequence object must be defined. All sequence matches are stored in the similar way as user annotations and there are the same features available as well. See *Sequence Tools* chapter for more information about sequence editing and processing.

➡ **To add new sequence:**
Press [+] button from the bottom toolbar and select New Sequence, or choose Sequence → New Sequence from the main menu. See *Sequence Tools* chapter for more information.

➡ **To edit sequence:**
Double-click on the sequence title and *Sequence Editor* shows up. See *Sequence Tools* chapter for more information.

➡ **To delete sequence:**
Click on the sequence title and press Command+Backspace or Delete, or press [-] button from the bottom toolbar and choose Delete Sequence.

➡ **To edit sequence match:**
Double-click on the sequence match to show up annotation dialog and edit the annotation.

➡ **To delete sequence match:**
Right-click on any sequence match and select Delete Match, or press [-] button from the bottom toolbar and choose Delete Match.

➡ **To delete all sequence matches:**
Right-click on any sequence match or the sequence title and select Delete All Matches, or press [-] button from the bottom toolbar and choose Delete All Matches.

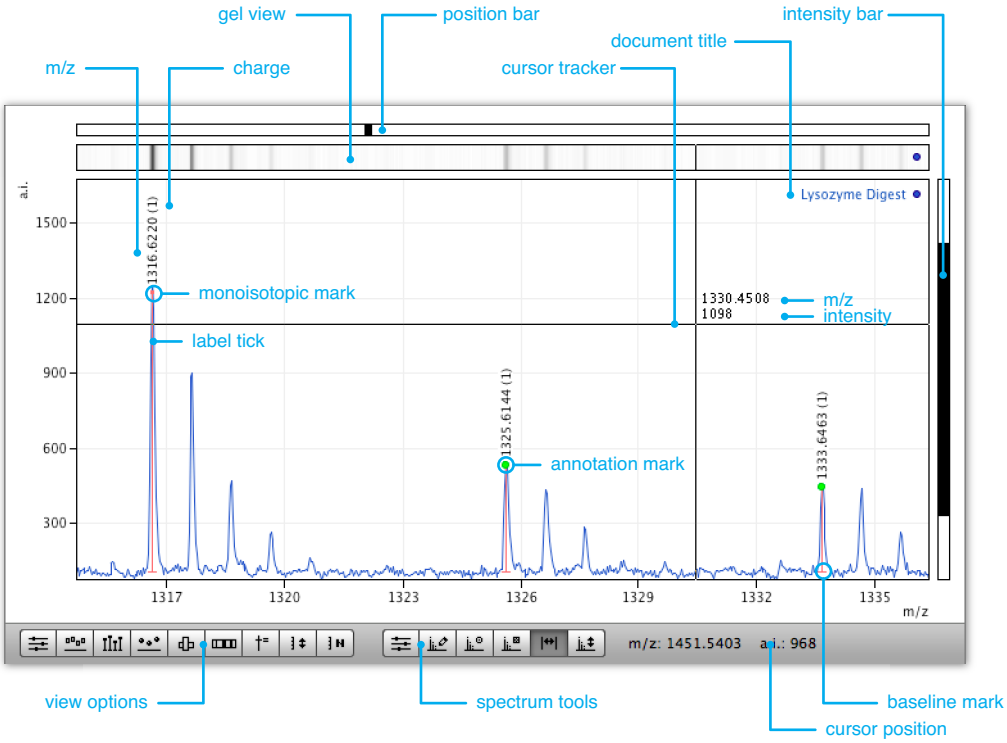
➡ **To highlight sequence match in spectrum viewer:**
Click on the sequence match and spectrum moves to the m/z value. Small red arrow shows up on m/z axis of the spectrum. Current zoom range remains the same.

➡ **To show isotopic pattern of sequence match:**
Right-click on the sequence match and select Show Isotopic Pattern. *Mass Calculator* panel shows up with the peptide formula and corresponding peak charge. See *Mass Calculator* chapter for more information.

➡ **To re-calibrate data using sequence matches:**
Right-click on any single match or sequence title and select Calibrate by Matches. All the matches will be send to *Calibration* panel. See *Calibration* chapter for more information.

5.5. Spectrum Viewer

Since most time in data interpretation is spent manipulating spectra (e.i. moving, shifting, scaling, zooming etc.), I aimed to make these functions as easy and user friendly as possible. There are no specific buttons or menu items hidden deep inside an application menu just to zoom spectrum. Everything is accessible by mouse, keyboard or combination of both. Vertical flipping, spectrum offset and gel view can be used to effectively compare your samples with any standard or blank spectrum. In addition, *Spectrum Viewer* not only provides for spectrum visualization, but also offers some other useful features such as peak labeling and distance measurements.



Spectrum Viewer panel.

Spectrum Manipulations

➡ **To zoom spectrum range:**
Select the m/z range with right or middle mouse button pressed. (Use Ctrl key to substitute right mouse button on Mac OS X.)

➡ **To zoom continuously from cursor position:**
Move the mouse cursor to desired m/z position and scroll the mouse wheel while holding Alt or Ctrl key.

➡ **To zoom from the center of current view:**
Use Left and Right arrows keys on your keyboard while holding Alt key.

➡ **To zoom from the start of current view:**
Drag the m/z axis horizontally with right mouse button pressed.

➡ **To move spectrum horizontally:**
Scroll the mouse wheel or drag the m/z axis horizontally with left mouse button pressed. If you prefer using keyboard, use Left, Right, PageUp, PageDown, Home and End keys.

➡ **To scale intensity axis:**
Scroll the mouse wheel while holding Shift key or drag the intensity axis vertically with right mouse button pressed.

➡ **To scale intensity axis automatically to fit current spectrum range:**
Press button from the bottom toolbar, or choose View → Autoscale Intensity from the main menu.

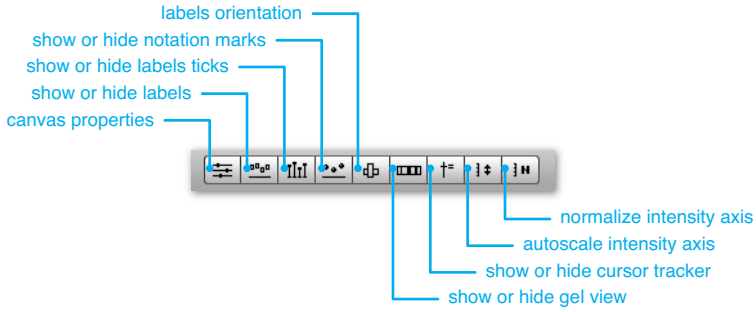
➡ **To show full mass range:**
Double-click on the m/z axis.

➡ **To show full intensity range:**
Double-click on the intensity axis.

➡ **To show full spectrum:**
Double-click anywhere in the spectrum.

View Options

There are different view options available for *Spectrum Viewer*. Those commonly used are available directly from the bottom toolbar, others can be accessed via the application main menu View.



Bottom toolbar with the most common Spectrum Viewer options.

➡ **To show or hide gridlines:**
Choose View → Show/Hide Gridlines from the main menu.

➡ **To show or hide legend:**
Choose View → Show/Hide Legend from the main menu.

➡ **To show or hide legend in gel view:**
Choose View → Show/Hide Gel Legend from the main menu.

➡ **To show or hide position bar:**
Choose View → Show/Hide Position Bar from the main menu.

➡ **To show or hide intensity bar:**
Choose View → Show/Hide Intensity Bar from the main menu.

➡ **To show or hide gel view:**
Press button from the bottom toolbar, or choose View → Show/Hide Gel from the main menu.

➡ **To show or hide cursor tracker:**
Press button from the bottom toolbar, or choose View → Show/Hide Cursor Tracker from the main menu.

➡ **To show or hide labels:**
Press button from the bottom toolbar, or choose View → Show/Hide Labels from the main menu.

➡ **To show or hide labels ticks:**
Press button from the bottom toolbar, or choose View → Show/Hide Labels Ticks from the main menu.

➡ **To show or hide charge in labels:**
Choose View → Show/Hide Labels Charge from the main menu.

➡ **To show or hide solid background for labels:**
Choose View → Show/Hide Labels Background from the main menu.

➡ **To show or hide notation marks:**
Press button from the bottom toolbar, or choose View → Show/Hide Notation Marks from the main menu.

➡ **To change labels orientation:**
Press button from the bottom toolbar, or choose View → Horizontal/Vertical Labels from the main menu.

➡ **To prevent overlapping labels:**
Choose View → Non-Overlapping Labels from the main menu.

➡ **To show labels in all documents:**
Choose View → Labels in All Documents from the main menu. Only labels from the selected document will be shown if this feature is disabled.

➡ **To enable or disable data points:**
Choose View → Show/Hide Data Points from the main menu. Data points are typically visible on detailed zoom only.

➡ **To enable intensity autoscale:**
Press button from the bottom toolbar, or choose View → Autoscale Intensity from the main menu.

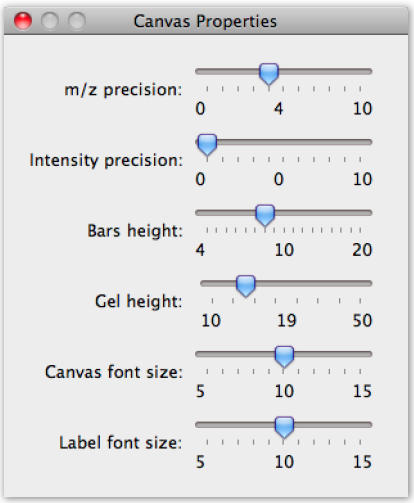
➡ **To enable intensity normalization:**
Press button from the bottom toolbar, choose View → Normalize Intensity from the main menu.

➡ **To flip spectrum vertically:**
Right-click on the document title in *Documents Panel* and choose Flip Spectrum.

➡ **To offset spectrum intensity:**
Right-click on the document title in *Documents Panel* and choose Offset Spectrum, or choose View → Offset Spectrum from the main menu to show up offset dialog. Set *Intensity offset* and press Offset button.

➡ **To clear spectrum offset:**
Right-click on the document title and choose Clear Offset. Choose View → Clear Offsets from the main menu to clear offset for all documents.

Please note that normalization and spectrum offset are just a visualization tools and no data are changed.



Canvas Properties dialog.

➡ **To set m/z precision (number of digits):**
Press button from the bottom toolbar, or choose View → Canvas Properties from the main menu to show up *Canvas Properties* dialog and move the *m/z precision* slider. This settings is used for all occurrences of mass throughout the application.

➡ **To set intensity precision (number of digits):**
Press button from the bottom toolbar, or choose View → Canvas Properties from the main menu to show up *Canvas Properties* dialog and move the *Intensity precision* slider. This settings is used for all occurrences of intensity throughout the application.

➡ **To set gel height:**
Press button from the bottom toolbar, or choose View → Canvas Properties from the main menu to show up *Canvas Properties* dialog and move the *Gel height* slider.

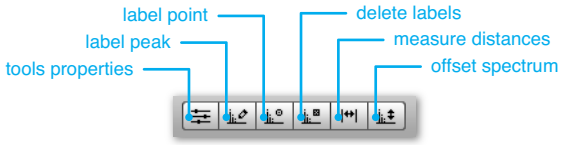
➡ **To set position and intensity bars height:**
Press button from the bottom toolbar, or choose View → Canvas Properties from the main menu to show up *Canvas Properties* dialog and move the *Bars height* slider.

➡ **To set axis and legend font size:**
Press button from the bottom toolbar, or choose View → Canvas Properties from the main menu to show up *Canvas Properties* dialog and move the *Canvas font size* slider.

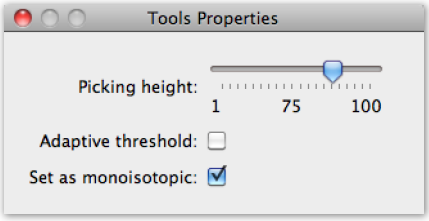
➡ **To set label font size:**
Press button from the bottom toolbar, or choose View → Canvas Properties from the main menu to show up *Canvas Properties* dialog and move the *Label font size* slider.

Spectrum Tools

There are several mouse tools available for *Spectrum Viewer* such as *Label Peak, Label Point, Delete Labels, Measure Distances* and *Offset Spectrum*.



Bottom toolbar with Spectrum Viewer tools.



Tools Properties dialog.

➡ **To label peak:**
Press button from the bottom toolbar and select desired peak in the spectrum. Only the most intense peak in the selection will be labeled. See *Data Processing* chapter for more information.

➡ **To label point:**
Press button from the bottom toolbar and click at desired point in the spectrum. Small cross mark tracks the spectrum until you release the mouse button.

➡ **To delete labels:**
Press button from the bottom toolbar and select area where the labels should be deleted. Only those peaks/labels where its m/z and intensity values fall into the selected area will be deleted.

➡ **To set peak picking height:**
Press button from the bottom toolbar to show up *Tools Properties* dialog and move the *Picking height* slider. See *Data Processing* chapter for more information.

➡ **To calculate baseline level from peak vicinity rather then from entire spectrum:**
Press button from the bottom toolbar to show up *Tools Properties* dialog and check *Adaptive threshold* checkbox. See *Data Processing* chapter for more information.

➡ **To automatically set labeled peak as monoisotopic:**
Press button from the bottom toolbar to show up *Tools Properties* dialog and check *Set as monoisotopic* checkbox.

➡ **To measure distances in spectrum:**
Press button from the bottom toolbar and drag mouse in the spectrum with left mouse button pressed. Distance shows in the bottom toolbar and next to the cursor if *Cursor Tracker* is enabled.

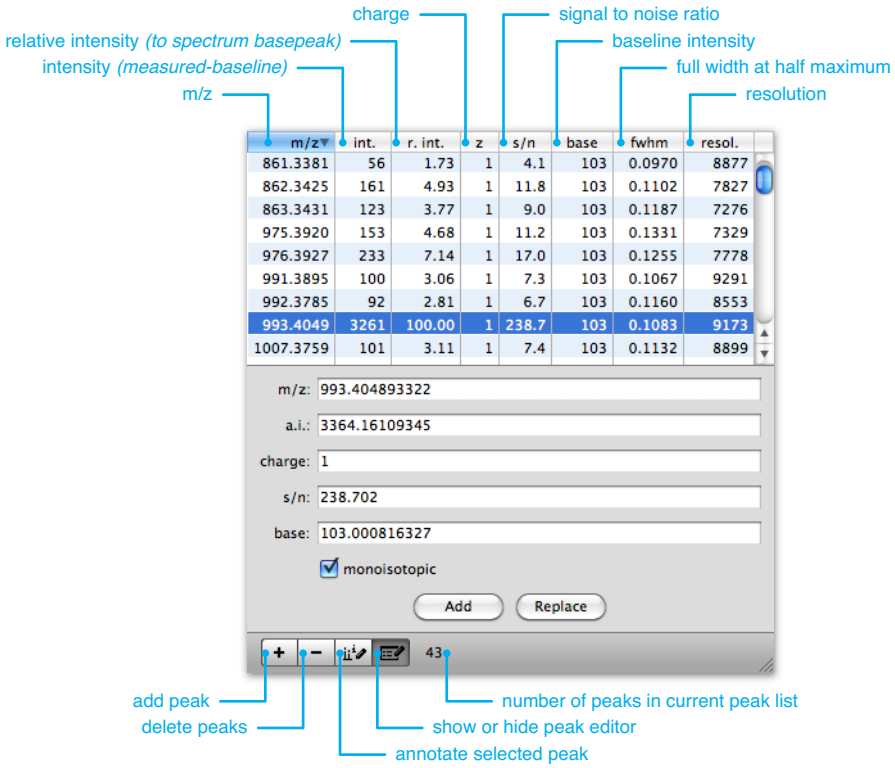
➡ **To offset spectrum intensity:**
Press button from the bottom toolbar and drag mouse in the spectrum with left mouse button pressed. Distance shows in the bottom toolbar and next to the cursor if *Cursor Tracker* is enabled. Current spectrum will be shifted after releasing the mouse button. Choose View → Offset Spectrum from the main menu to set spectrum offset manually.

Please note that spectrum offset is just a visualization tool and no real data are changed.

Please note that spectrum offset cannot be applied when normalized view is turned on.

5.6. Peaklist Panel

Peaklist Panel provides a table of all labeled peaks in selected document. For each peak, its *m/z, corrected intensity* (real intensity - baseline), *relative intensity, charge, signal to noise ratio, baseline intensity, fwhm* and *resolution* are shown. From this panel, any peak can be added, annotated, edited or removed. A simple peak editor can be easily used to create your own peak list manually.



Peaklist Panel with peak editor enabled.

➡ **To manually add new peak:**
Press + button from the bottom toolbar to show and clear peak editor, fill-up the peak parameters and press Add button.

➡ **To edit peak parameters:**
Press button from the bottom toolbar to show peak editor and click on the peak. Edit peak parameters and press Replace button.

➡ **To copy peak with different parameters:**
Press button from the bottom toolbar to show peak editor and click on the peak. Change peak parameters and press Add button.

➡ **To delete peaks:**
Select the peaks you want to delete and press Command+Backspace or Delete, or press − button from the bottom toolbar and choose Delete Selected. You can use *Delete Labels* tool in *Spectrum Viewer* as well.

➡ **To delete peaks by threshold:**
Press − button from the bottom toolbar and choose Delete by Threshold to show up threshold dialog. Set *Minimal value* and *Threshold type* and press Delete button. Another way is to sort peak list by specific value, selecting and deleting unwanted peaks.

➡ **To delete all peaks:**
Press − button from the bottom toolbar and choose Delete All.

➡ **To annotate peak:**
Double-click the peak or press button in the bottom toolbar to show up annotation dialog and type your annotation.

➡ **To highlight peak in spectrum viewer:**
Click on the peak and spectrum moves to the m/z value. Small red arrow shows up on m/z axis of the spectrum. Current zoom range remains the same.

➡ **To copy peaks into clipboard:**
Select the peaks you want to copy, press Command+C (Ctrl+C on MS Windows and Linux) and column selection dialog shows up. Select the columns you'd like to copy and press Copy.

➡ **To export peak list:**
Press button from the main toolbar, or choose File → Export from the main menu to show up *Export* dialog, and select *Export Peaklist Data* tool. See *Export* chapter for more information.

⚠ *Please note that "a.i." value in the peak editor represents absolute peak intensity without any baseline correction, while corrected intensity is shown in the peak list table.*

6. Document Basics

6.1. Supported Formats

mMass supports several mass spectrometry formats. Popular XML-based formats like *mzData* (http://www.psidev.info), *mzXML* (http://tools.proteomecenter.org) and *mzML* (http://www.psidev.info), which are open source and well documented are fully supported. Mass spectra and peak list data can also be imported from an *ASCII* file consisting of two columns (*m/z* and *intensity* pairs) separated by a *tab*, *space*, *comma* or *semicolon*.

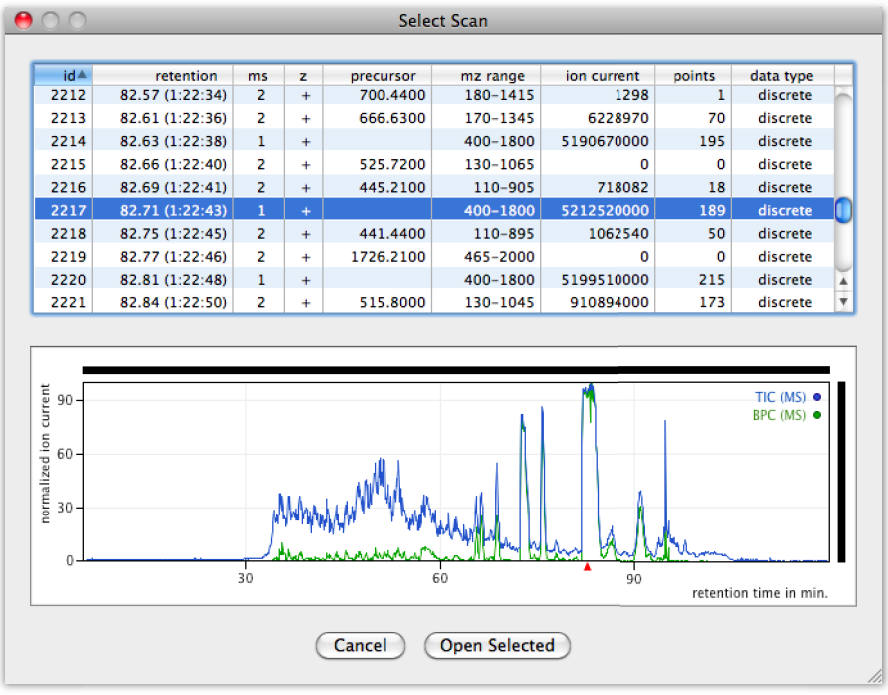
Since it is often impossible to obtain the manufacturer's description of their native file formats, they are not currently supported. However, if you have a *Bruker's CompassXport* tool installed on your computer it is automatically used to convert and open a raw data from all *Bruker's* instruments. This tool is available for free at www.bdal.de, unfortunately, for MS Windows platform only. In *mMass's* preferences you can specify whether *mzData*, *mzXML* or *mzML* format will be used for conversion and whether profile spectrum or peak list only will be extracted. By default, converted file is not deleted after successful import but this can be changed in *mMass's* preferences.

mMass is so-called a *"single spectrum editor"* therefore experiments such as LC-MS runs cannot be fully analyzed by *mMass*. However, it is possible to open any selected scan from such runs to analyze it separately. Sure, it does not make sense for many LC-MS experiments but it can be useful in many cases.

6.2. Open Document

➡ **To open document:**
Drag the document file into *mMass's* main window or choose File → Open from the main menu.

➡ **To open selected scan from LC-MS run:**
Drag the document file into *mMass's* main window or choose File → Open from the main menu. If document contains more scans, *Select Scan* dialog shows up. Select scan(s) you'd like to open and press Open button. *Total ion chromatogram* and *base peak chromatogram* is available if corresponding parameters are found in the data.



Select Scan dialog.

➡ **To open spectrum from Bruker's instruments:**
Drag the spectrum folder into *mMass's* main window or choose File → Open from the main menu and locate the *analysis.baf*, *analysis.yep* or *fid* file. You need to have *CompassXport* tool installed. This function is currently available for MS Windows platform only.

For *ASCII XY* and some *mzXML* documents *mMass* is unable to determine whether the document contains spectrum points or just centroides of peaks and chooses spectrum as default. If this decision isn't correct you can swap the data between line spectrum and peak list by choosing Processing → Swap Data from the main menu.

Please note that CompassXport tool does not allow non-ascii characters in a document path.

6.3. Blank Document

One of the unique features of *mMass* is the ability to make a blank document and manually create peak list. This feature is particularly useful in those cases where raw spectrum is unavailable, and user has only a spectrum image or printed list of labelled peaks. Such is often the situation in laboratories that do not have their own instruments and have to send their samples to other laboratories. This feature gives such laboratories the chance to analyze the data themselves. Once the peak list is prepared, all interpretation tools can be used. See *Peaklist Panel* chapter for more information about peak list editing.

Blank documents can also be used for protein digest or peptide fragmentation simulations or to make a personal database of sequences which can be easily imported into any document.

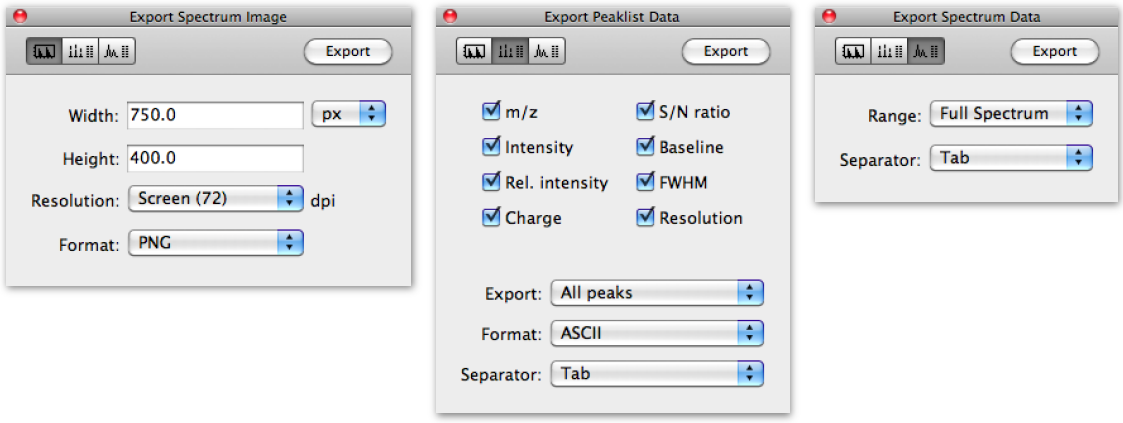
➡ **To open blank document:**
Press + button from the bottom toolbar and select New Document or choose File → New from the main menu.

6.4. Save Document

To retain all the information related to analysis such as protein sequence or user's annotations *mMass* has its own document format to store the data (*mSD* format). This format is XML-based to be easily processed by other software.

➡ **To save document:**
Select the document in *Documents Panel* and choose File → Save from the main menu.

6.5. Export



Export tools.

➡ **To export spectrum image:**
Press button from the main toolbar or choose File → Export from the main menu to show up *Export* dialog, and select *Export Spectrum Image* tool. Specify export parameters and press Export button.

➡ **To export spectrum points:**
Press button from the main toolbar or choose File → Export from the main menu to show up *Export* dialog, and select *Export Spectrum Data* tool. Specify export parameters and press Export button.

➡ **To export peak list:**
Press button from the main toolbar or choose File → Export from the main menu to show up *Export* dialog and select *Export Peaklist Data* tool. Specify export parameters and press Export button.

On MacOS X and Linux platform you can use native support for PDF creation to export spectrum into vector format. From the main menu choose File → Print and select PDF. On MS Windows you need to have some PDF convertor installed first.

To export spectrum images for monitor only, use 72 dpi. To export large spectrum images for printing or publications use larger resolution to thicken-up the lines and fonts. Is is often the case that for smaller images, font size became too big. Use *Canvas Properties* dialog and set the font size.

6.6. Print Spectrum

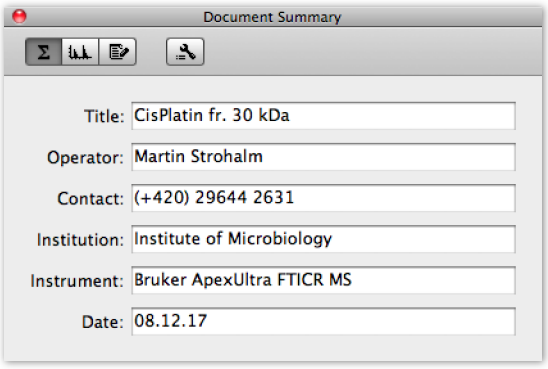
➡ **To print spectrum:**
Choose File → Print Spectrum from the main menu and current *Spectrum Viewer* contents will be printed.

6.7. Document Info

Document Info panel provides some information about selected document and place to write your own description of the sample, analysis and results. It is generally good idea to fill up this information if you want to share the analysis with other people.

Document Summary

In the *Document Summary* part of *Document Info* panel you can specify document *Title*, *Operator's* name, *Contact* and *Institution*, used *Instrument* and measurement *Date*. You can save current values as a presets to use it later again.



Document Summary.

➡ **To show document summary:**
Press button from the main toolbar or choose File → Document Info from the main menu to show up *Document Info* panel. Then press Σ button from the panel toolbar.

➡ **To save current values as presets:**
Write the information you'd like to save as presets. Press button from the panel toolbar and choose Save as Presets. In the dialog write presets name and press Save button.

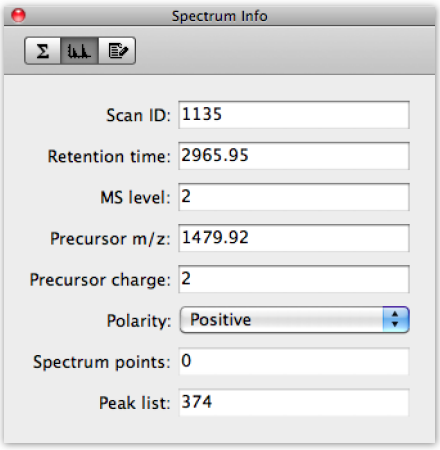
➡ **To use saved presets:**
Press button from the panel toolbar and choose any of your presets from the pup-up menu.

➡ **To delete saved presets:**
Choose Libraries → Presets from the main menu to show up *Presets Library* editor. Choose the presets you'd like to delete and press Delete button.

➡ **To rename saved presets:**
Choose Libraries → Presets from the main menu to show up *Presets Library* editor. Choose the presets you'd like to rename, type the new name and press Rename button.

Spectrum Info

In the *Spectrum Info* part of *Document Info* panel you can specify *Scan ID, Retention time, MS level Precursor m/z, Precursor charge* and *Polarity*. In addition, number of spectrum points and total number of peaks in peak list are shown.



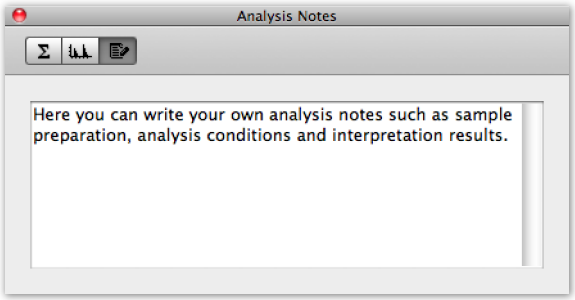
Spectrum Info.

➡ **To show spectrum info:**
Press button from the main toolbar or choose File → Document Info from the main menu to show up *Document Info* panel. Then press button from the panel toolbar.

⚠ *Please note that if you are importing a document from mzML format, Scan ID value does not correspond to the real scan number. Unfortunately, it is not possible to get the scan number value from mzML due to its non-uniform formatting. For both, mzXML and mzData formats, Scan ID corresponds to particular scan number.*

Analysis Notes

Analysis Notes provides a place to type you personal notes about sample preparation, sample analysis and interpretation results. These information will be also shown in analysis report. See *Analysis Report* chapter for more information.

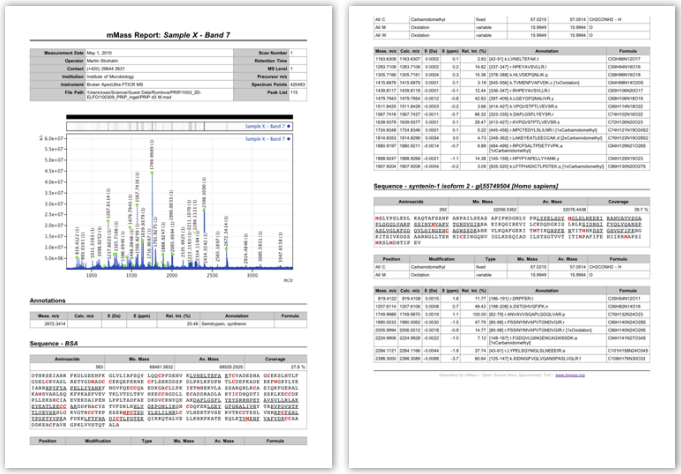


Analysis Notes.

➡ **To show analysis notes:**
Press button from the main toolbar or choose File → Document Info from the main menu to show up *Document Info* panel. Then press button from the panel toolbar.

6.8. Analysis Report

Analysis report can be generated from selected document and all available information such as document info, current *Spectrum Viewer* contents, user's notes and annotations, sequence, modifications and matches will be included. This report is generated in *HTML* format and automatically shows up in your web browser.



Analysis report.

➡ **To make analysis report:**
Press button from the main toolbar or choose File → Analysis Report from the main menu. Report shows up in your web browser.

➡ **To sort data in report tables:**
Click on appropriate column header in the report. Please note that this feature needs to have *JavaScript* enabled in your web browser.

It is generally good practice to write your analysis notes and results into document using *Document Info* tool prior to report generation. See *Document Info* chapter for more information.

On MacOS X and Linux platform you can use native support for PDF creation to make PDF report. When the report shows up in your web browser choose File → Print and select PDF. On MS Windows you need to have some PDF convertor installed first.

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7. Data Processing

mMass offers number of common data processing functions such as mathematical operations, data crop, baseline correction, smoothing, peak picking, charging and deisotoping. In order to avoid permanent changing of parameters and speed up the processing of data from different instruments you can define your own processing presets and use it frequently. For math operations, smoothing and baseline correction a preview is available and recommended to use before modifying your data. Your last processing step can be undone.

➡ **To open data processing tool:**
On Mac OS X press button from the main toolbar. Separate buttons for different processing tools are available on other platforms. All the tools can be reached via Processing menu as well.

➡ **To undo last processing step:**
From the main menu choose Processing → Undo.

➡ **To save current values as presets:**
Press button from the panel toolbar and choose Save as Presets. In the dialog type the presets name and press Save button.

➡ **To use saved presets:**
Press button from the panel toolbar and choose any of your presets from the pup-up menu.

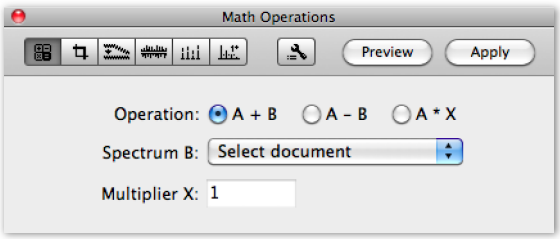
➡ **To delete saved presets:**
Choose Libraries → Presets from the main menu to show up *Presets Library* editor. Choose the presets you'd like to delete and press Delete button.

➡ **To rename saved presets:**
Choose Libraries → Presets from the main menu to show up *Presets Library* editor. Choose the presets you'd like to rename, type the new name and press Rename button.

⚠ *Please note that every presets contains parameters from all the processing tools. If you load any presets, parameters for all the tools will be changed. This is especially important for Peak Picking tool where parameters from other panels are used (Smoothing and Deisotoping).*

7.1. Math Operations

Simple math operations are available to add or subtract two documents, or to multiply current document by a specified factor. If you combine two documents containing spectrum points, operation is applied on the spectrum points only and document peak list (if any) is erased. Only the spectrum points can be subtracted. Multiplying is applied on both, spectrum points and peak list as well.



Math Operations tool.

- *Operation* - math operation to be applied.
- *Spectrum B* - spectrum to be added or subtracted from current document.
- *Multiplier* - multiplying factor.

➡ **To open math operation tool:**
On Mac OS X press button from the main toolbar, then press button from the panel toolbar. On other platforms press button from the main toolbar. You can choose Processing → Math Operations from the main menu as well.

➡ **To add spectrum to selected document:**
Select a document in the *Documents Panel*. In the *Math Operations* tool select *"A+B"* and the document to be added (*Spectrum B*). Press Preview button to see the results as a temporary (red) spectrum or Apply button to apply operation on selected document.

➡ **To subtract spectrum from selected document:**
Select a document in the *Documents Panel*. In the *Math Operations* tool select *"A-B"* and the document to be subtracted (*Spectrum B*). Press Preview button to see the results as a temporary (red) spectrum or Apply button to apply operation on selected document.

➡ **To multiply selected document:**
Select a document in the *Documents Panel*. In the *Math Operations* tool select *"A*X"* and specify multiplier factor (*Multiplier X*). Press Preview button to see the results as a temporary (red) spectrum or Apply button to apply operation on selected document.

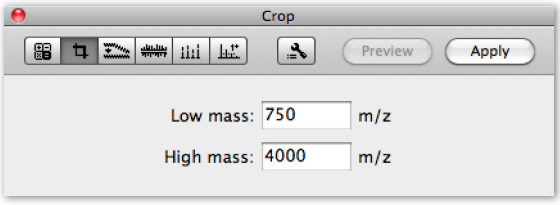
Please note that *Preview* is not available for peak list processing.

To be able to sum-up or subtract two spectra, both must have the same x-raster. Unfortunately, this is not often the case, therefore additional points must be added and resulted spectrum can easily became very huge and processing time extremely long! Since x-raster is mostly changed by different calibrations, it is generally good idea to apply this processing prior to any re-calibration step.

Please note that while the spectrum and peak list are changed by math operations, all the user's annotations and sequence matches remains the same and especially the intensity value can therefore be inaccurate. It is up to your decision if you prefer to retain or to remove such items. (It is generally good idea to apply this processing function prior to any data interpretation.)

7.2. Crop

This function simply discards all the spectrum data points, labeled peaks, annotations and sequence matches which are out of the m/z range specified by *Low mass* and *High mass* parameters.



Crop tool.

- *Low mass* - data below this limit will be removed.
- *High mass* - data above this limit will be removed.

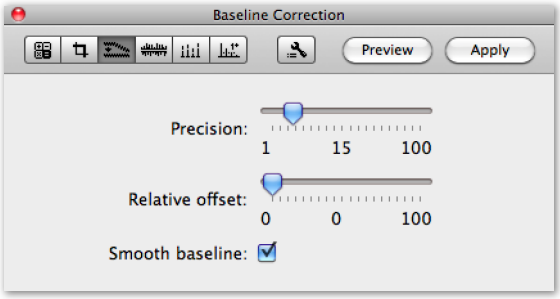
➡ **To open crop tool:**
On Mac OS X press button from the main toolbar, then press button from the panel toolbar. On other platforms press button from the main toolbar. You can choose Processing → Crop from the main menu as well.

➡ **To crop data:**
Using *Low mass* and *High mass* values specify the m/z range to keep and press Apply button.

Using *Crop* tool to remove "matrix area" from MALDI-TOF mass spectra can significantly reduce number of spectrum data points and speed up other processing.

7.3. Baseline Correction

Especially for MALDI-TOF mass spectra of proteins a strong baseline distortion is common problem which needs to be corrected quite often. Using *Baseline Correction* tool, this processing step can be done very easily. Baseline is calculated from the spectrum noise as a median of all data points minus noise width (median of absolute deviations). Using *Precision* slider, baseline can be composed from 1 to 100 segments to trace spectrum shape precisely. In addition, you can specify *Relative offset* to move baseline down a bit. *Smooth baseline* to eliminate local extremes. After setting all the parameters you can see a preview prior to applying baseline correction to your data.



Baseline Correction tool.

- *Precision* - number of baseline segments (1 = straight line).
- *Relative offset* - baseline intensity shift.
- *Smooth baseline* - applies smoothing to baseline.

➡ **To open baseline correction tool:**
On Mac OS X press button from the main toolbar, then press button from the panel toolbar. On other platforms press button from the main toolbar. You can choose Processing → Smooth Spectrum from the main menu as well.

➡ **To preview corrected data:**
Specify all the parameters and press Preview button. A temporary (red) corrected spectrum appears in *Spectrum Viewer*.

➡ **To subtract baseline from data:**
Specify all the parameters and press Apply button.

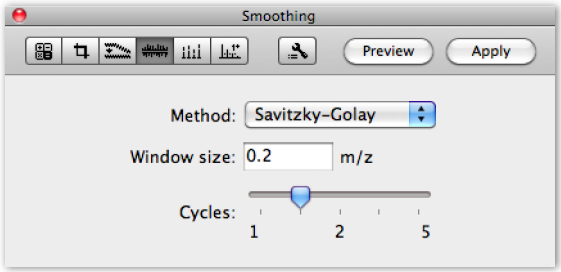
Please note that calculated baseline is shows in *Spectrum Viewer* while moving *Precision* or *Relative offset* slider. This feature can be very helpful to set baseline precisely.

Please note that current peak list will be removed after applying baseline correction.

Please note that while the spectrum and peak list are changed by baseline correction, all the user's annotations and sequence matches remains the same and especially the intensity value is therefore inaccurate. It is up to your decision if you prefer to retain or to remove such items. (It is generally good idea to apply this processing function prior to any data interpretation.)

7.4. Smoothing

You can use this function to smooth the noise which distorts peak shape. There are two different smoothing *Methods* available - *Moving Average* and *Savitzky-Golay*. In general, *Moving Average* is much faster but causes intensity loss for sharp peaks. This method should be preferentially used to smooth high-mass spectra where peaks are broader. On the other hand, *Savitzky-Golay* filter is very slow but intensity loss is lower. This method should be preferentially used to smooth low-mass spectra where peaks are sharp. After setting all the parameters you can see a preview prior to processing your data.



Smoothing tool.

- *Method* - smoothing algorithm.
- *Window size* - smoothing window.
- *Cycles* - number of smoothing repetitions.

➡ **To open smooth tool:**
On Mac OS X press button from the main toolbar, then press button from the panel toolbar. On other platforms press button from the main toolbar. You can choose Processing → Smooth Spectrum from the main menu as well.

➡ **To preview smoothed data:**
Specify all the parameters and press Preview button. A temporary (red) smoothed spectrum appears in *Spectrum Viewer*.

➡ **To smooth data:**
Specify all the parameters and press Apply button.

For *Moving Average* method the *Window size* value should be about 1/3 of the peak width and 1/2 for *Savitzky-Golay* method.

Always check the intensity loss for different peaks along the entire mass range. Use smaller *Window size* if the intensity loss is too strong.

Please note that at least 2 and 4 data points within the smoothing window are needed for Moving Average and Savitzky-Golay method respectively. No smoothing is applied if Window size is too narrow.

Please note that current peak list will be removed after applying smoothing.

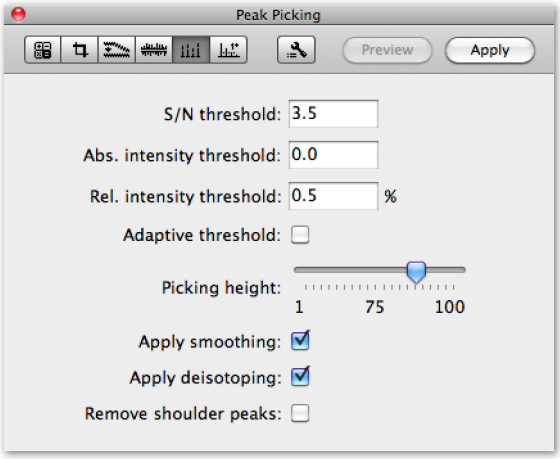
Please note that while the spectrum and peak list are changed by smoothing, all the user's annotations and sequence matches remains the same and especially the intensity value is therefore inaccurate. It is up to your decision if you prefer to retain or to remove such items. (It is generally good idea to apply this processing function prior to any data interpretation.)

7.5. Peak Picking

As mentioned earlier in *Spectrum Viewer* chapter, there is a specific tool to label peaks manually. However, this could be very annoying especially for data-rich spectra like those from FTICR MS or Orbitrap. Fortunately, an algorithm is incorporated into *mMass* to facilitate automatic peak picking. There are couple of basic steps in the peak picking algorithm:

- *Pre-smoothing* - if enabled, raw spectrum data are pre-smoothed to eliminate peak noise.
- *Searching for local maxima* - local maxima are temporarily labeled as potential peaks.
- *Filtering by intensity threshold* - peaks bellow user intensity threshold are being removed.
- *Centroides calculation* - peaks centroides are calculated and unresolved peaks are grouped together.
- *Filtering by intensity threshold* - peaks bellow user intensity threshold are being removed.
- *Removing shoulder peaks* - if enabled, "shoulder peaks" for FTMS data are being removed.
- *Deisotoping* - if enabled, deisotoping is applied to remove isotopes and calculate charges.

To get relevant intensities, for each peak its baseline is calculated. For a flat spectrum with constant noise along entire mass range a global noise level is used as the baseline for all peaks. This approach is very fast but generally not applicable for spectra with uneven baseline. In that cases, peak baselines can be calculated separately for each peak using the noise level from its surroundings using *Adaptive threshold*. This approach is slower but can be essential for protein mass spectra.



Peak Picking tool.

- *S/N threshold* - peaks bellow the signal to noise threshold will not be labeled.
- *Abs. intensity threshold* - peaks bellow the absolute intensity (peak intensity - baseline) threshold will not be labeled.
- *Rel. intensity threshold* - peaks bellow the relative intensity threshold will not be labeled.
- *Adaptive threshold* - each peak baseline will be calculated from its surroundings.
- *Picking height* - picking height for centroides.
- *Apply smoothing* - data will be smoothed prior to peak picking using current smoothing settings. See *Smoothing* chapter for more information.
- *Apply deisotoping* - peak isotopes will be removed and charge calculated using current deisotoping settings. See *Deisotoping* chapter for more information.
- *Remove shoulder peaks* - small surrounding peaks called "shoulder peaks" occurring in FTMS data will be removed.

➡ **To open peak picking tool:**
On Mac OS X press button from the main toolbar, then press button from the panel toolbar.

On other platforms press button from the main toolbar. You can choose Processing → Peak Picking from the main menu as well.

➡ **To label peaks:**
Specify all the parameters and press Apply button.

Use pre-smoothing for MALDI-TOF data of any kind.

If pre-smoothing is enabled, don't forget to check intensity loss for different peaks along the spectrum.

Smoothing significantly decreases number of local maxima, therefore speeds up further processing.

Using *Adaptive threshold* without pre-smoothing can sometimes be very slow.

⚠ *If smoothing or deisotoping is enabled, don't forget to check their settings in corresponding panels.*

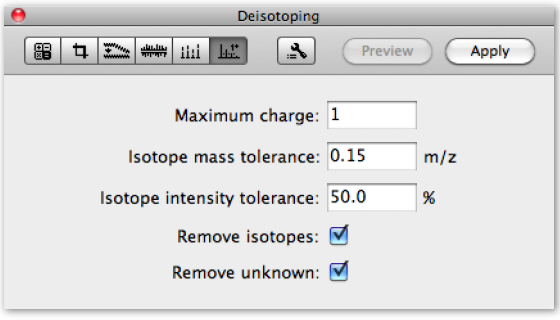
⚠ *Please note that while the peak list is changed, all the user's annotations and sequence matches remains the same and the m/z and intensity values are therefore inaccurate. It is up to your decision if you prefer to retain or to remove such items. (It is generally good idea to apply this processing function prior to any data interpretation.)*

7.6. Deisotoping

The main purpose of this tool is to remove unwanted peak isotopes after peak picking. However, in order to find the isotopes a peak charge needs to be calculated, therefore this tool can be used for charge determination as well.

Starting from specified *Maximum charge*, for every peak its isotopes are searched using corresponding isotopic mass shift *(1.00287/abs(z))* ± *Isotope mass tolerance*. If at least one isotope is found, parent peak is set as the monoisotopic with current charge state. If no isotope is found, current charge state is decreased *(abs(z) - 1)* and search cycle starts again for the same peak.

Because of possible peak overlaps, theoretical isotopic pattern needs to be taken into account. Intensity of every isotope is compared with its theoretical value. If the intensity is matching theoretical value ± *Isotope intensity tolerance*, corresponding isotope is discarded from any subsequent search cycle. If the difference is over tolerance, corresponding isotope will be used as possible parent (monoisotopic) peak in subsequent search cycle. Since *mMass* is mostly used for proteomic data interpretation, *the averagine (C4.9384 N1.3577 O1.4773 S0.0417 H7.7583)* is used to calculate theoretical isotopic patterns.



Deisotoping tool.

- *Maximum charge* - maximum charge state to be searched.
- *Isotope mass tolerance* - tolerance for mass difference between adjacent isotopes.
- *Isotope intensity tolerance* - tolerance for intensity check between theoretical and measured isotope.
- *Remove isotopes* - all identified isotopes will be removed after processing.
- *Remove unknown* - all unknown peaks will be removed after processing.

➡ **To open deisotoping tool:**
On Mac OS X press button from the main toolbar, then press button from the panel toolbar. On other platforms press button from the main toolbar. You can choose Processing → Deisotoping from the main menu as well.

➡ **To deisotope peaks:**
Specify all the parameters and press Apply button.

➡ **To apply deisotoping automatically after peak picking:**
In *Peak Picking* tool enable *Apply deisotoping*.

➡ **To edit peak charge:**
Press in the *Peaklist Panel* bottom toolbar to show peak editor and click on the peak in the list. Set the new charge and press Replace button.

➡ **To manually set peak as monoisotopic:**
Press in the *Peaklist Panel* bottom toolbar to show peak editor and click on the peak in the list. Check *monoisotopic* checkbox and press Replace button.

⚠ *Please note the relationship between Maximum charge and Isotope mass tolerance. Isotope mass tolerance must be lower than 1.00287×(1/(z-1) - 1/z) to successfully distinguish z and z-1 charge.*

⚠ *Please note that the combination of averagine intensity distribution and higher Isotope intensity tolerance is generally applicable to wide range of organic compounds but can be very problematic if atoms like Cl, Fe, Hg, Pt etc. are incorporated.*

7.7. Utilities

Normalize Data

To compare data between two different instruments it is sometimes necessary to normalize the data to a same intensity level.

➡ **To normalize data:**
Choose Processing → Normalize Data from the main menu.

Swap Data

For *ASCII XY* and some *mzXML* documents *mMass* is unable to determine whether document contains line spectrum points or just centroides of peaks and chooses line spectrum as default. If this decision isn't correct you can swap the data between line spectrum and peak list.

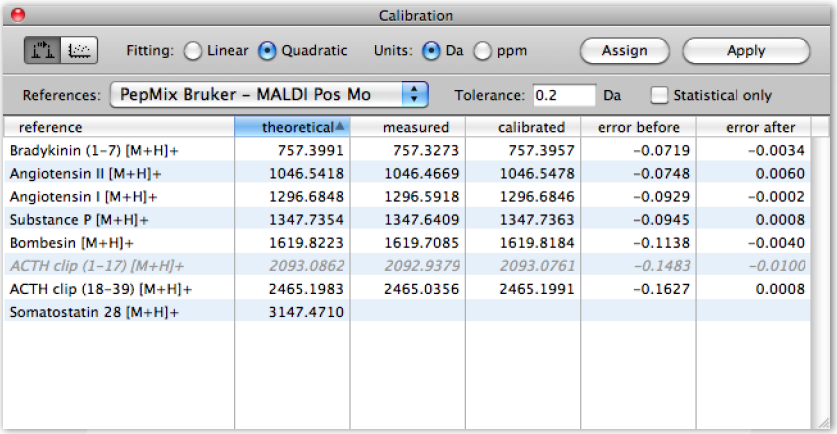
➡ **To swap data between spectrum and peak list:**
Choose Processing → Swap Data from the main menu.

8. Calibration

In order to re-calibrate you data *mMass* enables two principal approaches - standard calibration and statistical calibration. In the case of standard calibration any reference list must be selected first and reference values must be assigned to measured peaks. Reference values are assigned automatically using *Tolerance* value. You can use either *Linear* or *Quadratic* fitting to calculate calibration constants. In general, linear fitting is much safer if you want to re-calibrate an m/z range outside of your assigned references. Always see a calibration plot before recalculating your data.

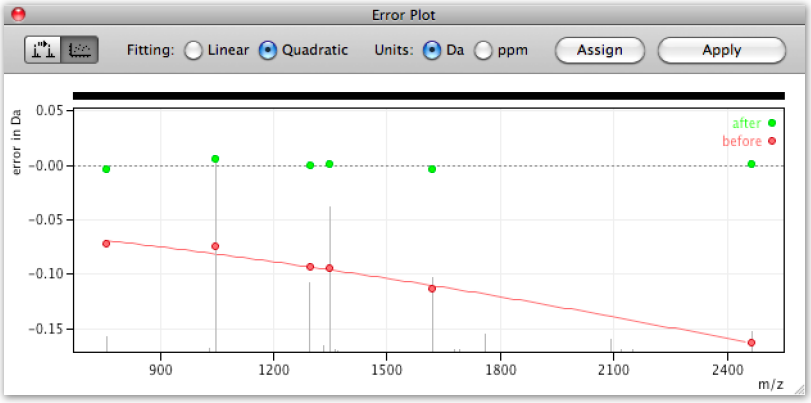
Statistical calibration, sometimes called "self-calibration" is a special method for peptide mass spectra only. It does not need any external reference points since it is based on the fact that monoisotopic masses of peptides are distributed in a very regular way. Decimal fraction of the peptide mass can be calculated with sufficient accuracy just by multiplying their integral part by factor *1.00048*. For this method, every peak above 700 m/z limit is recalculated and used as reference mass.

It is sometimes good to use other known peaks as internal calibration standards. Once you have the theoretical masses defined within your annotations or sequence matches, you can use them to re-calibrate your data. Please be careful while using this feature!



reference	theoretical	measured	calibrated	error before	error after
Bradykinin (1–7) [M+H]+	757.3991	757.3273	757.3957	–0.0719	–0.0034
Angiotensin II [M+H]+	1046.5418	1046.4669	1046.5478	–0.0748	0.0060
Angiotensin I [M+H]+	1296.6848	1296.5918	1296.6846	–0.0929	–0.0002
Substance P [M+H]+	1347.7354	1347.6409	1347.7363	–0.0945	0.0008
Bombesin [M+H]+	1619.8223	1619.7085	1619.8184	–0.1138	–0.0040
ACTH clip (1–17) [M+H]+	*2093.0862*	*2092.9379*	*2093.0761*	*–0.1483*	*–0.0100*
ACTH clip (18–39) [M+H]+	2465.1983	2465.0356	2465.1991	–0.1627	0.0008
Somatostatin 28 [M+H]+	3147.4710				

Calibration tool.



Calibration Error Plot.

➡ **To show calibration tool:**
Press button from the main toolbar or choose Processing → Calibration from the main menu.

➡ **To show error plot:**
Press button from the panel toolbar.

➡ **To assign reference masses:**
Specify *Tolerance* value and *Units* and press Assign button.

➡ **To exclude assigned reference from calculation:**
Double-click on the reference in the list. Corresponding line turns grey and italic.

➡ **To highlight reference mass in spectrum viewer:**
Click on the reference in the list and spectrum moves to theoretical m/z value. Small red arrow shows up on m/z axis of the spectrum. Current zoom range remains the same.

➡ **To use statistical calibration:**
Check *Statistical only* checkbox. Reference masses and calibration constants are automatically calculated from the current peak list.

➡ **To define new reference list:**
Choose Libraries → Calibration Masses from the main menu to show up *Calibration Masses Library* editor. See *Libraries* chapter for more information.

➡ **To re-calibrate data by user annotations:**
Right-click on any single annotation or the annotations root in *Documents Panel* and select Calibrate by Annotations. All the user annotations will be send to *Calibration* panel. Please note that only those annotations with specified theoretical m/z value can be used.

➡ **To re-calibrate data by sequence matches:**
Right-click on any single match or sequence title in *Documents Panel* and select Calibrate by Matches. All the matches will be send to *Calibration* panel.

➡ **To apply same calibration to multiple documents:**
Once the calibration is calculated you can apply it to multiple documents. Simply select another document in *Documents Panel* and press Apply Recent button.


Always check *Error plot* to see whether the calibration is correct.


In general, use *Linear* fitting if assigned references do not cover entire m/z range you'd like to calibrate.


Single-point calibration can be used for linear fitting.


User annotations and sequence matches are re-calibrated as well.


Please note that at least 3 reference mass points are needed for quadratic fitting.


Please note that the calibration is calculated using absolute m/z errors. Therefore shown calibration curve cannot be liner if you have "ppm" units selected, even if linear model is used.


Please note that statistical calibration can be used for peptides only! Any non-peptide contamination or modification could have disturbing effect to the calibration and should be discarded from calculations.

9. Mass Calculator

Mass Calculator provides a tools for calculation of molecular masses of compounds, generation of ion series and isotopic pattern simulation. Molecular formula can be typed manually or can be sent from various *mMass's* tools such as *Protein Digest, Peptide Fragmentation* etc. Theoretical isotopic profile can be easily overlaid with measured data or stored as regular document.

➡ **To show mass calculator:**
Press button from the main toolbar or choose Tools → Mass Calculator from the main menu.

9.1. Formula Syntax

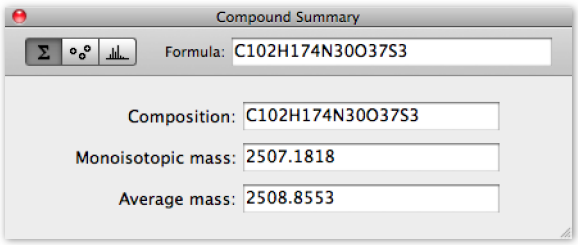
All known elements and their isotopes are defined within *mMass's* library and can be used to define any compound. Use the following syntax rules to specify compound formula:

- Use common syntax to type simple formula: C16H32O2.
- Use parenthesis "()" to define groups: CH3(CH2)14COOH
- Use negative "-" values to remove atoms: CH3(CH2)14COOH(NaH-1)
- Use braces "{}" to define specific isotope of the element: C{13}16H32O2

⚠ *Please note that using negative values for groups such as C16H32O2(OH)-1 does not work.*

9.2. Compound Summary

Compound Summary panel provides a fast preview of the compound defined in *Formula* field. *Composition*, *Monoisotopic* and *Average masses* are shown.

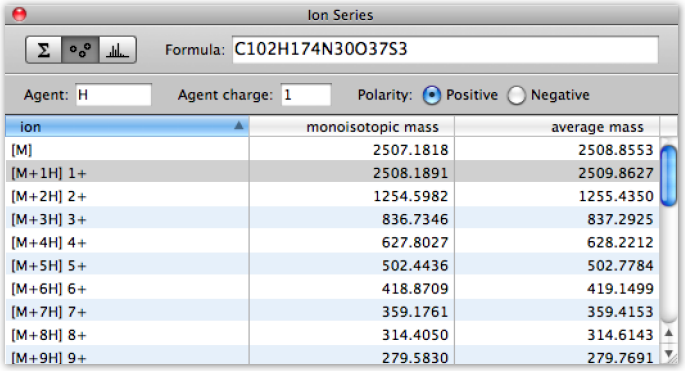


Compound Summary.

➡ **To show compound summary:**
Press button from the main toolbar or choose Tools → Mass Calculator from the main menu to show up *Mass Calculator* panel. Then press Σ button from the panel toolbar and write your compound into *Formula* field.

9.3. Ion Series

Using *Ion Series* panel you can see all the ions for the compound defined in *Formula* field. Corresponding monoisotopic and average masses are calculated with respect to polarity settings. By default, a proton is used as a "charging agent" but you can specify your own formula or *"e"* for radical ions.



Ion Series.

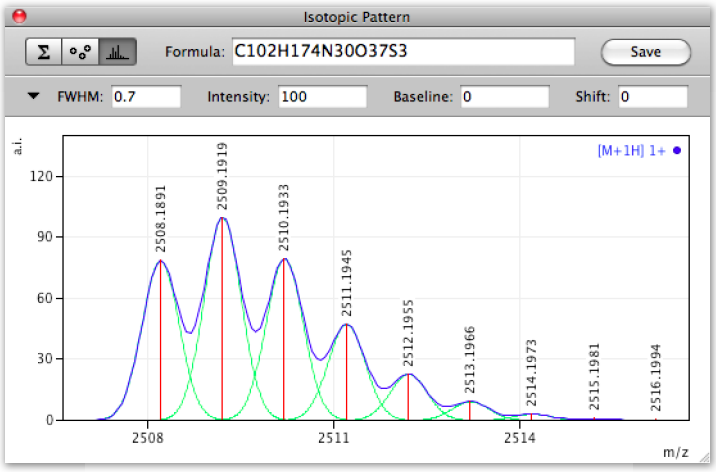
➡ **To show ion series:**
Press button from the main toolbar or choose Tools → Mass Calculator from the main menu to show up *Mass Calculator* panel. Then press button from the panel toolbar and type your compound into *Formula* field. Ions are generated automatically.

➡ **To copy ion series into clipboard:**
Click into the ions list and press Command+C (Ctrl+C on MS Windows and Linux).

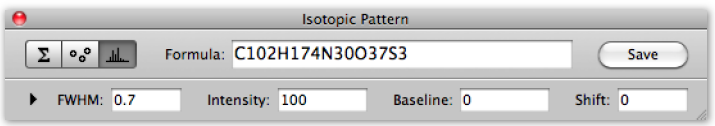
9.4. Isotopic Pattern

Isotopic Pattern panel provides a simple tool for generating theoretical isotopic pattern from compound formula. Isotopes are calculated and grouped together with respect to specified *Peak width*. For each isotope, Gaussian-shape peak is modeled and final profile is calculated as a sum of all the peaks.

Theoretical isotopic profile can be overlaid with measured data and positioned precisely using *FWHM, Intensity, Baseline* and m/z *Shift*. You can save theoretical profile as regular document as well.



Isotopic Pattern within Mass Calculator tool.



Collapsed version of Isotopic Pattern panel.

➡ **To show isotopic pattern:**
Press button from the main toolbar or choose Tools → Mass Calculator from the main menu to show up *Mass Calculator* panel. Then press button from the panel toolbar and type your compound into *Formula* field.

➡ **To change the ion type for current isotopic patter:**
Press button from the panel toolbar and select desired ion type in the list.

➡ **To overlay isotopic pattern with measured data:**
Press button from the panel toolbar and select desired ion type in the list. Theoretical pattern is then overlaid with measured data. Set *Intensity, Baseline* and *Shift* values to position the pattern precisely.

➡ **To save current isotopic pattern as regular document:**
Press Save button from the panel toolbar.

➡ **To collapse pattern panel:**
Press the small triangle on the left side of the panel toolbar.

Use the same spectrum manipulation conventions in isotopic pattern window as in the main *Spectrum Viewer*.

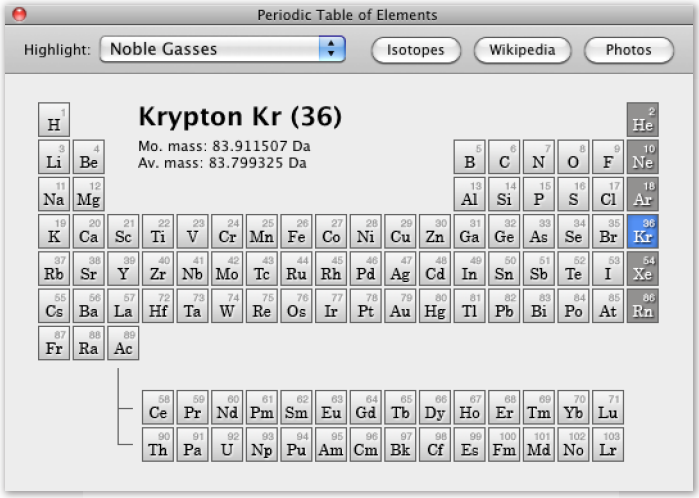
On Mac OS X you can change pattern parameters using a mouse scroll as well.

Use collapsed panel while overlaying theoretical profile and acquired data. This provides you more space to look at your data but all the positioning parameters are still available.

⚠ *Please note that when overlaying theoretical profile and acquired data, offset and flipping is applied automatically according to selected document.*

10.Periodic Table of Elements

Periodic Table of Elements provides some basic information about the elements. Different groups can be highlighted and element name, mass and isotopic pattern can be shown. For each element its detailed information can be seen on *Wikipedia* (en.wikipedia.org/wiki/Periodic_table) or *The Photographic Periodic Table of the Elements* (www.periodictable.com) using direct links.



Periodic Table of Elements.

➡ **To show periodic table:**
Choose Tools → Periodic Table from the main menu.

➡ **To highlight group of elements:**
Select the group name from the *Highlight* combo box.

➡ **To see element name and mass:**
Press the element button.

➡ **To see isotopic pattern of element:**
Select the element in the table and press Isotopes button. Element pattern will be shown in *Mass Calculator* tool.

➡ **To see detailed information about element:**
Select the element in the table and press Wikipedia button. Corresponding wiki page shows up in your web browser.

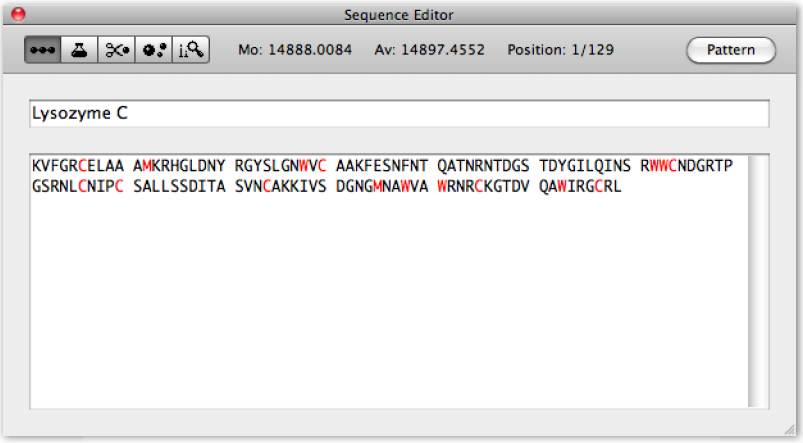
➡ **To see element photos:**
Select the element in the table and press Photos button. Corresponding photo page shows up in your web browser.

11. Sequence Tools

mMass provides an internal *Sequence Editor*, which can be used to make any protein or peptide sequence available for other tools. Any modification can be applied either as fixed or variable. *Protein Digest* tool can be used to generate a list of peptides resulting from *in silico* enzymatic or chemical digestion of specified protein sequence. Similarly, *Peptide Fragmentation* tool generates a list of common peptide fragments. In both cases, all possible combinations of variable modifications are calculated and results can be easily compared with measured data. In addition, sequence can be searched for a peptide mass by *Mass Search* tool to identify any non-specific cleavages.

11.1. Sequence Editor

Internal *Sequence Editor* provides a tool to define protein or peptide sequence to be available for other tools. Sequence can be manually typed, pasted from clipboard or imported from any *mMass* or *FASTA* document. Every input is checked automatically to contain only amino acids defined in *mMass's* library. Some basic information about the sequence are shown in the panel toolbar and theoretical isotopic pattern can be generated as well. If any modification is set, modified amino acids are shown in red.



Sequence Editor.

➡ **To add new sequence:**
Press + button from the *Documents Panel* bottom toolbar and select New Sequence or choose Sequence → New from the main menu. *Sequence Editor* shows up. Type your sequence manually or use copy/paste.

➡ **To import sequence:**
Choose Sequence → Import from the main menu and select your sequence file. If more than one sequence are available in the file, a selection dialog shows up. Select one or more sequence and press Import button. *mMass* and *FASTA* documents are currently supported.

➡ **To edit sequence:**
Double-click on the sequence title in *Documents Panel* and *Sequence Editor* shows up.

➡ **To delete sequence:**
Click on the sequence title in *Documents Panel* and press Command+Backspace or Delete, or press - button from the *Documents Panel* bottom toolbar and choose Delete Sequence.

➡ **To generate isotopic pattern from a whole sequence:**
In *Sequence Editor* press Pattern button.

If a sequence is pasted from the clipboard all white spaces and numbers are removed automatically. This can be very useful if you copy/paste a sequence from web sites.

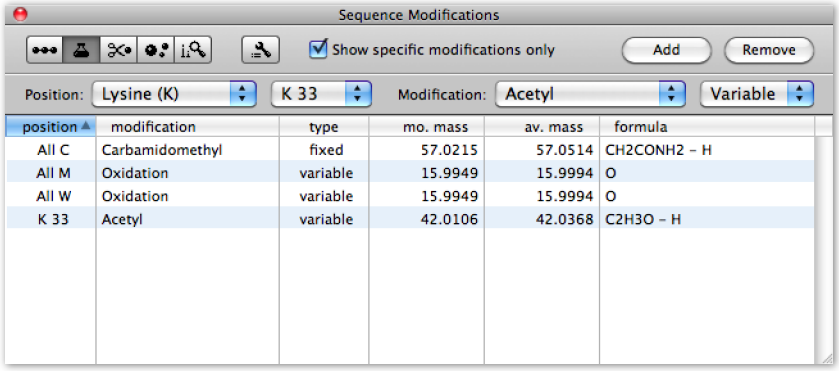
If you are using some sequences frequently, save them into *mMass* document as a sequence library.

Please note that only valid sequences are show in the import dialog and can be imported.

Please note that calculated sequence mass includes all fixed and variable modifications.

11.2. Modifications

In *Sequence Modifications* panel any post-translational modification can be set to a single amino acid or to selected type. Beside a position, for each modification you can specify whether it should be *Fixed* or *Variable* and all possible variants are then calculated in the sequence related tools. In order to avoid permanent assignment of the same modification set you can define your own presets and use it frequently.



Sequence Modifications.

- *Show specific modifications only* - show modifications specific for selected amino acid.
- *Position* - amino acid type and position.
- *Modification* - modification name and type.

➡ **To add modification:**
Press button from the *Sequence* panel toolbar to show up *Sequence Modifications*. Select amino acid type, position, modification and modification type and press Add button.

➡ **To remove modification:**
Press button from the *Sequence* panel toolbar to show up *Sequence Modifications*. Select desired modification in the list and press Remove button.

➡ **To edit modification:**
Choose Libraries → Modifications from the main menu to show up *Modifications Library* editor. See *Libraries* chapter for more information.

➡ **To define new modification:**
Choose Libraries → Modifications from the main menu to show up *Modifications Library* editor. See *Libraries* chapter for more information.

➡ **To save current global modifications as presets:**
Press button from the panel toolbar and choose Save as Presets. In the dialog type the presets name and press Save button.

➡ **To use saved presets:**
Press button from the panel toolbar and choose any of your presets from the pup-up menu.

➡ **To delete saved presets:**
Choose Libraries → Presets from the main menu to show up *Presets Library* editor. Choose the presets you'd like to delete and press Delete button.

➡ **To rename saved presets:**
Choose Libraries → Presets from the main menu to show up *Presets Library* editor. Choose the presets you'd like to rename, type the new name and press Rename button.

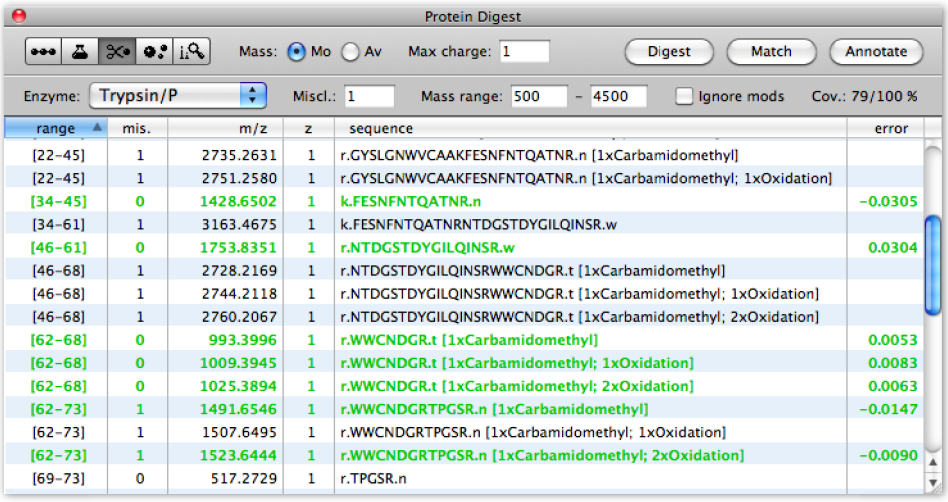
By default, only specific modifications for selected amino acid are shown, however, all available modifications can be enabled by unchecking *Show specific modifications only* checkbox.

Please note that multiple modifications on a single residue are not allowed.

Please note that only global modifications can be stored in presets.

11.3. Protein Digest

Many experiments, involving detection of modifications, protein validation etc., apply the specific enzymatic digestion of a protein with a known sequence. *Protein Digest* panel provides a tool which can be used to generate a list of peptides resulting from *in silico* digestion of a sequence. Masses of these peptides can then be compared with current peak list within a specified tolerance to see any matches. In addition, theoretical isotopic patterns can be generated and overlaid with the data to validate matches.



range	mis.	m/z	z	sequence	error
[22-45]	1	2735.2631	1	r.GYSLGNWVCAAKFESNFNTQATNR.n [1xCarbamidomethyl]	
[22-45]	1	2751.2580	1	r.GYSLGNWVCAAKFESNFNTQATNR.n [1xCarbamidomethyl; 1xOxidation]	
[34-45]	0	1428.6502	1	k.FESNFNTQATNR.n	-0.0305
[34-61]	1	3163.4675	1	k.FESNFNTQATNRNTDGSTDYGILQINSR.w	
[46-61]	0	1753.8351	1	r.NTDGSTDYGILQINSR.w	0.0304
[46-68]	1	2728.2169	1	r.NTDGSTDYGILQINSRWWCNDGR.t [1xCarbamidomethyl]	
[46-68]	1	2744.2118	1	r.NTDGSTDYGILQINSRWWCNDGR.t [1xCarbamidomethyl; 1xOxidation]	
[46-68]	1	2760.2067	1	r.NTDGSTDYGILQINSRWWCNDGR.t [1xCarbamidomethyl; 2xOxidation]	
[62-68]	0	993.3996	1	r.WWCNDGR.t [1xCarbamidomethyl]	0.0053
[62-68]	0	1009.3945	1	r.WWCNDGR.t [1xCarbamidomethyl; 1xOxidation]	0.0083
[62-68]	0	1025.3894	1	r.WWCNDGR.t [1xCarbamidomethyl; 2xOxidation]	0.0063
[62-73]	1	1491.6546	1	r.WWCNDGRTPGSR.n [1xCarbamidomethyl]	-0.0147
[62-73]	1	1507.6495	1	r.WWCNDGRTPGSR.n [1xCarbamidomethyl; 1xOxidation]	
[62-73]	1	1523.6444	1	r.WWCNDGRTPGSR.n [1xCarbamidomethyl; 2xOxidation]	-0.0090
[69-73]	0	517.2729	1	r.TPGSR.n	

Protein Digest tool.

- *Mass* - mass type to be used for calculations.
- *Max charge* - maximum charge to be calculated.
- *Enzyme* - enzyme to be used to simulate digestion.
- *Miscl.* - maximum number of enzyme miss cleavages.
- *Mass range* - m/z range for peptides to be calculated.
- *Ignore mods* - ignore modifications in cleavage site.
- *Cov.* - matched / theoretical sequence coverage.

➡ **To digest protein:**
Double-click on the sequence title in *Documents Panel* to show up *Sequence* tools and press button for *Protein Digest* tool. Specify all the parameters and press Digest button.

➡ **To highlight peptide mass in spectrum viewer:**
Click on the peptide and spectrum moves to theoretical m/z value. Small red arrow shows up on m/z axis of the spectrum. Current zoom range remains the same.

➡ **To show isotopic pattern of peptide:**
Double-click on the peptide to show up *Mass Calculator* panel. Peptide formula appears in *Formula* field and corresponding ion type is selected. See *Mass Calculator* chapter for more information.

➡ **To match peptides to peak list:**
Generate theoretical peptides and press Match button in the panel toolbar to show up *Match Peptides* panel. Matched peptides shows green and bold in the list. See *Data Matching* chapter for more information.

➡ **To annotate peaks by matched peptides:**
Press Annotate button in the panel toolbar. All matches show up in *Documents Panel* under current sequence.

➡ **To copy peptide sequence into clipboard:**
Right-click on any peptide and choose *Copy Selected Sequence* from pop-up menu.

➡ **To copy peptides into clipboard:**
Click into the list and press Command+C (Ctrl+C on MS Windows and Linux) or use pop-up menu.

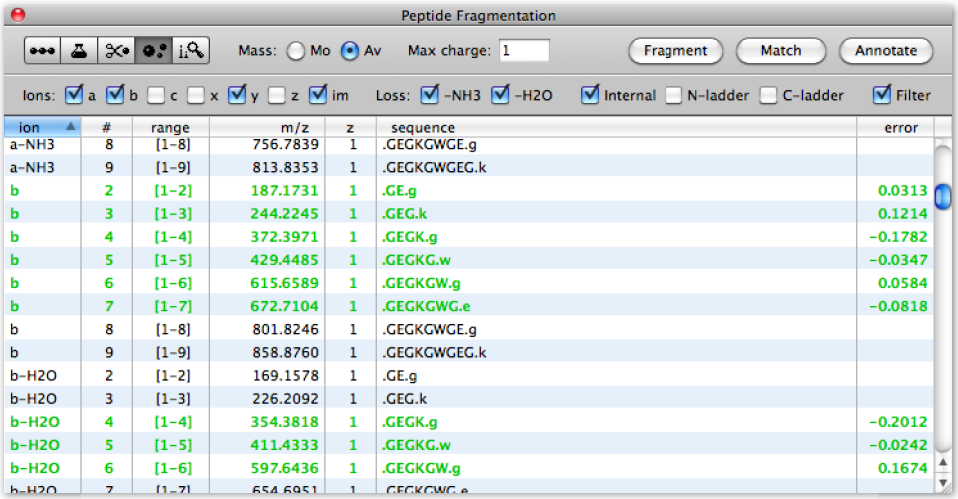
➡ **To see matched/unmatched peptides only:**
Right-click into the list and select view option from pop-up menu.

All variants are calculated for peptides with variable modifications.

Use theoretical sequence coverage to select the right enzyme for particular protein and mass range.

11.4. Peptide Fragmentation

Different types of fragmentation techniques can be used for the validation of a peptide sequence, as well as for the detection, localization and characterization of post-translational modifications. For these types of experiments, common fragments of a peptide sequence can be generated *in silico* using *Peptide Fragmentation* tool. Depending on a fragmentation technique used, different fragments can be generated. Some of the peptide fragments are theoretical only and can be filtered using *Filter* check box. Such fragments are shown in grey and italic when filtering is disabled.



ion	#	range	m/z	z	sequence	error
a-NH3	8	[1-8]	756.7839	1	.GEGKGWGE.g	
a-NH3	9	[1-9]	813.8353	1	.GEGKGWGEG.k	
b	2	[1-2]	187.1731	1	.GE.g	0.0313
b	3	[1-3]	244.2245	1	.GEG.k	0.1214
b	4	[1-4]	372.3971	1	.GEGK.g	-0.1782
b	5	[1-5]	429.4485	1	.GEGKG.w	-0.0347
b	6	[1-6]	615.6589	1	.GEGKGW.g	0.0584
b	7	[1-7]	672.7104	1	.GEGKGWG.e	-0.0818
b	8	[1-8]	801.8246	1	.GEGKGWGE.g	
b	9	[1-9]	858.8760	1	.GEGKGWGEG.k	
b-H2O	2	[1-2]	169.1578	1	.GE.g	
b-H2O	3	[1-3]	226.2092	1	.GEG.k	
b-H2O	4	[1-4]	354.3818	1	.GEGK.g	-0.2012
b-H2O	5	[1-5]	411.4333	1	.GEGKG.w	-0.0242
b-H2O	6	[1-6]	597.6436	1	.GEGKGW.g	0.1674
b-H2O	7	[1-7]	654.6951	1	.GEGKGWG.e	

Peptide Fragmentation tool.

- *Mass* - mass type to be used for calculations.
- *Max charge* - maximum charge to be calculated.
- *Ions* - common fragment types to be calculated.
- *Loss* - common losses to be calculated.
- *Internal* - calculate internal fragments.
- *N-ladder* - calculate N-ladder fragments.
- *C-ladder* - calculate C-ladder fragments.
- *Filter* - filter nonsense fragments.

➡ **To fragment peptide:**
Double-click on the sequence title in *Documents Panel* to show up *Sequence* tools and press button for *Peptide Fragmentation* tool. Specify all the parameters and press Fragment button.

➡ **To highlight fragment mass in spectrum viewer:**
Click on the fragment and spectrum moves to theoretical m/z value. Small red arrow shows up on m/z axis of the spectrum. Current zoom range remains the same.

➡ **To show isotopic pattern of fragment:**
Double-click on the fragment to show up *Mass Calculator* panel. Fragment formula appears in *Formula* field and corresponding ion type is selected. See *Mass Calculator* chapter for more information.

➡ **To match fragments to peak list:**
Generate theoretical fragments and press Match button in the panel toolbar to show up *Match Fragments* panel. Matched fragments shows green and bold in the list. See *Data Matching* chapter for more information.

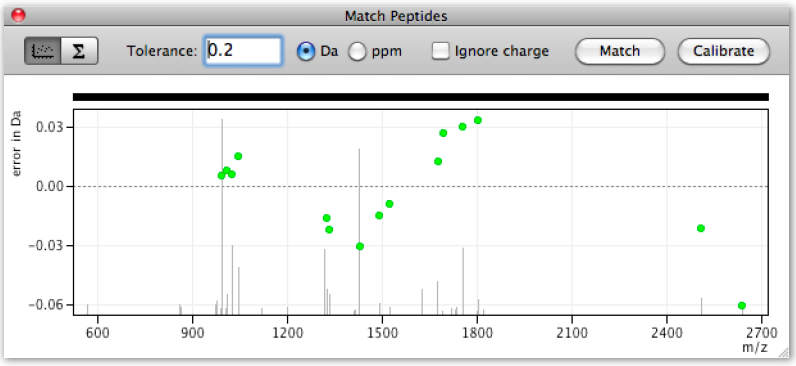
➡ **To annotate peaks by matched fragments:**
Press Annotate button in the panel toolbar. All matches show up in *Documents Panel* under current sequence.

➡ **To copy fragments into clipboard:**
Click into the list and press Command+C (Ctrl+C on MS Windows and Linux) or use pop-up menu.

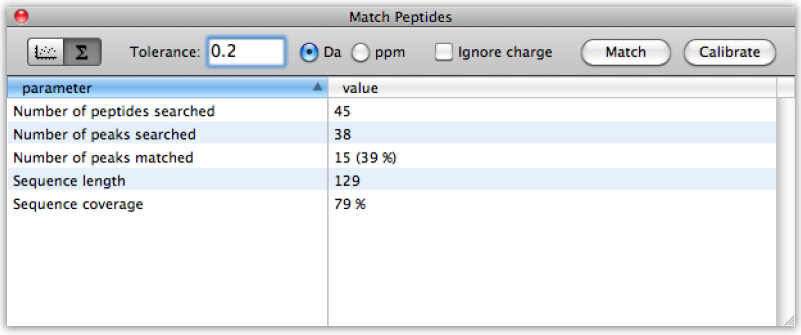
➡ **To see matched/unmatched fragments only:**
Right-click into the list and select view option from pop-up menu.

11.5. Data Matching

Both, theoretical peptides and fragments lists can be compared with peak list of current document by pressing Match button in corresponding tool. If some of the peptides or fragments are matched successfully you can use them for data recalibration.



Match tool.



Match summary.

- *Tolerance* - mass tolerance for data matching.
- *Da, ppm* - units for tolerance value.
- *Ignore charge* - ignore peak charge while data matching.

➡ **To match peptides to peak list:**
Generate theoretical peptides in *Protein Digest* tool and press Match button in the panel toolbar to show up *Match Peptides* panel. Specify the parameters and press Match button. Matched peptides shows green and bold in the peptides list.

➡ **To match fragments to peak list:**
Generate theoretical fragments in *Peptide Fragmentation* tool and press Match button in the panel toolbar to show up *Match Fragments* panel. Specify the parameters and press Match button. Matched fragments shows in green and bold in the fragments list.

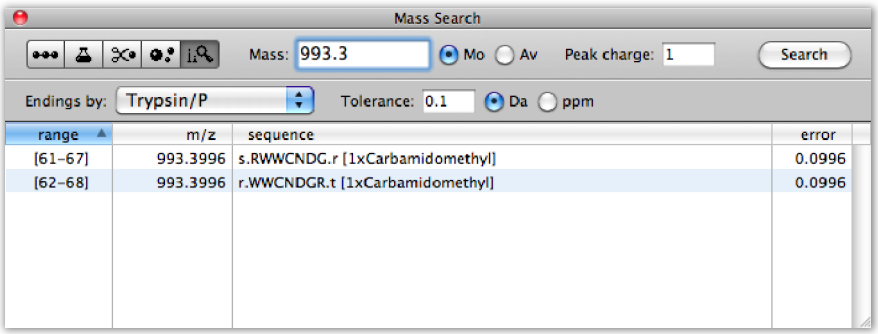
➡ **To ignore peak charge and use only m/z value while data matching:**
Check *Ignore charge* checkbox.

➡ **To re-calibrate data using matches:**
Press Calibrate button in the panel toolbar to send matched items into *Calibration* tool. See *Calibration* chapter for more information. Please be se careful while using this feature!

Use the same spectrum manipulation conventions in the error plot as in the main *Spectrum Viewer*.

11.6. Mass Search

Using sequence *Mass Search* tool you can search a sequence for any peptide of specified m/z. This tool can be very useful for identification of the peaks resulting from non-specific cleavage of a protein.



Mass Search tool.

- *Mass* - peptide mass to be searched.

- *Mo, Av* - mass type to be searched.
- *Max charge* - maximum charge to be calculated for peptides.
- *Endings by* - peptide "caps" (e.g. H and OH).
- *Tolerance* - mass tolerance for searching.
- *Da, ppm* - units for tolerance value.

➡ **To search sequence:**
Double-click on the sequence title in *Documents Panel* to show up *Sequence* tools and press button for *Mass Search* tool. Specify all the parameters and press Search button. List of matched peptides will be shown.

➡ **To highlight peptide mass in spectrum viewer:**
Click on the peptide and spectrum moves to theoretical m/z value. Small red arrow shows up on m/z axis of the spectrum. Current zoom range remains the same.

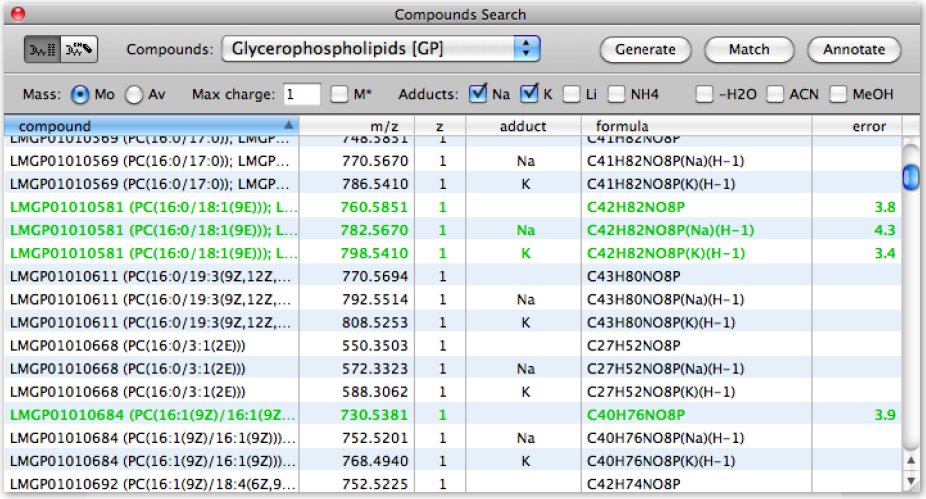
➡ **To show isotopic pattern of peptide:**
Double-click on the peptide to show up *Mass Calculator* panel. Peptide formula appears in *Formula* field and corresponding ion type is selected. See *Mass Calculator* chapter for more information.

➡ **To copy peptide sequence into clipboard:**
Right-click on any peptide and choose *Copy Selected Sequence* from pop-up menu.

➡ **To copy peptides into clipboard:**
Click into the list and press Command+C (Ctrl+C on MS Windows and Linux) or use pop-up menu.

12.Compounds Search

Using *Compounds Search* tool you can search for any user-specified compound or even a list of compounds in a peak list. Every compound is specified in *mMass's* library as molecular formula, title and description, therefore both monoisotopic or average masses can be search with any charge. In addition common adducts can be searched automatically as well. All the matched peaks can be annotated and then shown or printed within analysis report.



compound	m/z	z	adduct	formula	error
LMGP01010569 (PC(16:0/17:0)); LMGP...	770.5670	1	Na	C41H82NO8P(Na)(H-1)	
LMGP01010569 (PC(16:0/17:0)); LMGP...	786.5410	1	K	C41H82NO8P(K)(H-1)	
LMGP01010581 (PC(16:0/18:1(9E))); L...	760.5851	1		C42H82NO8P	3.8
LMGP01010581 (PC(16:0/18:1(9E))); L...	782.5670	1	Na	C42H82NO8P(Na)(H-1)	4.3
LMGP01010581 (PC(16:0/18:1(9E))); L...	798.5410	1	K	C42H82NO8P(K)(H-1)	3.4
LMGP01010611 (PC(16:0/19:3(9Z,12Z,...	770.5694	1		C43H80NO8P	
LMGP01010611 (PC(16:0/19:3(9Z,12Z,...	792.5514	1	Na	C43H80NO8P(Na)(H-1)	
LMGP01010611 (PC(16:0/19:3(9Z,12Z,...	808.5253	1	K	C43H80NO8P(K)(H-1)	
LMGP01010668 (PC(16:0/3:1(2E)))	550.3503	1		C27H52NO8P	
LMGP01010668 (PC(16:0/3:1(2E)))	572.3323	1	Na	C27H52NO8P(Na)(H-1)	
LMGP01010668 (PC(16:0/3:1(2E)))	588.3062	1	K	C27H52NO8P(K)(H-1)	
LMGP01010684 (PC(16:1(9Z)/16:1(9Z...	730.5381	1		C40H76NO8P	3.9
LMGP01010684 (PC(16:1(9Z)/16:1(9Z)))...	752.5201	1	Na	C40H76NO8P(Na)(H-1)	
LMGP01010684 (PC(16:1(9Z)/16:1(9Z)))...	768.4940	1	K	C40H76NO8P(K)(H-1)	
LMGP01010692 (PC(16:1(9Z)/18:4(6Z,9...	752.5225	1		C42H74NO8P	

Compounds Search tool.

- *Compounds* - compounds list to be searched.
- *Formula* - compound formula to be searched.
- *Mass* - mass type to be searched.
- *Max charge* - maximum charge to be calculated.
- *M** - calculate radical ions.
- *Adducts* - type of adduct to be searched.

➡ **To search for list of compounds:**
Press button from the main toolbar or choose Tools → Compounds Search from the main menu and select tool in the panel toolbar. Select *Compounds* list name, set the parameters and press Generate button. Then press Match button to show up *Match Compounds* tool.

➡ **To search for specified formula:**
Press button from the main toolbar or choose Tools → Compounds Search from the main menu and select tool in the panel toolbar. Type compound *Formula*, set the parameters and press Generate button. Then press Match button to show up *Match Compounds* tool. See *Mass Calculator* chapter for more information about formula syntax.

➡ **To highlight compound mass in spectrum viewer:**
Click on the compound and spectrum moves to theoretical m/z value. Small red arrow shows up on m/z axis of the spectrum. Current zoom range remains the same.

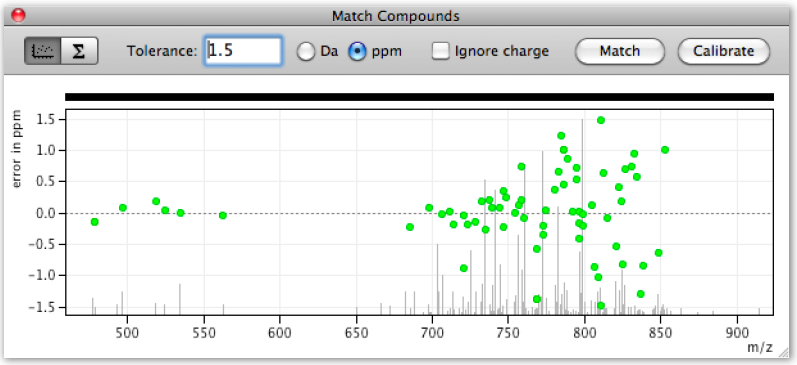
➡ **To show isotopic pattern of compound:**
Double-click on the compound to show up *Mass Calculator* panel. Compound formula appears in *Formula* field and corresponding ion type is selected automatically. See *Mass Calculator* chapter for more information.

➡ **To copy compounds into clipboard:**
Click into the list and press Command+C (Ctrl+C on MS Windows and Linux).

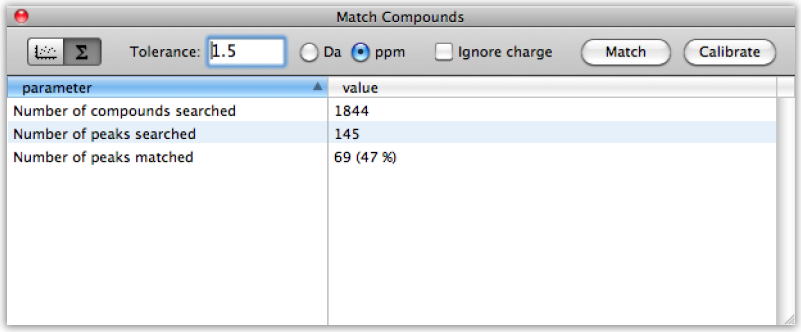
➡ **To see matched/unmatched compounds only:**
Right-click into the list and select view option from pop-up menu.

➡ **To define a new list of compounds:**
Choose Libraries → Compounds from the main menu to show up *Compounds Library* editor. See *Libraries* chapter for more information.

➡ **To match compounds to peak list:**
Generate theoretical compounds and press Match button in the panel toolbar to show up *Match Compounds* panel. Matched compounds shows in green and bold.



Compounds match tool.



Compounds match summary.

- *Tolerance* - mass tolerance for data matching.
- *Da, ppm* - units for tolerance value.
- *Ignore charge* - ignore peak charge while data matching.

➡ **To annotate peaks by matched compounds:**
Press Annotate button in panel toolbar. All matches show up in *Documents Panel* under *Annotations*.

➡ **To ignore peak charge while data matching:**
Check *Ignore charge* checkbox.

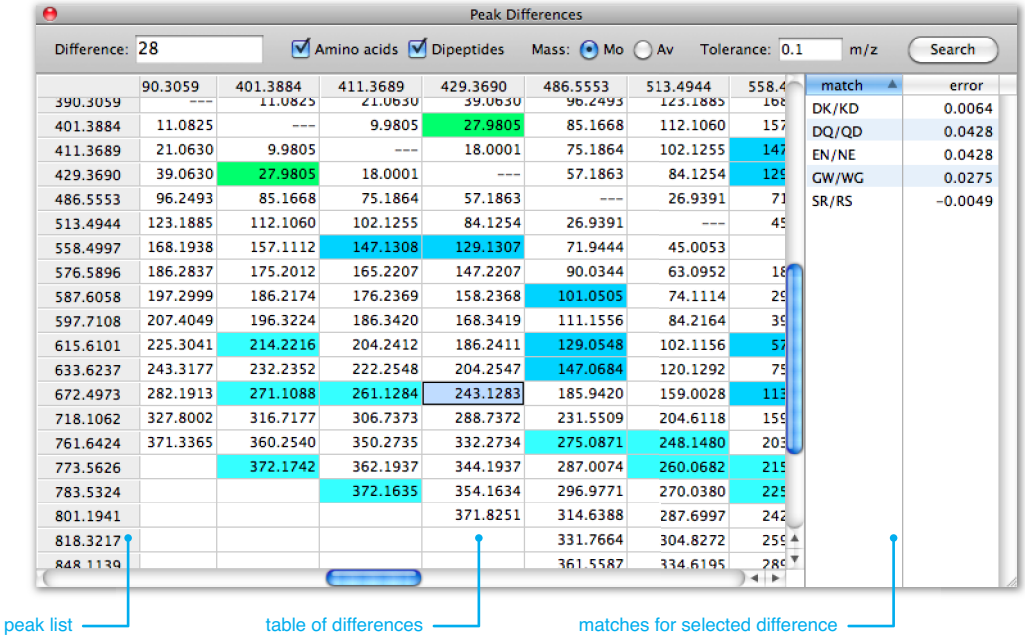
➡ **To re-calibrate data using matches:**
Press Calibrate button in the panel toolbar to send matched items into *Calibration* tool. See *Calibration* chapter for more information. Please be se careful while using this feature!

Use the same spectrum manipulation conventions in the error plot as in the main *Spectrum Viewer*.

See match summary panel for more information about current match.

13.Peak Differences

Interpretation of mass spectra typically involves a seemingly never-ending check of the differences between all peaks in a spectrum. However, *Peak Differences* tool is able to simply generate a table of all the differences between the peaks in the peak list. This table can then be used to automatically compare, within a specified tolerance, each difference with the respective masses of all amino acids, calculated dipeptides or specified m/z value. *Peak Differences* tool therefore provides a useful utility for *de novo* peptide sequencing or PTM search.



Peak Differences tool.

- *Difference* - user defined m/z difference to searched.
- *Amino acids* - all available amino acids will be searched.
- *Dipeptides* - all calculated dipeptides will be searched.
- *Mass* - mass type to be used for amino acids and dipeptides calculation.
- *Tolerance* - mass tolerance for searching.

➡ **To show peak differences tool:**
Press button from the main toolbar or choose Tools → Peak Differences from the main menu.

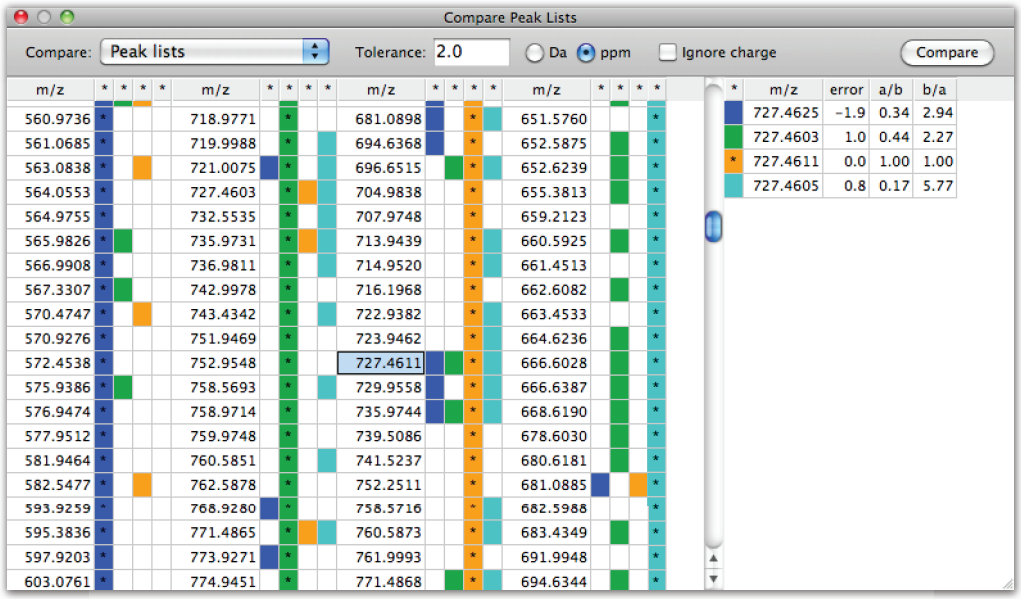
➡ **To search:**
Specify all the parameters and press Search button from the panel toolbar. Click on any highlighted differences to see corresponding matches.

If the specified mass is matched, corresponding difference turns green. If at least one amino acid is matched, corresponding difference turns dark blue. If at least one dipeptide is matched, corresponding difference turns light blue.

Please note that the differences which does not make sense for current mass range (for specified Difference, Amino acids and Dipeptides) are not shown for better readability.

14.Compare Peak Lists

Similarly as the *Peak Differences* tool, the *Compare Peak Lists* tool can easily be utilized to compare peak lists or annotations between multiple documents. Using this tool, one of the most typical and annoying manual task can be automatically performed within a few clicks. Once the tool is shown, all of the opened documents are loaded and marked by its own spectrum color and can be compared within the specified mass tolerance. For each peak identified in a different document, corresponding document color is shown next to the *m/z* value. By selecting any *m/z* value in the peak lists table, all the matched peaks are shown followed by error and intensity ratios (*a* - selected peak, *b* - matched peak).



Compare Peak Lists tool.

- *Compare* - data type to be compared.
- *Tolerance* - mass tolerance for comparison.
- *Da, ppm* - units for tolerance value.
- *Ignore charge* - ignore peak charge while comparing peaks.

➡ **To show compare peak lists tool:**
Press button from the main toolbar or choose Tools → Compare Peak Lists from the main menu.

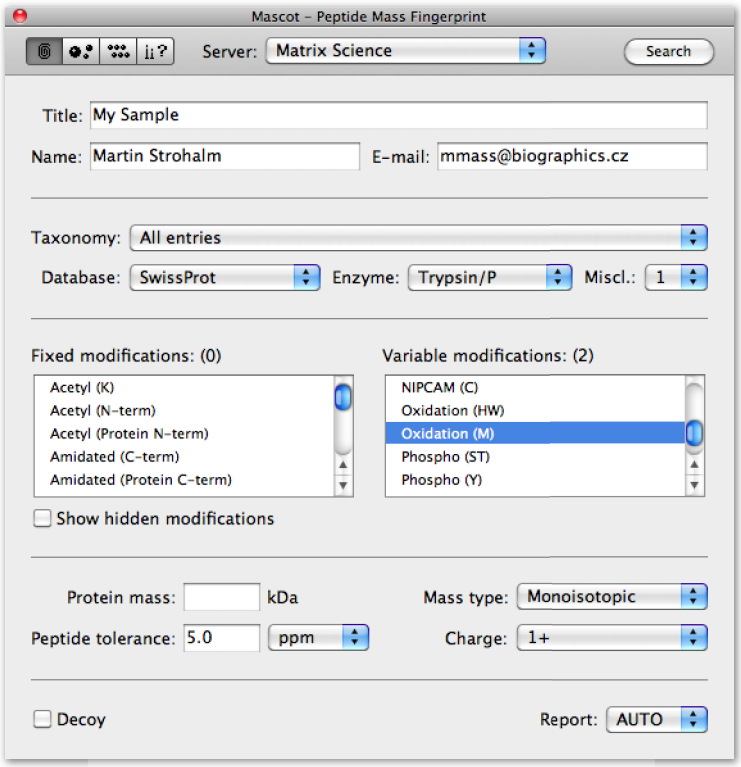
➡ **To compare:**
Specify all the parameters and press Compare button from the panel toolbar. Click on any *m/z* value in the peak lists table to see corresponding matches.

➡ **To remove peak list temporarily:**
Disable document by clicking the corresponding document bullet in the main *Documents Panel*.

➡ **To copy tables into clipboard:**
Click into the table you'd like to copy and press Command+C (Ctrl+C on MS Windows and Linux).

15.Mascot Search

mMass provides an interface that allows data to be directly sent to the main tools available on *Mascot* website (http://www.matrixscience.com); *Peptide Mass Fingerprint, Sequence Query* and *MS/MS Ion Search*. When Search button is pressed, temporary *HTML* page is generated containing all the parameters and using *JavaScript*, the page is automatically sent to selected server. Please see the *Mascot* website for more information about the tools and the form fields.



Peptide Mass Fingerprint search tool.

➡ **To show peptide mass fingerprint tool:**
Press button from the main toolbar to show Mascot tools and press button from the panel toolbar or choose Tools → Mascot Peptide Mass Fingerprint from the main menu.

➡ **To show MS/MS ion search tool:**
Press button from the main toolbar to show Mascot tools and press button from the panel toolbar or choose Tools → Mascot MS/MS Ion Search from the main menu.

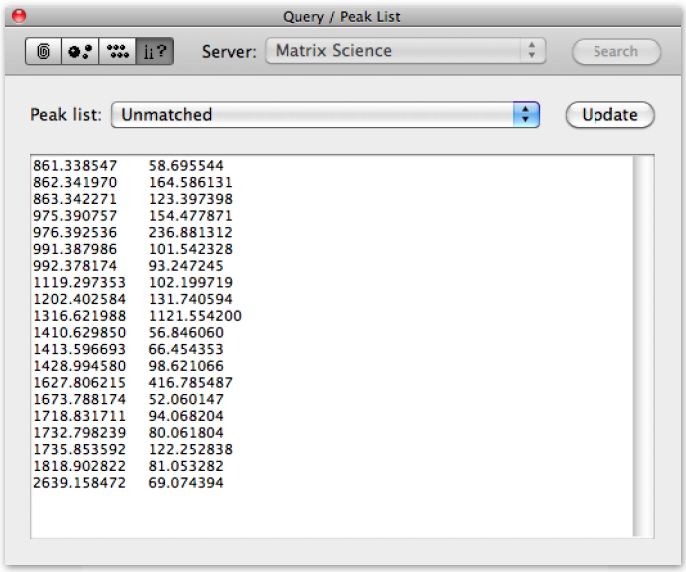
➡ **To show sequence query tool:**
Press button from the main toolbar to show Mascot tools and press button from the panel toolbar or choose Tools → Mascot Sequence Query from the main menu.

➡ **To change server:**
Select the *Server* in the panel toolbar.

➡ **To send data to server:**
Specify all the parameters and press Send button in the panel toolbar. *HTML* page will be generated and sent to specified server. Results show up in your default web browser.

➡ **To define new server:**
Choose Libraries → Mascot Servers from the main menu to show up *Mascot Servers Library* editor. See *Libraries* chapter for more information.

➡ **To specify peak list or query:**
Press from the panel toolbar and type your query manually or use *Peak list* selection.



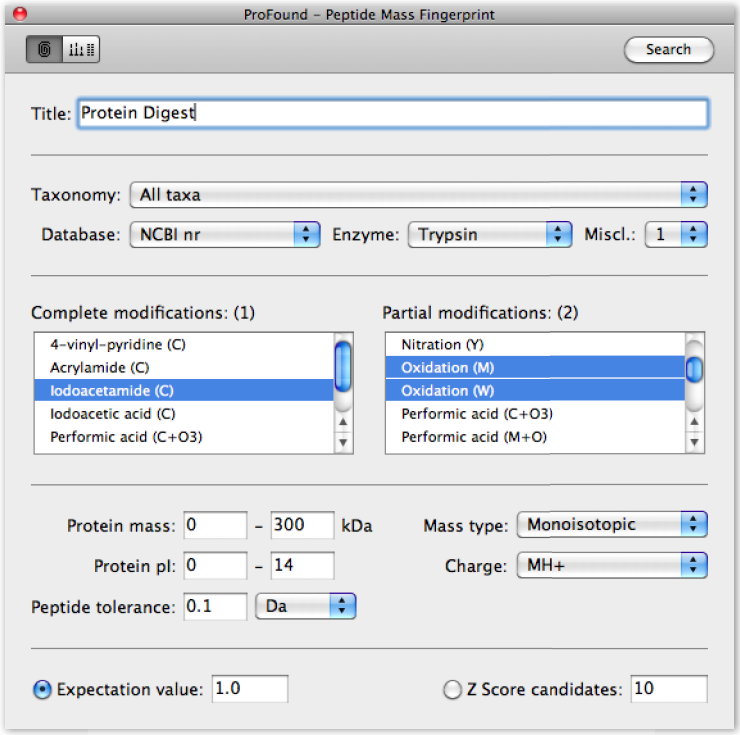
Query / Peak List.

See http://www.matrixscience.com website for more information about *Mascot* tools and form parameters.

Please note that while changing server, most of the form fields changed as well. Check if the form is filled correctly.

16.ProFound Search

mMass provides an interface that allows data to be directly sent to *ProFound* search tool available on a website of Professor Brian T. Chait group (http://prowl.rockefeller.edu). When Search button is pressed, temporary *HTML* page is generated containing all the parameters and using *JavaScript*, the page is automatically sent to *ProFound* server. Please see the *ProFound* website for more information about the tool and the form fields.



ProFound search tool.

➡ **To show ProFound tool:**
Press PRO FOUND button from the main toolbar or choose Tools → ProFound from the main menu.

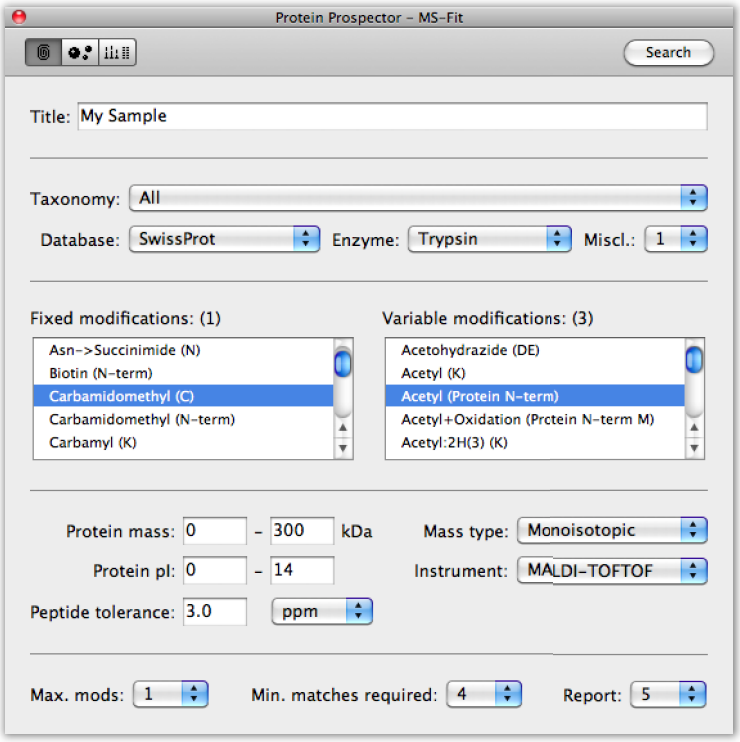
➡ **To send data to server:**
Specify all the parameters and press Send button in the panel toolbar. *HTML* page will be generated and sent to *ProFound* server. Results show up in your default web browser.

➡ **To specify peak list:**
Press from the panel toolbar and use *Peak list* selection.

See http://prowl.rockefeller.edu website for more information about *ProFound* tool and form parameters.

17.Protein Prospector Search

mMass provides a simplified interface that allows data to be directly sent to the main tools available on *Protein Prospector* website (http://prospector.ucsf.edu); *MS-Fit* and *MS-Tag*. When Search button is pressed, temporary *HTML* page is generated containing all the parameters and using *JavaScript*, the page is automatically sent to *Protein Prospector* server. Please see the *Protein Prospector* website for more information about the tools and the form fields.



MS-Fit search tool.

➡ **To show MS-Fit tool:**
Choose Tools → Protein Prospector MS-Fit from the main menu.

➡ **To show MS-Tag tool:**
Choose Tools → Protein Prospector MS-Tag from the main menu.

➡ **To send data to server:**
Specify all the parameters and press Send button in the panel toolbar. *HTML* page will be generated and sent to *Protein Prospector* server. Results show up in your default web browser.

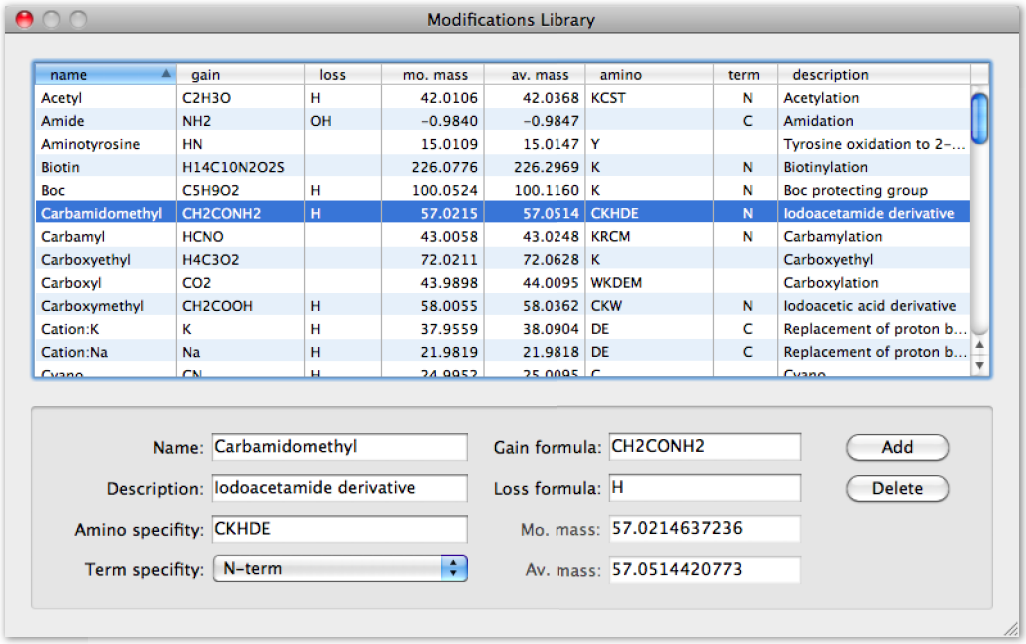
➡ **To specify peak list:**
Press from the panel toolbar and use *Peak list* selection.

See http://prospector.ucsf.edu website for more information about *ProteinProspector* tools and form parameters.

18. Libraries

All *mMass's* libraries and configuration files are located within a single configuration folder having different locations, depending on your platform. On Mac OS X, all configuration files can be found under *"~/Library/Application Support/mMass/"*. On MS Windows and Linux systems, all configuration files can be found under *"configs"* folder, located directly under the *mMass's* main folder. All files are in XML-based formats and can be easily edited manually, however, it is strongly recommended to use dedicated *mMass's* tools.

18.1. Modifications



Modifications Library editor.

- *Name* - unique modification name.
- *Description* - brief description.
- *Amino specifity* - amino acids which can be modified.
- *Term specifity* - sequence terminus which can be modified.
- *Gain formula* - formula to be added to a sequence.
- *Loss formula* - formula to be removed from a sequence.
- *Mo. mass* - resulting monoisotopic mass.
- *Av. mass* - resulting average mass.

➡ **To show modification library editor:**
Choose Libraries → Modifications from the main menu.

➡ **To add modification:**
Open *Modifications Library* editor, specify all the modification parameters and press Add button.

➡ **To edit modification:**
Open *Modifications Library* editor, select the modification you'd like to edit, change the parameters and press Add button. If the *Name* remains the same you will be asked to Replace modification definition.

➡ **To rename modification:**
Open *Modifications Library* editor, select the modification you'd like to rename, change the *Name* and press Add button. New modification will be added and the old one can be deleted.

➡ **To delete modification:**
Open *Modifications Library* editor, select the modification you'd like to delete and press Delete button. It is not possible to delete modification which is used in one of the opened documents.

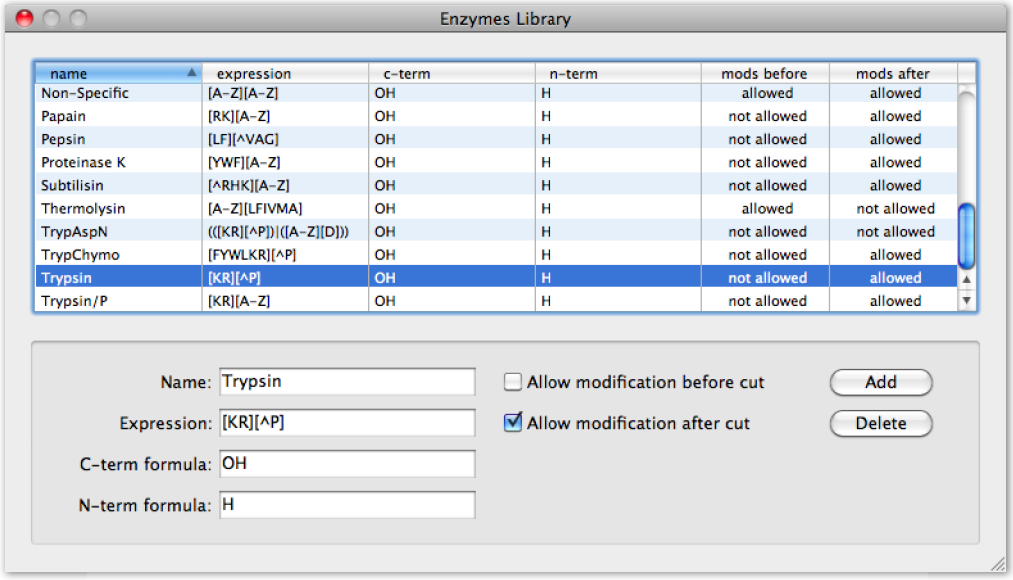

See *Mass Calculator* chapter for more information about formula syntax.


Monoisotopic and average masses are calculated automatically as you type the formula.


If you open a document with undefined modification this modification is added into your library automatically, however, the *Amino specifity* is set to ACDEFGHIKLMNPQRSTVWY.


Please note that the modification name must be unique for each modification.

18.2. Enzymes



Enzymes Library editor

- *Name* - unique enzyme name.
- *Expression* - enzyme regular expression.
- *C-term formula* - formula to be added at new C-terminus.
- *N-term formula* - formula to be added at new N-terminus.
- *Allow modification before cut* - allow modifications before cleavage site.
- *Allow modification after cut* - allow modifications after cleavage site.

➡ **To show enzymes library editor:**
Choose Libraries → Enzymes from the main menu.

➡ **To add enzyme:**
Open *Enzymes Library* editor, specify all the enzyme parameters and press Add button.

➡ **To edit enzyme:**
Open *Enzymes Library* editor, select the enzyme you'd like to edit, change the parameters and press Add button. If the *Name* remains the same you will be asked to Replace enzyme definition.

➡ **To rename enzyme:**
Open *Enzymes Library* editor, select the enzyme you'd like to rename, change the *Name* and press Add button. New enzyme will be added and the old one can be deleted.

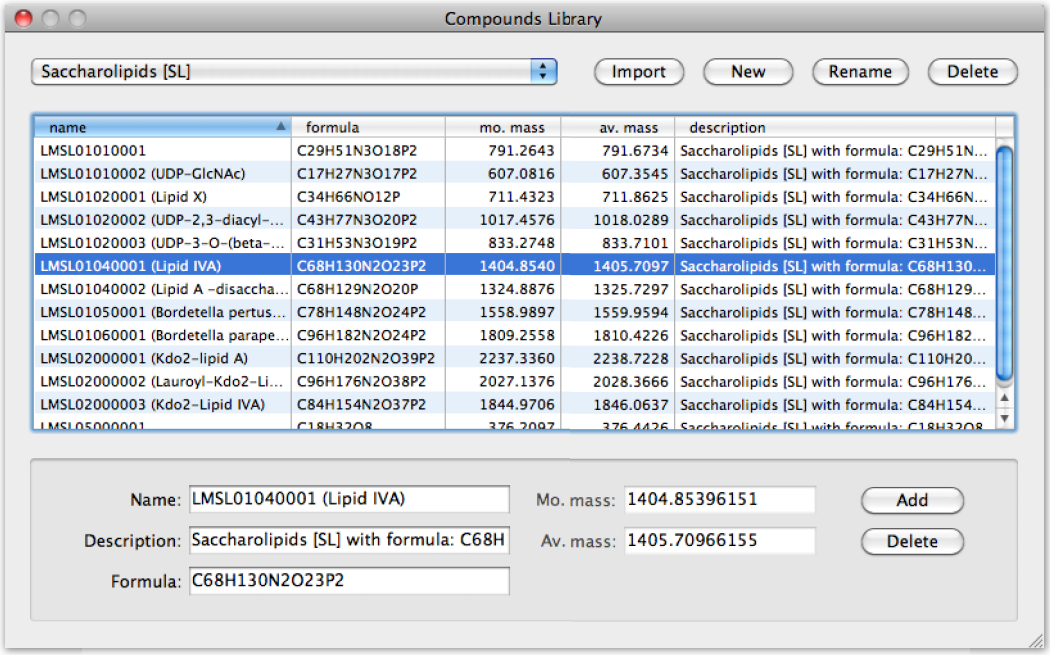
➡ **To delete enzyme:**
Open *Enzymes Library* editor, select the enzyme you'd like to delete and press Delete button.

The enzyme expression uses regular expression syntax where both, amino acids before and after cleavage must be defined. For example *[KR][A-Z]* for the Trypsin/P, where *[KR]* means that lysine or arginine must be before cleavage and *[A-Z]* means that any amino acid (i.e. character in the sequence) is allowed after cleavage. To block any amino acid use "^" like in the regular Trypsin *[KR][^P]*. See the http://docs.python.org/howto/regex.html#regex-howto for more information about regular expression syntax.

See *Mass calculator* chapter for more information about formula syntax.

Please note that the enzyme name must be unique for each enzyme.

18.3. Compounds



Compounds Library editor.

- *Name* - unique compound name.
- *Description* - brief description.
- *Formula* - compound formula
- *Mo. mass* - resulting monoisotopic mass.
- *Av. mass* - resulting average mass.

➡ **To show compounds library editor:**
Choose Libraries → Compounds from the main menu.

➡ **To import compounds lists:**
Open *Compounds Library* editor and press Import button on top of the panel. Select your compounds library and press Open button. Select compounds lists you'd like to import and press Import button. See above for location of all the libraries on your system.

➡ **To add new compounds list:**
Open *Compounds Library* editor and press New button on top of the panel. Type the name and press OK button.

➡ **To rename compounds list:**
Open *Compounds Library* editor, select the list you'd like to rename and press Rename button on top of the panel. Type the name and press OK button.

➡ **To delete compounds list:**
Open *Compounds Library* editor, select the list you'd like to delete and press Delete button on top of the panel.

➡ **To add compound:**
Open *Compounds Library* editor and select the list for the compound. Specify all the compound parameters and press Add button down on the panel.

➡ **To edit compound:**
Open *Compounds Library* editor and select the list containing the compound you'd like to edit. Change the compound parameters and press Add button down on the panel.

➡ **To rename compounds:**
Open *Compounds Library* editor and select the list containing the compound you'd like to rename. Change the *Name* and press Add button. New compound will be added and the old one can be deleted.

➡ **To delete compound:**
Open *Compounds Library* editor, select the list containing the compound you'd like to delete and press Delete button down on the panel.

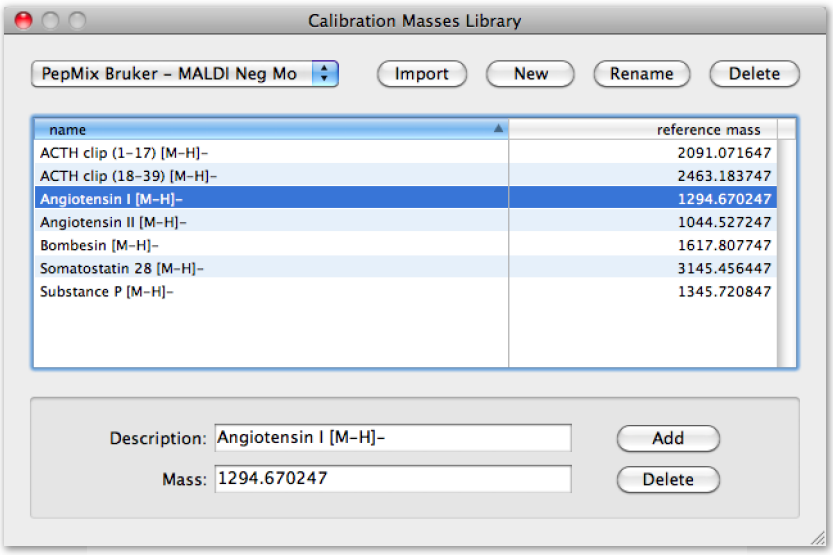

See *Mass Calculator* chapter for more information about formula syntax.


Monoisotopic and average masses are calculated automatically as you type the formula.


Please note that the group name must be unique for each group.


Please note that the compound name must be unique for each compound.

18.4. Calibration Masses



Calibration Masses editor.

- *Description* - calibrant name.
- *Mass* - reference mass.

➡ **To show calibration masses library editor:**
Choose Libraries → Calibration Masses from the main menu.

➡ **To import reference lists:**
Open *Calibration Masses Library* editor and press Import button on top of the panel. Select your references library and press Open button. Select references lists you'd like to import and press Import button. See above for location of all the libraries on your system.

➡ **To add new reference list:**
Open *Calibration Masses Library* editor and press New button on top of the panel. Type the name and press OK button.

➡ **To rename reference list:**
Open *Calibration Masses Library* editor, select the list you'd like to rename and press Rename button on top of the panel. Type the name and press OK button.

➡ **To delete reference list:**
Open *Calibration Masses Library* editor, select the list you'd like to delete and press Delete button on top of the panel. Type the name and press OK button.

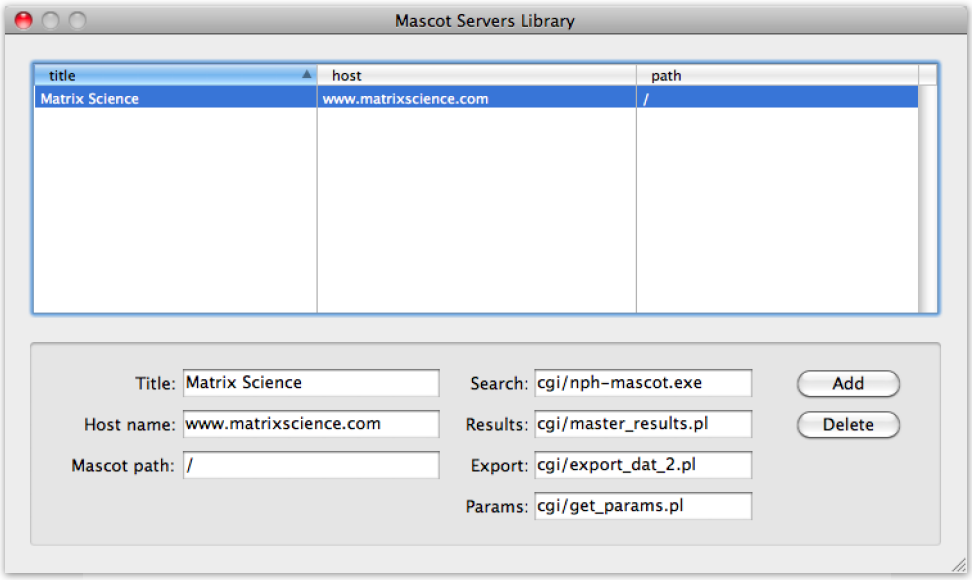
➡ **To add calibration mass:**
Open *Calibration Masses Library* editor and select the list for the calibration mass. Specify all the calibration mass parameters and press Add button down on the panel.

➡ **To edit calibration mass:**
Open *Calibration Masses Library* editor and select the list containing the calibration mass you'd like to edit. Change the calibration mass parameters and press Add button down on the panel.

➡ **To rename calibration mass:**
Open *Calibration Masses Library* editor and select the list containing the calibration mass you'd like to rename. Change the *Name* and press Add button. New calibration mass will be added and the old one can be deleted.

➡ **To delete calibration mass:**
Open *Calibration Masses Library* editor, select the list containing the calibration mass you'd like to delete and press Delete button down on the panel.

18.5. Mascot Servers



Mascot Servers Library editor.

- *Title* - server title.
- *Host name* - IP address or domain.
- *Mascot path* - path to the Mascot's main folder ("/" or "/mascot/" etc.).
- *Search* - path to the main search script (relative to the Mascot's main folder).
- *Results* - path to the results viewer script (relative to he Mascot's main folder).
- *Export* - path to the results export script (relative to he Mascot's main folder).
- *Params* - path to the form parameters values (relative to he Mascot's main folder).

➡ **To show mascot servers library editor:**
Choose Libraries → Mascot Servers from the main menu.

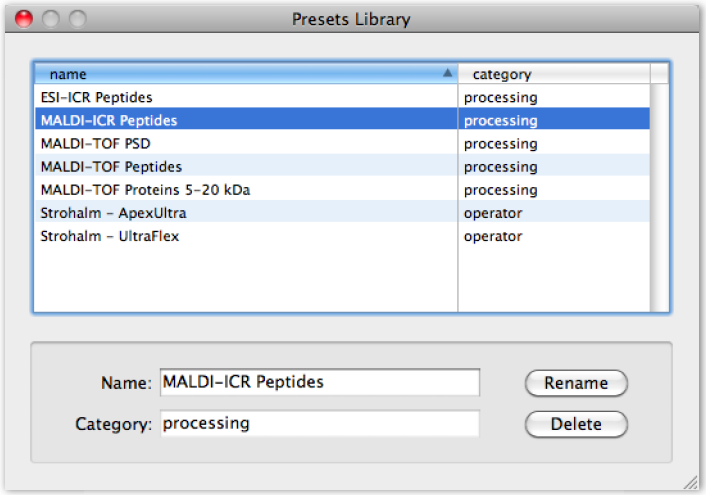
➡ **To add server:**
Open *Mascot Servers Library* editor, specify all the server parameters and press Add button.

➡ **To edit server:**
Open *Mascot Servers Library* editor, select the server you'd like to edit, change the parameters and press Add button. If the *Title* remains the same you will be asked to Replace server definition.

➡ **To rename server:**
Open *Mascot Servers Library* editor, select the server you'd like to rename, change the *Title* and press Add button. New server will be added and the old one can be deleted.

➡ **To delete server:**
Open *Mascot Servers Library* editor, select the server you'd like to delete and press Delete button.

18.6. Presets



Presets Library editor.

- *Name* - presets name.
- *Category* - presets category.

➡ **To show presets library editor:**
Choose Libraries → Presets from the main menu.

➡ **To rename presets:**
Open *Presets Library* editor, select the presets you'd like to rename, change the *Name* and press Rename button.

➡ **To delete presets:**
Open *Presets Library* editor, select the presets you'd like to delete and press Delete button.

19.Appendix

19.1. Elements

Configuration file *"elements.xml"* contains all the elements available for formula definitions.

```
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  <element symbol="As" name="Arsenic" atomicNumber="33">
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```

```
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    <isotope massNumber="132" mass="131.905056" abundance="0.00101" />
    <isotope massNumber="134" mass="133.904503" abundance="0.02417" />
    <isotope massNumber="135" mass="134.905683" abundance="0.06592" />
    <isotope massNumber="136" mass="135.90457" abundance="0.07854" />
    <isotope massNumber="137" mass="136.905821" abundance="0.11232" />
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    <isotope massNumber="150" mass="149.917271" abundance="0.0738" />
    <isotope massNumber="152" mass="151.919728" abundance="0.2675" />
    <isotope massNumber="154" mass="153.922205" abundance="0.2275" />
  </isotopes>
</element>
<element symbol="Sn" name="Tin" atomicNumber="50">
  <mass monoisotopic="119.9021966" average="118.710110491" />
  <isotopes>
    <isotope massNumber="112" mass="111.904821" abundance="0.0097" />
    <isotope massNumber="114" mass="113.902782" abundance="0.0066" />
    <isotope massNumber="115" mass="114.903346" abundance="0.0034" />
    <isotope massNumber="116" mass="115.901744" abundance="0.1454" />
    <isotope massNumber="117" mass="116.902954" abundance="0.0768" />
    <isotope massNumber="118" mass="117.901606" abundance="0.2422" />
    <isotope massNumber="119" mass="118.903309" abundance="0.0859" />
    <isotope massNumber="120" mass="119.9021966" abundance="0.3258" />
    <isotope massNumber="122" mass="121.9034401" abundance="0.0463" />
    <isotope massNumber="124" mass="123.9052746" abundance="0.0579" />
  </isotopes>
</element>
<element symbol="Sr" name="Strontium" atomicNumber="38">
  <mass monoisotopic="87.9056143" average="87.6166462926" />
  <isotopes>
    <isotope massNumber="84" mass="83.913425" abundance="0.0056" />
    <isotope massNumber="86" mass="85.9092624" abundance="0.0986" />
    <isotope massNumber="87" mass="86.9088793" abundance="0.07" />
    <isotope massNumber="88" mass="87.9056143" abundance="0.8258" />
  </isotopes>
</element>
<element symbol="Ta" name="Tantalum" atomicNumber="73">
  <mass monoisotopic="180.947996" average="180.947875936" />
  <isotopes>
    <isotope massNumber="180" mass="179.947466" abundance="0.00012" />
    <isotope massNumber="181" mass="180.947996" abundance="0.99988" />
  </isotopes>
</element>
<element symbol="Tb" name="Terbium" atomicNumber="65">
  <mass monoisotopic="158.925343" average="158.925343" />
  <isotopes>
    <isotope massNumber="159" mass="158.925343" abundance="1.0" />
  </isotopes>
</element>
<element symbol="Tc" name="Technetium" atomicNumber="43">
  <mass monoisotopic="97.907216" average="97.907216" />
  <isotopes>
    <isotope massNumber="97" mass="96.906365" abundance="0.0" />
```

```
    <isotope massNumber="98" mass="97.907216" abundance="1.0" />
    <isotope massNumber="99" mass="98.9062546" abundance="0.0" />
  </isotopes>
</element>
<element symbol="Te" name="Tellurium" atomicNumber="52">
  <mass monoisotopic="129.9062228" average="127.603125354" />
  <isotopes>
    <isotope massNumber="120" mass="119.90402" abundance="0.0009" />
    <isotope massNumber="122" mass="121.9030471" abundance="0.0255" />
    <isotope massNumber="123" mass="122.904273" abundance="0.0089" />
    <isotope massNumber="124" mass="123.9028195" abundance="0.0474" />
    <isotope massNumber="125" mass="124.9044247" abundance="0.0707" />
    <isotope massNumber="126" mass="125.9033055" abundance="0.1884" />
    <isotope massNumber="128" mass="127.9044614" abundance="0.3174" />
    <isotope massNumber="130" mass="129.9062228" abundance="0.3408" />
  </isotopes>
</element>
<element symbol="Th" name="Thorium" atomicNumber="90">
  <mass monoisotopic="230.0331266" average="765.802546733" />
  <isotopes>
    <isotope massNumber="230" mass="230.0331266" abundance="2.320381" />
    <isotope massNumber="232" mass="232.0380504" abundance="1.0" />
  </isotopes>
</element>
<element symbol="Ti" name="Titanium" atomicNumber="22">
  <mass monoisotopic="47.9479471" average="47.8667498036" />
  <isotopes>
    <isotope massNumber="46" mass="45.9526295" abundance="0.0825" />
    <isotope massNumber="47" mass="46.9517638" abundance="0.0744" />
    <isotope massNumber="48" mass="47.9479471" abundance="0.7372" />
    <isotope massNumber="49" mass="48.9478708" abundance="0.0541" />
    <isotope massNumber="50" mass="49.9447921" abundance="0.0518" />
  </isotopes>
</element>
<element symbol="Tl" name="Thallium" atomicNumber="81">
  <mass monoisotopic="204.974412" average="204.383317015" />
  <isotopes>
    <isotope massNumber="203" mass="202.972329" abundance="0.29524" />
    <isotope massNumber="205" mass="204.974412" abundance="0.70476" />
  </isotopes>
</element>
<element symbol="Tm" name="Thulium" atomicNumber="69">
  <mass monoisotopic="168.934211" average="168.934211" />
  <isotopes>
    <isotope massNumber="169" mass="168.934211" abundance="1.0" />
  </isotopes>
</element>
<element symbol="U" name="Uranium" atomicNumber="92">
  <mass monoisotopic="233.039628" average="792.730599067" />
  <isotopes>
    <isotope massNumber="233" mass="233.039628" abundance="2.3802891" />
    <isotope massNumber="234" mass="234.0409456" abundance="5.5e-05" />
    <isotope massNumber="235" mass="235.0439231" abundance="0.0072" />
    <isotope massNumber="236" mass="236.0455619" abundance="0.0" />
    <isotope massNumber="238" mass="238.0507826" abundance="0.992745" />
  </isotopes>
</element>
<element symbol="V" name="Vanadium" atomicNumber="23">
  <mass monoisotopic="50.9439637" average="50.9414716978" />
  <isotopes>
    <isotope massNumber="50" mass="49.9471628" abundance="0.0025" />
    <isotope massNumber="51" mass="50.9439637" abundance="0.9975" />
  </isotopes>
</element>
<element symbol="W" name="Tungsten" atomicNumber="74">
  <mass monoisotopic="183.9509326" average="183.841778628" />
  <isotopes>
    <isotope massNumber="180" mass="179.946706" abundance="0.0012" />
    <isotope massNumber="182" mass="181.948206" abundance="0.265" />
    <isotope massNumber="183" mass="182.9502245" abundance="0.1431" />
```

```
      <isotope massNumber="184" mass="183.9509326" abundance="0.3064" />
      <isotope massNumber="186" mass="185.954362" abundance="0.2843" />
    </isotopes>
  </element>
  <element symbol="Xe" name="Xenon" atomicNumber="54">
    <mass monoisotopic="131.9041545" average="131.292480845" />
    <isotopes>
      <isotope massNumber="124" mass="123.9058958" abundance="0.0009" />
      <isotope massNumber="126" mass="125.904269" abundance="0.0009" />
      <isotope massNumber="128" mass="127.9035304" abundance="0.0192" />
      <isotope massNumber="129" mass="128.9047795" abundance="0.2644" />
      <isotope massNumber="130" mass="129.9035079" abundance="0.0408" />
      <isotope massNumber="131" mass="130.9050819" abundance="0.2118" />
      <isotope massNumber="132" mass="131.9041545" abundance="0.2689" />
      <isotope massNumber="134" mass="133.9053945" abundance="0.1044" />
      <isotope massNumber="136" mass="135.90722" abundance="0.0887" />
    </isotopes>
  </element>
  <element symbol="Y" name="Yttrium" atomicNumber="39">
    <mass monoisotopic="88.9058479" average="88.9058479" />
    <isotopes>
      <isotope massNumber="89" mass="88.9058479" abundance="1.0" />
    </isotopes>
  </element>
  <element symbol="Yb" name="Ytterbium" atomicNumber="70">
    <mass monoisotopic="173.9388581" average="173.037691736" />
    <isotopes>
      <isotope massNumber="168" mass="167.933894" abundance="0.0013" />
      <isotope massNumber="170" mass="169.934759" abundance="0.0304" />
      <isotope massNumber="171" mass="170.936322" abundance="0.1428" />
      <isotope massNumber="172" mass="171.9363777" abundance="0.2183" />
      <isotope massNumber="173" mass="172.9382068" abundance="0.1613" />
      <isotope massNumber="174" mass="173.9388581" abundance="0.3183" />
      <isotope massNumber="176" mass="175.942568" abundance="0.1276" />
    </isotopes>
  </element>
  <element symbol="Zn" name="Zinc" atomicNumber="30">
    <mass monoisotopic="63.9291466" average="65.3955665657" />
    <isotopes>
      <isotope massNumber="64" mass="63.9291466" abundance="0.4863" />
      <isotope massNumber="66" mass="65.9260368" abundance="0.279" />
      <isotope massNumber="67" mass="66.9271309" abundance="0.041" />
      <isotope massNumber="68" mass="67.9248476" abundance="0.1875" />
      <isotope massNumber="70" mass="69.925325" abundance="0.0062" />
    </isotopes>
  </element>
  <element symbol="Zr" name="Zirconium" atomicNumber="40">
    <mass monoisotopic="89.9047037" average="91.2236472138" />
    <isotopes>
      <isotope massNumber="90" mass="89.9047037" abundance="0.5145" />
      <isotope massNumber="91" mass="90.905645" abundance="0.1122" />
      <isotope massNumber="92" mass="91.9050401" abundance="0.1715" />
      <isotope massNumber="94" mass="93.9063158" abundance="0.1738" />
      <isotope massNumber="96" mass="95.908276" abundance="0.028" />
    </isotopes>
  </element>
</mspyElements>
```

19.2. Amino acids

Configuration file *"aminoacids.xml"* contains all the amino acids available for sequence editing.

```
<?xml version="1.0" encoding="utf-8" ?>
<mspyAminoacids version="1.0">
  <aminoacid symbol="A" name="Alanine" abbr="Ala" formula="C3H5NO" />
  <aminoacid symbol="C" name="Cysteine" abbr="Cys" formula="C3H5NOS" />
  <aminoacid symbol="D" name="Aspartic Acid" abbr="Asp" formula="C4H5NO3" />
  <aminoacid symbol="E" name="Glutamic Acid" abbr="Glu" formula="C5H7NO3" />
```

```
  <aminoacid symbol="F" name="Phenylalanine" abbr="Phe" formula="C9H9NO" />
  <aminoacid symbol="G" name="Glycine" abbr="Gly" formula="C2H3NO" />
  <aminoacid symbol="H" name="Histidine" abbr="His" formula="C6H7N3O" />
  <aminoacid symbol="I" name="Isoleucine" abbr="Ile" formula="C6H11NO" />
  <aminoacid symbol="K" name="Lysine" abbr="Lys" formula="C6H12N2O" />
  <aminoacid symbol="L" name="Leucine" abbr="Leu" formula="C6H11NO" />
  <aminoacid symbol="M" name="Methionine" abbr="Met" formula="C5H9NSO" />
  <aminoacid symbol="N" name="Asparagine" abbr="Asn" formula="C4H6O2N2" />
  <aminoacid symbol="P" name="Proline" abbr="Pro" formula="C5H7NO" />
  <aminoacid symbol="Q" name="Glutamine" abbr="Gln" formula="C5H8N2O2" />
  <aminoacid symbol="R" name="Arginine" abbr="Arg" formula="C6H12N4O" />
  <aminoacid symbol="S" name="Serine" abbr="Ser" formula="C3H5NO2" />
  <aminoacid symbol="T" name="Threonine" abbr="Thr" formula="C4H7NO2" />
  <aminoacid symbol="V" name="Valine" abbr="Val" formula="C5H9NO" />
  <aminoacid symbol="W" name="Tryptophan" abbr="Trp" formula="C11H10N2O" />
  <aminoacid symbol="Y" name="Tyrosine" abbr="Tyr" formula="C9H9NO2" />
</mspyAminoacids>
```

19.3. Fragments

Configuration file *"fragments.xml"* contains all the fragments definitions for peptides fragmentation.

```
<?xml version="1.0" encoding="utf-8" ?>
<mspyFragments version="1.0">
  <fragment name="a" terminus="N" specifity="ACDEFGHIKLMNPQRSTVYW">
    <formula nTerm="" cTerm="C-1O-1H-1" neutralLoss="" />
    <termFilter nTerm="1" cTerm="1" />
  </fragment>
  <fragment name="a-H2O" terminus="N" specifity="STED">
    <formula nTerm="" cTerm="C-1O-1H-1" neutralLoss="H2O" />
    <termFilter nTerm="1" cTerm="1" />
  </fragment>
  <fragment name="a-NH3" terminus="N" specifity="RKQN">
    <formula nTerm="" cTerm="C-1O-1H-1" neutralLoss="NH3" />
    <termFilter nTerm="1" cTerm="1" />
  </fragment>
  <fragment name="b" terminus="N" specifity="ACDEFGHIKLMNPQRSTVYW">
    <formula nTerm="" cTerm="H-1" neutralLoss="" />
    <termFilter nTerm="1" cTerm="1" />
  </fragment>
  <fragment name="b-H2O" terminus="N" specifity="STED">
    <formula nTerm="" cTerm="H-1" neutralLoss="H2O" />
    <termFilter nTerm="1" cTerm="1" />
  </fragment>
  <fragment name="b-NH3" terminus="N" specifity="RKQN">
    <formula nTerm="" cTerm="H-1" neutralLoss="NH3" />
    <termFilter nTerm="1" cTerm="1" />
  </fragment>
  <fragment name="c" terminus="N" specifity="ACDEFGHIKLMNPQRSTVYW">
    <formula nTerm="" cTerm="NH2" neutralLoss="" />
    <termFilter nTerm="1" cTerm="1" />
  </fragment>
  <fragment name="c-ladder" terminus="N" specifity="ACDEFGHIKLMNPQRSTVYW">
    <formula nTerm="" cTerm="OH" neutralLoss="" />
    <termFilter nTerm="0" cTerm="1" />
  </fragment>
  <fragment name="im" terminus="S" specifity="ACDEFGHIKLMNPQRSTVYW">
    <formula nTerm="H" cTerm="C-1O-1H-1" neutralLoss="" />
    <termFilter nTerm="1" cTerm="0" />
  </fragment>
  <fragment name="int" terminus="I" specifity="ACDEFGHIKLMNPQRSTVYW">
    <formula nTerm="H" cTerm="H-1" neutralLoss="" />
    <termFilter nTerm="0" cTerm="0" />
  </fragment>
  <fragment name="int-CO" terminus="I" specifity="ACDEFGHIKLMNPQRSTVYW">
    <formula nTerm="H" cTerm="C-1O-1H-1" neutralLoss="" />
    <termFilter nTerm="0" cTerm="0" />
  </fragment>
```

```
  <fragment name="int-H2O" terminus="I" specifity="STED">
    <formula nTerm="H" cTerm="H-1" neutralLoss="H2O" />
    <termFilter nTerm="0" cTerm="0" />
  </fragment>
  <fragment name="int-NH3" terminus="I" specifity="RKQN">
    <formula nTerm="H" cTerm="H-1" neutralLoss="NH3" />
    <termFilter nTerm="0" cTerm="0" />
  </fragment>
  <fragment name="n-ladder" terminus="C" specifity="ACDEFGHIKLMNPQRSTVYW">
    <formula nTerm="H" cTerm="" neutralLoss="" />
    <termFilter nTerm="1" cTerm="0" />
  </fragment>
  <fragment name="x" terminus="C" specifity="ACDEFGHIKLMNPQRSTVYW">
    <formula nTerm="COH-1" cTerm="" neutralLoss="" />
    <termFilter nTerm="0" cTerm="1" />
  </fragment>
  <fragment name="y" terminus="C" specifity="ACDEFGHIKLMNPQRSTVYW">
    <formula nTerm="H" cTerm="" neutralLoss="" />
    <termFilter nTerm="1" cTerm="0" />
  </fragment>
  <fragment name="y-H2O" terminus="C" specifity="STED">
    <formula nTerm="H" cTerm="" neutralLoss="H2O" />
    <termFilter nTerm="1" cTerm="0" />
  </fragment>
  <fragment name="y-NH3" terminus="C" specifity="RKQN">
    <formula nTerm="H" cTerm="" neutralLoss="NH3" />
    <termFilter nTerm="1" cTerm="0" />
  </fragment>
  <fragment name="z" terminus="C" specifity="ACDEFGHIKLMNPQRSTVYW">
    <formula nTerm="N-1H-1" cTerm="" neutralLoss="" />
    <termFilter nTerm="1" cTerm="0" />
  </fragment>
</mspyFragments>
```

19.4. Enzymes

Configuration file *"enzymes.xml"* contains all the enzymes definitions for protein digestion.

```
<?xml version="1.0" encoding="utf-8" ?>
<mspyEnzymes version="1.0">
  <enzyme name="Arg-C">
    <expression><![CDATA[[R][A-Z]]]></expression>
    <formula nTerm="H" cTerm="OH" />
    <allowMods before="0" after="1" />
  </enzyme>
  <enzyme name="Asp-N">
    <expression><![CDATA[[A-Z][D]]]></expression>
    <formula nTerm="H" cTerm="OH" />
    <allowMods before="1" after="0" />
  </enzyme>
  <enzyme name="Bromelain">
    <expression><![CDATA[[KAY][A-Z]]]></expression>
    <formula nTerm="H" cTerm="OH" />
    <allowMods before="0" after="1" />
  </enzyme>
  <enzyme name="CNBr-HSerLac">
    <expression><![CDATA[[M][A-Z]]]></expression>
    <formula nTerm="H" cTerm="O-1C-1H-3" />
    <allowMods before="0" after="1" />
  </enzyme>
  <enzyme name="Cathepsin B">
    <expression><![CDATA[[R][A-Z]]]></expression>
    <formula nTerm="H" cTerm="OH" />
    <allowMods before="0" after="1" />
  </enzyme>
  <enzyme name="Cathepsin D">
    <expression><![CDATA[[LF][^VAG]]]></expression>
    <formula nTerm="H" cTerm="OH" />
```

```
  <allowMods before="0" after="1" />
</enzyme>
<enzyme name="Cathepsin G">
  <expression><![CDATA[[YWF][A-Z]]]></expression>
  <formula nTerm="H" cTerm="OH" />
  <allowMods before="0" after="1" />
</enzyme>
<enzyme name="Chymotrypsin">
  <expression><![CDATA[[YWFL][^P]]]></expression>
  <formula nTerm="H" cTerm="OH" />
  <allowMods before="0" after="1" />
</enzyme>
<enzyme name="Clostripain">
  <expression><![CDATA[[R][^P]]]></expression>
  <formula nTerm="H" cTerm="OH" />
  <allowMods before="0" after="1" />
</enzyme>
<enzyme name="Elastase">
  <expression><![CDATA[[AVLIGS][A-Z]]]></expression>
  <formula nTerm="H" cTerm="OH" />
  <allowMods before="0" after="1" />
</enzyme>
<enzyme name="Glu-C Bic">
  <expression><![CDATA[[E][A-Z]]]></expression>
  <formula nTerm="H" cTerm="OH" />
  <allowMods before="0" after="1" />
</enzyme>
<enzyme name="Glu-C Phos">
  <expression><![CDATA[[ED][A-Z]]]></expression>
  <formula nTerm="H" cTerm="OH" />
  <allowMods before="0" after="1" />
</enzyme>
<enzyme name="Hydroxylamine">
  <expression><![CDATA[[N][G]]]></expression>
  <formula nTerm="H" cTerm="OH" />
  <allowMods before="0" after="0" />
</enzyme>
<enzyme name="Lys-C">
  <expression><![CDATA[[K][A-Z]]]></expression>
  <formula nTerm="H" cTerm="OH" />
  <allowMods before="0" after="1" />
</enzyme>
<enzyme name="Lys-N">
  <expression><![CDATA[[A-Z][K]]]></expression>
  <formula nTerm="H" cTerm="OH" />
  <allowMods before="1" after="0" />
</enzyme>
<enzyme name="Non-Specific">
  <expression><![CDATA[[A-Z][A-Z]]]></expression>
  <formula nTerm="H" cTerm="OH" />
  <allowMods before="1" after="1" />
</enzyme>
<enzyme name="Papain">
  <expression><![CDATA[[RK][A-Z]]]></expression>
  <formula nTerm="H" cTerm="OH" />
  <allowMods before="0" after="1" />
</enzyme>
<enzyme name="Pepsin">
  <expression><![CDATA[[LF][^VAG]]]></expression>
  <formula nTerm="H" cTerm="OH" />
  <allowMods before="0" after="1" />
</enzyme>
<enzyme name="Proteinase K">
  <expression><![CDATA[[YWF][A-Z]]]></expression>
  <formula nTerm="H" cTerm="OH" />
  <allowMods before="0" after="1" />
</enzyme>
<enzyme name="Subtilisin">
  <expression><![CDATA[[^RHK][A-Z]]]></expression>
  <formula nTerm="H" cTerm="OH" />
```

```
    <allowMods before="0" after="1" />
  </enzyme>
  <enzyme name="Thermolysin">
    <expression><![CDATA[[A-Z][LFIVMA]]]></expression>
    <formula nTerm="H" cTerm="OH" />
    <allowMods before="1" after="0" />
  </enzyme>
  <enzyme name="TrypAspN">
    <expression><![CDATA[(([KR][^P])|([A-Z][D]))]]></expression>
    <formula nTerm="H" cTerm="OH" />
    <allowMods before="0" after="0" />
  </enzyme>
  <enzyme name="TrypChymo">
    <expression><![CDATA[[FYWLKR][^P]]]></expression>
    <formula nTerm="H" cTerm="OH" />
    <allowMods before="0" after="1" />
  </enzyme>
  <enzyme name="Trypsin">
    <expression><![CDATA[[KR][^P]]]></expression>
    <formula nTerm="H" cTerm="OH" />
    <allowMods before="0" after="1" />
  </enzyme>
  <enzyme name="Trypsin/P">
    <expression><![CDATA[[KR][A-Z]]]></expression>
    <formula nTerm="H" cTerm="OH" />
    <allowMods before="0" after="1" />
  </enzyme>
</mspyEnzymes>
```