
libraryeditor 4.0

Reference Manual



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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. LibraryEditor also supports NIST and NIST user libraries created by other programs containing spectra from other vendors.

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

2 FILE MENU

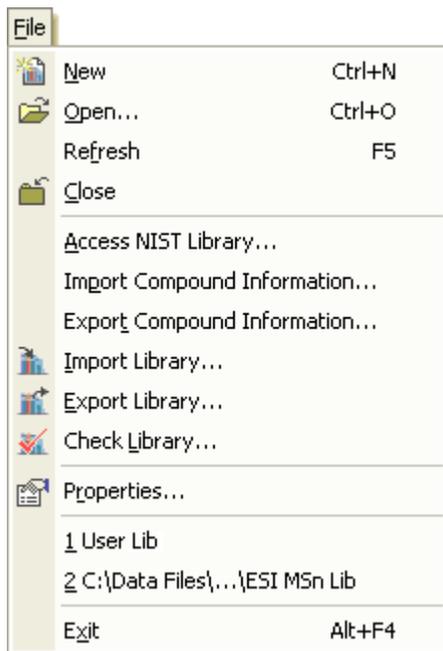


Figure 2-1 File menu (for a writable library being active)

The **File** menu offers the following commands:

New	Creates a new library.
Open	Opens an existing library.
Refresh	Refreshes the active library.
Close	Closes the active library.
Access NIST Library	Accesses an existing NIST user library.
Import Compound Information	Imports the selected compound information into the active library.
Export Compound Information	Exports compound information of the active library.
Import Library	Imports the selected library into the active library.
Export Library	Exports the active library to ASCII Library File format (*.library) or Library File format (*.mlb).
Check Library	Checks and rebuilds the selected user library.
Properties	Shows properties of the active library.
Recent file	Opens the selected recent file.
Exit	Closes LibraryEditor.

2.1 New Command

The **New** command is used to create a new library of the Libraries Files format (*.mlb) which can be used with LibraryEditor.

Each library must be placed in a separate folder. This is necessary since the various data files which are generated during a 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 new library and save it in the respective folder.

The command opens the **Create New Library** dialog. If you have not yet set up a new folder for the library you want to create, first create the respective folder. For this, click  and enter the name of the new folder. Then open this folder and create the new library.

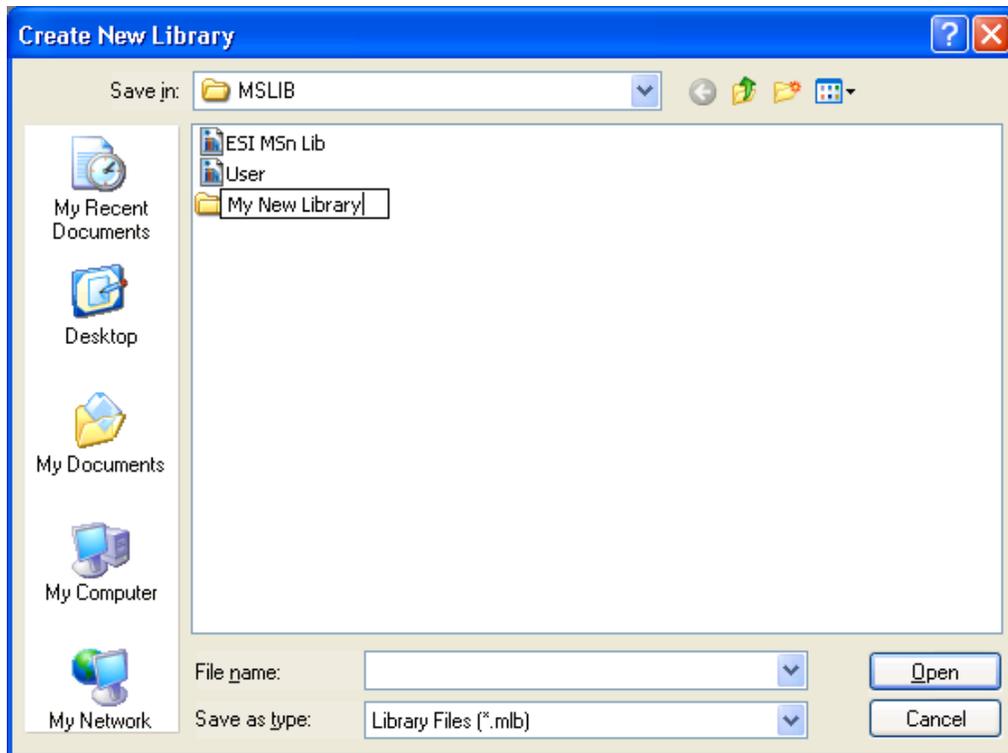


Figure 2-2 Create New Library dialog: Creating a new folder for the library to be set up

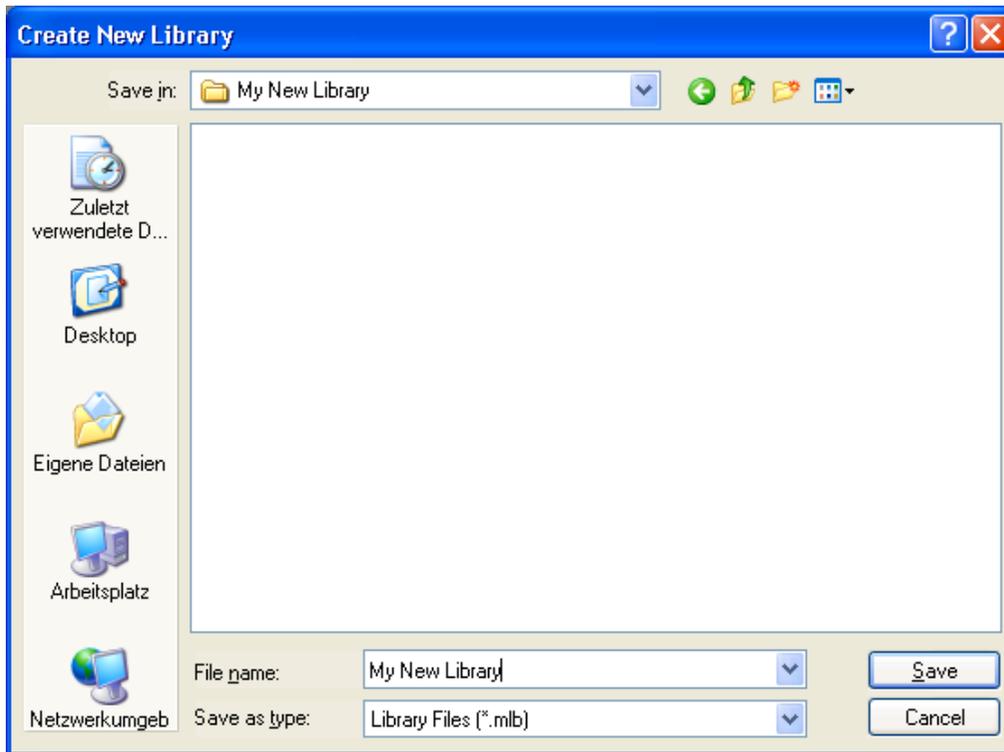


Figure 2-3 Create New Library dialog: Creating a library

Look in and folder list

Navigate to the drive and folder to which the new library should be saved. If the desired folder has not been set up yet, click , enter the new folder name in the appearing frame and then double-click the new folder.

File name

Enter the name of the new library you want to create.

Files of type

Select the file format the new library is to be saved to.

Library Files (*.mlb). Creates files of the Library Files format.

Save

Creates the new library, saves the data files set up for this library to the selected folder and opens the new library.

Shortcuts

Button: 
Keys: Ctrl+N

2.2 Open Command

The **Open** command is used to open an existing library having the Library Files format (*.mlb).

The command opens the resizable **Open Library** dialog, which allows you to specify the name and location of the library you want to open.

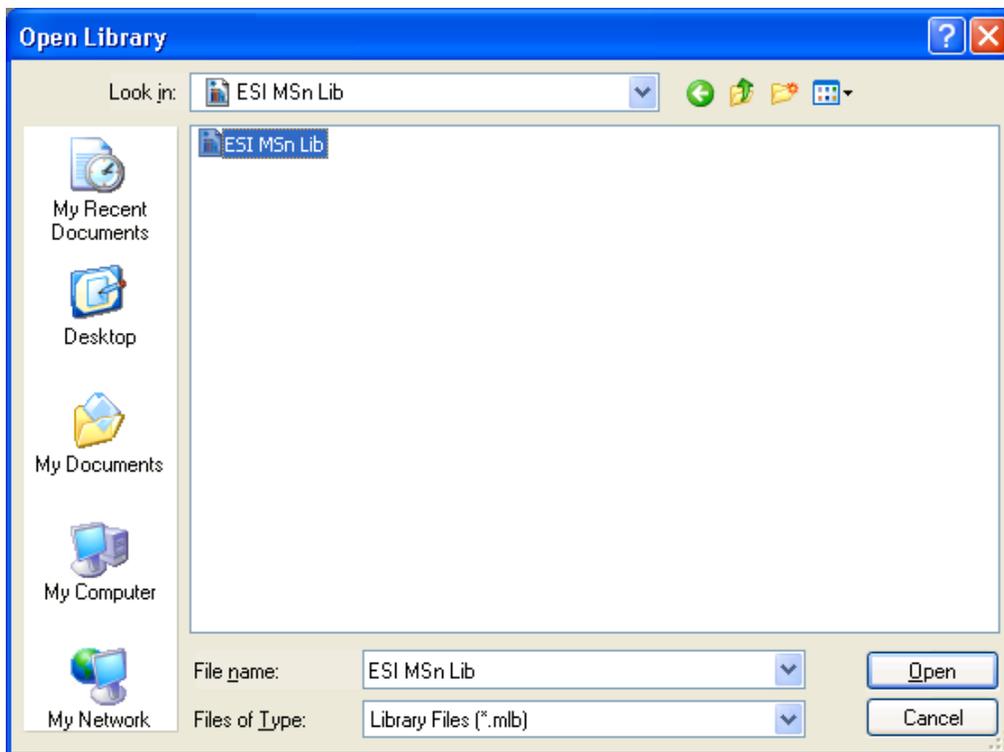


Figure 2-4 Open Library dialog

Look in and folder list

Navigate to the drive and folder that contains the library you want to open. Double-click the library or select it and click **Open**.

File name

Enter the file name or select it from the folder list.

Files of type

Select the type of files to be shown in the folder list.

Library Files (*.mlb). Lists all files of the Library Files format.

All (*.*). Lists all files available.

Open

If a library file is selected, it opens the respective library and displays the data of the first compound contained in this library.

If a folder is selected, it opens the folder and displays its contents in the folder list.

Shortcuts

Button:



Keys: Ctrl+O

2.3 Refresh Command

The **Refresh** command is used to 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.

2.4 Close Command

The **Close** command is used to close the active library. If on closing a library changes made to its currently selected compound have not been saved yet, a confirmation request appears asking you about saving these changes. After answering this request, the respective library is closed.

2.5 Access NIST Library Command

The **Access NIST Library** command is used to access the selected NIST user library (named 'User.dbu') that does not have the Library Files format (*.mlb) required by LibraryEditor yet. Performing this command generates the corresponding *.mlb file ('library name'.mlb) allowing you to open and process the respective library in LibraryEditor. Information about mass spectrum acquisition (e.g. ion polarity, MS/MS stage, precursor ion, product ion) that is stored in the respective NIST user library is entered automatically in Acquisition Parameter of the corresponding mass spectrum if Library-

Editor can read this information from the user library. The generated library automatically gets the name of the folder the User.dbu is contained in (in the example shown below this will be 'MSMSLib.mlb').

Additionally, you can optionally specify the location of the NIST main library via this command. Giving this location will enable chemical structures of the NIST user libraries to be resolved from the NIST main library.

The command opens the **Access NIST User Library** dialog, which allows you to select the user library you wish to get access to.

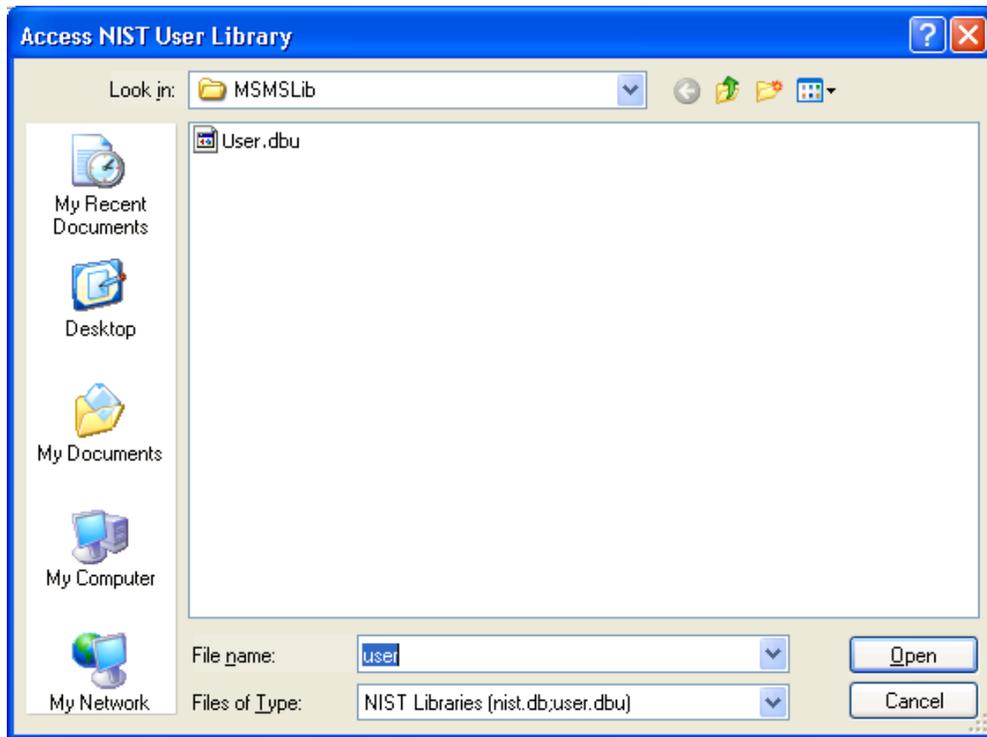


Figure 2-5 Access to NIST User Library dialog

Look in and folder list

Navigate to the drive and folder that contains the user library you want to get access to. Double-click the desired User.dbu file or select it and click **Open**.

File name

Automatically contains the file name User.dbu.

Files of type

Select the type of files to be shown in the folder list.

NIST Libraries Files (nist.db;user.dbu). Lists all files of the NIST Libraries Files format.

Open

If a folder is selected, opens the folder and displays its contents in the folder list. If a user.dbu file is selected and the location of the NIST main library is known, generates the corresponding *.mlb file for the selected user.dbu. A dialog informs you about successfully creating additional files for accessing NIST (user) library and asks you if you want to open the library now. Click **Yes** if you want to.

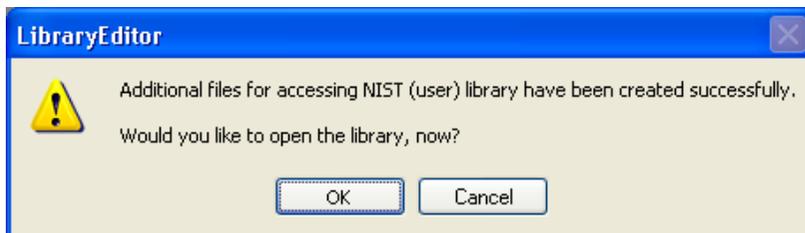


Figure 2-6 Information on creation of access file(s)

If a user.dbu file is selected but the location of the NIST main library has not been specified yet, the **NIST Library** dialog appears. Via this dialog, you can enter the location of the NIST main library as an option. This allows chemical structures from NIST user libraries to be resolved from the NIST main library. For this, enter the respective path or click and select it in the appearing **NIST Main Library** dialog. Clicking **OK** saves the location of the NIST main library and generates the corresponding *.mlb file for the selected user library. Clicking **Cancel** also generates the *.mlb file but does not save any NIST main library location.

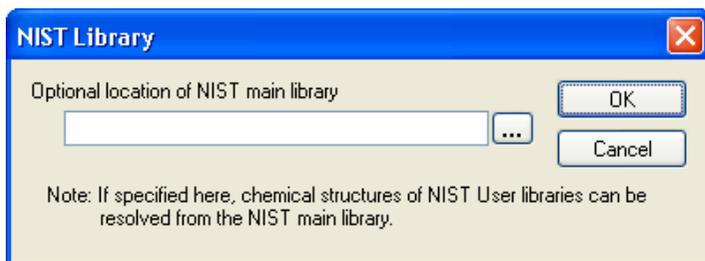


Figure 2-7 NIST Library dialog

2.6 Import Compound Information Command

The **Import Compound Information** command to 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 (Section 2.6.1). A 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 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.

The command opens the **Import Compound Information** dialog, which allows you to select the compound information file to be imported into the active library.

Look in and folder list

Navigate to the drive and folder that contains the compound information file you want to import. Double-click the file or select it and click **Open**.

File name

Enter the file name or select it from the folder list.

Files of type

Select the type of files to be shown in the folder list.

Comma Separated Values Files (*.csv). Lists Comma Separated Values Files.

Tab Separated Values Files (*.tsv). Lists Tab Separated Values Files.

Structure Data Files (SDfiles) (*.sdf). Lists Structure Data Files.

All Files (*.*). Lists all files present.

Open

If a compound information file is selected, it imports the respective information into the active library and overwrites that existing compound information that corresponds to matched compound names by the imported compound information.

If a folder is selected, it opens the folder and displays its contents in the folder list.

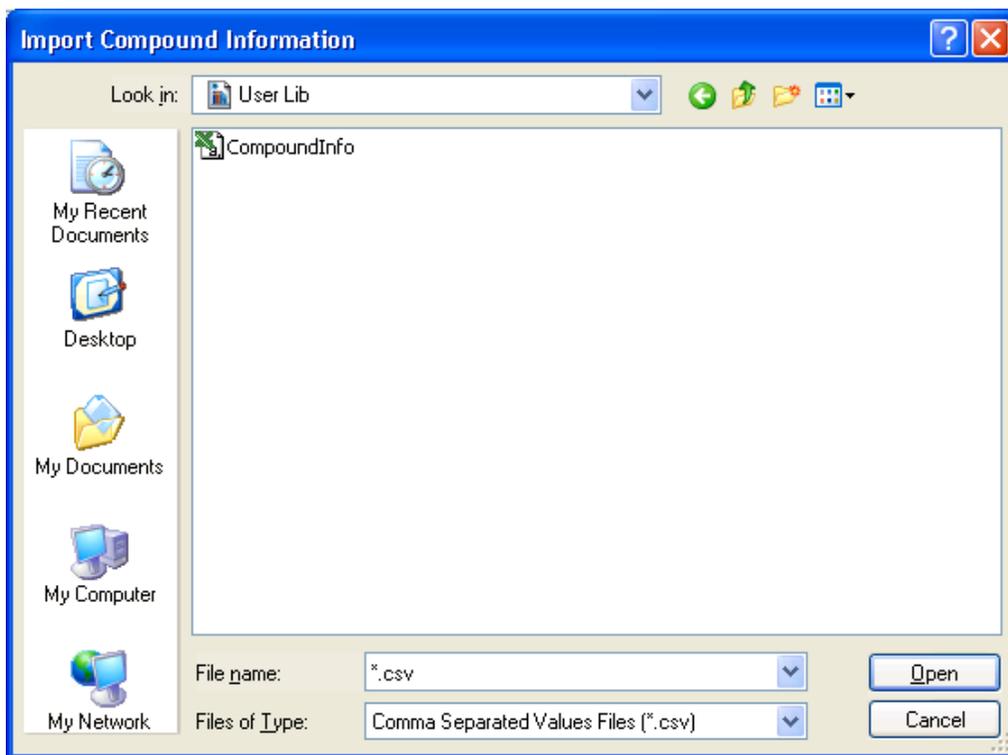


Figure 2-8 Import Compound Info dialog

2.6.1 Requirements for Creating Compound Information Containing *.csv or *.tsv Files

A compound information containing Comma Separated Values Files (*.csv) or Tab Separated Values Files (*.tsv) file must meet specific requirements concerning the data that may be contained and how this data has to be entered.

The first not empty row (which not necessarily must be the first row in the file) has to contain a kind of string, which may include the following tokens. These will be recognized neglecting capital/small letters:

- Name
- Formula
- Comment
- NominalMass
- CASNo
- NISTNo

- UNNo
- Synonym

The following rules have to be followed:

- The first token must be the 'Name' token, which, therefore, is mandatory.
- The 'Synonym' token can be contained several times.
- If the 'Name' token is present, multiple times the last token must be 'Name' again. This will ensure that the corresponding compound will be renamed to the second occurrence of 'Name'.
- All other tokens are allowed to be present only once.
- In a *.csv file the tokens must be comma separated, in a *.tsv file tab separated. Empty spaces before and after the separators will be neglected. Aside from the different separators used *.csv and *.tsv files behave quite equivalent.

For example, a valid CSV format string could look as follows:

Name, Synonym, casNO, SYNONYM, NAME

This format string is understood as follows: Subsequently a list of (any number of) rows will follow having the following format: First the compound name is given for which all following information is to be entered (since it is allowed that several compounds within a library have the same compound name the following actions will be performed on all compounds of the library having the respective compound name). This is followed by a new synonym to be added to the compound's synonym list if not already present. After that a CAS number comes that is to be entered for this compound; if a CAS number is already present this will overwrite the previous CAS number. Then an additional synonym follows to be also entered in the synonym list if not already present. Finally, a new compound name for the respective compound comes that will replace the old one.

After this format string row, the program expects any number of rows supplying information according to the above format. Intervening empty rows will be ignored. Optional entries of the format (except for the format string and the compound name) can be left out. This is a legal possibility to omit entries you do not want to make. Such "empty entries" result in the old entries remaining unchanged. For example, a row could look as follows:

Phenol, Hydroxybenzol, , , xyz

This row will have the following effects: The currently active library is searched for the presence of compounds named "Phenol". Depending on whether such a compound is found the following happens:

- If (a) compound(s) named "Phenol" is/are found, "Hydoxybenzol" is added to all corresponding synonym lists if not already present. All "Phenol" entries are renamed to "xyz". Since the entries for CAS number and the second synonym have been left out (empty entries), the old CAS number remains unchanged.

- If no compound named “Phenol” is found, nothing will happen. No new compound named “Phenol” will be added to the library.

2.7 Export Compound Information Command

The **Export Compound Information** command is used to export the compound information of the active library to Comma Separated Values Files (*.csv) or Tab Separated Values Files (*.tsv) format which can be loaded e.g. into Excel. The exported file includes information about each compound of the library concerning its name, formula, nominal mass, CAS number, and comment, if available.

The command opens the **Export Compound Information** dialog to select the file format and target folder where you want to save the exported file.

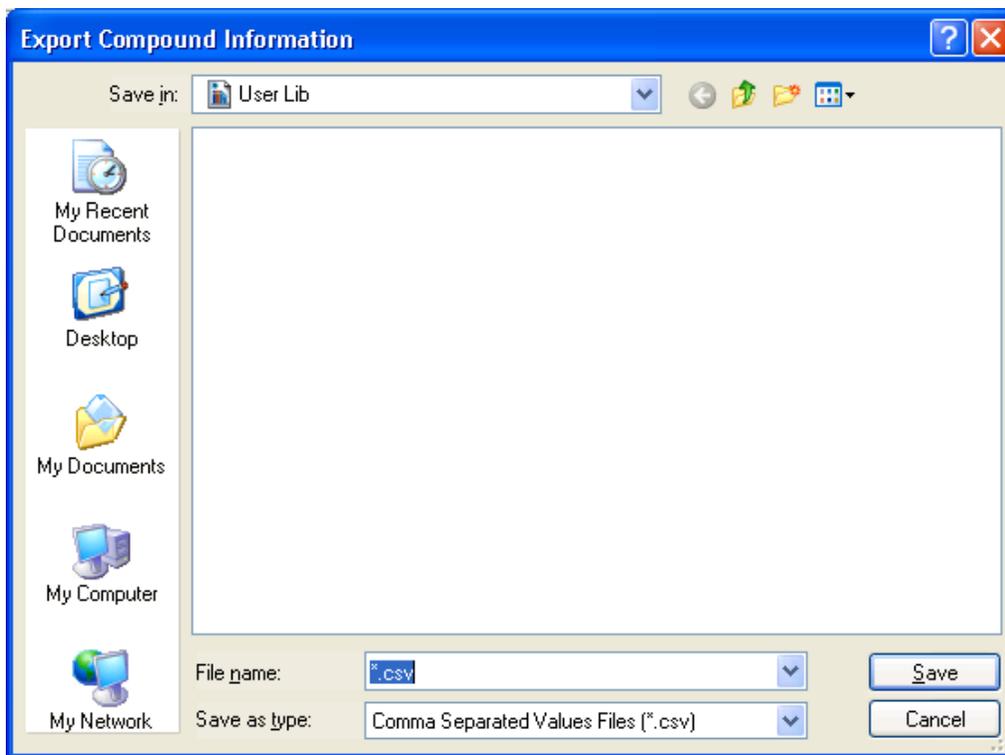


Figure 2-9 Export Compound Information dialog

Save in and folder list

Navigate to the drive and folder in which you want to save the exported file.

File name

Enter a new file name or select an existing name from the folder list.

Save as type

Select the format the compound information should be converted to.

Comma Separated Values Files (*.csv). Converts to Comma Separated Values Files format.

Tab Separated Values Files (*.tsv). Converts to Tab Separated Values Files format.

All Files (*.*). Lists all files present.

Save

Converts the compound information of the active library into the selected file format and saves it under the specified name in the selected folder. If you have chosen an already existing file name, confirm the appearing request for overwriting the existing file.

2.8 Import Library Command

The **Import Library** command is used to import the selected library having the Library Files format (*.mlb) into the active library in order to add the compounds and/mass spectra contained in the import library to the active library.

When 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 are being added to the latter as new compound entries whereas the mass spectra of those 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.

The command opens the **Import Library** dialog, which allows you to select the library you want to import into the active library.

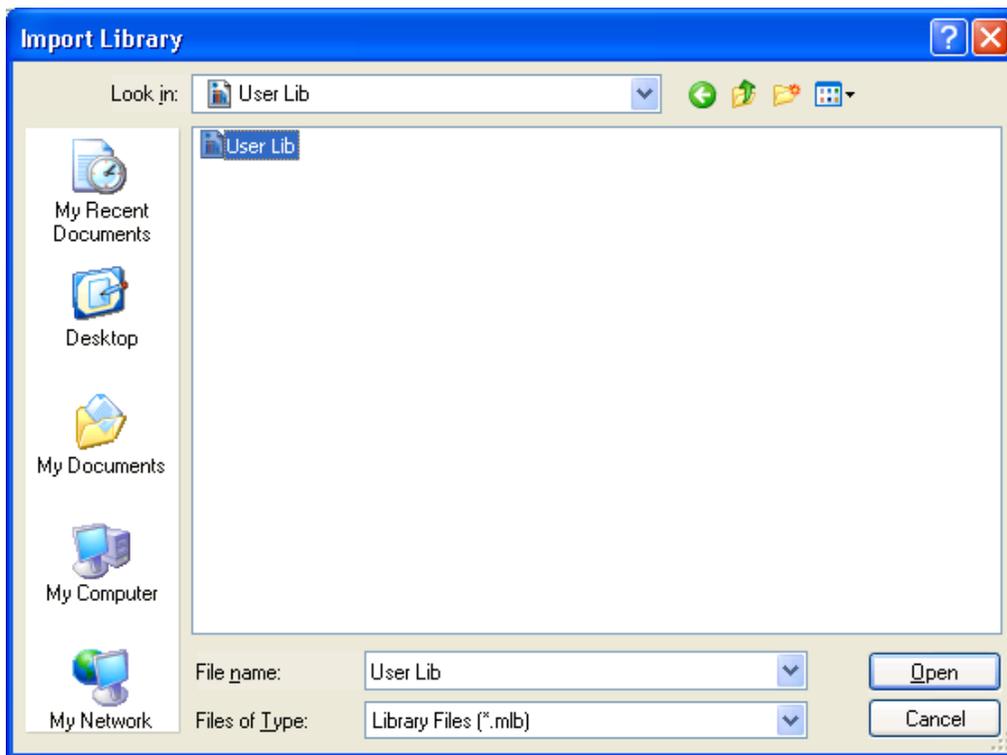


Figure 2-10 Import Library dialog with the library to be imported being selected

Look in and folder list

Navigate to the drive and folder that contains the library you want to import. Double-click the library or select it and click **Open**.

File name

Enter the file name or select it from the folder list.

Files of type

Select the type of files to be shown in the folder list.

Library Files (*.mlb). Lists all files of the Library Files format.

Open

If a folder is selected, it opens the folder and displays its contents in the folder list.

If a library file is selected, it imports the selected library into the active library. Information on the import process and progress appears. This dialog lists at its end all compound ID's of the active library, which got new spectra. To close this information, click **Close**.

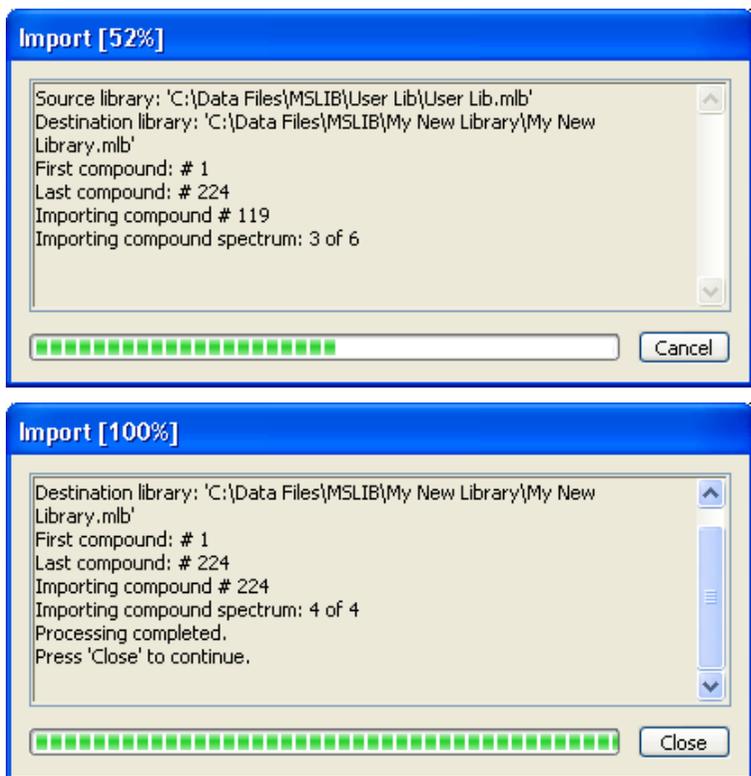


Figure 2-11 Information about import process and progress during (above) and after import is finished (below)

2.9 Export Library Command

The **Export Library** command is used to export the active library to ASCII Library Files (*.library) or Library Files (*.mlb) format.

The ASCII Library Files format (*.library) is fully NIST compatible and, therefore, allows for loading the exported library into the NIST. It is almost identical with the ASCII MS Spectrum Files format (*.spectrum) with the one difference that the *.library format can contain any number of mass spectra but the *.spectrum format only a single one. The specification of the ASCII Spectrum Files format (*.spectrum) is given with the description of the **Import** command from the **Spectrum** menu.

The command opens the **Export Library** dialog, which allows you to select the name for the library file to be exported and where it is to be saved.

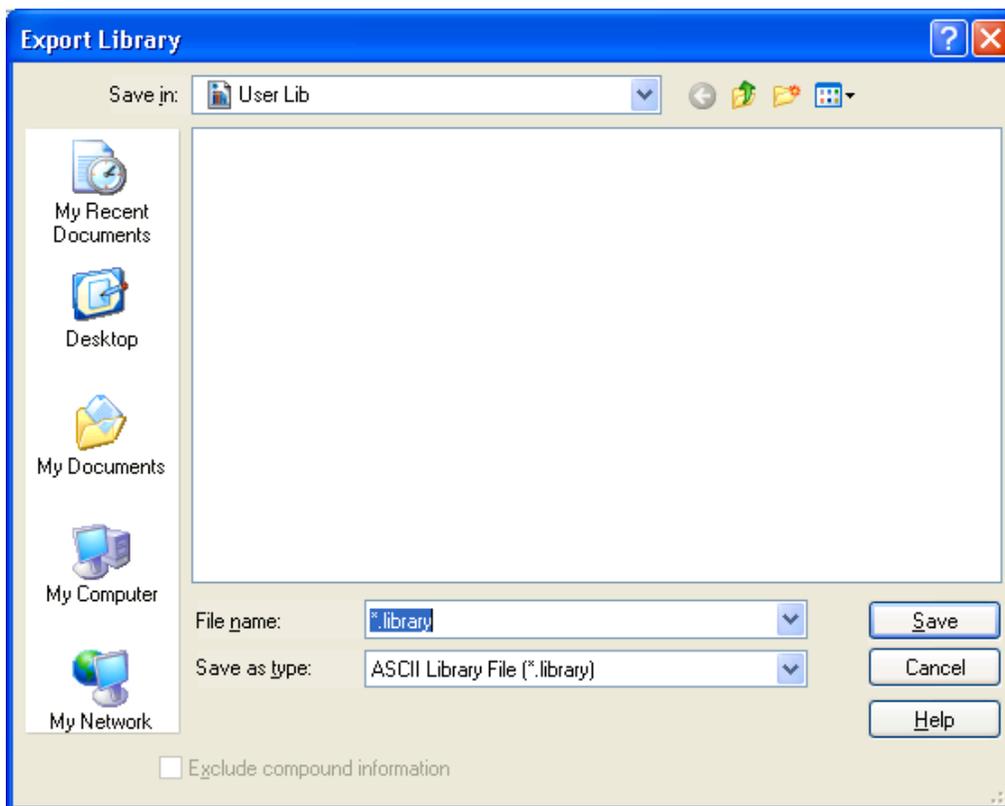


Figure 2-12 Export Library dialog

Save in and folder list

Navigate to the drive and folder in which you want to save the exported file.

File name

Enter a new file name or select an existing name from the folder list.

Save as type

Select the file format the library should be converted to:

ASCII Library File (*.library). Converts to ASCII Library File format.

Library File (*.mlb). Converts to the Library File format.

Exclude compound information

If the **Library File (*.mlb)** format is selected, check this option if compound information should be excluded from being exported. This results in the exported library containing only compound names but no additional compound information. If this option is not checked, full compound information is included. Default is unchecked.

Save

Converts the active library into the selected file format and saves it under the specified name in the selected folder. If you have chosen an already existing file name, confirm the appearing request for overwriting the existing file.

2.10 Check Library Command

The **Check Library** command is used to check and rebuild the selected library having the Library Files format (*.mlb). This is required if corresponding error messages have appeared when performing library search 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.

The command opens the **Check Library** dialog, which allows you to select the library you want to check.

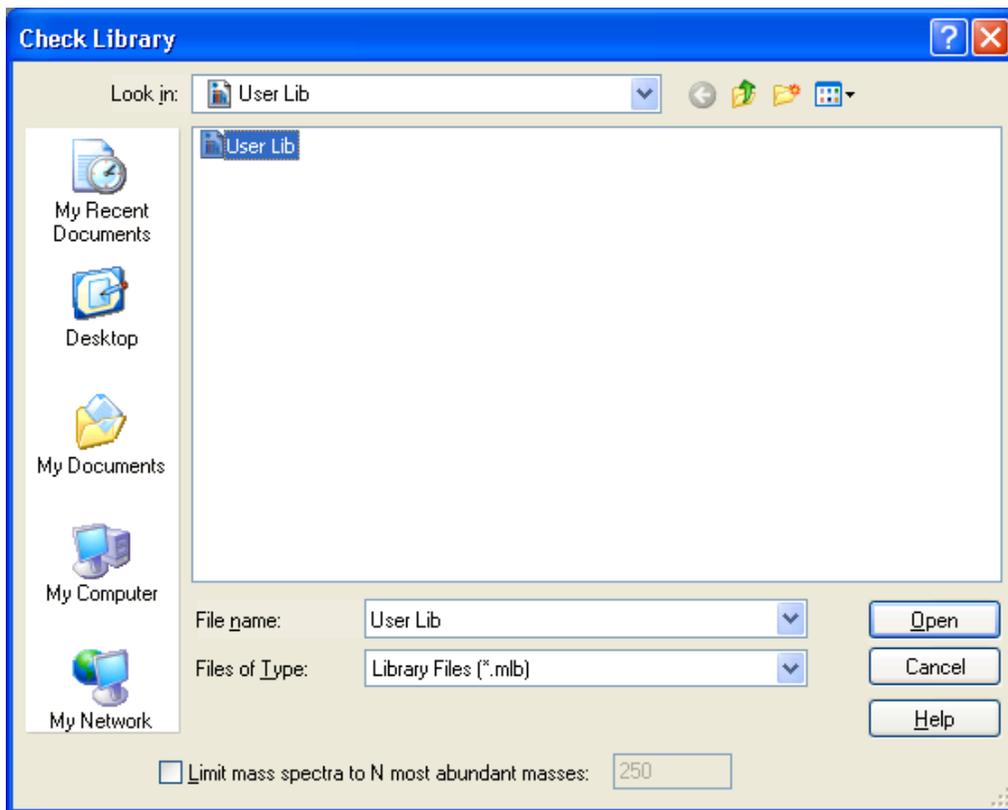


Figure 2-13 Check Library dialog

Look in and folder list

Navigate to the drive and folder that contains the library you want to check. Double-click the desired library file (*.mlb) or select it and click **Open**.

File name

Enter the file name or select it from the folder list.

Files of type

Displays the type of files to be shown in the folder list.

Libraries Files (*.mlb). Lists all files of the Library Files format.

Limit mass spectra to N most abundant masses

Check this option if mass spectra should be limited to a specified number of most abundant masses and enter the desired number in the box to the right. Default is unchecked. Default setting for 'N' is '250'.

Open

Checks and rebuilds the selected library and creates a new, rebuilt library file. If the option for limiting mass spectrum masses is set, the spectra currently containing more masses than the maximum number set are reduced to the specified number of most abundant masses.

First a temporary 'YYMMDDhhmmss' subfolder is created to which a copy of the original library is saved. Then the rebuild is performed. While this process is running, the **Check Library Progress** dialog informs you about the progress of rebuild.

After rebuild is finished, the new, rebuilt library file is saved according to the status (writable or read-only) of the original library. For writable libraries, a backup-subfolder of the general name 'BAK' or 'BAK_n' ($n \geq 2$) is created to which a backup of the original library is saved. Then the rebuilt library replaces the original library and the 'YYMMDDhhmmss' subfolder is removed. For read-only libraries, the original library remains unchanged and the rebuilt library is saved to the 'YYMMDDhhmmss' subfolder which is kept.

Click **Close** to close the dialog.

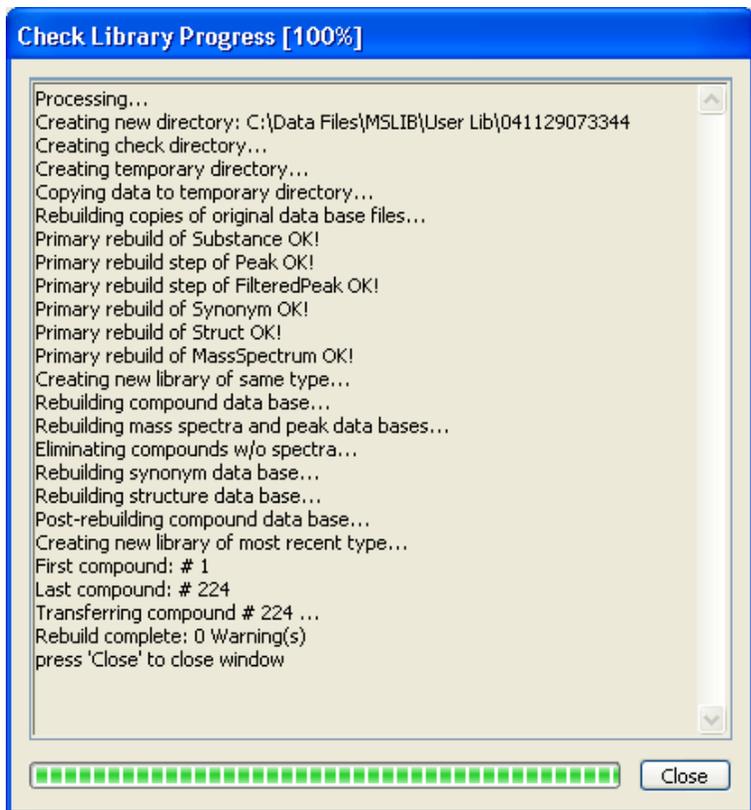


Figure 2-14 Check Library Progress dialog after rebuild of a writable library has been completed

2.11 Properties Command

The **Properties** command is used to show properties of the active library concerning library name and path, status, number of compounds and spectra contained, and version number.

The command opens the **Library Properties** dialog, which informs you about certain properties of the active library.

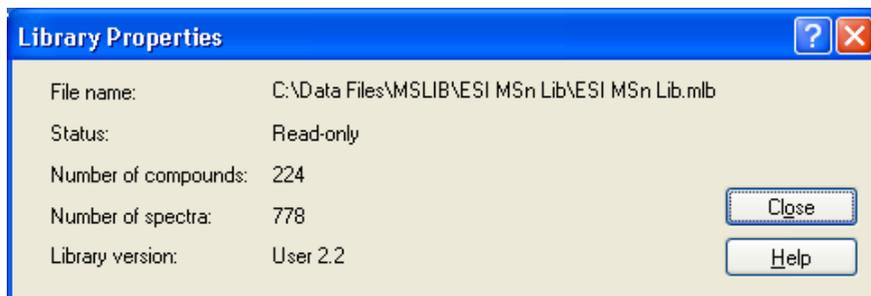


Figure 2-15 Library Properties dialog

Information about the following library properties is displayed:

File name

Displays file name and path of the active library.

Status

Displays the status of the library, **Read-only** or **Writable**.

Number of compounds

Displays the number of compounds currently contained in the library.

Number of spectra

Displays the number of spectra currently contained in the library.

Library version

Displays the version number of the library.

2.12 Recent File List

You can use the numbers and library file names listed in the recent file list at the bottom of the **File** menu to open quickly one of the last closed libraries. Select the number that corresponds to the library file you want to open.

When pointing on a recent file, corresponding full path name is displayed in a tool tip.

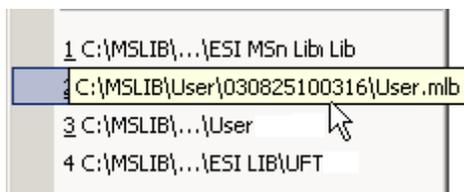


Figure 2-16 Tool tip displaying full path name of selected recent file

2.13 Exit Command

The **Exit** command closes your current LibraryEditor session. The current user interface settings are automatically stored for the current user logged into Windows. If on closing LibraryEditor changes made to the selected compound of the open library have not been saved yet, a confirmation request appears asking you about saving these changes. After answering this request, LibraryEditor is closed.

Shortcuts

Keys: ALT+F4

Button: Click  or double-click .

3 EDIT MENU



Figure 3-1 Edit menu

The **Edit** menu offers the following commands:

- Undo** Undoes the last editing action performed on the selected compound of the active library.
- Cut** Cuts the current selection in an entry field and puts it onto the Clipboard.
- Copy** Copies the current selection in an entry field and puts it onto the Clipboard.
- Paste** Inserts current Clipboard contents in the selected, editable entry field of the active library.

3.1 Undo Command

The **Undo** command undoes the last editing action you have performed in an editable entry field of the selected compound in the active library. This applies to compound and spectrum data fields.

Shortcut

Keys: Ctrl+Z

3.2 Cut Command

The **Cut** command cuts the current selection in an entry field and puts it onto the Clipboard. This applies to compound and spectrum data fields. Using the **Paste** command from the **Edit** menu, you can paste this data to a selected position in an editable entry field of the same or another library.

Shortcuts

Button: 

Keys: Ctrl+X

3.3 Copy Command

The **Copy** command copies the current selection in an entry field and puts it onto the Clipboard. This applies to compound and spectrum data fields. Using the **Paste** command from the **Edit** menu, you can paste this data to a selected position in an editable entry field of the same or another library.

Shortcuts

Button: 

Keys: Ctrl+C

3.4 Paste Command

The **Paste** command pastes the current Clipboard contents to the selected position in an entry field of the active library. This applies to compound and spectrum data entry fields. The command will be active for editable entry fields only.

Shortcuts

Button: 

Keys: Ctrl+V

4 COMPOUND MENU



Figure 4-1 Compound menu

The **Compound** menu offers the following commands:

Find Compound	Searches the active library for the compound specified.
Import Structure	Imports structure for the selected compound.
Export Structure	Exports structure of the selected compound.
Delete Structure	Deletes structure from the selected compound.
First	Selects the first compound of the active library.
Previous	Selects the previous compound in the active library.
Next	Selects the next compound in the active library.
Last	Selects the last compound of the active library.

4.1 Find Compound Command

The **Find Compound** command is used to search the active library for a particular compound. The compound can be specified by its compound ID number, one of its spectrum ID(s), name, CAS number, nominal mass, chemical formula or UN number.

This command allows you to select quickly a particular compound, which you know to be contained in the active library. In the case of large libraries, this can keep you from time-consuming clicking systematic through the compounds contained until you will reach the desired one. Additionally, you can search a library for a particular compound if you do not know whether it is contained in the respective library.

The command opens the **Find Compound** dialog, which allows you to specify the compound you want to find.

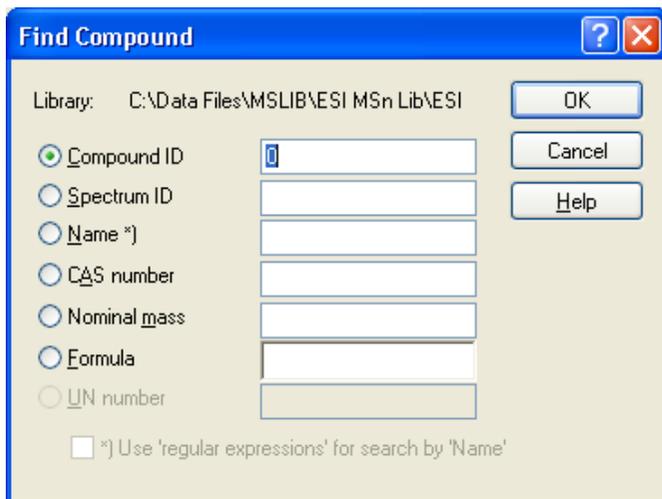


Figure 4-2 Find Compound dialog

Select the search criterion to be used to search the active library and enter the desired number or name.

Note: An entry made in one of the text boxes will become effective only if the corresponding option is checked.

Library

Displays path and name of the active library. If due to a longer path the library name is not shown (completely), click the entry and press the End key to get to the library name.

Compound ID

(Default) Select this option to search for a compound using a specified compound ID number. Enter the respective ID number in the box on the right.

Spectrum ID

Select this option to search for a compound using a specified spectrum ID number. Enter the respective ID number in the box on the right.

Name

Select this option to search for a compound using a specified compound name. Enter the respective name in the box on the right.

With new libraries (library version 2.2 number), the compound search routine also finds compounds with similar names. Thus, compounds can be found without their names being entered completely and perfectly right. For example, this allows for searching a

library for all compound names starting with e.g. "Methyl" or "Desmethyl" (see example below) which may be helpful especially when searching larger libraries.

Also using simple wildcards as well as 'regular expressions' (for description see 4.1.1) is supported. If you want to use regular expressions, you have to check the **Use 'regular expressions' for search by 'Name'** option.

CAS number

Select this option to search for a compound using a specified CAS number. Enter the respective CAS number in the box on the right.

Nominal mass

Select this option to search for a compound using a specified nominal mass. Enter the respective mass in the box on the right.

Formula

Select this option to search for a compound using a specified chemical formula. Enter the respective formula in the box on the right.

UN number

Select this option to search for a compound using a specified UN number. Enter the respective UN number in the box on the right.

Note: This option will be enabled for the original NIST library only.

Use 'regular expressions' for search by 'Name'

Check this option if you want to use 'regular expressions' (for description see 4.1.1) for compound search by 'Name'. Default is unchecked.

OK

Searches the selected library for the specified compound. Depending on whether one or more compounds is/are found which meet(s) the specified criterion one of the following occurs:

- If only one compound is found, this 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 corresponding **Compound ID**, **Name**, **CAS number** and **Chemical formula** if available.
To show one of these compounds, select the desired compound from this list and click **Show**.

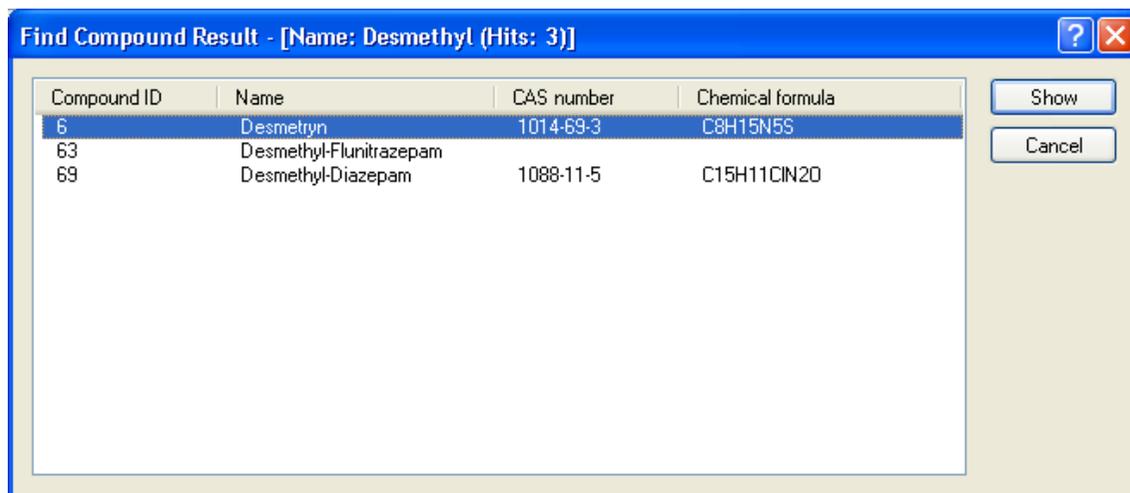


Figure 4-3 Find Compound Result – [‘Criterion’: ‘entry’(Hits:‘number’)] dialog listing all compounds found in a search by ‘Name’ meeting the specified criterion und entry

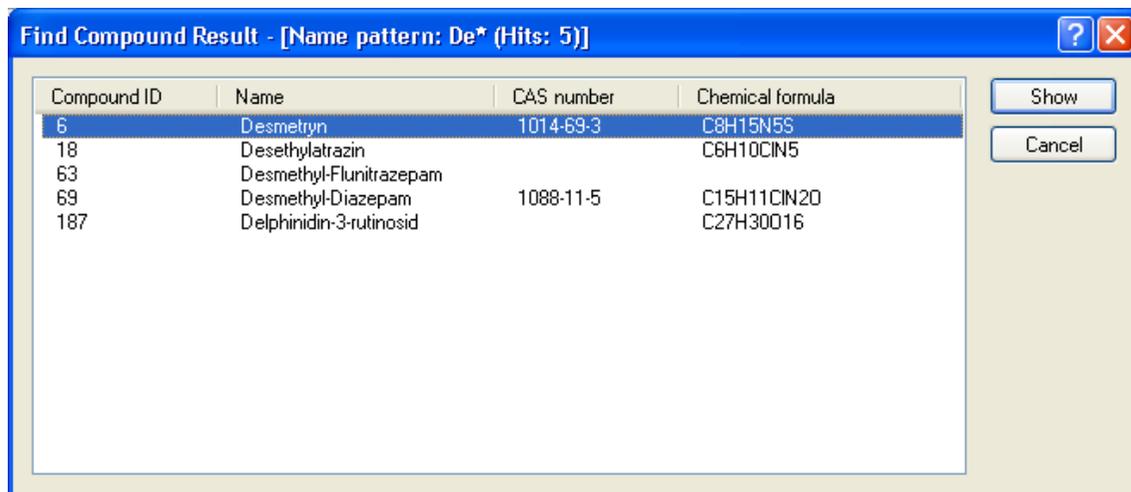


Figure 4-4 Result of compound search by ‘Name’ with using a simple wildcard (without *Use ‘regular expressions’ for search by ‘Name’* option set)

- 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 the message, the **Find Compound** dialog appears again showing the previous search entry.

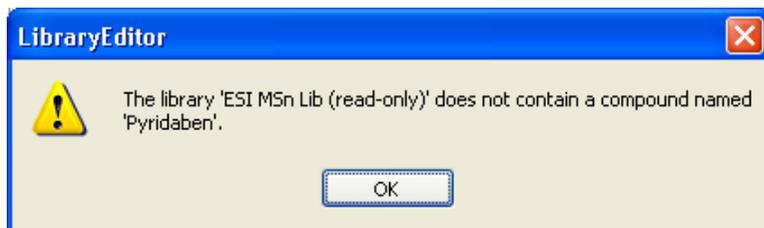


Figure 4-5 Message about named compound is not contained in searched library

Shortcuts

Button:



Keys: Alt+F3

4.1.1 Regular Expressions for Compound Search by 'Name'

To search for compounds by 'Name' you can use 'regular expressions' (= special wild-cards). For this, you have to check the **Use 'regular expressions' for search by 'Name'** option found in the **Find Compound** dialog.

Regular expressions represent notations for patterns of text rather than the literal character. They are a concise and flexible notation for finding patterns of text. The provided expressions conform to the POSIX extended syntax, but with locale specific collation disabled, and escape characters inside set declarations enabled. Additionally to that, the matching is performed case insensitively.

Expressions for matching characters or digits:

The following expressions can be used to match characters or digits in your search string:

<u>Expression</u>	<u>Syntax</u>	<u>Description</u>
Any character	.	Matches any single character except a line break.
Maximal — zero or more	*	Matches zero or more occurrences of the preceding expression.
Maximal — one or more	+	Matches at least one occurrence of the preceding expression.
Minimal — zero or more	?	Matches zero or one occurrences of the preceding expression.
Set of characters	[]	Matches any one of the characters within the []. To specify a range of characters, list the starting and

		ending character separated by a dash (-), as in [a-z].
Character not in set	[^...]	Matches any character not in the set of characters following the ^.
Grouping	()	Groups a subexpression.
Or		Matches the expression before or after the OR symbol (). Mostly used within a group. For example, (sponge mud) bath matches "sponge bath" and "mud bath."
Escape	\	Matches the character following the backslash (\). This allows you to find characters used in the regular expression notation, such as { and ^. For example, \^ Searches for the ^ character.
Range for the number of matches	{}	Matches a range of valid occurrences of the preceding expression.
Alphanumeric character in sets	[:alnum:]	[:alnum:] matches the expression ([a-zA-Z0-9]).
Word character	[:word:]	[:word:] matches the expression ([a-zA-Z0-9_]).
Alphabetic character	[:alpha:]	[:alpha:] matches the expression ([a-zA-Z]).
Decimal digit	[:digit:]	[:digit:] matches the expression ([0-9]).
Hexadecimal digit	[:xdigit:]	[:xdigit:] matches any hexadecimal digit character ([0-9a-fA-F]).
Blanks	[:blank:]	[:blank:] matches any blank character, either a space or a tab.
Space	[:space:]	[:space:] matches any whitespace character (Space, vertical tab, horizontal tab, form feed, newline)

Some useful aliases of regular expressions:

The following table lists some useful aliases of several regular expressions:

<u>Expression</u>	<u>Syntax</u>	<u>Alias</u>
Decimal digit	\d	[:digit:]
No decimal digit	\D	[^:digit:]
Space	\s	[:space:]
Non-space	\S	[^:space:]
Word character	\w	[:word:]
Non-word character	\W	[^:word:]

Further explanations:

The escape "\" character makes the following character to a simple literal and thus allows to search for characters which are actually part of the regular expression syntax. Special characters which have to be „literalized“ for their search are ".", "|", "*", "?", "+", "(", ")", "{", "}", "[", "]", "^", "\$" and "\".

Character classes are denoted using the syntax "[:classname:]" and are valid only within a set declaration, for example "[[:space:]]" is the set of all whitespace characters.

Some examples:

"ba*" will match all of "b", "ba", "baaa" etc.

"ba." will match "baa" or "ba5" for example but not "b", "ba", or "baaa"

(**Note:** The regular expression "." corresponds to "?" of simple wildcards, while the regular expression ".*" corresponds to "*" of simple wildcards.)

"ba+" will match "ba" or "baaaa" for example but not "b".

"ba?" will match "b" or "ba".

"ba{2,4}" will match "baa", "baaa" and "baaaa".

"ba{2,}" will match all of "baa", "baaa", "baaaa", "baaaaa", "baaaaaa" etc.

"a(b|c)" could match "ab" or "ac".

"abc|def" could match "abc" or "def".

"(H.*o)s(p.*e)" could match "Hello people" or "ho pe" for example. (Beware of the case insensitiveness and the spaces.)

4.2 Import Structure Command

The **Import Structure** command is used to import a chemical structure having the Mol Files format (*.mol) for the selected compound. This assigns the respective structure to the selected compound and saves it in the active library. After importing, the respective structure will be shown in the spectrum display. Once you have imported a structure you can export or delete it.

If a chemical structure is currently 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.

The command opens the **Import Mol File** dialog, which allows you to select the *.mol file for the compound currently selected in the active library.

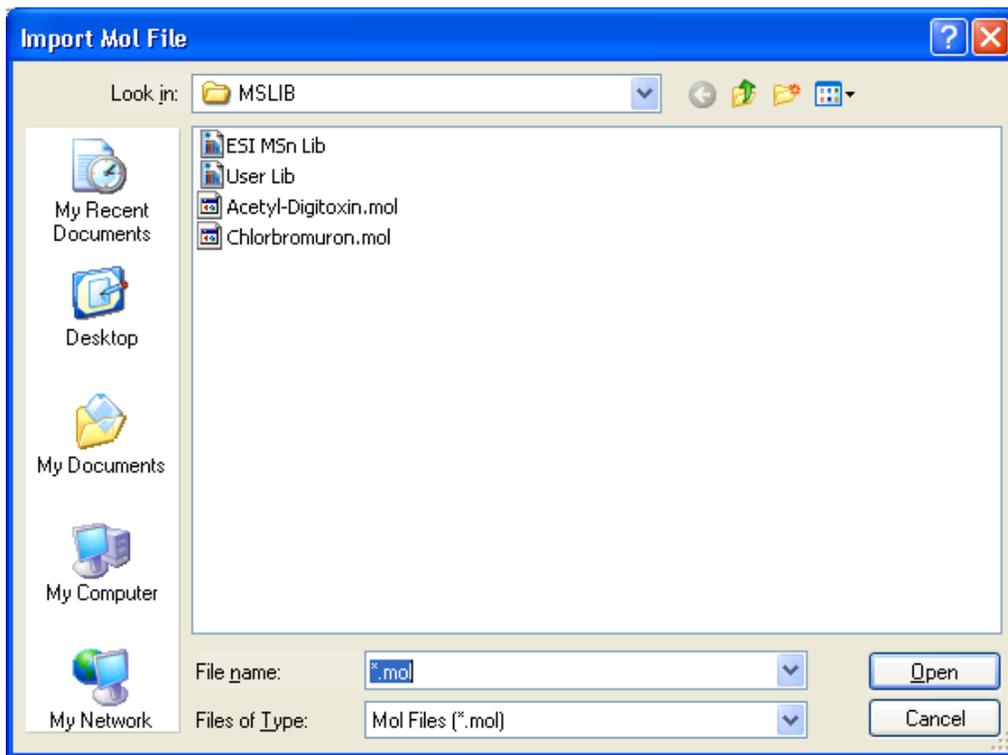


Figure 4-6 Import Mol File dialog

Look in and folder list

Navigate to the drive and folder that contains the *.mol file you want to import. Double-click the file or select it and click **Open**.

File name

Enter the file name or select it from the folder list.

Files of type

Displays the type of files to be shown in the folder list.

Mol Files (*.mol). Lists all files of the Mol Files format.

Open

If a *.mol file is selected, it imports the respective chemical structure, assigns the structure to the currently selected compound of the active library and shows it in the spectrum display.

If a folder is selected, it opens the folder and displays its contents in the folder list.

4.3 Export Structure Command

The **Export Structure** command is used to export the chemical structure currently assigned to the selected compound to Mol File format (*.mol).

The command opens the **Export Mol File** dialog, which allows you to select the name for the *.mol file to be exported and where it should be saved.

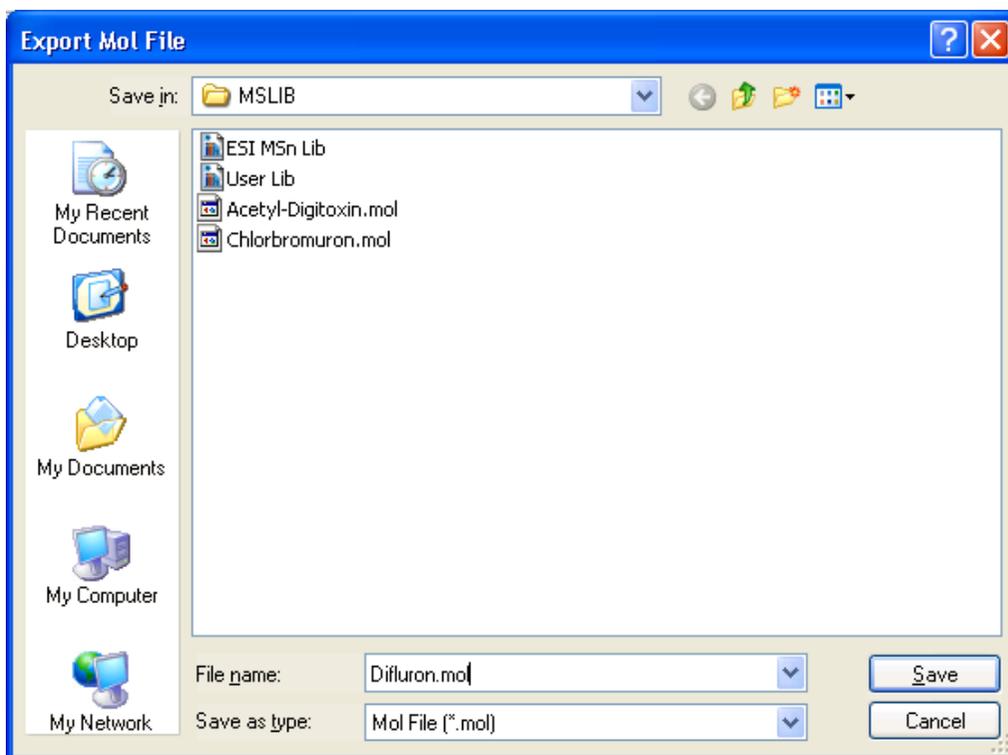


Figure 4-7 Export Mol File dialog

Save in and folder list

Navigate to the drive and folder in which you want to save the exported file.

File name

Enter a new file name or select an existing name from the folder list.

Files of type

Select the file format into which the structure should be exported:

Mol File (*.mol). Exports in the Mol File format.

Save

Exports the chemical structure in *.mol file format and saves it under the specified name in the selected folder. If you have chosen an already existing file name, confirm the appearing request for overwriting the existing file.

4.4 Delete Structure Command

The **Delete Structure** command deletes the chemical structure currently assigned to the selected compound of the active library.

4.5 First Command

The **First** command goes to the first compound in the active library. If changes made to the currently selected compound have not been saved yet, first a confirmation request appears asking you about saving these changes. After answering this question, the first compound appears.

Shortcuts

Button:



Keys:

Alt+Home

4.6 Previous Command

The **Previous** command goes to the previous compound in the active library. If changes made to the currently selected compound have not been saved yet, first a confirmation request appears asking you about saving these changes. After answering this question, the previous compound appears.

Shortcuts

Button:



Keys:

Alt+Left

4.7 Next Command

The **Next** command goes to the next compound in the active library. If changes made to the currently selected compound have not been saved yet, first a confirmation request appears asking you about saving these changes. After answering this question, the next compound appears.

Shortcuts

Button:



Keys: Alt+Right

4.8 Last Command

The **Last** command goes to the last compound in the active library. If changes made to the currently selected compound have not been saved yet, first a confirmation request appears asking you about saving these changes. After answering this question, the last compound appears.

Shortcuts

Button:



Keys: Alt+End

5 SPECTRUM MENU

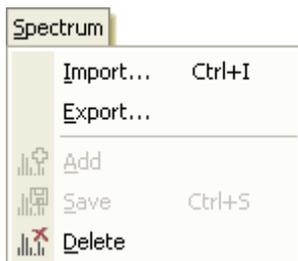


Figure 5-1 Spectrum menu

The **Spectrum** menu offers the following commands:

Import	Imports the selected mass spectrum.
Export	Exports the selected mass spectrum.
Add	Adds the imported mass spectrum as a new compound entry to the library or as a new mass spectrum to the selected compound.
Save	Saves the changes made to the selected mass spectrum.
Delete	Deletes the selected mass spectrum from the selected compound, which will result in deleting the respective compound from the active library if no mass spectrum is left for this compound.

5.1 Import Command

The **Import** command is used to import a mass spectrum from the file system in order to add this mass spectrum either as a new compound entry to the active library or as an additional mass spectrum to a selected compound. You can import mass spectra of the ASCII MS Spectrum Files format (*.spectrum) which were exported from either DataAnalysis or LibraryEditor or mass spectra of the NIST ASCII MS Spectrum Files format (*.msp) which were exported from the NIST main library.

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. If you want to add the respective mass spectrum to the active library, you must perform the **Add** command from the **Spectrum** menu and add the imported spectrum as either a new compound entry or a new (additional) mass spectrum to an existing compound. The **Add** command becomes enabled by performing a spectrum import.

The command opens the **Import Spectrum** dialog to select the mass spectrum to be imported.

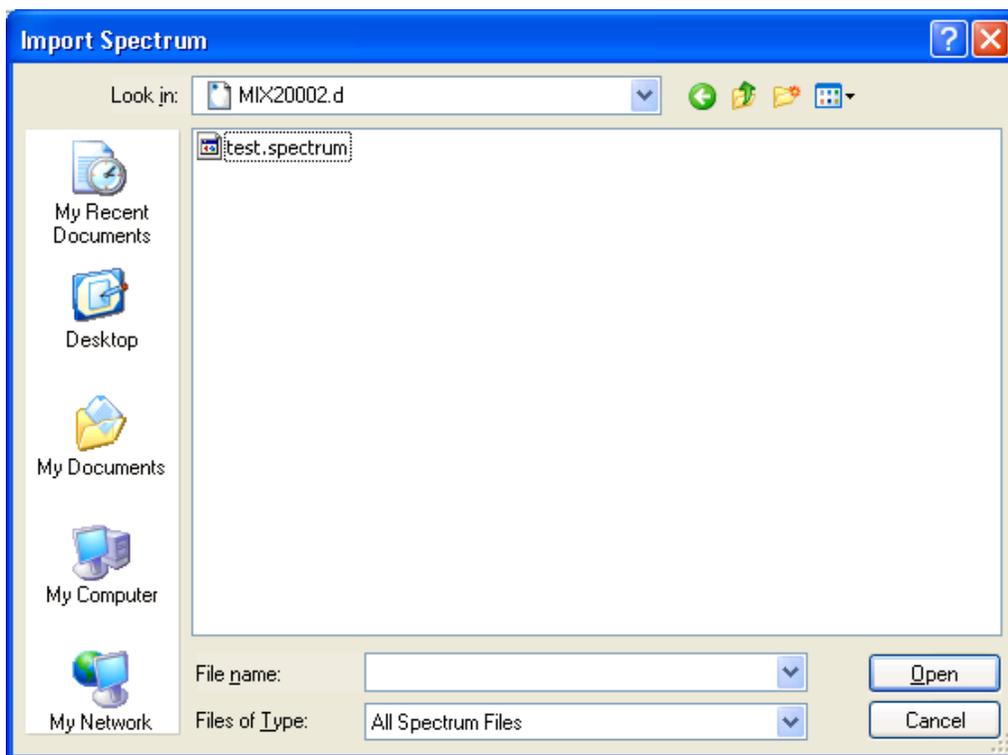


Figure 5-2 Import Spectrum dialog

Look in and folder list

Navigate to the drive and folder that contains the mass spectrum you want to import. Double-click the desired mass spectrum or select it and click **Open**.

File name

Enter the file name or select it from the folder list.

Files of type

Select the type of files to be shown in the folder list.

All Spectrum Files. Lists all files of the following formats.

ASCII MS Spectrum Files (*.spectrum). Lists all *.spectrum files exported from DataAnalysis (for description of file format see 5.1.1).

NIST ASCII MS Spectrum Files (*.msp). Lists all *.msp files exported from the NIST main library.

Open

If a mass spectrum file is selected, it imports the respective mass spectrum into LibraryEditor and displays the corresponding data without a **Compound ID** given and with 'unnamed' entered in **Name**. For adding this new mass spectrum, you have to select the **Add** command from the **Spectrum** menu.

If a folder is selected, opens the folder and displays its contents in the folder list.

Shortcuts

Keys: Ctrl+I

5.1.1 **ASCII MS Spectrum File Format (*.spectrum)**

The ASCII MS Spectrum File format (*.spectrum) is fully compatible to the NIST mass spectra file format and has the following specifications:

Each row of the file is introduced by a special case-insensitive keyword, which is immediately followed by a colon, separating the key from the corresponding value(s). Spaces or other characters between the keyword and the colon are not allowed. Some keywords can be abbreviated; the optional part is listed in parentheses in the table below.

The order of the keywords is irrelevant, but the first one must be the *Name* keyword and the last one must be the *Num Peaks* keyword. Other keywords are optional, but may appear only once (except for the *Synonym* keyword).

Note: Some keywords accept only predefined arguments, which are listed in braces.

Keyword	Description
<i>Name</i>	This entry is required, only ASCII characters between ' ' (ASCII no. 32) and '~' (ASCII no. 126) are allowed, see table II a below. For Greek characters see table II b below.
<i>CAS</i>	The chemical abstracts registry number (with or without '-').
<i>NIST</i>	The database entry number of NIST libraries.
<i>UN</i>	The four-digit <i>United Nations</i> number of the compound.
<i>MW</i>	The molecular weight in the sense of a nominal mass (an integer number).
<i>Form(ula)</i>	The chemical formula.
<i>Syn(onym)</i>	A synonym for the compound. This entry can appear multiply.
<i>Com(ment)</i>	Any comment.
<i>Struc(ture)</i>	The hexadecimally coded structure information of an MDL [®] MOL file, continuously written in the same line. Each single

byte value is a two-digit number, where each digit must be a hexadecimal number (0..9,A..F,a..f).

Example: The first five bytes of some arbitrary MDL MOL file with the molecule name H2O in the first line should start with

Structure: 48324F0D0A...

<i>Cont(ributor)</i>	Contributor, recommended as "Name, Organization".
<i>InstType</i>	Type of instrument. Recognized symbols are: {IT, TQ, Q, TOF, ICR, FTMS, ESI-TOF} .
<i>InstName</i>	Any description for the instrument.
<i>IoniMethod</i>	Method of ionization. Recognized symbols are: {EI, CI, APCI, ESI, nano-ESI, TS, MALDI, CAESIUM, APMALDI, APPI} .
<i>IonPol(arity)</i>	Ion polarity. The following symbols are recognized: {neg or 0 for negative, pos or 1 for positive, -1 for undefined polarity, both or 2 for both polarities}.
<i>MSMS(Stage)</i>	An integer number <i>n</i> describing the MS ^{<i>n</i>} stage.
<i>Prelon</i>	A comma-separated list of precursor ions in <i>m/z</i> (floating-point numbers). Although not obligatory, it is recommended to provide a list of <i>n-1</i> precursor ions, if the MSMS stage was specified to be of order <i>n</i> .
<i>ProdIon</i>	A floating-point number describing the product ion in <i>m/z</i> .
<i>TrapDrive</i>	A floating-point number describing the trap drive value of the <i>esquire</i> instruments.
<i>Skim1</i>	A floating-point number describing the skim 1 value of the <i>esquire</i> instruments.
<i>FragAmpl</i>	A floating-point number describing the fragmentation amplitude value in <i>V</i> .
<i>IsolWidth</i>	A floating-point number describing the isolation width value in <i>m/z</i> .
<i>TargetGas</i>	Any identifier for the target gas.
<i>TargetGasPres(sure)</i>	A floating-point number describing the target gas pressure in <i>hPa</i> .
<i>ReagentIon</i>	Any identifier for the reagent ion.
<i>ReagentGasPres(sure)</i>	A floating-point number describing the reagent gas pressure in <i>hPa</i> .
<i>ColEnergy</i>	A floating-point number describing the collision energy in <i>eV</i> .
<i>PeakWidth</i>	A floating-point number describing the original mass spectral peak width of the raw spectrum in <i>m/z</i> .
<i>Ref(lector)</i>	Integer number describing the reflector mode as linear {0} or reflector {1} .

<i>PSD</i>	Integer number describing whether the spectrum is a post source decay spectrum {0, 1}.
<i>ChargeDecon(volved)</i>	Integer number denoting whether the spectrum has been charge deconvoluted into the singly charged state {0, 1}.
<i>Date</i>	Date and time of the analysis given as a local time in the ISO 8601 format: <code>YYYY-MM-DD[T]HH:MM:SS[+ -]hh:mm</code> <i>Each item is presented as an integer value, hh:mm corresponds to the time offset between local time and the Coordinated Universal Time (UTC), such that UTC = local time - hh:mm</i>
<i>Column</i>	Any description of the chromatographic column.
<i>RetTime</i>	A floating-point number describing the retention time of the spectrum in analysis in seconds.
<i>SSID</i>	Unique software system ID of the analysis (Bruker-specific).
<i>AnaIID</i>	Unique ID of the analysis (Bruker-specific).
<i>AnaName</i>	Any descriptive identifier of the analysis.
<i>Mass(Range)</i>	Two comma-separated floating-point numbers describing the lowest and the highest mass values of the MS measurement range.
<i>Num(Peaks)</i>	This item is obligatory and must be the last one of the list. The format is as follows: An integer number of peaks followed by pairs of mass (floating-point) and intensity (floating-point) values delimited by characters of the set " \n,;:'(){}".

List of ASCII symbols allowed in the *Name* field:

SPACE	!	"	#	\$	%	&	'	()
*	+	,	-	.	/	0-9	:	;	<
=	>	?	@	A-Z	[\]	^	_
`	a-z	{		}	~				

Greek characters in the *Name* and *Synonym* fields can be embedded by placing their English transcription between dots:

.alpha.	.beta.	.gamma.	.delta.	.epsilon.	.zeta.
.eta.	.theta.	.iota.	.kappa.	.lambda.	.mu.
.nu.	.xi.	.omicron.	.pi.	.rho.	.sigma.
.tau.	.upsilon.	.phi.	.chi.	.psi.	.omega.

5.2 Export Command

The **Export** command is used to export a single mass spectrum to the ASCII MS Spectrum Files format (*.spectrum) to the file system. This e.g. allows importing the mass spectrum into another library opened in LibraryEditor.

The command opens the **Export Spectrum** dialog to select the name and target folder for the mass spectrum to be exported.

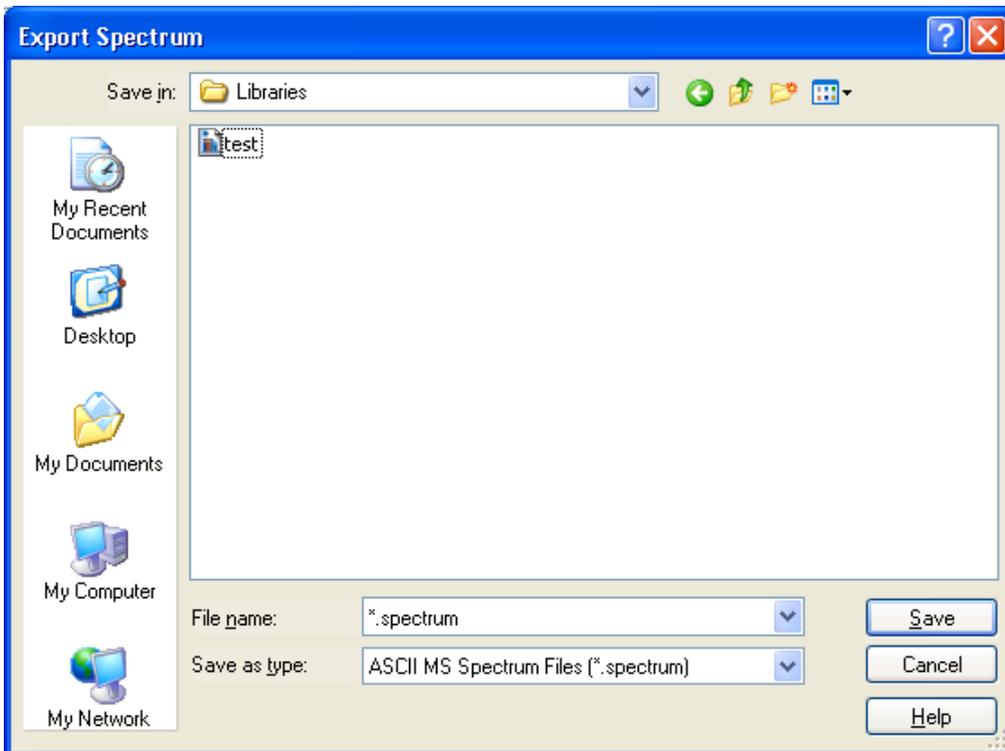


Figure 5-3 Export Spectrum dialog

Save in and folder list

Navigate to the drive and folder in which you want to save the exported file.

File name

Enter a new file name or select an existing name from the folder list.

Save as type

Select the file format the library should be converted to:

ASCII MS Spectrum Files (*.spectrum). Converts to the ASCII MS Spectrum Files format.

Save

Converts the active mass spectrum into the selected file format and saves it under the specified name in the selected folder. If you have chosen an already existing file name, confirm the appearing request for overwriting the existing file.

5.3 Add Command

The **Add** command is used to add the mass spectrum you have previously imported. You can add this spectrum to the active library as either new compound entry or new (additional) spectrum for an existing compound. Additionally, you can use this command to re-add a previously deleted mass spectrum. This operation is possible until you select another compound in the same library.

On selecting this command, the program first checks whether the active library already contains a compound of the specified **Name**. Depending on the result of checking, one of the following appears:

- If the library does not contain compound of this name, the mass spectrum is added to the library as a new compound entry, automatically getting a **Compound ID** number.
- If a compound with the same name is found, the **Add New Spectrum** dialog appears informing you that the **New compound** 'name' already exists in the library and lists the respective compounds with their compound IDs and names. In this case, you have to decide whether the new mass spectrum is to be added as a new compound entry to the library, or as a new mass spectrum to an existing compound, which you have to select from the list.

If the **Add New Spectrum** dialog appears, define how to add the mass spectrum:

New compound

Displays the compound name currently assigned to the mass spectrum to be added. If you want to add the mass spectrum as a new compound entry, change the compound name shown and click **New**. You are also allowed to use the same compound name, which will result in two compound entries having the same name. Otherwise, leave the entry unchanged.

(Compound list)

Lists the compounds currently contained in the active library having the same compound name with the corresponding compound ID in front.

If you want to add the mass spectrum as a new mass spectrum to an existing compound, select the respective compound from this list and click **Add to**.

New

Adds the mass spectrum as a new compound entry to the library using the compound name specified in **New compound**.

Add to

Adds the mass spectrum as a new spectrum to the compound selected in the compound list.

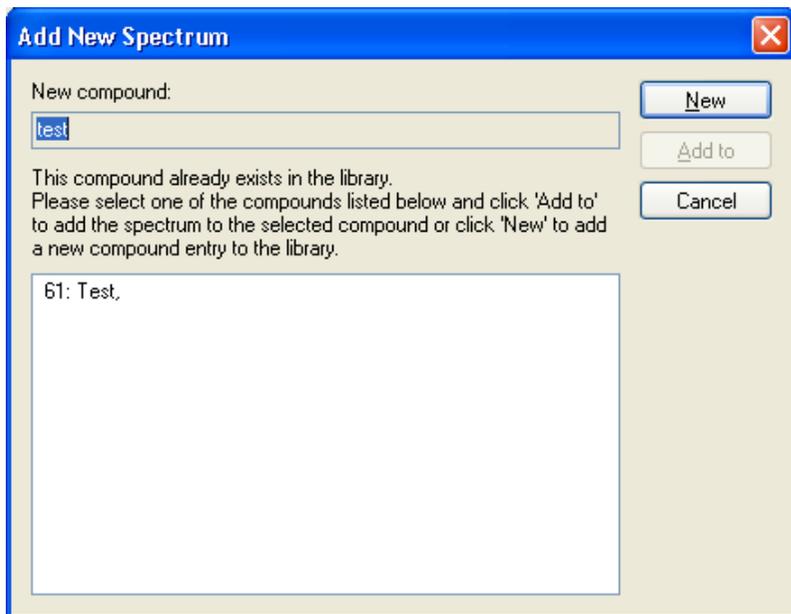


Figure 5-4 Add new spectrum dialog

Shortcut

Button:



5.4 Save Command

The **Save** command saves the changes made to the selected mass spectrum or compound e.g., by editing a mass spectrum's Mass List or the compound's synonym list.

Shortcut

Button:



5.5 Delete Command

The **Delete** command is used to delete the selected mass spectrum from the corresponding compound. If the selected mass spectrum is the only mass spectrum available for this compound, then deleting the mass spectrum will result in deleting the compound from the library.

Deleting a mass spectrum occurs in two steps. By selecting this command, 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 add the respective mass spectrum back to either the compound it derives from or as a new compound entry using the enabled **Add** command from the **Spectrum** menu, e.g., if you have deleted the respective mass spectrum by mistake. Deletion is only completed when you select another compound of the active library.

Selecting this command puts the respective mass spectrum to memory. The compound ID number disappears and the **Add** command becomes enabled. Deletion becomes effective on selecting another compound of the active library.

Shortcut

Button:



6 VIEW MENU

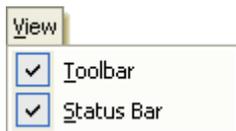


Figure 6-1 View menu

The **View** menu offers the following commands:

- Toolbar** Shows/Hides the toolbar.
Status Bar Shows/Hides the status bar.

6.1 Toolbar Command

The **Toolbars** command hides the toolbar when currently visible or shows it when currently hidden.

6.2 Status Bar Command

The **Status Bar** command hides the status bar when currently visible or shows it when currently hidden.

7 WINDOW MENU

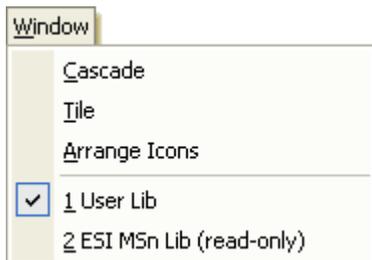


Figure 7-1 Window menu

The **Window** menu offers the following commands:

Cascade	Arranges multiple library windows in cascade view.
Tile	Arranges multiple library windows in tile view.
Arrange Icons	Arranges the icons of minimized libraries.
Open library list	Activates the selected library and displays its window on top.

7.1 Cascade Command

The **Cascade** command arranges the open library windows currently not minimized in cascade view. All windows have the same default size but they are shifted by a title bar height and an angle of 45°. The active library displays on top with its title bar being highlighted.

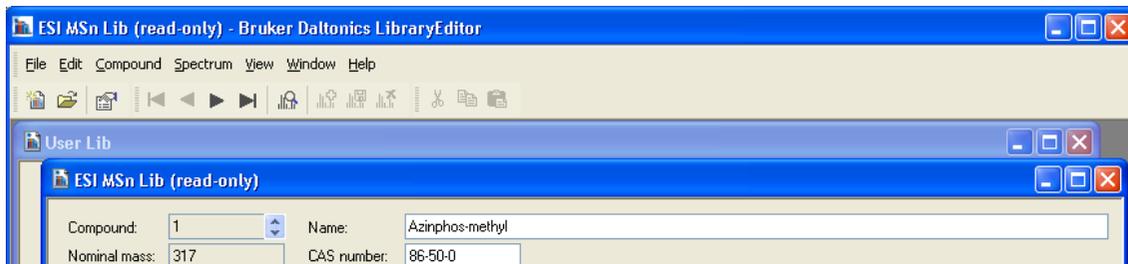


Figure 7-2 Two library windows arranged in cascade view

7.2 Tile Command

The **Tile** command arranges the open library windows currently not minimized in tile view. Selecting this command shows the window of the currently active library covering the full width of the LibraryEditor's user interface. When you activate another library, then its window is laid like a tile onto the window of the previously active library. The active library displays on top with its title bar being highlighted.

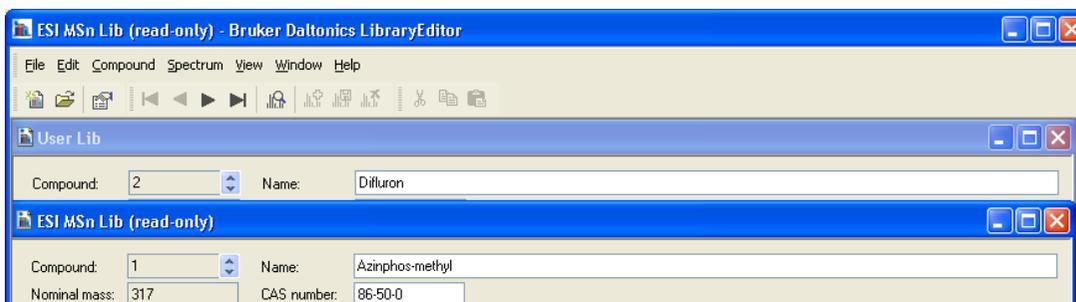


Figure 7-3 Two library windows arranged in tile view

7.3 Arrange Icons Command

The **Arrange Icons** command arranges the icons of libraries whose windows are currently minimized within a straight line at the bottom of the LibraryEditor window.



Figure 7-4 Arrangement of icons before (top) and after (bottom) selecting the Arrange Icons command

7.4 Open Library List

If more than one library is open, you can use the open library list to activate a library currently not active. The currently active library is indicated by a check mark in front of the library name. Selecting another library from this list activates that library and shows its library window according to the current display mode. If you select a library currently minimized, this library is shown again either maximized or on top of the other open library windows.

8 HELP MENU

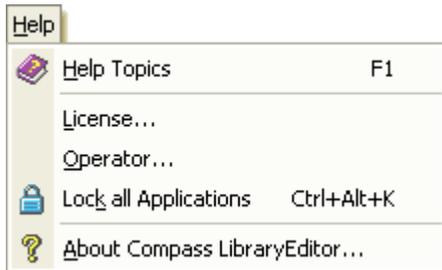


Figure 8-1 Help menu (when in Compliance mode)

The **Help** menu offers the following commands:

Help Topics	Starts LibraryEditor Help.
License	Licenses your present LibraryEditor installation and displays license information.
Operator	Logs in the specified operator.
Lock All Applications	Locks all Bruker Daltonics applications.
About Compass LibraryEditor	Provides information about your present LibraryEditor copy.

8.1 Help Topics Command

The **Help Topics** command starts LibraryEditor Help in order to get information about specific topics. LibraryEditor Help is used like other help applications running under Windows.

Shortcuts

Button:



Key: F1

8.2 License Command

The **License** command is used to view, add and/or delete licenses for Bruker Daltonics applications. The command opens the **Bruker Daltonics LicenseManager** dialog that shows any license currently available for any of the Bruker Daltonics applications and how long it will be valid.

To add a new license, enter the license key you received in **New license key** and click **Add**. A new line is added to **Existing licenses** with the key you have entered, the product name and the date until the license will be valid. To delete an existing license select it in **Existing licenses**, click **Delete** and confirm the corresponding request.

Note: If LibraryEditor is running in Compliance mode, only operators who have the special right can add and delete licenses.

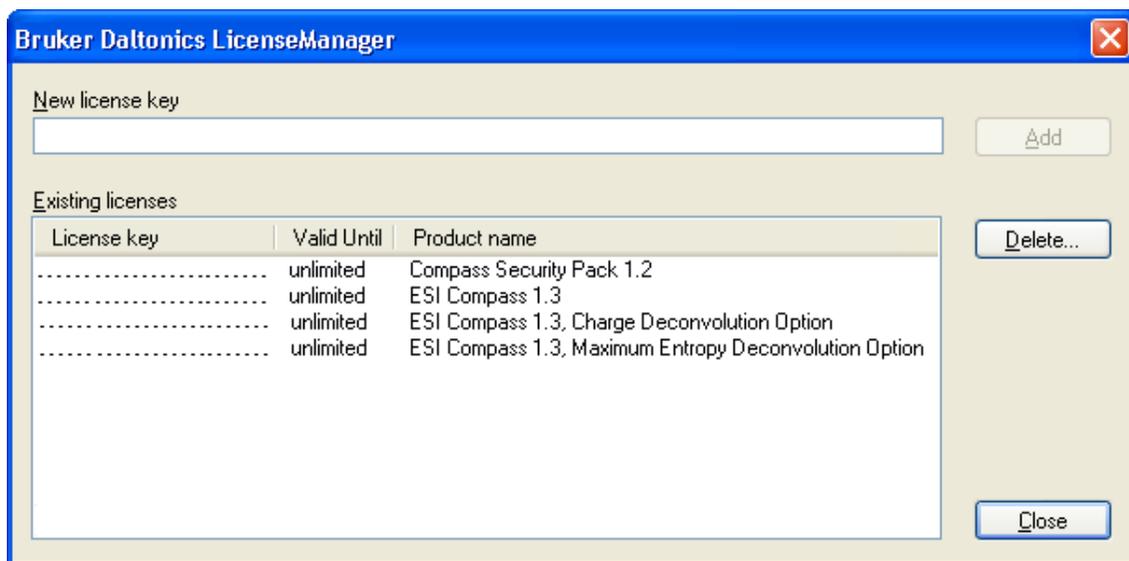


Figure 8-2 Bruker Daltonics LicenseManager dialog with 'ESI Compass 1.3' license needed for LibraryEditor being present (example)

New license key

Enter the submitted license key. This enables the **Add** button.

Existing licenses

Lists already existing licenses.

License key

Lists the license keys for the existing licenses.

Valid until

Permanent licenses are indicated as 'unlimited'.

For temporary licenses, the date until the respective license is valid is shown. An expiration warning will inform you automatically about the forthcoming expiration of a temporary license firstly 30 days before the respective expiration will expire. If for one product more than one license is present, this warning concerns to the longest valid license. An expiration warning will appear once per 24 hours and can be skipped by the operator.

Product name

Lists the names of the products for which licenses already exist.

Add

When in Non-Compliance mode, adds the license key entered in **New license key** to the list of existing licenses and licenses the corresponding product.

When in Compliance mode, opens the **Re-enter Your Password** dialog (see below) to enter again the password for the current operator account. The license key will be added after re-entering the correct password and if the operator has the required right. This button becomes enabled after the license key has been entered completely.

Delete

When in Non-Compliance mode, deletes the license key selected in the **Existing licenses** list after affirming corresponding confirmation request.

When in Compliance mode, opens, after affirming confirmation request, the **Re-enter Your Password** dialog to enter again the password for the current operator account. The license key will be deleted after re-entering the correct password and if the operator has the required right.

Re-enter Your Password dialog

This dialog is used to re-enter the password for the current operator account.



Figure 8-3 Re-enter Your Password dialog

Password

Enter the password for the current operator account.

OK

If the password is correct for the current operator account and the operator has the right to add/delete licenses the entered license key is added to or the selected license key is deleted from the LicenseManager's **Existing licenses** list.

If the password is incorrect or the operator does not have the required right, a corresponding error message will inform you.

8.3 Operator Command

The **Operator** command is used to change the operator during a running LibraryEditor session. When LibraryEditor is running in Compliance mode, you can also use this command to change your current password.

Note: There is always only one operator logged into Bruker Daltonics applications on a specific computer at a time.

The command opens the **LibraryEditor** dialog, which allows you to log in and/or change your password. Depending on the current mode, Non-Compliance or Compliance, this dialog looks something different. In Non-Compliance mode, you can log in without identifying whereas in Compliance mode you have to identify by operator name and password.

Note: This dialog appears automatically on each start-up of your LibraryEditor application unless you are currently logged in another Bruker Daltonics application (for both Non-Compliance and Compliance mode) or the corresponding option for skipping this dialog is set (for Non-Compliance mode only).

Operator

Enter your operator ID. The ID of the current operator will automatically be entered if the UserManagement administrator has set the corresponding option. The operator ID is not case-sensitive.

Password

Enter your password. The password is not displayed as you type it.

Note: Passwords are case-sensitive. Successive wrong inputs will cause locking of the operator when the number of wrong login tries exceeds the number of wrong logins allowed by the UserManagement administrator. Only the UserManagement administrator can unlock a locked operator.

Note: This entry field is available in Compliance mode only.

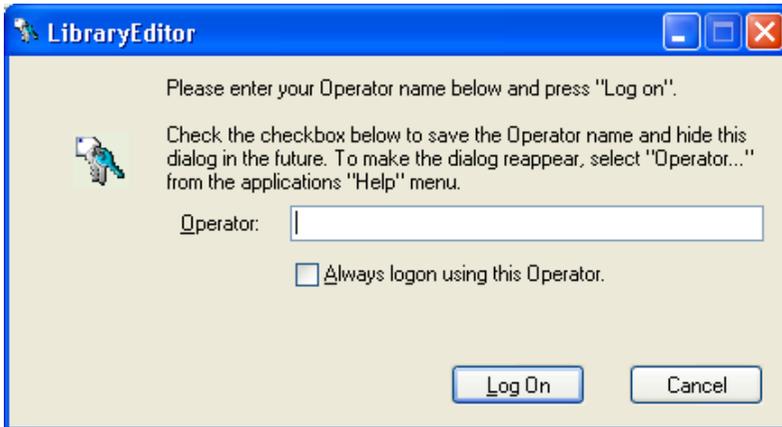


Figure 8-4 LibraryEditor dialog for logging in the operator when in Non-Compliance mode



Figure 8-5 LibraryEditor dialog for logging in the operator when in Compliance mode

Always login using this Operator

Check this option if the operator named in **Operator** should be logged in automatically. This will skip this dialog when starting LibraryEditor in future.

Note: This check box is available in Non-Compliance mode only.

Change Password

Allows you to change your current password before logging in. Opens the **Change Password** dialog (see below).

Note: This button is available in Compliance mode only.

Log On

Logs in the (specified) operator.

In Compliance mode, log in will be successful only if operator ID and password match.

If both do not match an error message will appear. Successive wrong password inputs can cause locking of an operator by UserManagement. If a new created operator tries to log into a Bruker Daltonics application the first time, the program requires for changing the password. Quitting the request opens the **Change Password** dialog (see below).

Change Password dialog

This dialog is used to change the current password for the operator named in **Operator**. The new password must comply with the password policy settings defined by the UserManagement administrator.



Figure 8-6 Change Password dialog

Operator

Displays the ID of the operator whose password can be changed. If the password for another operator should be changed, click **Cancel** and enter the desired operator in the previous dialog.

Old password

Enter your current password. The password is not displayed as you type it.

Note: Passwords are case-sensitive.

New password

Enter the new password. The password is not displayed as you type it.

Note: Passwords are case-sensitive. Make sure, that the new password complies with the current password policy settings.

Confirm new password

Confirm your new password. You must enter the same password as above.

OK

If the new password and its repetition are the same and the new password complies with the current password policy settings, it changes the password. A dialog informs

you about successful password change. Quitting this dialog returns you to the **Library-Editor** dialog.

If the new password and its repetition are different or the chosen password does not comply with the current password policy settings, a corresponding message appears. Quit the message and in the **Change Password** dialog make again desired entries.

If the old password is incorrect, a message about denying password change appears. Quitting this message returns you to the **LibraryEditor** dialog.

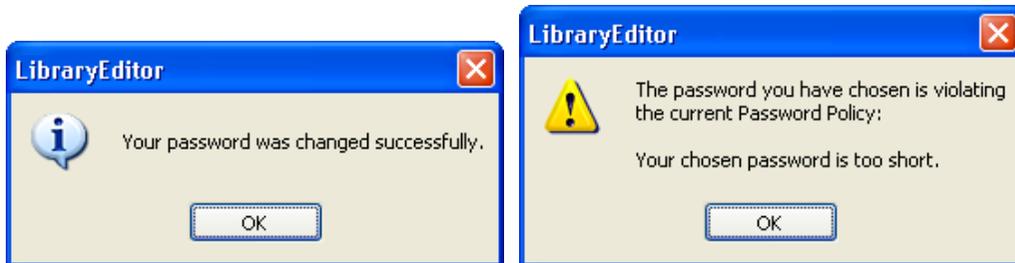


Figure 8-7 Messages on successful password change (left) and chosen password is violating password policy (right)

8.4 Lock All Applications Command

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

The **Lock All Applications** command is used to lock all Bruker Daltonics applications. This includes LibraryEditor as well as all other Bruker Daltonics applications currently installed on your system.

Note: Only the previous operator or someone with the special right to unlock applications can unlock a locked application.

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.

The command opens the **LibraryEditor** dialog, which informs you that LibraryEditor has been locked, by whom (displays the full name of the operator) and how it can be unlocked.



Figure 8-8 LibraryEditor dialog when LibraryEditor has been locked

Operator

Enter the operator ID of the operator who has locked LibraryEditor. The respective operator ID will automatically be entered if the UserManagement administrator has set the corresponding option.

If not the previous operator but someone else wants to unlock the applications, enter the respective operator ID.

Note: This respective operator must have the right to unlock applications.

Password

Enter the corresponding password.

Note: Passwords are case-sensitive. Successive wrong password inputs will cause locking of the operator.

Change Password

Allows you to change your current password before logging in. Opens the **Change Password** dialog.

Log On

If operator ID and password match, and the respective operator is allowed to unlock applications, it unlocks Bruker Daltonics applications and logs in the specified operator.

Shortcuts

Button: 

Key: Ctrl+Alt+K

8.5 About Compass LibraryEditor Command

Use the **About Compass LibraryEditor** command to display the version number of your present copy of LibraryEditor with the copyright notice, the user-specific license information, as well as how to contact Bruker Daltonik GmbH. The command opens the **About Bruker Daltonics LibraryEditor** dialog.



Figure 8-9 About Bruker Daltonics LibraryEditor dialog

Shortcut

Button:



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