
libraryeditor 4.0

User Manual



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Document History

LibraryEditor User Manual, Version 4.0 (March 2008)

Part #: 253269

First edition: June 2000

Printed in Germany

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1 **PREFACE**

The *Bruker Compass LibraryEditor 4.0* application (referred to as 'LibraryEditor') is the state-of-art Windows XP application for managing mass spectral libraries.

The LibraryEditor creates and edits the most advanced MS and MSn libraries for use with *Bruker Compass DataAnalysis*. Unlike any other mass spectral library it contains mass spectra with full mass precision and essential acquisition parameters. The search algorithm from DataAnalysis makes full use of this information. Structural formulas can be added to the compounds. The LibraryEditor also supports NIST and NIST user libraries created by other programs containing spectra from other vendors.

The LibraryEditor User Manual describes how to work with LibraryEditor 4.0. For reference on LibraryEditor 4.0 menus and commands, please refer to the LibraryEditor Reference Manual that is available as PDF document with your installation.

2 GETTING STARTED

2.1 Installing and Uninstalling LibraryEditor

The LibraryEditor 4.0 application installs automatically when the *Bruker Compass DataAnalysis 4.0* application is installed on your system. The LibraryEditor application is automatically uninstalled when the DataAnalysis application is uninstalled from your system. To work with LibraryEditor, a valid 'ESI Compass 1.3' license must be present.

2.2 Compliance Modes and UserManagement

2.2.1 Running LibraryEditor in Compliance or Non-Compliance Mode

LibraryEditor can be operated in 'Compliance' or 'Non-Compliance' mode. Working in Compliance mode can support you to meet *FDA 21 CFR Part 11* (FDA's rule on electronic signatures and records) requirements. To run LibraryEditor in Compliance mode, the *Bruker Daltonics Compass Security Pack* program providing *Bruker Daltonics UserManagement* needs to be installed either on this computer or preferably on a central server. When the 'Compass Security Pack' license is present, LibraryEditor is running in Compliance mode automatically. Otherwise, LibraryEditor is running in Non-Compliance mode.

Note: Compliance mode in the context of Compass Security Pack exclusively means the availability of Compass Security Pack tools and functionalities, which can be used to support the user to meet 21 CFR Part 11 requirements. Neither Compliance mode nor Compass Security Pack can assure full compliance with 21 CFR Part 11 requirements.

Compliance mode

The Compliance mode offers the following features for LibraryEditor:

- Only operators created by the customer's UserManagement administrator can log into LibraryEditor after identification by operator ID and password.
- The UserManagement administrator can administer access to LibraryEditor by assigning individual rights to the operators he creates. These rights concern the actions the operator is allowed to perform in LibraryEditor.

- All Bruker Daltonics applications that are installed on the operator's computer can be locked and unlocked by the operator.

Note: The features above apply to any application supported by the Bruker Daltonics UserManagement.

Non-Compliance mode

When LibraryEditor is running in Non-Compliance mode:

- Anybody can log into LibraryEditor; no identification by operator ID and password is needed.
- Operators having different LibraryEditor rights do not exist.
- LibraryEditor and other Bruker Daltonics applications cannot be locked.

2.2.2 Bruker Daltonics UserManagement

When LibraryEditor is running in Compliance mode LibraryEditor uses the *Bruker Daltonics UserManagement* application.

UserManagement enables you to administer access to Bruker Daltonics applications and manage individual action rights based on operator ID and password. Creating operators and assigning rights to them is performed using the *Bruker Daltonics UserManagement Administration Tool* application. Only the customer's UserManagement default administrator and perhaps further UserManagement administrators (if having the 'UserManagement Administration Tool: Administrate Operators' right) have the right to create operators which should use LibraryEditor and assign individual rights to them concerning the actions these operators are allowed to perform in LibraryEditor.

Before anybody apart from the UserManagement default administrator can log into LibraryEditor when in Compliance mode, the UserManagement administrator has to create (an) desired operator(s) specified by operator ID and password. To become effective an operator must be assigned to an operator group having specific rights included. The UserManagement administrator can use the auto-generated operator groups or he can define new groups to customize right assignments according to his own requirements. All members within a group will have the same rights. In addition, the UserManagement administrator can modify the default password policy and timeout settings as desired.

Note: For detailed information on how to create operators and assign rights, please refer to the UserManagement help tools.

UserManagement is client-server based. On the server PC the database defining operators and their rights is installed, on the client PC the Bruker Daltonics applications are installed.

2.2.2.1 LibraryEditor Operating Rights in UserManagement

In UserManagement specific rights for performing actions in LibraryEditor exist that can be assigned to an operator group and, therefore, to an operator. If an operator wants to perform an action without having the respective right corresponding information will appear.

The rights existing in LibraryEditor are listed below (in alphabetical order). In most cases, several actions are associated with a single right, which an operator having this right is allowed to perform in LibraryEditor. The **Open library** right is the lowest right somebody must have to view data with LibraryEditor.

| | |
|-------------------------------|--|
| Right: | <i>Allows performing actions concerning the following subjects:</i> |
| • Change configuration | Configuring LibraryEditor and customizing user interface. |
| • Create library, add spectra | Creating new libraries, adding spectra, exporting libraries. |
| • Delete spectra | Deleting spectra. |
| • Modify spectra | Modifying spectra e.g., importing libraries and compound information, checking and rebuilding libraries, importing and deleting chemical structures, changing spectra. |
| • Open library | Opening, refreshing and closing libraries, accessing NIST library, importing spectra, finding compounds. |

2.2.2.2 Auto-Generated Operator Groups and Their Right Assignments in LibraryEditor

In UserManagement various so-called 'auto-generated' operator groups are predefined with each of them having specific rights for performing actions in LibraryEditor included. The UserManagement administrator can assign a new operator to one of these auto-generated groups if he does not want to define own groups but he cannot change the right assignment of the predefined groups.

The following operator groups are predefined in UserManagement (in alphabetical order):

- Administrators (auto-generated)
- Operators (auto-generated)
- Project Managers (auto-generated)
- Scientists (auto-generated)
- Service (auto-generated)

Which LibraryEditor rights are assigned to the auto-generated operator groups is shown below (the figures show the respective sections in the UserManagement Administration Tool). No difference exists between an operator of the ‘Administrators (auto-generated)’ and the ‘Project Managers (auto-generated)’ group; both have all rights that are available for this application. An operator of the ‘Scientists (auto-generated)’ group lacks the **Delete spectra** and **Modify spectra** rights. An operator of the ‘Operators (auto-generated)’ group also lacks the **Create library, add spectra** right. The ‘Service (auto-generated)’ group is needed for service purposes of the manufacturer.

‘Administrator’

Group

Administrators [auto-generated] ▼

Rights included in group:

- Change configuration
- Create library, add spectra
- Delete spectra
- Modify spectra
- Open library

‘Project Manager’

Group

Project Managers [auto-generated] ▼

Rights included in group:

- Change configuration
- Create library, add spectra
- Delete spectra
- Modify spectra
- Open library

‘Scientist’

Group

Scientists [auto-generated] ▼

Rights included in group:

- Change configuration
- Create library, add spectra
- Open library

‘Operator’

Group

Operators [auto-generated] ▼

Rights included in group:

- Change configuration
- Open library

Figure 2-1 LibraryEditor rights assignments of the predefined operator groups

2.3 Starting LibraryEditor

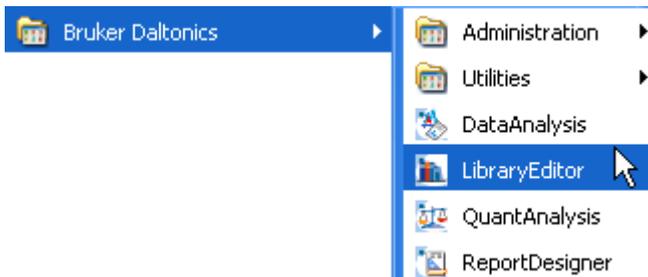
You can start LibraryEditor from the Windows **Start** menu. During installation of the Bruker Daltonics applications package, a **Bruker Daltonics** folder was created automatically in the **Start** menu’s **Programs** folder. This folder contains the respective applications. Alternatively, you can start LibraryEditor via Windows Explorer by double-clicking an existing library file (*.mlb) that automatically starts LibraryEditor and opens the respective library. You can also start it from DataAnalysis.

On starting LibraryEditor, a dialog appears that requests you to log unless you are currently logged in another Bruker Daltonics application (for Compliance as well as Non-Compliance mode) or the corresponding option for skipping this dialog is set (for Non-Compliance mode only).

After log in is performed, LibraryEditor starts with the user interface displayed according to the settings stored for the user currently logged into Windows. The currently logged in operator is displayed in the status bar of the LibraryEditor window.

To start LibraryEditor via the Windows Start menu:

1. Click .
2. Click **Programs**.
3. Click **Bruker Daltonics**.
4. Click **LibraryEditor**. This starts LibraryEditor and opens the **LibraryEditor** dialog.



5. Log in if requested.

To start LibraryEditor via Windows Explorer with opening the selected library:

1. Start Windows **Explorer**.
2. Navigate to the library file you want to open.
3. Double-click the library file. This starts LibraryEditor and opens the **LibraryEditor** dialog.
4. Log in if requested.

To start LibraryEditor from DataAnalysis:

1. Start DataAnalysis.
2. From the **Tools** menu, select **LibraryEditor**. This starts LibraryEditor and opens the **LibraryEditor** dialog.
3. Log in if requested.

2.4 Logging an Operator into LibraryEditor

When LibraryEditor is running in Compliance mode, only operators created by the UserManagement administrator can log into LibraryEditor after being identified by their operator ID and password. Multiple successive wrong logons will cause locking of the operator. The UserManagement administrator defines the maximum number of false attempts allowed. When LibraryEditor is running in Non-Compliance mode, any operator can log in after entering an operator ID. Identification by password is not required.

Note: Only one operator can be logged into Bruker Daltonics applications on a specific computer at a time.

Log in must be performed after starting LibraryEditor unless you are currently logged in another Bruker Daltonics application (for both Non-Compliance and Compliance mode). When LibraryEditor is running in Non-Compliance mode an option for automatic log in of a specified operator can be set.

In Compliance mode, if LibraryEditor is the first Bruker Daltonics application into which you want to log after the UserManagement administrator has defined you as a new operator, you will be required by the program to change your password.

When LibraryEditor is running, the currently logged in operator is identified in the status bar.

To log into LibraryEditor:

1. Start LibraryEditor or when in a running session select **Operator** from the **Help** menu. This opens the **LibraryEditor** dialog that corresponds to the mode in which LibraryEditor is currently running.
2. In **Operator**, enter your operator ID. The operator ID is not case-sensitive.
3. In Non-Compliance mode, check **Always log in using this operator** if you want the specified **Operator** to be logged in the next time automatically without showing the log on dialog again.
4. In Compliance mode, enter your password in **Password**.
Note: Passwords are case-sensitive. Be careful, too many successive wrong inputs will cause locking.
5. Click **Log On**. In Compliance mode, log in will be successful only if operator ID and password match.
6. If you are required to change your password, change it in the **Change Password** dialog and then repeat steps 4 and 5.

2.5 Changing the Operator's Password

When LibraryEditor is running in Compliance mode, the operator who wants to log in has to identify by password.

The program will require you to change your password when you log into a Bruker Daltonics application supporting UserManagement the first time after the UserManagement administrator has defined you as new operator. You must also change your password after the administrator has changed your password or has forced a password change on you. Apart from this, you can change your password whenever you want either when logging into LibraryEditor or during a running LibraryEditor session. The new password must comply with the current password policy settings defined by the UserManagement administrator.

To change an operator's password:

1. Start LibraryEditor or when in a running session, select **Operator** from the **Help** menu. This opens the **LibraryEditor** dialog.
2. In **Operator**, enter your name.
Note: The operator ID does not distinguish between capital and small letters.
3. Click **Change Password**. This opens the **Change Password** dialog.
4. In **Operator**, the ID of the operator whose password can be changed is identified. If the password for another operator should be changed, click **Cancel** to return to the **LibraryEditor** dialog and repeat steps 2 and 3.
5. In **Old password**, enter your current password. The password will not be displayed as you type it.
Note: Passwords are case-sensitive.
6. In **New password**, enter the new password.
Note: Make sure, that the new password complies with the current password policy settings.
7. In **Confirm new password**, enter your new password again.
8. Close the message confirming a successful password change. If an error message appears, repeat the corresponding steps.

2.6 Locking and Unlocking an Operator

The UserManagement can lock an operator after entering too many wrong passwords in succession. The UserManagement administrator defines how many wrong inputs are allowed. Furthermore, an operator can be locked by direct UserManagement administrator action. The operator will get information about being locked after locking has occurred.

A locked operator cannot log into any Bruker Daltonics application supporting UserManagement. Only the UserManagement administrator can unlock a locked operator.

2.7 Locking and Unlocking LibraryEditor and All Other Bruker Daltonics Applications

When LibraryEditor is running in Compliance mode, you can lock LibraryEditor and all other Bruker Daltonics applications currently installed on your system. Only the previous operator or someone with the special right to unlock applications can unlock a locked application.

Note: The **Lock All Applications** command is only available when LibraryEditor is running in Compliance mode.

Note: Automatic locking of all UserManagement using Bruker Daltonics applications will occur if one of these applications has not been used for a certain period defined by the UserManagement administrator.

To lock all Bruker Daltonics applications:

1. Click . Or press the Ctrl+Alt+K keys. Or from the **Help** menu, select **Lock All Applications**. This opens the **LibraryEditor** dialog that informs you that LibraryEditor is currently locked and how it can be unlocked.

To unlock all Bruker Daltonics applications:

1. In the **LibraryEditor** dialog, enter in **Operator** your operator ID. The dialog displays the name of the previous operator who has locked Bruker Daltonics applications. The respective ID will automatically be entered if the UserManagement administrator has set the corresponding option. Anyone other than the previous operator who wants to unlock the applications must enter the operator ID.
Note: The operator must have the right to unlock applications.
2. If you want to change your password before logging in, click **Change Password** and change it as desired.

3. In **Password**, enter the password for the operator named in **Operator**.
Note: Passwords are case-sensitive. Successive wrong password inputs will cause locking of the operator.
4. Click **Log On**. If operator ID and password match and if the respective operator is allowed to unlock applications, LibraryEditor is unlocked and the operator is logged in.

2.8 Closing LibraryEditor

You can close LibraryEditor when you have finished your current session. Upon closing, the current user interface settings are automatically stored for the user currently logged into Windows.

To close LibraryEditor:

1. Click the application's **Close**  or from the **File** menu, select **Exit**.
2. Answer the confirmation request for saving the unsaved processing state of the open library/libraries if a message appears.

3 LIBRARYEDITOR USER INTERFACE

The LibraryEditor user interface consists of the title bar, menu bar, toolbar, status bar and one to several library windows. LibraryEditor supports multi-library operation, which means that you can have several libraries opened at a time with one being active. Libraries, which are simultaneously open, display in multiple windows that you can manipulate with respect to their size, position and arrangement. You can customize the user interface according to your requirements.

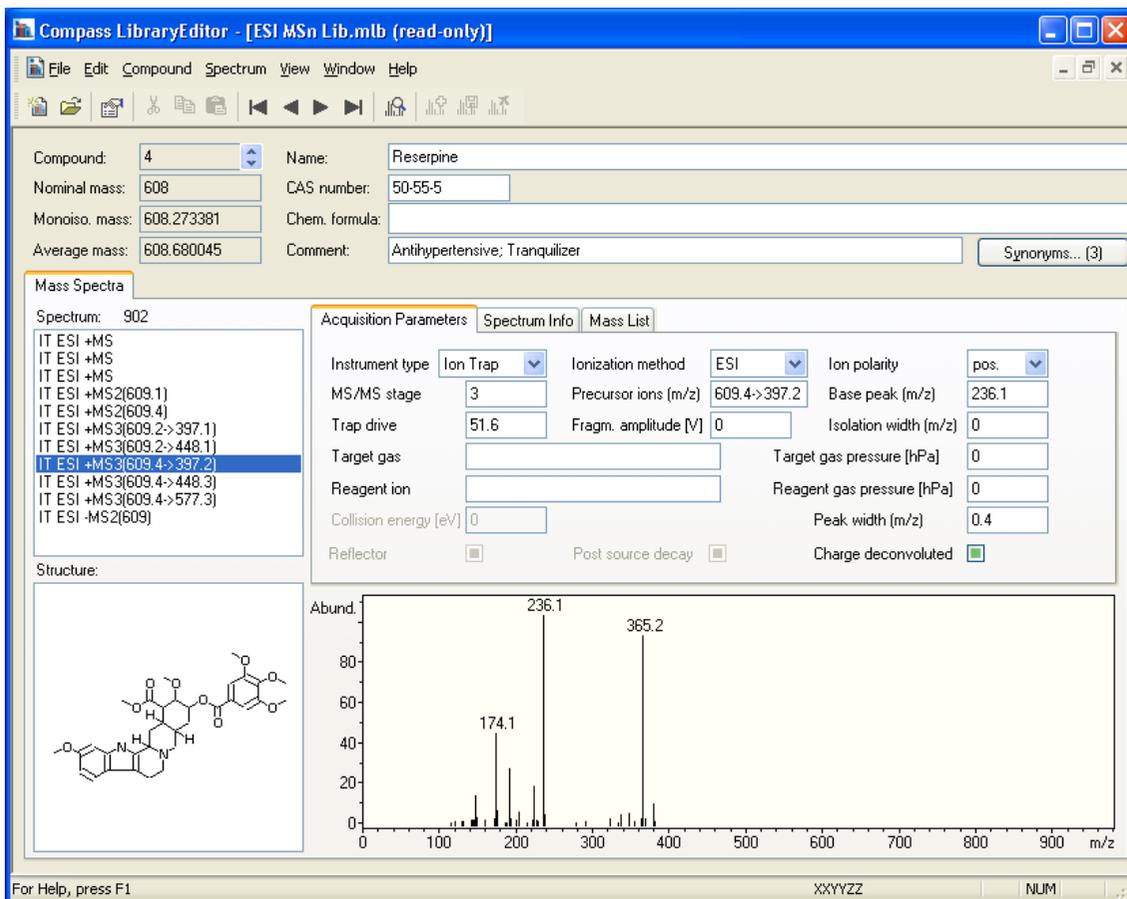


Figure 3-1 LibraryEditor user interface showing data for a compound in the library indicated in the title bar (library window displays in maximized mode)

The library window displays the data, which is currently available for the selected compound of the respective open library whose name is shown in the window's title bar. If this library is write-protected, a [read-only] appendix indicates this. The Compound

Data field shows compound-specific information such as the running index number, name, or chemical formula and allows opening the Synonym list. The Mass Spectra Data field shows the mass spectral information that is currently available for the selected compound. This includes the mass spectra contained for this compound in the library and the corresponding acquisition parameters, analysis info, Mass List and line spectrum. The Structure window displays the chemical structure of the selected compound if available.

3.1 Compound Data

3.1.1 Compound Data Field

The Compound data field displays compound-related data for the selected compound of the active library.

| | | | |
|----------------|------------|----------------|---|
| Compound: | 4 | Name: | Reserpine |
| Nominal mass: | 608 | CAS number: | 50-55-5 |
| Monoiso. mass: | 608.273381 | Chem. formula: | C ₃₃ H ₄₀ N ₂ O ₉ |
| Average mass: | 608.680045 | Comment: | Antihypertensive; Tranquillizer |
| | | | Synonyms... (3) |

Figure 3-2 Compound data

Compound

Compound ID of the compound. The compound ID is automatically given by the system when the compound is added to the library. This box is always read-only.

Nominal mass

Nominal mass of the compound. The nominal mass has to be entered by the user. Entering a value is only possible if no chemical formula is entered in **Chem(ical) formula** since entering a chemical formula will result in the **Nominal mass** box becoming read-only with the current nominal mass value being kept. No nominal mass calculation will occur from the chemical formula entered.

Monoiso(topic) mass

Monoisotopic mass of the compound. This is calculated by the system from the chemical formula currently entered in **Chem(ical) formula**. If no chemical formula is entered, no monoisotopic mass is given. This box is always read-only.

Average mass

Average mass of the compound. This is calculated by the system from the chemical formula currently entered in **Chem(ical) formula**. If no chemical formula is entered, no average mass is given. This box is always read-only.

Name

Name currently assigned to the compound. On adding a new compound by importing a mass spectrum from the file system into LibraryEditor, this box will show a name made up from the analysis name and the retention time. If a mass spectrum is exported from the *Bruker Compass DataAnalysis* application directly into LibraryEditor, the compound name specified in the corresponding DataAnalysis dialog will appear. The compound name can be changed.

CAS number

CAS number of the compound provided such a number exists for the respective compound and has already been entered.

NIST number

NIST number of the compound.

Note: This entry box is only present if the original NIST library is loaded.

UN number

UN number of the compound.

Note: This entry box is only present if the original NIST library is loaded.

Chem(ical) formula

Chemical formula of the compound if already entered. From this formula the system calculates the corresponding **Monoiso(topic) mass** and **Average mass**. Entering a chemical formula will result in the **Nominal mass** box becoming read-only.

Comment

Comment currently entered for the compound.

Synonyms

Opens the **Edit Synonyms** dialog, which lists the synonyms currently available for the compound and allows you to edit the synonym list. The number of synonyms currently contained in the synonym list is indicated on this button (e.g. '(2)').

3.1.2 Synonym List (Edit Synonyms Dialog)

The Synonym list contains all synonyms already entered for the selected compound of the active library in alphabetical order. You can edit this synonym list.

The Synonym list is opened by clicking the **Synonyms** button in the Compound Data field, which indicates the number of synonyms currently edited. It is displayed in the **Edit Synonyms** dialog. You can edit the Synonym list of the selected compound e.g., by adding new synonyms or changing or deleting already existing synonyms.

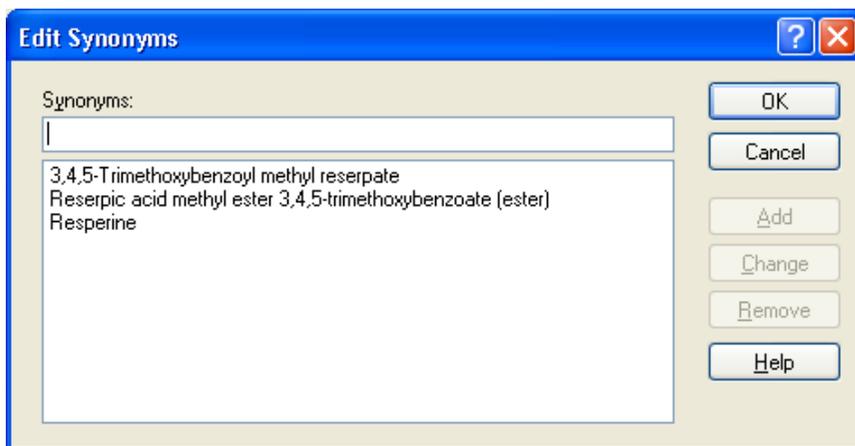


Figure 3-3 Edit Synonyms dialog listing the synonyms already entered for the selected compound

Synonyms

Displays the synonym that is selected in the synonym list below.

To add a new synonym enter its name and click **Add**. To change the selected synonym, change it as desired and click **Change**.

(Synonym list)

Lists all synonyms currently available for the selected compound. On selecting a synonym from this list, its name is shown in **Synonyms**.

Add

Adds the synonym entered in **Synonyms** to the synonym list.

Change

Changes the selected synonym according to the changes made in **Synonyms**.

Remove

Removes the selected synonym from the synonym list.

3.1.3 Structure Window

The Structure window displays the chemical structure for the selected compound if available in the active library.

If the library does not contain this structure data, you can import the corresponding *.mol file to display it. Deleting the structure will result in the structure is removed from this window.

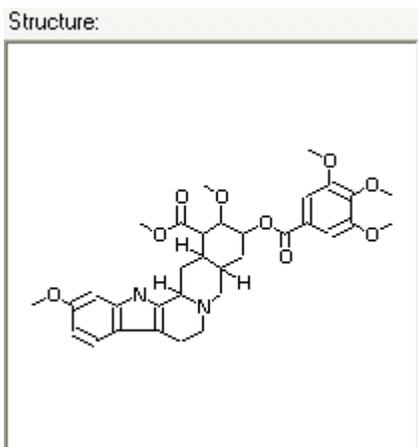


Figure 3-4 Structure window displaying the chemical structure of the selected compound

3.2 Mass Spectra Data

3.2.1 Mass Spectra Data Field

The Mass Spectra data field displays the mass spectral data currently contained for the selected compound in the active library. This field includes the Mass Spectra list, **Acquisition Parameter** tab, **Spectrum Info** tab, **Mass List** tab and Mass Spectrum window. The Structure window is placed in this area, too.

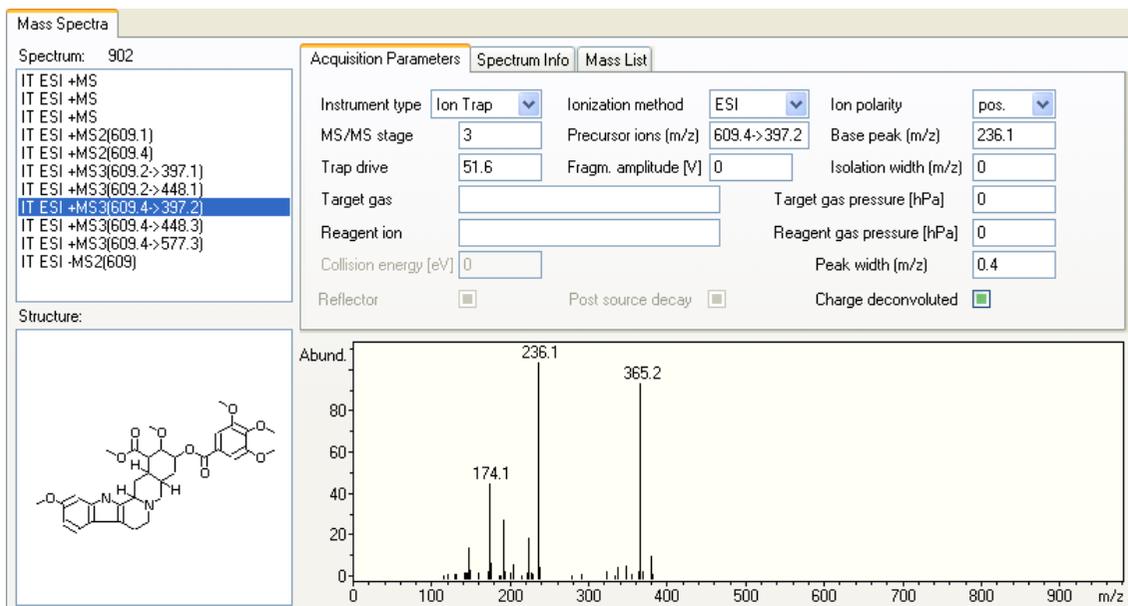


Figure 3-5 Mass Spectra data field displaying the data available for the selected spectrum

3.2.2 Mass Spectra List

The Mass Spectra list itemizes all mass spectra currently contained for the selected compound in the active library. The mass spectra are listed in sequence of their adding to the library. Each mass spectrum is represented by a short description indicating the instrument type, ionization method, ion polarity and MS/MS stage that was used in acquiring the mass spectrum.

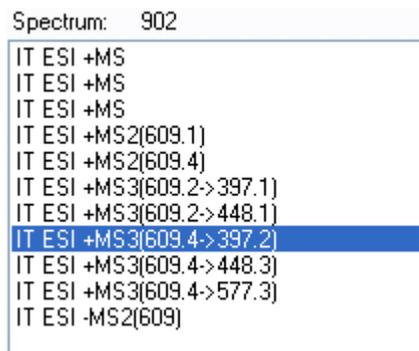


Figure 3-6 Mass Spectra list showing the spectra currently available for the selected compound in the active library

When selecting a mass spectrum from this list, its **Spectrum ID** is shown above the list and its line spectrum is displayed in the Mass spectrum window. Corresponding information is displayed in the **Acquisition Parameters**, **Spectrum Info** and **Mass List** tabs.

3.2.3 Mass Spectrum Window

The Mass Spectrum window displays the line spectrum that corresponds to the mass spectrum selected in the Mass Spectrum list. It shows the masses present and their relative abundances with regard to the base peak (100% mass). A common mass axis range is used for all mass spectra of a compound.

The corresponding m/z and abundance values can be read from the **Mass List** tab. The Mass List can be edited which will result in the displayed line spectrum automatically being changed accordingly.

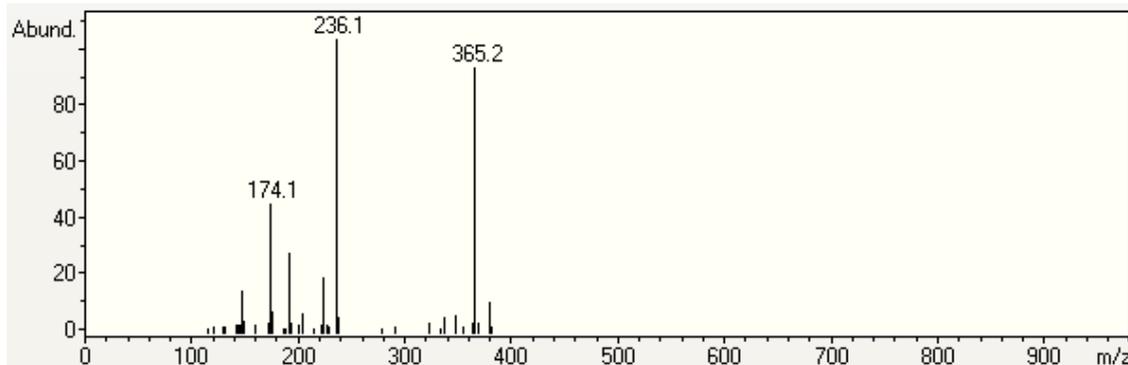


Figure 3-7 Display of the line spectrum that corresponds to the selected mass spectrum

3.2.4 Acquisition Parameters Tab

The **Acquisition Parameters** tab displays information about the acquisition parameters that were used in acquiring the mass spectrum selected in the Mass Spectra list.

Some of this data is automatically entered when a mass spectrum is added to the library (e.g. **Instrument type**, **Ionization method**, **Ion polarity**, **MS/MS stage**, **Precursor ions [m/z]** (for MS>1), **Base peak [m/z]**, **Peak width [m/z]**, if being **Charge deconvoluted**) if LibraryEditor can read the corresponding information from the respective data file. You can enter additional acquisition information on the respective mass spectrum in the corresponding parameter boxes.

| Acquisition Parameters | | | Spectrum Info | Mass List | |
|------------------------|--------------------------|----------------------------|--------------------------|-----------------------|-------------------------------------|
| Instrument type | Ion Trap | Ionization method | ESI | Ion polarity | pos. |
| MS/MS stage | 3 | Precursor ions (m/z) | 609.4->397.2 | Base peak (m/z) | 236.1 |
| Trap drive | 51.6 | Fragm. amplitude [V] | 0 | Isolation width (m/z) | 0 |
| Target gas | | Target gas pressure [hPa] | 0 | | |
| Reagent ion | | Reagent gas pressure [hPa] | 0 | | |
| Collision energy [eV] | 0 | Peak width (m/z) | 0.4 | | |
| Reflector | <input type="checkbox"/> | Post source decay | <input type="checkbox"/> | Charge deconvoluted | <input checked="" type="checkbox"/> |

Figure 3-8 Acquisition Parameter tab displaying the acquisition parameters used in acquiring the selected mass spectrum

3.2.5 Spectrum Info Tab

The **Spectrum Info** tab displays general information about the mass spectrum selected in the Mass Spectra list.

| Acquisition Parameters | | | Spectrum Info | Mass List |
|------------------------|-------------------|----------------------|---------------------|-----------|
| Analysis name | Reser004.d | | | |
| Instrument name | Bruker Esquire-LC | Date | 27.01.2003 14:09:00 | |
| Operator name | Peter Sander | Change date | 17.12.2003 16:13:18 | |
| Column | | Retention time [min] | 0 | |
| Contributor | | | | |
| Comment | | | | |

Figure 3-9 Spectrum Info tab displaying information about the selected mass spectrum

The data shown in **Analysis name**, **Instrument name**, **Date**, **Operator name** and **Change date** is entered by the system and cannot be edited by the operator.

Analysis name

Name and path of the analysis the mass spectrum originates from.

Note: Name and full path of an analysis are only shown for a new mass spectrum added to a new library (library version number 2.2).

Instrument name

Name of the instrument on which the analysis the mass spectrum originates from was acquired.

Date

Date and time the analysis the mass spectrum originates from was acquired.

Operator name

Name of the operator who has last processed the mass spectrum e.g., by adding it to the active library or changing its Mass List or spectrum info.

Note: **Operator** is only filled in new libraries (library version number 2.2) when a new spectrum is added or an existing spectrum is changed.

Change date

Date and time the mass spectrum has been processed last.

Note: **Change date** is only filled in new libraries (library version number 2.2) when a new spectrum is added or an existing spectrum is changed.

Optionally, you can enter following information about:

Column

Column used for acquiring the analysis.

Retention time [min]

Retention time of the mass spectrum. This data is entered by the system but can be edited.

Contributor

Name of the contributor who has acquired the mass spectrum.

Comment

Comment e.g. on the mass spectrum or analysis.

3.2.6 Mass List Tab

The **Mass List** tab displays the Mass List of the mass spectrum selected in the Mass Spectra list. The corresponding line spectrum is displayed in the Mass Spectrum window.

The Mass List tab lists all masses currently present in the line spectrum and their corresponding abundances. You can edit the Mass List e.g., by adding new masses or changing or removing existing masses. Each change results in the line spectrum displayed is immediately altered accordingly.

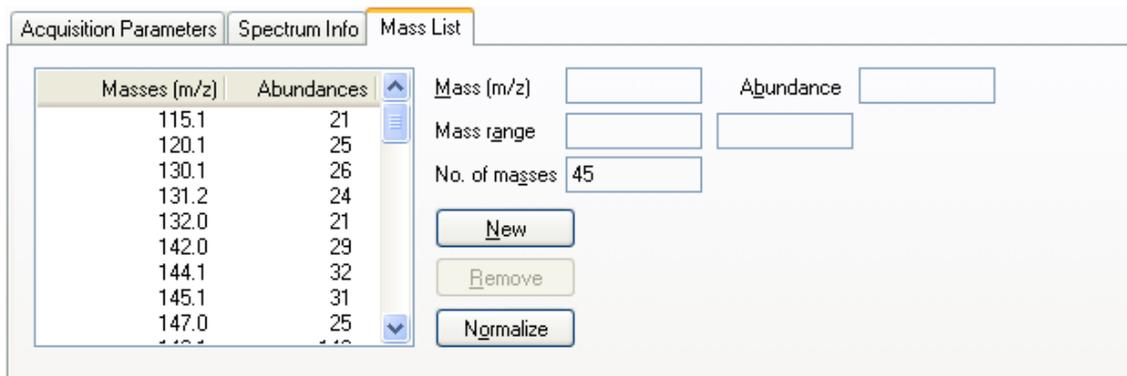


Figure 3-10 Mass List tab displaying the Mass List of the selected mass spectrum

Masses [m/z]

Current masses of the selected mass spectrum.

Abundances

Corresponding abundances of the masses listed.

Mass

Mass value of the mass currently selected in **Masses [m/z]**.

Abundance

Abundance of the mass currently selected in **Masses [m/z]** with the abundance of the base peak being set to '999'.

Mass range

Acquired mass range of the mass spectrum.

Note: **Mass range** is only filled for a new mass spectrum added to a new library (library version number 2.2).

No. of masses

Number of masses contained in the mass spectrum.

New

Adds the mass currently specified in **Mass** and **Abundance** as a new mass.

Remove

Removes the mass currently selected in **Masses [m/z]**.

Normalize

Normalizes the line spectrum displayed in the Mass Spectrum window e.g. if the 100% mass has been removed.

3.3 Customizing the User Interface

You can customize the user interface with respect to the current display state of the toolbar and status bar, which both are shown by default. Since LibraryEditor supports multi-library operation using multiple windows, you can toggle between different display modes showing only either the window of the active library or the windows of all libraries currently open simultaneously. In the latter case, you can resize and move the individual library windows or minimize single windows to icons.

3.3.1 Showing and Hiding the Toolbar

The toolbar is positioned below the menu bar by default. You can hide the toolbar and show it again.

To show or hide the toolbar:

1. From the **View** menu, select **Toolbar**.

3.3.2 Showing and Hiding the Status Bar

The status bar is positioned at the bottom of the LibraryEditor window by default. You can hide the status bar and show it again.

To show or hide the status bar:

1. From the **View** menu, select **Status Bar**.

3.3.3 Manipulating Library Windows

LibraryEditor supports multi-library operation, meaning that you can have several libraries open at a time displayed in multiple windows.

On opening a library, by default, it displays in a window being maximized with the library name shown in brackets in the LibraryEditor window's title bar and its window size depends on the current size of the LibraryEditor window.

If you have more than one library open at a time you can switch from the maximized mode showing only the active library to display modes showing also the windows of the other open libraries. In the multiple windows mode each library is displayed in a separate window having its own title bar indicating the name of the respective library.

The active library is always shown on top with its title bar being highlighted. You can arrange multiple windows in different ways as well as resize and move them within the current borders of the LibraryEditor window. In addition, you can minimize such a window if you wish to keep the respective library open but temporarily exclude its window from being displayed among the other library windows.

3.3.3.1 Moving a Library Window

You can move a library window to another position on the user interface. This may result in only part of the library window being shown.

To move a library window to another position:

1. Position the mouse pointer on the title bar of the library window you want to move.
2. Drag the window, with the left mouse button depressed, to the desired new position and release the mouse button.

3.3.3.2 Resizing a Library Window

You can change the size of the active library window by dragging its borders. The program sets a minimum permissible size whereas the maximum possible size depends on the current size of the LibraryEditor window.

In addition, you can minimize a library window or maximize it by clicking its  but maximizing will result in changing the display mode to show only the active library, but not several libraries simultaneously.

To resize the width of a library window:

1. Click the library window you want to resize.
2. Position the mouse pointer on the left or right window border so it changes to .
3. Drag the border, with the left mouse button depressed, to the left or right until the desired or the minimum/maximum window size is reached. Then release the mouse button.

To resize the height of a library window:

1. Click the library window you want to resize.
2. Position the mouse pointer on the upper or lower window border so that it changes to .
3. Drag the border with the left mouse button depressed up or down until the desired or minimum/maximum window size is reached. Then release the mouse button.

3.3.3.3 Arranging Library Windows

The library windows will be arranged and sized by default. In the case of the cascade view, each of the respective windows has the same default size but is shifted by title bar height and an angle of 45°. In the tile view, the windows are sized according to the current size of the LibraryEditor window, provided this does not remain under the minimum allowed size set for a library window.

You can switch the display to show the library windows of all open, currently not minimized libraries in cascade or tile view. If desired, you can move the windows to new positions and/or resize them. When switching to another view, changed window sizes will be reset to the default values.

To arrange multiple windows in cascade view:

1. From the **Window** menu, select **Cascade**.

To arrange multiple windows in tile view:

1. From the **Window** menu, select **Tile**.

3.3.3.4 Minimizing Library Windows and Arranging Icons

You can minimize a library window to an icon and arrange the icons present in a straight line at the bottom of the LibraryEditor user interface. Minimizing a library window keeps the corresponding library open but excludes the respective window from being displayed among the other multiple windows.

To minimize a library window:

1. Click the library window's . This minimizes the active library window to an icon
e.g. .

To arrange icons of minimized library windows:

1. From the **Window** menu, select **Arrange Icons**.

4 CREATING AND MANAGING LIBRARIES

To perform a library search on acquired, unknown mass spectra LibraryEditor allows you to build appropriate mass spectral libraries containing MS and MS/MS spectra of the compounds you are interested in. How a new library is created and how an existing library can be managed is described in this section. This includes creating, opening, activating, saving, refreshing, exporting and checking libraries as well as accessing NIST user libraries. Chapter 5 describes how a library can be build, i.e. is filled with data.

4.1 Creating a New Library

You can create a new library having the Library Files format (*.mlb). This is required for building a new library e.g., by importing and adding mass spectra or importing other libraries.

Each library must be placed in a separate folder. This is necessary since the various data files which are generated during library set up will have identical names for all libraries created, except for the library file (*.mlb) whose name you select. Therefore, when creating a new library, first set up a new folder with the name of the library you want to create and then create the library and save it in the respective folder.

On saving a new library, the specified *.mlb file as well as the specific corresponding data files are set up and saved to the selected folder. The library is automatically opened.

To create a new library:

1. Click  or select **New** from the **File** menu.
3. Navigate to the folder the new library should be saved to.
2. Click  to create a subfolder for the library you want to set up.
3. Enter the folder name in the appearing frame.
4. Double-click the new subfolder to open it.
5. In **File name**, enter the name of the new library.
6. Click **Save**.
7. Build the newly created library.

4.2 Opening a Library

LibraryEditor uses Windows conventions for opening library files. You can open a library either from LibraryEditor or from Windows Explorer. LibraryEditor supports the drag-and-drop functionality, i.e. you can open a library by dragging its file name (*.mlb) from Windows Explorer into the LibraryEditor window. On opening a library, the library displays in a new library window with the first compound shown that is contained in respective library.

To open a library from LibraryEditor:

1. Start LibraryEditor.
2. Click  or select **Open** from the **File** menu.
3. In **Look in** and the folder list, navigate to that folder that contains the library file (*.mlb) you want to open.
4. Double-click the desired library file. Or click the library file and click **Open**.

Tip: You can quickly open a library you have recently processed by clicking the respective recent file list name at the bottom of the **File** menu.

To open a library from Windows Explorer using drag and drop:

1. Start LibraryEditor.
2. Start Windows **Explorer**.
3. Navigate to the folder which contains the library file (*.mlb) you want to open.
4. Click the desired library file and drag it with left mouse button depressed in the LibraryEditor window. Then release the mouse button.

To open a library from Windows Explorer by double-clicking it:

1. Start Windows **Explorer**.
2. Navigate to the folder, which contains the desired library file (*.mlb).
3. Double-click the library file. This starts LibraryEditor and opens the respective library.

4.3 Activating a Library

If more than one library is opened at a time, you have to activate the respective library you want to view and/or process. All currently open libraries are listed in the open library list at the bottom of the **Window** menu. The active library is indicated by a check mark in front of its name.

If the maximized window mode is active, i.e. only the active library is shown with its

corresponding library window being maximized, you can activate another library only by selecting it from the open library list. If multiple windows are simultaneously displayed and cover each other only partially, e.g. when the cascade view or tile view is active, you can activate the desired library by just clicking the respective library window. This puts the respective library window on top.

To activate an open library:

- 1 From the **Window** menu, select the desired library from the open library list. Or click the respective library window if visible.

4.4 Refreshing a Library

You can refresh the active library. This is required if at least two computers within a network access the same library. For example, on computers A and B the library X is open; computer A is viewing entries and computer B is writing into the library. For computer B, the library is refreshed automatically whereas Computer A will see the changes made by computer B not automatically but after performing a refresh on the library. Computer A will also see these changes after deactivating (= activating another application) and re-activating LibraryEditor since this will cause an automatic refresh.

To refresh a library:

1. Activate the library you want to refresh.
2. From the **File** menu, select **Refresh**.

4.5 Saving Changes Made to a Library

The program will automatically save changes you made to the active library by adding or deleting mass spectra. In contrast, if you have altered the currently selected compound concerning its current compound or mass spectrum data e.g., by editing a mass spectrum's Mass List or the compound's synonym list, you can decide whether these changes should be saved. Use this procedure to save the changes you have made to the compound data of the selected compound or to one of its mass spectra.

If you made changes to the current compound or its selected mass spectrum but have not saved them yet, the program will ask you about saving these changes each time you try to select another mass spectrum. Affirm this confirmation request if you want the changes to be saved.

To save changes made to a compound or its mass spectrum:

1. Click  or from the **Spectrum** menu, select **Save**.

4.6 Showing Library Properties

You can show the properties of the active library concerning the library name and path, status, number of compounds and spectra contained, and version number.

To show properties of a library:

1. Activate the library whose properties you want to show.
2. From the **File** menu, select **Properties**.

4.7 Exporting a Library

You can export the active library to Library File format (*.mlb) or to ASCII Library File format (*.library) which is fully NIST compatible. The *.library format allows loading the exported library into the NIST. It is almost identical with the ASCII MS Spectrum File format (*.spectrum) with the one difference that the *.library format can hold any number of mass spectra but the *.spectrum format only a single one.

To export a library:

1. Activate the library you want to export.
2. From the **File** menu, select **Export Library**.
3. In **Save in** and the folder list, navigate to the folder to which the exported *.library file should be saved.
4. In **Name**, enter the name for the *.library file to be exported or select a name from the folder list.
5. In **Save as type**, select the format the library should be converted to.
6. If **Library File (*.mlb)** is selected, check **Exclude compound information** if only compound names but no additional compound information should be included in the exported library.
7. Click **Save**.
8. If you have chosen an existing file name, affirm the appearing confirmation request on overwriting the existing file.

4.8 Accessing a NIST User Library and Locating the NIST Main Library

LibraryEditor allows you to access a NIST user library (named User.dbu) not yet having the Library Files format (*.mlb) required by LibraryEditor. Access creates the corre-

sponding *.mlb file ('library name'.mlb) that can be opened and processed in LibraryEditor. Information about mass spectrum acquisition (e.g. polarity, MS/MS stage, precursor ion, production) that is stored in the respective NIST user library is automatically entered in **Acquisition Parameter** of the corresponding mass spectrum if LibraryEditor can read this information from the user library.

Additionally, you can specify the location of the NIST main library as an option, which allows chemical structures from the NIST user libraries to be resolved from the NIST main library.

To access a NIST user library w/o specifying location of the NIST main library:

1. From the **File** menu, select **Access NIST Library**. This opens the **Access NIST User Library** dialog.
2. In **Look in** and the folder list navigate to the respective NIST user library folder and open it.
3. Double-click the User.dbu file or select it and click **Open**.
4. If the location of the NIST main library has not been specified yet, the **NIST Library** dialog appears which allows you to enter the location as an option. If you want to, enter the respective path or click  to select it in the appearing **NIST Main Library** dialog. Then click **OK**. Otherwise, click **Cancel**.
5. A message informs you about successful creation of access file(s) and asks if you want to open the library now. If you want to, click **OK**.

4.9 Checking and Rebuilding a Library with Converting to the New Library Format

You can check and rebuild a selected library having the Library Files format (*.mlb). This is necessitated if error messages have appeared when performing library searches in DataAnalysis and/or when browsing the respective library in LibraryEditor.

In addition, you can use library check and rebuild to convert libraries created with LibraryEditor 3.1 or below to the new library format supported since LibraryEditor 3.2, which provides additional properties for mass spectra. It is recommended to convert existing libraries set up with a previous LibraryEditor version (library version number 2.0 or 2.1) to the new library format to make use of the new properties additionally available for mass spectra. The version number of a library can be examined from the **Properties** command from the **File** menu.

Note: A prerequisite is that all installations containing a 'LibraryEditor' and all computers containing mass-spectral libraries are updated at least to 'esquire 5.2', 'DataAnalysis 3.2', or 'LibraryServer 1.2', including any higher version of those.

You can also use library check and rebuild to reduce mass spectra consisting of a huge number of masses to the most abundant ones. Rebuilding then creates a library containing only spectra with at most the specified number of masses. The number of masses a selected spectrum consists of you can examine from the **Mass List** tab.

Checking and rebuilding a library creates a new, rebuilt library having the version number 2.2 while the original library is still preserved. Depending on whether the original library is writable or read-only, library check and rebuild proceeds as follows: For writable libraries, the rebuilt library replaces the original one after this was saved to a new backup-subfolder named either 'BAK' or 'BAK_n' (with $n \geq 2$). For read-only libraries, the rebuilt library is saved to a new subfolder named 'YYMMDDhhmmss' (Y: year, M: month, D: day, h: hour, m: minute, s: second) with the original library remaining unchanged.

If the library you want to check and rebuild is open when check is prompted, the library is automatically closed and opened again after rebuild is finished, i.e. after you have clicked **Close** in the **Check Library Progress** dialog.

To check and rebuild a library:

1. From the **File** menu, select **Check Library**. This opens the **Check Library** dialog box.
2. In **Look in** and the folder list, navigate to the folder that contains the library file (*.mlb) you want to check.
3. Check **Limit mass spectra to N most abundant masses** if you want to reduce spectra containing a huge number of masses to a specified number of most abundant masses and enter the desired number in the box to the right.
4. Click **Open**. While library check and rebuild is running, the **Check Library Progress** dialog informs you about the progress of rebuild.
5. After rebuild is finished, click **Close**.

4.10 Closing a Library

You can close the active library if you do not want to have it open any longer. If changes made to the last selected compound have not been saved yet, a confirmation request will appear for saving these changes.

To close a library:

1. Activate the library you want to close.
2. From the **File** menu, select **Close**.

5 BUILDING LIBRARIES

LibraryEditor allows you to build specific MS and MS/MS libraries which you can use for library searching and mass spectrum identification to be performed in DataAnalysis. Such libraries can hold one to several MS and MS/MS spectra for each compound present. Filling a library with data includes adding mass spectra by importing single spectra or a complete library and then editing the compound and/or mass spectrum data

Building a library includes the following major steps:

- Creating a new library (Section 4.1)
- Adding mass spectra to this library
- Processing the compounds and their mass spectra present in the library

5.1 Adding Mass Spectra to a Library

For building a new library, you have to add MS and MS/MS spectra to this library. This can be done by first importing a mass spectrum from the file system and then specifying whether the respective spectrum should be added as a new compound entry to the active library or as a new (additional) spectrum to a compound already existing in the respective library. Alternatively, you can add a new mass spectrum or compound directly from DataAnalysis to an existing library. Or you can import another library into the active library with all compounds not yet present in the target library being added automatically as new compound entries and all mass spectra belonging to already existing compounds being added as additional spectra to the respective compounds.

After adding, you can process a new compound or mass spectrum e.g. by editing the corresponding data.

5.1.1 Importing a Mass Spectrum

You can import a mass spectrum of the ASCII MS Spectrum Files format (*.spectrum) or NIST ASCII MS Spectrum Files format (*.msp) from the file system. This allows adding the respective mass spectrum to the active library as either new compound entry or new (additional) spectrum for an existing compound.

On importing, the respective mass spectrum is loaded in LibraryEditor without getting compound and spectrum ID numbers. Corresponding data is shown in the library window. A compound name is entered automatically in **Name** consisting of the name of analysis the spectrum derives from and corresponding retention time. For adding the

imported mass spectrum to the active library, you can change the compound name to the desired name and perform the **Add** command from the **Spectrum** menu, which becomes enabled on importing a mass spectrum.

To import a mass spectrum:

1. Activate the library into which you want to import a mass spectrum.
2. From the **Spectrum** menu, select **Import**.
3. In **Files of Type**, select the file format of the data files to be shown in the folder list.
4. In **Look in** and the folder list, navigate to the folder that contains the mass spectrum you want to import.
5. Double-click the respective mass spectrum. Or click the respective mass spectrum and click **Open**.
6. Add the imported mass spectrum as a new compound entry or as a new mass spectrum to an existing compound.

5.1.2 Adding a Mass Spectrum as New Compound Entry

A mass spectrum you have previously imported can be added to the active library as new compound entry. This requires assigning the spectrum to a compound name not yet existing in the active library.

On adding a mass spectrum as new compound entry, a new compound is added to the active library getting a compound ID number for the library. The respective spectrum is added as the compound's first spectrum getting a spectrum ID number. Afterwards, you can add additional mass spectra to such a new compound.

To add a mass spectrum as new compound entry:

1. Import the mass spectrum you want to add to the active library as new compound entry.
2. In compound **Name**, enter a compound name not yet existing in the library.
3. Click  or select **Add** from the **Spectrum** menu.
4. If the **Add New Spectrum** dialog appears because you have used an already existing compound name, enter the desired new name in **New Compound** and then click **New**.

5.1.3 Adding a Mass Spectrum as New Spectrum for an Existing Compound

A mass spectrum you have previously imported can be added to the active library as new (additional) spectrum for an already existing compound. This requires assigning the spectrum to a compound name already existing in the active library. On adding a mass spectrum to a compound, the respective spectrum is added to the specified compound as additional spectrum getting a spectrum ID number.

To add a mass spectrum as new spectrum for an existing compound:

1. Import the mass spectrum you want to add to the active library as additional spectrum for an existing compound.
2. In compound **Name**, enter the name of the compound you want to add the mass spectrum to.
3. Click  or select **Add** from the **Spectrum** menu,.
4. In the compound list, select the compound the mass spectrum should be added to.
5. Click **Add to**.

5.1.4 Adding a Mass Spectrum Directly from DataAnalysis

You can also add a mass spectrum directly from DataAnalysis to an existing library using the appropriate DataAnalysis command. This adding operation can be performed when LibraryEditor is running as well as when it is closed. Line as well as profile spectra can be added. In contrast to line spectra for which all mass lines present will be exported to the target library, for profile spectra only the detected peaks will be exported. You can add a single mass spectrum or multiple selected mass spectra either of the same or of different compounds at once.

On selecting DataAnalysis' **Add to Library** command the tabbed **Add Spectra to Library** dialog will appear. In this, you have to specify the compound name of the mass spectrum/spectra to be added and the desired target library. The mass spectrum/spectra can be added either to a pre-existing compound in the chosen library or as a new compound entry. You can define how to proceed if the target library already contains a compound of the specified name. When a mass spectrum is added to a library, some specific data associated with the mass spectrum (e.g. instrument type, ionization method, MS/MS stage, precursor ions) are automatically entered as well as the compound details specified by the user.

If LibraryEditor is already running and the chosen target library is currently open when you perform this adding operation from DataAnalysis, you have to refresh the respective library to directly get access to the new added compound or mass spectrum.

To add a single or multiple selected mass spectra directly from DataAnalysis:

1. In DataAnalysis, select a single or several mass spectra to add them to a custom library.
2. Right-click the data window displaying the mass spectrum and select **Add to Library**. Alternatively, you can click  or select **Add to Library** from the **Identify** menu. This opens the **Spectra** tab of the **Add Spectra to Library** dialog. The selected mass spectrum/spectra will be listed in **Add compounds/spectra**.
3. Check **Auto-name** if the compound should be added under an auto-name consisting of the analysis name and the compound's retention time. This will automatically enter '**[analysis name]-[retention time]**' in **Compound name**. If mass spectra of different compounds are selected **Auto-name** will be checked automatically and disabled. Or leave **Auto-name** unchecked.
4. If **Auto-name** is unchecked, enter in **Compound name** the explicit compound name. This is only allowed for a single selected compound.
5. In **Library**, select the target library the spectrum/spectra is/are to be added to. Do one of the following:
 - Enter path and name of the desired library.
 - Click  and select the library in the **Select Library** dialog.
6. If a single mass spectrum is to be added, click the **Compound Details** tab if you want to enter information on the specified compound/mass spectrum. Do the desired entries and/or selections.
7. Click the **Options** tab and select the option that defines how to proceed if the specified compound name already exists in the chosen target library.
8. Click **OK**. This adds the spectrum/spectra and corresponding information to the chosen target library using the explicit name or an auto-name. If no compound of the specified name exists the spectrum is added as a new compound entry.
9. If the compound name already exists, adding is performed according to the settings currently defined in the **Options** tab. If **If compound exists, ask for action** is selected, the **Add New Spectrum** dialog will appear. In this case, do one of the following:
 - If you wish to add the spectrum/spectra as a new compound entry, specify its name in **New Compound** and click **New**.
 - If you wish to add the spectrum/spectra to a pre-existing compound, select the desired compound from the list of existing compounds and click **Add to**.
10. If LibraryEditor is already running and the chosen target library is currently open, refresh the respective library in LibraryEditor to get direct access to the new added compound or mass spectrum.

5.1.5 Importing a Library into another Library

You can import a library of the Library Files format (*.mlb) into the active library in order to add the compounds and/or mass spectra contained in the import library to the target library.

On importing a library into another library, this will result in those compounds of the imported library having names not yet contained in the active library being added to the latter as new compound entries whereas the mass spectra of the compounds having already existing names are being added as additional spectra to the respective existing compounds. To which compound ID's of the target library new spectra were added will be listed at the end of the appearing import progress information.

To import a library:

1. Activate the library, into which you want to import another library.
2. From the **File** menu, select **Import Library**.
3. In **Look in** and the **folder list**, navigate to the folder that contains the *.mlb file you want to import.
4. Double-click the desired *.mlb file. Or click the desired *.mlb file and click **Open**.
5. After import is finished, click **Close** in the import information displayed.

5.1.6 Exporting a Mass Spectrum

You can export the active mass spectrum to the ASCII MS Spectrum Files format (*.spectrum) which is fully NIST compatible. This allows importing the exported mass spectrum into another library opened in LibraryEditor.

To export a mass spectrum:

1. Activate the mass spectrum you want to export.
2. From the **Spectrum** menu, select **Export**.
3. In **Save in** and the folder list, navigate to the folder to which the exported *.spectrum file should be saved.
4. In **Name**, enter the name for the *.spectrum file to be exported or select a name from the folder list.
5. Click **Save**.
6. If you have chosen an existing file name, affirm the appearing confirmation request on overwriting the existing file.

5.2 Processing Compounds and Mass Spectra of a Library

You can process the compounds and mass spectra currently contained in a library.

For a compound, you can edit its compound data and synonym list and assign a structure formula to it that will be displayed in the spectrum display when the respective compound is selected. In addition, you can import compound information into a library or export it. For a mass spectrum, you can edit its Mass List, acquisition parameters and analysis info.

To process compound or mass spectrum data the respective compound or mass spectrum must be selected, i.e. its corresponding data must be displayed in the active library window.

5.2.1 Selecting a Compound of a Library

You have to select the compound you want to view or process. Only one compound of a library can be selected at a time. The selected compound displays in the active library window. There are two ways to select a desired compound. You can go step-by-step through the active library or you can directly select a compound by searching the library for it.

To select a compound by browsing the library:

1. Go step-by step through the active library using the respective button , , , or  until you have reached the desired compound.

To select a compound directly:

1. Click  or from the **Compound** menu, select **Find Compound**.
2. Select the search criterion you want to use e.g. **Compound ID** or **Name**.
3. For the search criterion selected, enter the respective number or name.
4. Click **OK**.

5.2.2 Selecting a Mass Spectrum of a Compound

A library can contain several mass spectra for one compound, e.g. from different MS/MS stages or ionization methods. To view a mass spectrum available for the active compound you have to select this spectrum from the compound's mass spectrum list. This will result in the data of the respective mass spectrum being displayed and allows

you to view and, if desired, process the respective mass spectrum.

To select a mass spectrum of a compound:

1. Select the desired compound.
2. In the Mass spectrum list, click the mass spectrum you wish to select.

5.2.3 Editing Compound Data

The compound data of the selected compound can be edited except for its compound ID which is given by the system. Additionally, you can set up and edit a synonym list for the respective compound. Compound information can be entered manually or automatically by importing an appropriate *.csv or *.tsv file.

To edit the compound data:

1. Select the compound whose compound data you want to edit.
2. Make new or change existing entries. This is possible in the **Name**, **Nominal mass**, **CAS number**, **NIST number**, **UN number**, **Chem. formula** and **Comment** boxes provided the respective box is available and not read-only.
3. Save changes.

5.2.4 Editing the Synonym List of a Compound

You can edit the synonym list of the selected compound by adding new synonyms or changing or removing already existing synonyms.

To add a synonym:

1. Select the compound whose synonym list you want to edit.
2. Click **Synonyms**.
3. In the **Synonyms** entry box, enter the new synonym name.
4. Click **Add**.
5. Repeat steps 3 and 4 for all synonyms you want to add.
6. Click **OK**.
7. Save changes.

To change a synonym:

1. Select the compound whose synonym list you want to edit.
2. Click **Synonyms**.

3. In the **Synonyms** list, select the synonym you want to change.
4. In the **Synonyms** entry box, change the selected synonym as desired.
5. Click **Change**.
6. Repeat steps 3 to 5 for all synonyms you want to change.
7. Click **OK**.
8. Save changes.

To remove a synonym:

1. Select the compound whose synonym list you want to edit.
2. Click **Synonyms**.
3. In the **Synonyms** list, double-click the synonym you want to remove. Or select it and click **Remove**.
4. Repeat step 4 for all synonyms you want to remove.
5. Click **OK**.
6. Save changes.

5.2.5 Importing Compound Information

You can import compound information stored in Comma Separated Values Files (*.csv), Tab Separated Values Files (*.tsv) or Structure Data File (SDfiles) (*.sdf) file format into the active library.

A CSV resp. TSV compound information file can contain information about one or several compounds concerning e.g. their chemical formula, nominal mass, CAS number, NIST number, UN number, synonym(s) or a comment. It must be created meeting specific requirements (see LibraryEditor Reference Manual). SDF compound information is a collection of mol files, which will be assigned to compounds by name.

When importing such a compound information file into the active library, the library is searched for all compounds having compound names identically to compound names contained in the imported file. If such a compound is found, its current compound data is supplied or replaced by the new compound information from the imported file. If no such compound is found importing of the compound information file will not have any effect on the respective library.

To import compound information:

1. Activate the library into which you want to import compound information.
2. From the **File** menu, select **Import Compound Information**.
3. In **Look in** and the folder list, navigate to the folder that contains the compound information file you want to import.

4. Double-click the respective *.csv or *.tsv or *.sdf file. Or select it and click **Open**.
5. Save changes.

5.2.6 Exporting Compound Information

You can export the compound information of the active library in either the Comma Separated Values Files (*.csv) or Tab Separated Values Files (*.tsv) format. This allows you to load the respective information e.g. in Excel. The exported file includes information about each compound of the library concerning its name, formula, nominal mass, CAS number and comment, if available.

To export compound information:

1. Activate the library of which you want to export compound information.
2. From the **File** menu, select **Export Compound Information**.
3. In **Save in** and the folder list, navigate to the folder to which you want to save the exported file.
4. In **Save as type**, select the file format into which the compound information should be converted.
5. In **File name**, enter the name for the export file, or select a name from the folder list.
6. Click **Save**.
7. If you have chosen an already existing file name, affirm the appearing confirmation request if you wish to overwrite the existing file.

5.2.7 Assigning Chemical Structures to Compounds

A chemical structure having the *.mol file format can be imported and assigned to the selected compound of the active library. The chemical structure will be displayed in the Structure window. In addition, you can export a chemical structure currently assigned to a compound or delete it from the compound.

Note: If you have already specified the location of the NIST main library, chemical structures from NIST user libraries can be resolved from the NIST main library.

5.2.7.1 Importing a Chemical Structure for a Compound

You can import a chemical structure having the Mol Files format (*.mol) and assign it to the selected compound of the active library. If a chemical structure is already assigned

to the respective compound, the imported structure will overwrite the current one.

Tip: Alternatively, you can use the **Import Compound Information** command from the **File** menu to import an appropriate Structure Data Files (*.sdf) file in the active library allowing you to assign chemical structures to several compounds in the library at once.

To import a chemical structure for a compound:

1. Select the compound for which you want to import a chemical structure.
2. From the **Compound** menu, select **Import Structure**.
3. In **Look in** and the folder list, navigate to the folder that contains the respective *.mol file you want to import.
4. Double-click the desired *.mol file or click the desired *.mol file and click **Open**.
5. Save changes.

5.2.7.2 Exporting the Chemical Structure of a Compound

The chemical structure that is currently assigned to the selected compound of the active library can be exported in the Mol Files format (*.mol).

To export a chemical structure of a compound:

1. Select the compound whose chemical structure you want to export.
2. From the **Compound** menu, select **Export Structure**.
3. In **Save in** and the folder list, navigate to the folder to which the exported *.mol file should be saved.
4. In **Name**, enter the name for the *.mol file to be exported or select a name from the folder list.
5. Click **Save**.
6. If you have chosen an existing file name, affirm the appearing confirmation request on overwriting the existing file.

5.2.7.3 Deleting the Chemical Structure from a Compound

You can delete the chemical structure assigned to the selected compound of the active library. This results in the structure being removed from the Structure window.

To delete a chemical structure from a compound:

1. Select the compound which chemical structure you want to delete.
2. From the **Compound** menu, select **Delete Structure**.
3. Save changes.

5.2.8 Editing Mass Spectrum Data

The mass spectrum data available for the selected mass spectrum of the active library can be edited and the changes saved to the compound the respective mass spectrum corresponds to. Editing mass spectrum data includes the Mass List of the mass spectrum, its acquisition parameters and analysis info.

Changes are not saved automatically but saving has to be induced either using the **Change** command from the **Spectrum** menu, or by affirming the respective appearing confirmation request.

5.2.8.1 Editing the Mass List of a Mass Spectrum

You can edit the Mass List of the selected mass spectrum displayed in the Mass List tab with respect to the masses present and their abundances. When a mass spectrum is imported into LibraryEditor either from the file system or directly from DataAnalysis the respective m/z and corresponding abundance values are automatically entered in the Mass List.

You can edit a Mass List by adding new and/or changing existing masses and corresponding abundances. In addition, you can remove existing masses from the Mass List. If you have removed the current base peak (100% mass) or changed its abundance below the abundance of another mass you can renormalize the Mass List accordingly. Changing the Mass List results in the line spectrum displayed in the Mass Spectrum window automatically being changed accordingly.

To add a new mass:

1. Select the mass spectrum of which you want to edit the Mass List.
2. Click the **Mass List** tab.
3. Click **New**.
4. In **Mass**, enter the m/z value to be added.
5. In **Abundance**, enter the corresponding abundance.
6. Click in the Mass List. This enters the new mass and its abundance in the Mass List.
7. Repeat steps 3 to 6 for all new masses you want to add.
8. Save changes.

To change the m/z value and/or abundance of a mass:

1. Select the mass spectrum of which you want to edit the Mass List.
2. Click the **Mass List** tab.
3. From the Mass List, select the mass whose m/z value and/or whose abundance

you want to change.

4. In **Mass**, enter the desired m/z value and/or in **Abundance**, enter the desired abundance.
5. Click in the Mass List. This changes the selected mass accordingly.
6. Repeat steps 3 to 5 for all masses you want to change.
7. If you have changed the abundance of the current 100% mass below the abundance of another mass, click **Normalize** to renormalize the Mass List. This sets the now most abundant mass to an abundance of '999' and changes the abundance values of the other masses accordingly.
8. Save changes.

To remove a mass:

1. Select the mass spectrum of which you want to edit the Mass List.
2. Click the **Mass List** tab.
3. From the Mass List, select the mass you want to remove.
4. Click **Remove**.
5. Repeat steps 3 and 4 for all masses you want to remove.
6. If you have removed the current 100% mass, click **Normalize** to renormalize the Mass List. This sets the now most abundant mass to an abundance of '999' and changes the abundance values of the other masses accordingly.
7. Save changes.

5.2.8.2 Editing the Acquisition Parameters of a Mass Spectrum

You can edit the acquisition parameters of the selected mass spectrum displayed in the Acquisition Parameters tab. When a mass spectrum is imported into LibraryEditor either from the file system or directly from DataAnalysis, the information on essential acquisition parameters that is contained in the imported file will automatically be entered. You can edit the acquisition parameters of a mass spectrum by making new entries and/or changing existing entries.

To edit the acquisition parameters of a mass spectrum:

1. Select the mass spectrum whose acquisition parameters you want to edit.
2. In the **Acquisition Parameters** tab, make the desired new entries or changes.
3. Save changes.

5.2.8.3 Editing the Spectrum Info of a Mass Spectrum

You can edit the spectrum info of the selected mass spectrum displayed in the Spectrum Info tab. When a mass spectrum is imported into LibraryEditor, either from the file system or directly from DataAnalysis, some information on the acquired analysis this spectrum derives from will automatically be entered as well as operator information.

You can edit the spectrum info except the read-only entries in **Analysis name**, **Instrument name**, **Date**, **Operator name** and **Change date** by adding new or changing existing entries.

To edit the spectrum info of a mass spectrum:

1. Select the mass spectrum whose acquisition parameters you want to edit.
2. Click the **Spectrum Info** tab
3. Make the desired new entries or changes, if allowed.
4. Save changes.

5.3 Deleting Mass Spectra and Compounds from a Library

You can delete mass spectra and compounds from a library if you do not need them any longer in the respective library. Deleting a mass spectrum occurs in two steps. First, the selected mass spectrum will be removed from the compound it corresponds to but it will be put to the memory. This allows you to re-add the respective spectrum to the compound it derives from e.g. if you have deleted it by mistake. Or you can add this spectrum as a new compound entry or to another compound of the active library. Deletion will only become permanent when you select another compound of the active library without having re-added the respective mass spectrum.

5.3.1 Deleting a Mass Spectrum from a Compound

Deleting the selected mass spectrum from the corresponding compound occurs in two steps. On selecting the **Delete** command from the **Spectrum** menu, firstly the selected mass spectrum will be removed from the compound it corresponds to but it will be put to the memory. This allows you to re-add the respective mass spectrum either to the compound it derives from or as a new compound entry using the enabled **Add** command from the **Spectrum** menu. Deletion will only become permanent when you select another compound of the active library without having re-added the respective mass spectrum.

If the mass spectrum you want to delete is the only mass spectrum available for the selected compound, deletion of this mass spectrum will result in deletion of the compound, too.

To delete a mass spectrum from a compound:

1. Select the mass spectrum you want to delete.
2. Click  or select **Delete** from the **Spectrum** menu.

5.3.2 Deleting a Compound from a Library

Deletion of the selected compound from the active library can be performed by deleting all mass spectra that are currently contained for this compound in the library. On deleting the last of its mass spectra, the respective compound will be deleted, too.

To delete a compound from a library:

1. Select the compound you want to delete.
2. Successively delete all mass spectra available for this compound.

6 BROWSING AND SEARCHING LIBRARIES

You can browse through the active library by scrolling through compounds contained in this library. Or you can directly search the active library for a compound that meets a given specification. For example, this allows you to quickly check whether a particular compound is already contained in the respective library.

6.1 Going to Compounds Contained in a Library

If you want to select a compound in the active library for viewing and, if desired, processing it you can use different ways to go to it. Alternatively, you can search for it directly e.g. by compound name.

Selecting the first compound of a library:

1. Click  or select **First** from the **Compound** menu.

Selecting the previous compound of a library:

1. Click the **Compound** box' down spin button. If the focus is set here, the mouse wheel can be used, too. Or click  or select **Previous** from the **Compound** menu.

Selecting the next compound of a library:

1. Click the **Compound** box' up spin button. If the focus is set here, the mouse wheel can be used, too. Or click  or select **Next** from the **Compound** menu.

Selecting the last compound of a library:

1. Click  or select **Last** from the **Compound** menu.

6.2 Searching a Library for a Certain Compound

You can search the active library for a certain compound which you have to specify by either its compound ID number, (one of) its spectrum ID number(s), compound name, CAS number, nominal mass, chemical formula or UN number. This allows you to search a library for the presence of a given compound or to select quickly a compound, which you know to be contained in the respective library. The latter is advantageous in the case of large libraries because it can keep you from time-consuming clicking

systematic through the compounds contained until you will reach the desired one.

With new libraries (library version 2.2 number), compound search by compound name also finds compounds with similar names. Thus, compounds can be found without their names being entered completely and perfectly right. This allows e.g. for searching a library for all compounds which names start with "Methyl" or "Desmethyl". Also, using simple wildcards as well as 'regular expressions' (= special wildcards) is supported (For the regular expressions that can be used, please refer to the LibraryEditor Reference Manual.).

Depending on whether or not one or more compounds is/are found that meet(s) the specified criterion one of the following will occur:

- If only one compound is found the respective compound is shown in the library window.
- If more than one compound is found, the **Find Compound Result** dialog appears which lists all compounds found with the corresponding **Compound ID, Name, CAS number** and **Chemical formula** if available. You can use the **Show** button to show the selected compound.
- If no compound is found, a corresponding message appears informing you that the library 'name' does not contain a compound of the specified criterion 'entry'. On quitting this message, the **Find Compound** dialog appears again.

To search a library for a certain compound:

1. Click  or select **Find Compound** from the **Compound** menu.
2. Select the search criterion you want to use.
3. If you want to search by '**Name**' and want to use 'regular expressions', check **Use 'regular expressions' for search by 'Name'**.
4. For the search criterion selected, enter the respective number or name.
5. Click **OK**. One of the following will occur:
 - If only one compound is found, this is shown in the library window.
 - If more than one compound is found, the **Find Compound Result** dialog appears. To show a compound of the list, select it and click **Show**.
 - If no compound is found, a corresponding message appears.
6. If compound search was not successful, repeat steps 2 to 5 if desired.

A APPENDIX

A.1 LibraryEditor 4.0 Toolbar

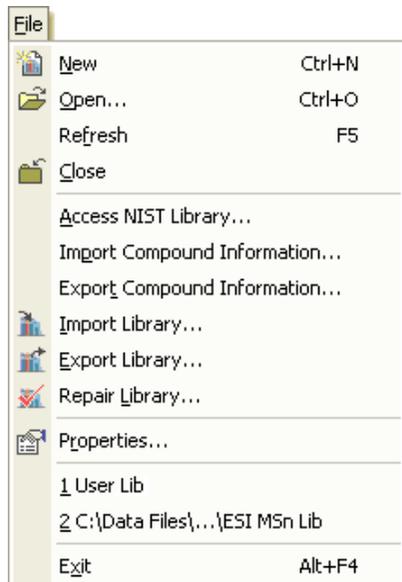
LibraryEditor 4.0 provides in its toolbar the following buttons:

| <u>Button</u> | <u>Menu - Command</u> | <u>Shortcut</u> | <u>Used to...</u> |
|---|--------------------------|-----------------|---|
|  | File – New | Ctrl+N | Create a new library. |
|  | File – Open | Ctrl+O | Open an existing library. |
|  | File – Properties | | Show properties of active library. |
|  | Compound – First | Alt*Home | Select first compound. |
|  | Compound – Previous | Alt+Left | Select previous compound. |
|  | Compound – Next | Alt+Right | Select next compound. |
|  | Compound – Last | Alt+End | Select last compound. |
|  | Compound – Find Compound | Alt+F3 | Specify a compound to search for. |
|  | Spectrum – Add | | Add selected spectrum to active library. |
|  | Spectrum – Save | Ctrl+S | Save the changes made to selected spectrum. |
|  | Spectrum – Delete | | Delete selected spectrum. |
|  | Edit – Cut | Ctrl+X | Cut selection. |
|  | Edit – Copy | Ctrl+C | Copy selection. |
|  | Edit – Paste | Ctrl+V | Paste Clipboard contents. |

A.2 LibraryEditor 4.0 Menus and Commands

LibraryEditor 4.0 provides the following menus and commands:

File menu



Commands

New
Open
Refresh
Close
Access NIST Library
Import Compound Information
Export Compound Information
Import Library
Export Library
Check Library
Properties
Recent file
Exit

Used to...

Create a new library.
Open an existing library.
Refresh the active library.
Close active library.
Access NIST library and user libraries.
Import selected compound information.
Export compound information of active library.
Import selected library into active library.
Export active library.
Check and rebuild selected library.
Show number of compounds and spectra of active library.
Open selected library.
Close LibraryEditor.

Edit menu



Commands

Undo
Cut
Copy
Paste

Used to...

Undo last performed editing operation.
Cut selection.
Copy selection.
Paste Clipboard contents.

Compound menu

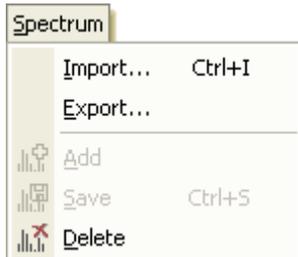


Commands

Find Compound
Import Structure
Export Structure
Delete Structure
First
Previous
Next
Last

Used to...

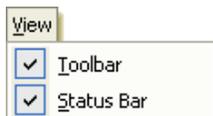
Specify a compound to search for.
Import structure of the compound.
Export structure of the compound.
Delete structure of the compound.
Select the first compound.
Select the previous compound.
Select the next compound.
Select the last compound.

Spectrum menuCommands

Import
Export
Add
Save
Delete

Used to...

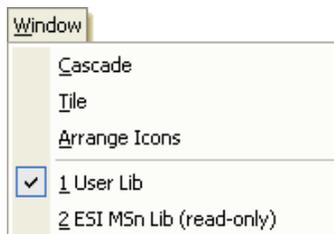
Import a mass spectrum.
Export selected amss spectrum.
Add imported mass spectrum.
Save changed mass spectrum.
Delete selected mass spectrum.

View menuCommands

Toolbar
Status Bar

Used to...

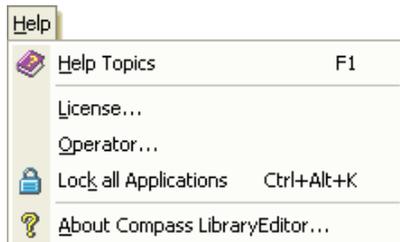
Show/Hide toolbar.
Show/Hide status bar.

Window menuCommands

Cascade
Tile
Arrange Icons
Open window list

Used to...

Arrange open library windows cascade-like.
Arrange open library windows tile-like.
Arrange icons of minimized library windows.
Select open library window to activate library.

Help menuCommands

Help Topics
License
Operator
Lock All Applications
About Compass LibraryEditor

Used to...

Start LibraryEditor help and list help topics.
License present LibraryEditor installation or view license information.
Log in specified operator.
Lock all Bruker Daltonics applications.
Show program information.

A.3 LibraryEditor 4.0 Shortcuts

LibraryEditor 4.0 provides the following shortcuts:

| <u>Shortcut</u> | <u>Menu – Command</u> | <u>Used to...</u> |
|-----------------|------------------------------|--|
| Alt+F3 | Compound – Find compound | Find compound. |
| Alt+F4 | File – Exit | Close LibraryEditor. |
| Alt+End | Compound – Last | Select the last compound. |
| Alt+Home | Compound – First | Select the first compound. |
| Alt+Left | Compound – Previous | Select the previous compound. |
| Alt+Right | Compound – Next | Select the next compound. |
| Ctrl+Alt+K | Help – Lock All Applications | Lock all Bruker Daltonics applications. |
| Ctrl+C | Edit – Copy | Copy selection. |
| Ctrl+I | Spectrum – Import | Import compound. |
| Ctrl+N | File – New | Create a new library. |
| Ctrl+O | File – Open | Open an existing library. |
| Ctrl+S | Spectrum – Save | Save changed mass spectrum. |
| Ctrl+V | Edit – Paste | Paste Clipboard contents. |
| Ctrl+X | Edit – Cut | Cut selection. |
| Ctrl+Z | Edit – Undo | Undo last performed editing operation. |
| F1 | Help – Help Topics | Start LibraryEditor help and list help topics. |

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