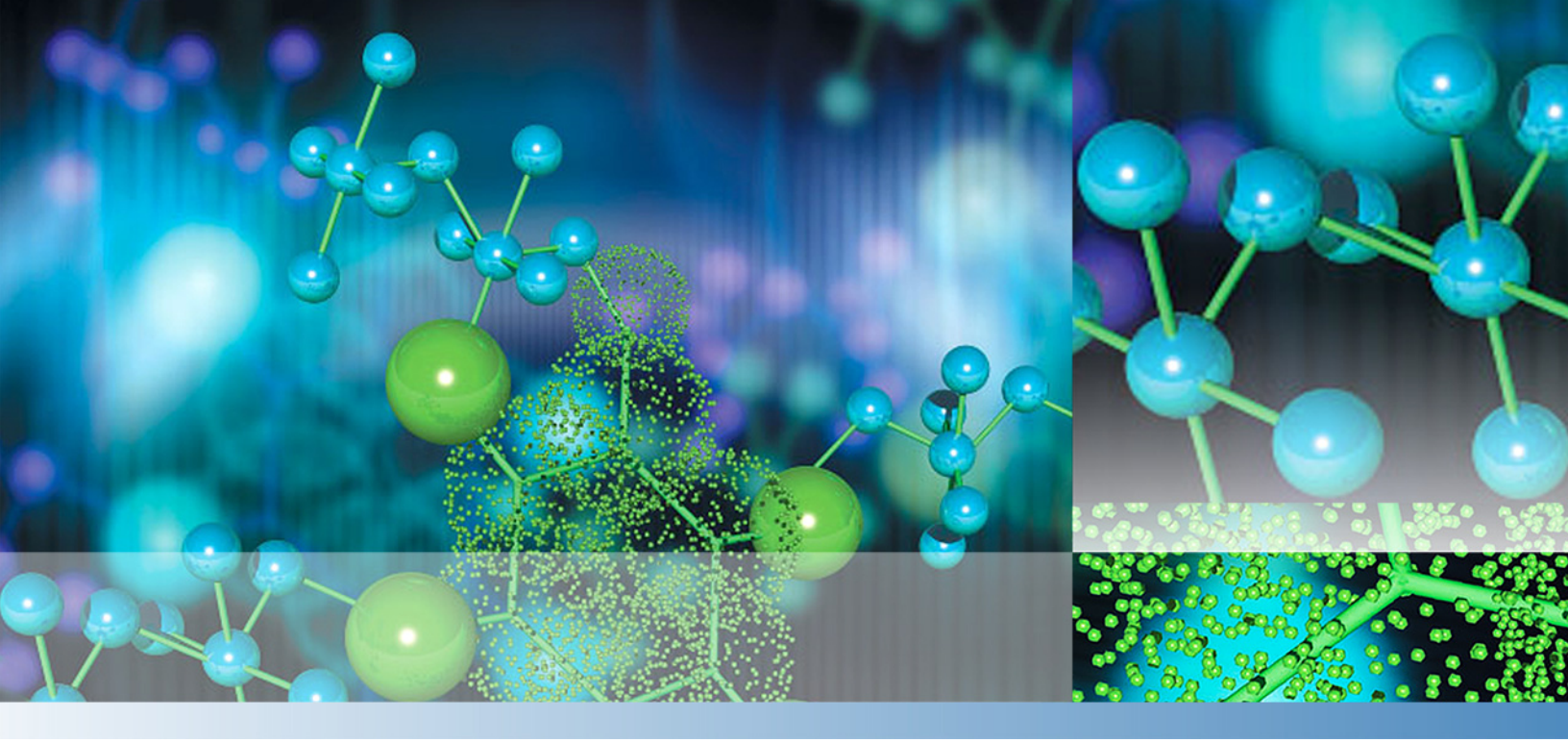

Thermo

Library Manager

User Guide

Software Version 3.0

XCALI-97750 Revision A July 2015

DOCUMENTATION SURVEY

Thermo SCIENTIFIC

Release history: Revision A July 2015

Software version: Library Manager 3.0

For Research Use Only. Not for use in diagnostic procedures.

Contents

Preface

This guide describes how to use the Thermo Library Manager™ application to add spectra to libraries of accurate mass data, delete spectra from these libraries, and search for a spectrum or spectra in these libraries.

Contents

Related Documentation

The Library Manager application includes complete documentation.

❖ To view the product manual

From the Microsoft™ Windows™ taskbar, do one of the following:

- Choose **Start > All Programs > Thermo Library Manager > Manuals > Library Manager User Guide**.
- From the Library Manager window, choose **Help > Manuals**.

For access to the application Help, follow this procedure.

❖ To view the Library Manager Help

From the application window, choose **Help > Library Manager Help**.

- If information about setting parameters is available for a specific view, page, or dialog box, click **Help** or press the F1 key for information about setting parameters.
- In applications that have a Communicator bar, click the field or parameter to display definitions, required actions, ranges, defaults, and warnings.

❖ To download user documentation from the Thermo Scientific website

1. Go to www.thermoscientific.com.
2. In the Search box, type the product name and press Enter.
3. In the left pane, select **Documents & Videos**, and then under Refine By Category, click **Operations and Maintenance**.
4. (Optional) Narrow the search results or modify the display as applicable:
   - For all related user manuals and quick references, click **Operator Manuals**.
   - For installation and preinstallation requirements guides, click **Installation Instructions**.
   - For documents translated into a specific language, use the Refine By Language feature.
   - Use the Sort By options or the Refine Your Search box (above the search results display).
5. Download the document as follows:
   a. Click the document title or click **Download** to open the file.
   b. Save the file.

System Requirements

In addition, ensure that the system meets these minimum requirements.

IMPORTANT Before you install the device driver, ensure that the data system computer has a compatible version of the Thermo Foundation™ platform as noted in the *Library Manager 3.0 Release Notes*.

System	Minimum requirements
Computer	• 1.6 GHz processor with 2.0 GB RAM • Dual-core processor • Video card and monitor capable of 1280 × 1024 resolution (XGA) • 30 GB available on the hard drive
Software	• Microsoft .NET Framework 4.0 Extended • Microsoft Windows 7 SP1 (32-bit or 64-bit) • Thermo Foundation 3.1 SP1 • Adobe™ Acrobat™ or Reader™

Cautions and Special Notices

Make sure you follow the cautions and special notices presented in this guide. Cautions and special notices appear in boxes; those concerning safety or possible system damage also have corresponding caution symbols.

This guide uses the following types of cautions and special notices.

CAUTION Highlights hazards to humans, property, or the environment. Each CAUTION notice is accompanied by an appropriate CAUTION symbol.

IMPORTANT Highlights information necessary to prevent damage to software, loss of data, or invalid test results; or might contain information that is critical for optimal performance of the system.

Note Highlights information of general interest.

Tip Highlights helpful information that can make a task easier.

Contacting Us

There are several ways to contact Thermo Fisher Scientific for the information you need. You can use your smartphone to scan a QR code, which opens your email application or browser.

Contact us	Customer Service and Sales	Technical Support
	(U.S.) 1 (800) 532-4752	(U.S.) 1 (800) 532-4752
	(U.S.) 1 (561) 688-8731	(U.S.) 1 (561) 688-8736
	us.customer-support.analyze@thermofisher.com	us.techsupport.analyze@thermofisher.com

Contact us	Customer Service and Sales	Technical Support

❖ **To find global contact information or customize your request**

1. Go to www.thermoscientific.com.
2. Click **Contact Us**, select the **Using/Servicing a Product** option, and then type the product name.
3. Use the phone number, email address, or online form.

❖ **To find product support, knowledge bases, and resources**

Go to www.thermoscientific.com/support.

❖ **To find product information**

Go to www.thermoscientific.com/lc-ms.

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- Send an email message to Technical Publications (techpubs-lcms@thermofisher.com).
- Complete a survey at www.surveymonkey.com/s/PQM6P62.

1

Getting Started

The Library Manager application searches libraries of accurate mass data for the desired spectrum or spectra. Accurate mass data is fine-resolution data (that is, data of four decimal places or more) produced by the Orbitrap™ and other mass spectrometers. You can use the Library Manager application to add spectra to or delete spectra from these libraries, open and create libraries, and view spectra in them. You can also filter spectra and add data that might not originally have been associated with the spectra.

Contents

When you install the TraceFinder™ application, you can optionally install the Library Manager application.

Opening the Library Manager Application

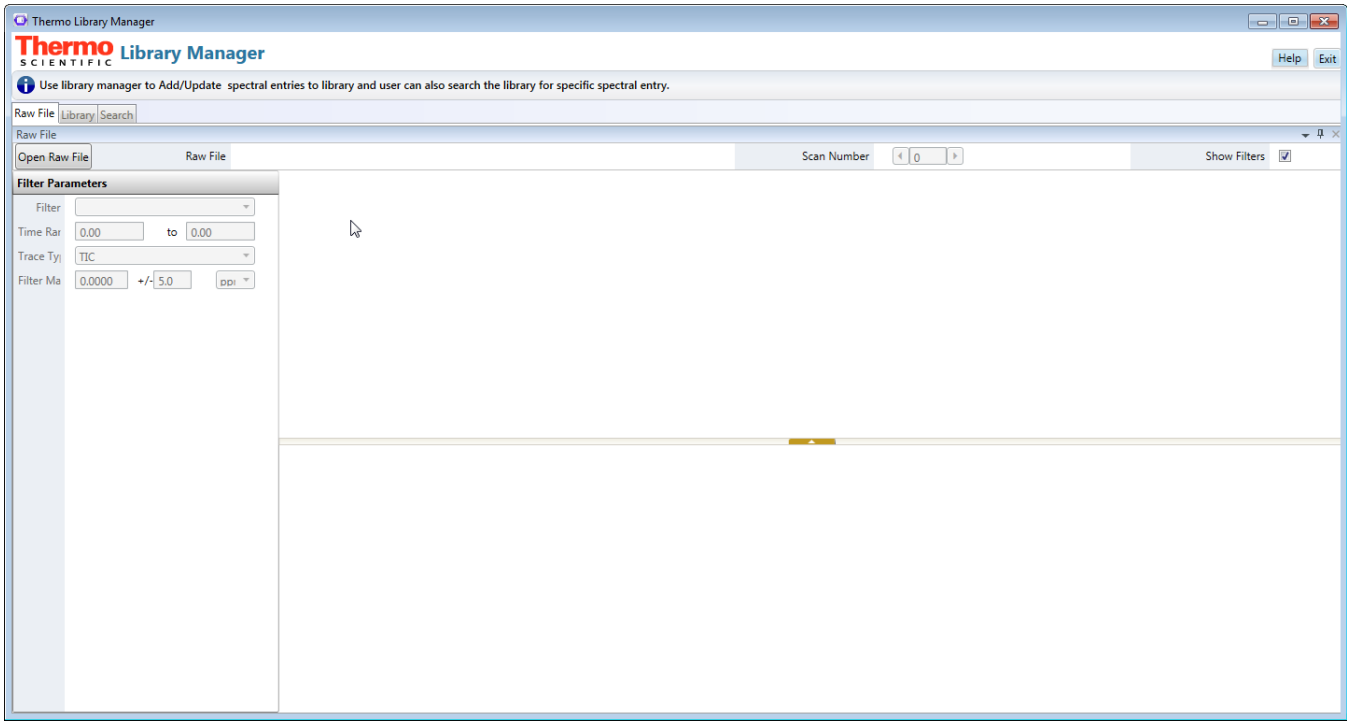
You can open the Library Manager application by clicking its corresponding desktop icon or choosing the appropriate Start menu command.

❖ **To open the Library Manager application**

Choose **Start > Programs > Thermo Library Manager**, or click the **Library Manager** icon,  .

The Library Manager window opens, as shown in Figure 1.

Figure 1. Library Manager window



Closing the Library Manager Application

The Library Manager application does not prompt you to confirm if you want to exit the application.

❖ **To close the Library Manager application**

Click **Exit** in the upper right corner of the Library Manager window.

Finding Help in the Library Manager Application

You can find information about Library Manager parameters and procedures from the Help menu.

❖ **To find information about aspects of the Library Manager application**

Click **Help** in the upper right corner of the Library Manager window.

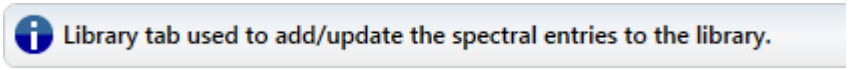
The Help menu contains the commands described in Table 1.

Table 1. Help menu

Command	Function
Help > Library Manager Help	Opens the Help for the application.
Help > Glossary	Opens the glossary in the Help.
Help > How to Use Online Help	Opens the How to Use Help page of the Help.
Help > About Library Manager	Displays the name and version number of the software and the copyright information.
Help > Library Manager User Guide	Opens the *Library Manager User Guide* as a PDF file.

In addition, when you click a tab in the Library Manager window, an explanation of the tab appears in the Communicator bar in the upper left following the information icon, , as shown in Figure 2 for the Library page.

Figure 2. Library Manager Communicator bar



Searching the Library for a Selected Spectrum

In searching a library for a spectrum, you load a raw data file, select the spectrum, load a library, and search the library for the selected spectrum.

Contents

Loading a Raw Data File

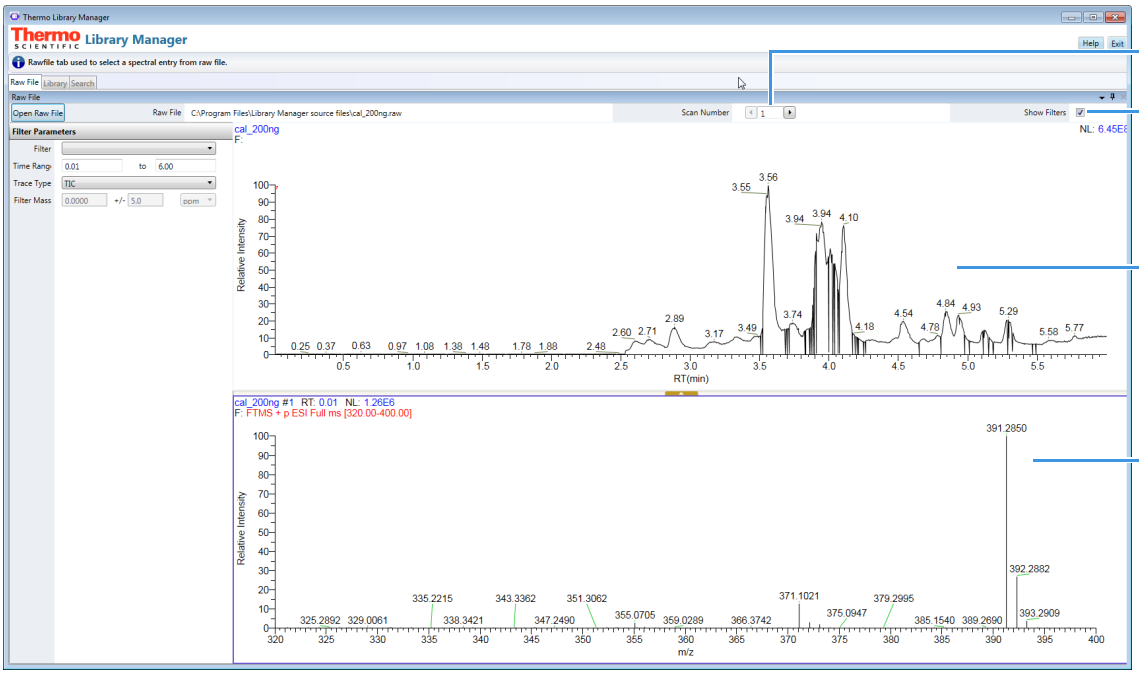
A raw data file contains spectra from a mass spectrometer. You must load a raw data file when you want to find spectra in the library (database) that match a spectrum in the raw data file.

❖ **To load a raw data file**

1. Click the **Raw File** tab if it is not already selected.
2. Click **Open Raw File**.
3. In the Open dialog box, browse to the raw data file and select it, or type its path and name in the File Name box, and click **Open**.

   The chromatogram of the data in the raw data file and the spectrum associated with the scan number in the raw data file now appear on the Raw File page, as shown in Figure 3. By default, the Library Manager application displays scan 1.

Figure 3. Loaded raw data file displayed on the Raw File page of the Library Manager window



For information on the parameters of the Raw File page, see "Raw File Page Parameters" on page 30.

❖ To control the mass spectrum that is displayed

1. Click the chromatogram to select a scan.
2. Use the arrows on either side of the Scan Number box at the top right of the Library Manager window to step through the scans matching the filter, or you can type in a number and press ENTER.

If you want to filter the spectra after you load them, see "Selecting the Spectrum" on page 7.

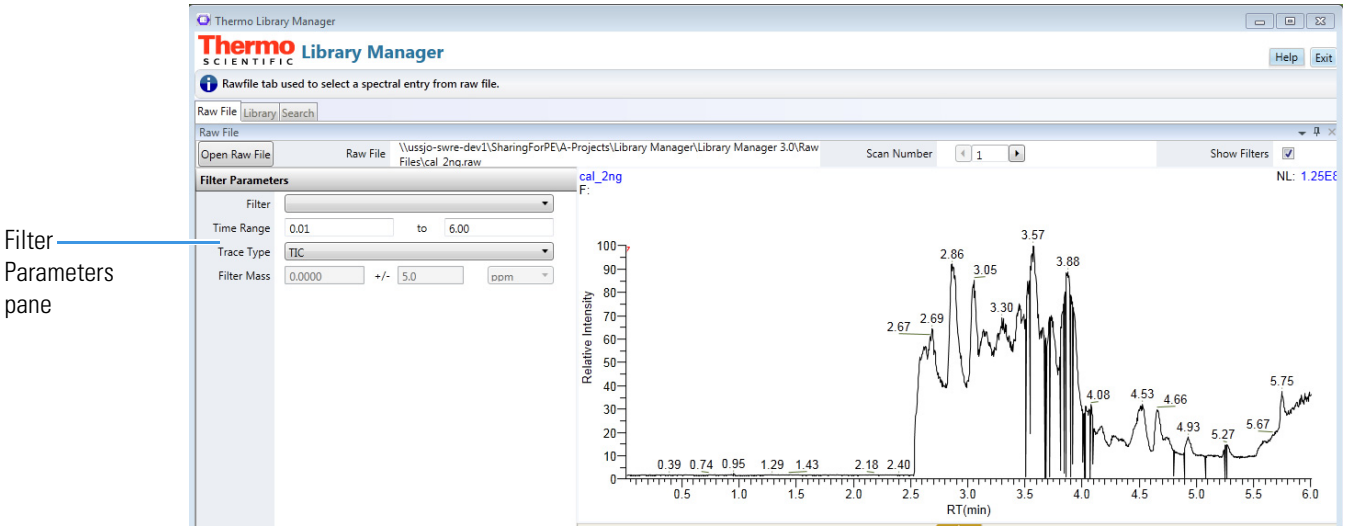
❖ To display or hide the Filter Parameters pane

Select the **Show Filters** check box if it is not already selected (it is selected by default).

The Filter Parameters pane now opens, as shown in Figure 4.

Clear the Show Filters check box to hide the Filter Parameters pane.

Figure 4. Filter Parameters pane on the Raw File page



Selecting the Spectrum

You might want to filter the chromatogram to display a single experiment, which can include multiple compounds. The chromatogram of all the data in the raw data file appears on the Raw File page in the Library Manager window. Below the chromatogram is the spectrum associated with a particular scan number in this raw data file. You can filter the chromatogram by using the parameters available in the Filter Parameters area of the Raw File page. You can also enlarge the chromatogram or the spectrum, then reset it to the original scaling.

❖ To zoom the chromatogram or the spectrum

1. Drag the cursor to the left or right over the area of the chromatogram or the spectrum that you want to enlarge.
2. To return to the original scaling, right-click the chromatogram or the spectrum and choose **Reset Scaling** from the shortcut menu.

❖ To copy a chromatogram or a spectrum

Right-click the chromatogram or the spectrum, and choose **Copy to Clipboard** from the shortcut menu.

❖ To select a spectrum

Place the cross-shaped cursor at the desired point in the chromatogram and click the mouse button.

The cursor changes to a red vertical line, the scan number in the Scan Number box changes to reflect the location of the new scan, and the Library Manager application updates the spectrum to the selected scan.

–or–

In the Scan Number box, enter the scan number corresponding to the desired spectrum location and press ENTER, or use the left and right arrow keys to select it.

A red vertical line appears at the location of the scan in the chromatogram, and beneath the chromatogram, the Library Manager application updates the spectrum to the selected scan.

❖ To select an MS/MS spectrum

1. Select the **Show Filters** check box if it is not already selected.
2. From the Filter list in the Filter Parameters pane, select a scan filter that contains data-dependent MS/MS data for the compound of interest.

   For example, Figure 5 shows the selection of the FTMS + ESI d Full ms2 344.16@hcd45.00 [50.00-370.00] scan filter.
3. Select the best scan, typically the scan with the highest intensity.

   In Figure 5, the best scan is 828.

Figure 5. Filter scan selected

This scan is now selected, and you can import it into a library or spectrum. For instructions on importing it into a library, see "Adding Data Records to a Library" on page 20. For instructions on importing it into a spectrum, see "Searching the Library" on page 13.

❖ To filter the chromatogram

1. Select the **Show Filters** check box in the upper right area of the Library Manager window to open the Filter Parameters pane.
2. In the Filter list in the Filter Parameters pane, specify the type of scans to filter by.

   The information in the list comes from the raw data file.
3. In the Time Range boxes, specify the retention time to filter by. Specify the beginning of the range of data to use in the first box and the end of the range in the second box.
4. From the Trace Type list, specify the type of chromatogram to filter by:

   - (Default) TIC: Displays a total ion current (TIC) chromatogram, which displays a point for every spectrum in the chromatogram, where the *x* axis displays the retention time of the spectrum, and the *y* axis displays the summed intensity of all peaks (TIC) in the spectrum.
   - Base Peak: Displays a base peak ion chromatogram. A base peak chromatogram is very similar to a total ion current chromatogram, but instead of the summed intensity of all peaks (TIC), it displays the intensity of the largest peak (base peak) in the spectrum on the *y* axis. The *x* axis displays the analysis data from the beginning of the analysis. The base peak chromatogram lists the detected peaks and the retention time associated with each peak.
   - Target Mass: Displays a subset of a mass chromatogram.

   The Filter Mass option becomes available when you select Target Mass in the Trace Type list.
5. If you selected Target Mass in the Trace Type list, specify the mass, tolerance, and unit to use for filtering the chromatogram in the Filter Mass boxes.
   a. In the first box, specify the mass to use for filtering the chromatogram.
   b. In the second box, specify the mass tolerance window for the filter mass to use for filtering the chromatogram.
   c. In the third box, specify the unit to display the mass in:
      - mmu: Millimass units (one thousandth of a mass unit)
      - (Default) ppm: Parts per million (one millionth of the filter mass)

Loading a Library

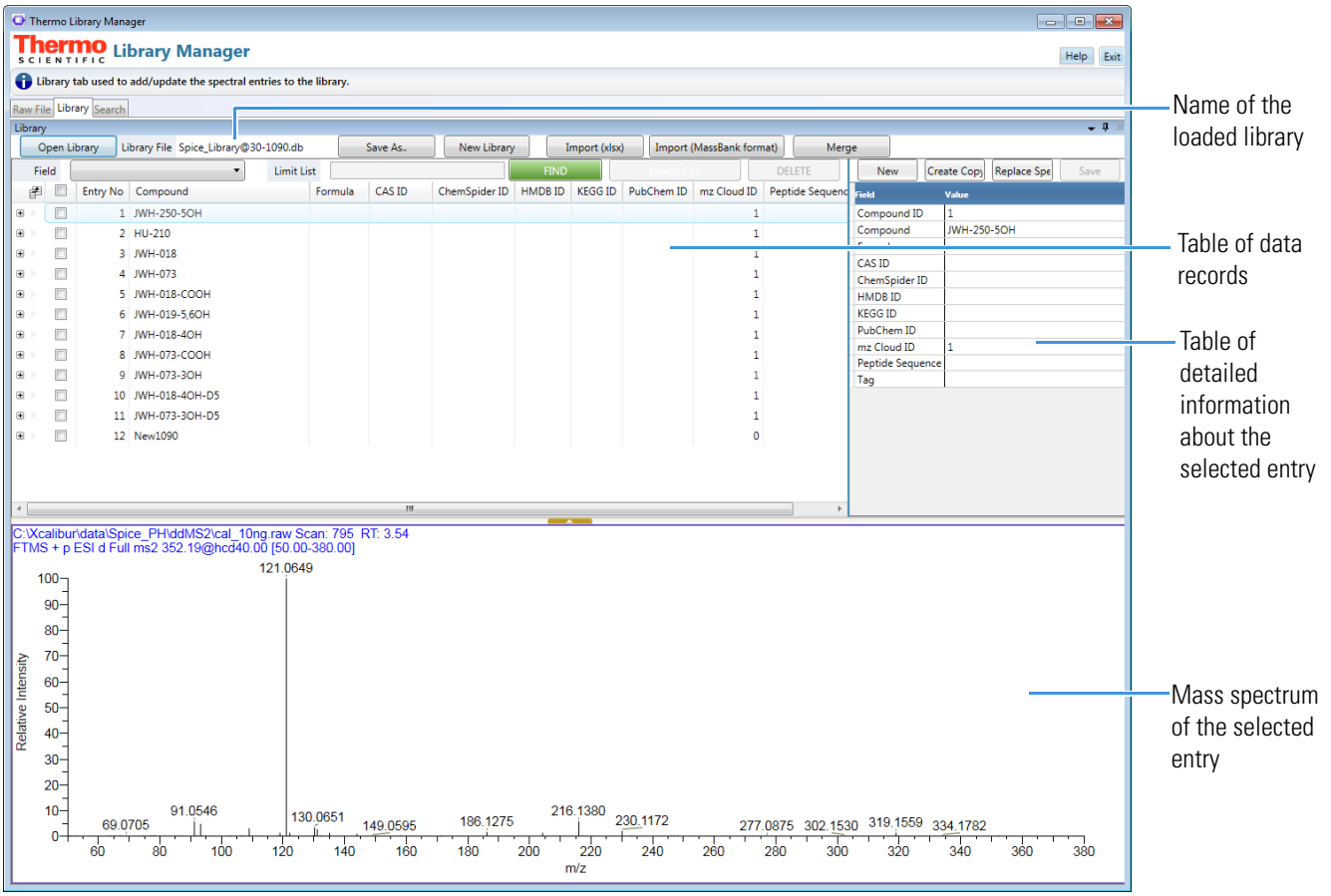
If you want to search a library for the spectrum in a loaded raw data file or add a spectrum to a library, the next step is to load the appropriate library (database) of accurate mass data.

❖ To load a library

1. Click the **Library** tab.
2. Click **Open Library**.
3. In the Open Existing File dialog box, browse to the appropriate library (.db) file and select it or type its name and path in the File Name box, and click **Open**.

   The databases in the library appear on the Library page of the Library Manager window, as shown in Figure 6.

Figure 6. Library page displayed in the Library Manager window



4. (Optional) For a large library, sort or filter its constituent databases with options in the Field list:

   - **Compound**: Sorts the databases by the name of the substance associated with the spectrum to search for in the library.
   - **Formula**: Sorts the databases by the chemical formula of the substance associated with the spectrum to search for in the library.

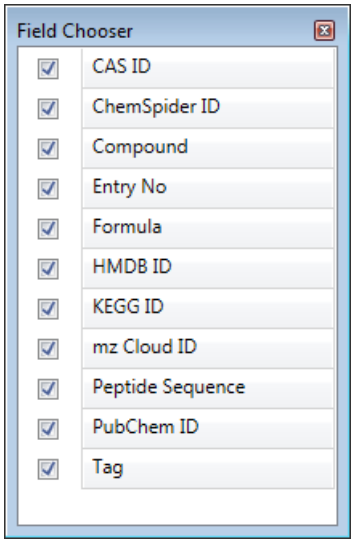
- **CASIDnumber**: Sorts the databases by the unique chemical registry number that the Chemical Abstracts Service™ assigns to the substance associated with the spectrum to search for in the library.
- **Filter**: Specifies the scan filter from the original raw data file.
- **PeptideSequence**: Sorts the databases by the amino acid sequence of a peptide or protein associated with the spectrum.

5. (Optional) Select the columns to display on the Library page:
   a. Click the **Field Chooser** icon, , in the upper left corner of the Library page.
   b. In the library Field Chooser dialog box, select the check boxes next to the names of the columns that you want to display on the Library page. Some columns might already be selected, as shown in Figure 7. Clear the check boxes next to the names of any columns that you do not want to display.

      The changes are visible immediately.

      For definitions of these columns, see "Library records" on page 33.

      Figure 7. Library Field Chooser dialog box

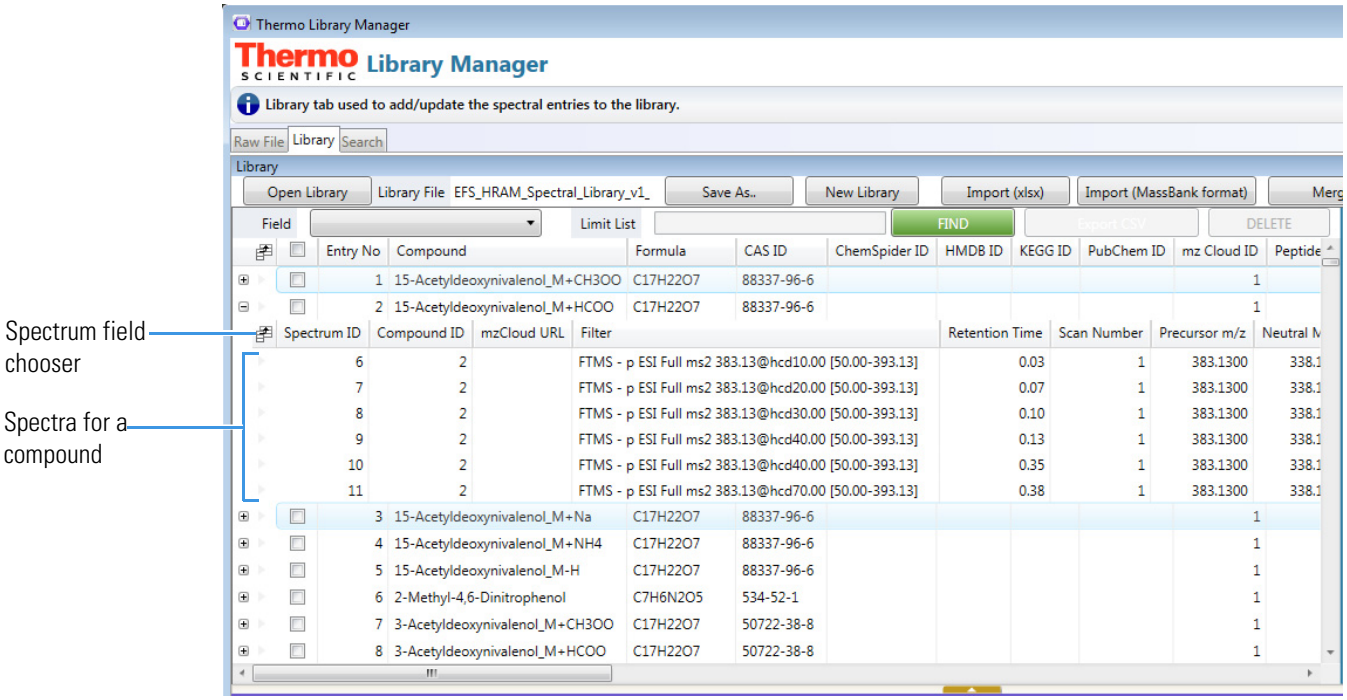


6. (Optional) Click the Expand icon (+) to the left of a check box to display the spectral information for a compound.

   This information is displayed in a table. For information on the columns of this table, see "Child records" on page 34.

   For example, Figure 8 shows all the spectra in the 15-Acetyldeoxynivalenol_M+HCOO compound.

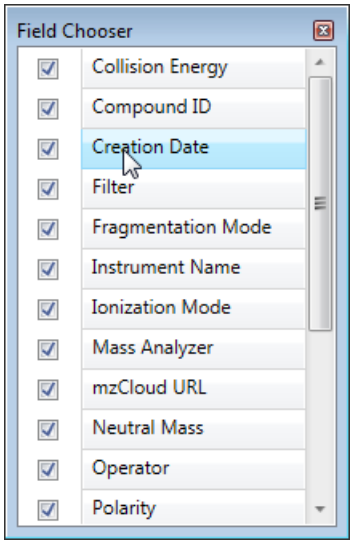
Figure 8. Spectral information displayed for a compound



7. Click the spectrum **Field Chooser** icon, , to open the spectrum Field Chooser dialog box, shown in Figure 9.

   The column names are listed in alphabetical order in the dialog box.

   Figure 9. Spectrum Field Chooser dialog box



8. Select the check boxes next to the names of the columns that you want to display for the spectrum. Some columns might already be selected. Clear the check boxes next to the names of any columns that you do not want to display.

The changes are visible immediately.

For definitions of these columns, see "Child records" on page 34.

Searching the Library

Once you load the raw data file and the library and select the spectrum to search for, you can search for the library for that spectrum.

❖ To search for a spectrum

1. Click the **Search** tab.
2. From the Field list, select the category of information to search for. You can select one of the following criteria:
   - **Compound**: Specifies the name of the substance associated with the spectrum to search for in the library.
   - **Formula**: Specifies the chemical formula of the substance associated with the spectrum to search for in the library.
   - **Precursor m/z**: Specifies the mass of the precursor ion of the spectrum to search for in the library. When you select this option, the Precursor m/z box becomes available.
   - **CASIDnumber**: Specifies the unique chemical registry number that the Chemical Abstracts Service assigns to the substance associated with the spectrum to search for in the library.
3. (Optional) If you selected Precursor m/z in the Field list, in the Precursor m/z box specify the value used to match individual peaks between the mass spectrum being searched and the library entries.

   You can specify up to four decimal places.

   Default: 0.000

   If you selected an MS/MS spectrum on the Raw File page, the application takes the default value from the scan.
4. (Optional) If you selected Precursor m/z in the Field list, in the Precursor Tolerance list, specify the tolerance to use for the mass of the precursor ion, in parts per million (PPM), daltons (Da), or millimass units (MMU).

   Valid range: Values with one decimal place from 0.1 to 1000.0

   Default: 5.0 PPM, 5.0 MMU, or 0.05 Da

5. (Optional) In the Fragment Tolerance box, specify a mass value, either absolute or relative, within which your observed masses must match the theoretical fragment mass in parts per million (PPM), daltons (Da), or millimass units (MMU).

   Default: 10.0 PPM, 10.0 MMU, or 0.05 Da

6. (Optional) In the Limit Search box, specify the terms to use to filter the selection you made in the Field list. For example, if you selected Compound in the Field list, you might specify a substance like myoglobin.

7. (Optional) In the Percent Cut-off (%) box, specify the percentage of the highest score below which to filter out results.

8. (Optional) Clear the check box to the right of the Intensity Threshold (%) box if you do not want to filter any peaks from the spectrum that are less than the value that is displayed or entered when you use the High Res algorithm. This algorithm calculates the score that indicates how well a spectrum matches a library spectrum.

   Default: 0.8

9. (Optional) In the Search Type area, select the search algorithm to use:

   - (Default) **Forward**: Searches the library for spectra similar to the spectrum displayed in the raw data file. Use a forward search when the unknown spectra are relatively pure or of high quality, such as those produced by precursor filtration or high-resolution chromatography.
   - **Reverse**: Attempts to determine if any library spectra are included in the unknown spectrum. Use a reverse search if the unknown spectrum contains many potential contaminant peaks, such as that produced with full-scan MS, for example, all ion fragmentation (AIF) or data-independent acquisition (DIA). A reverse search attempts to determine if any library spectra are included in the unknown spectrum.

10. (Optional) Select the **Remove Precursor Ion** check box if you want the Library Manager application to remove from the spectra any mass or intensity data that is within 2.2 Da of the precursor ion.

    In an MS/MS experiment, the precursor ion sometimes can appear and interfere with the scoring of the algorithm. This option corrects this problem.

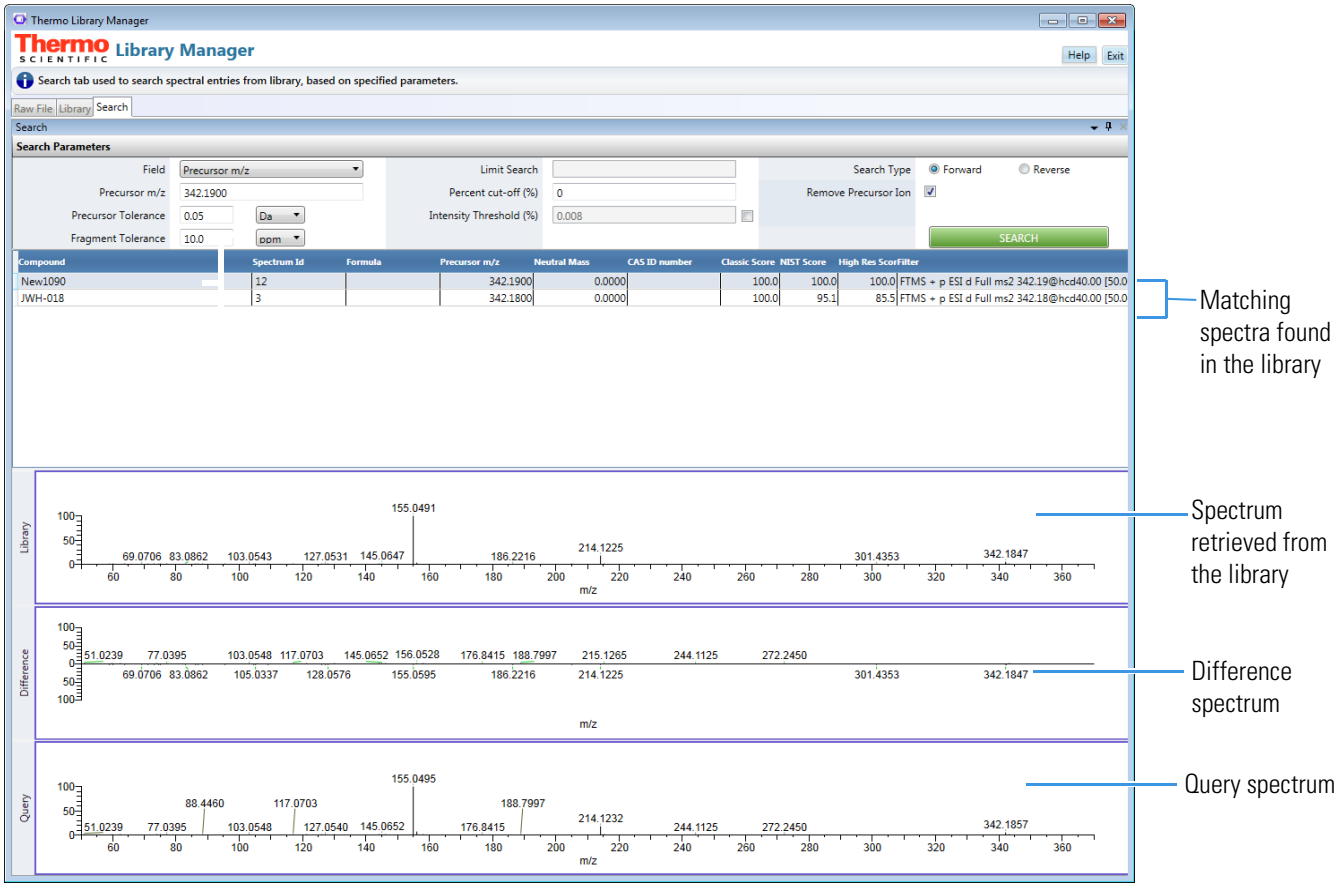
11. Click **Search**.

    The Library Manager application displays the search results in a table on the Search page, as shown in Figure 10. The results that most closely match the specified criteria are at the top. Three spectra appear beneath the search results table:

    - The Library pane shows the spectrum returned from the library.
    - The Difference pane shows the difference between the query spectrum from the raw data file and the library spectrum.
    - The Query pane shows the spectrum selected in the raw data file.

When you click an individual record in the search table, the spectra shown in the Library and Difference panes change accordingly.

Figure 10. Search results on the Search page



3

Managing Libraries

This chapter explains how to create and manage libraries in the Library Manager application.

Contents

Creating a Library

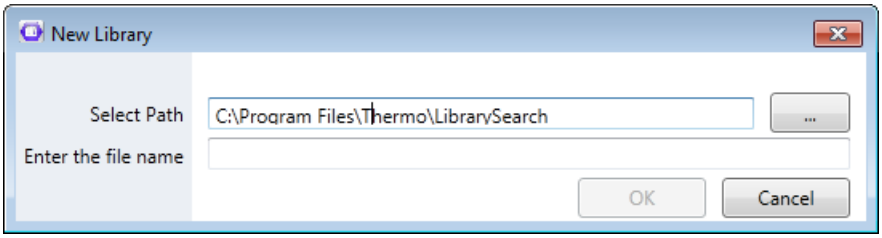
You can create a library and import data records into it or add data records manually one at a time. You might want to create a library when you have collected a body of information that you want to keep separate from other information.

❖ **To create a library**

1. Click the **Library** tab if the Library page is not already selected.
2. On the Library page, click **New Library**.

   The New Library dialog box appears, as shown in Figure 11.

Figure 11. New Library dialog box



3. In the Select Path box, type the path to the folder where the new library file will reside or click the **Browse** button (...) to browse to the location.
4. In the Enter the File Name box, type the name of the new library file.
5. Click **OK**.
6. Follow the procedure "Importing Data Records from Excel Files into a Library" on page 23 or "Adding Data Records to a Library" on page 20 to fill the library with data records.

Displaying a Subset of Records in the Data Records Table

You can filter the records to display a subset in the data records table on the Library page.

❖ **To select a subset of data records to display in the data records table**

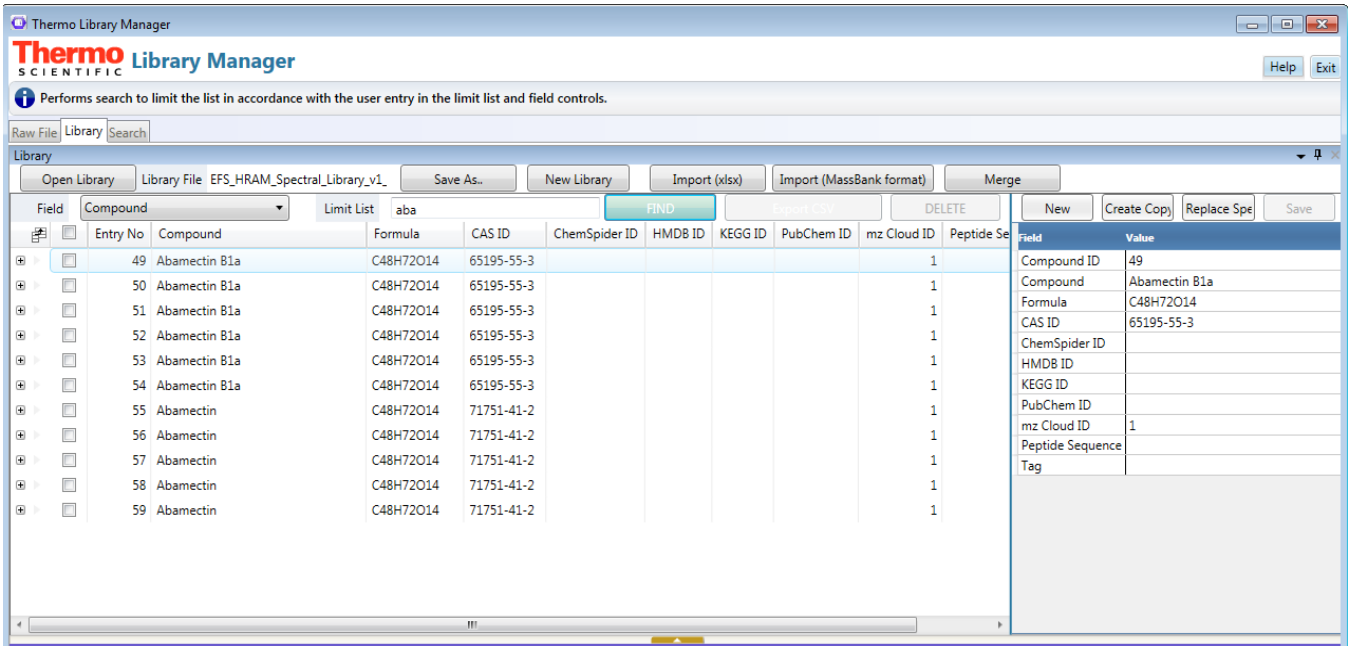
1. Click the **Library** tab if the Library page is not already selected.
2. From the Field list, select the category of information to filter by.

   For example, in Figure 12, the Compound category is selected. The list in the Limit List box now becomes available.
3. In the Limit List box, specify the terms to use to filter the selection you made in the Field list.

   For example, in Figure 12, the filter in the Limit List box is **aba**.
4. Click **Find**.

   The Library page displays all the data records that include the filter criterion in alphabetical order. In Figure 12, all the data records display "aba" in their names.

Figure 12. Filtered data records



❖ To redisplay all the records in the library

1. Delete the contents of the Limit List box on the Library page.
2. Click **Find**.

   The Library Manager application now redisplays all the records associated with the scan number.

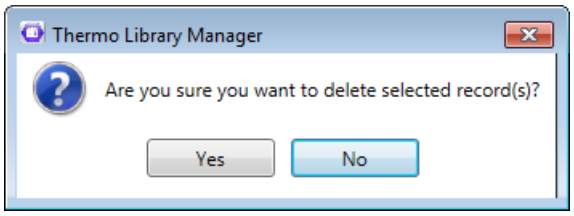
❖ To delete a data record in the library

1. Click the **Library** tab if the Library page is not already selected.
2. Select the check box to the left of the entry that you want to delete.

   The Delete button becomes available.
3. Click **Delete**.

   The confirmation box shown in Figure 13 appears.

Figure 13. Delete confirmation box



4. Click **Yes**.

   The Library Manager application deletes the record from the data records table.

Adding Data Records to a Library

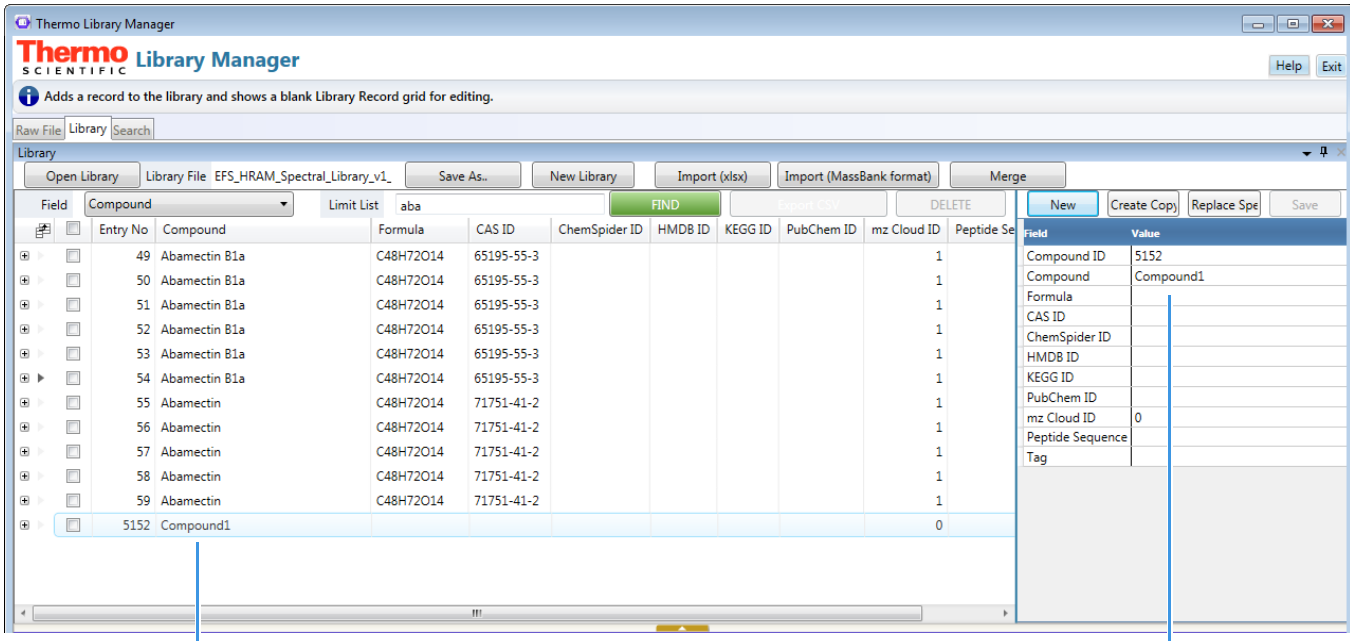
You can add data records to a library in two ways. You can add a new record directly to the library, or you can add a record to an existing compound in the library.

❖ To add a data record directly to a library

1. Open the appropriate raw data file by following the instructions in "Creating a Library" on page 17.
2. Open the appropriate library by following the instructions in "Loading a Library" on page 9.
3. Filter the chromatogram to find the appropriate spectrum by following the instructions in "Selecting the Spectrum" on page 7.
4. Click the **Library** tab.
5. On the Library page, click **New**.

   The Library Manager application adds a new data record called Compound1 that contains the currently selected mass spectrum to the end of the data records table and to the Compound row of the Value column, as shown in Figure 14.

Figure 14. New record added to a library



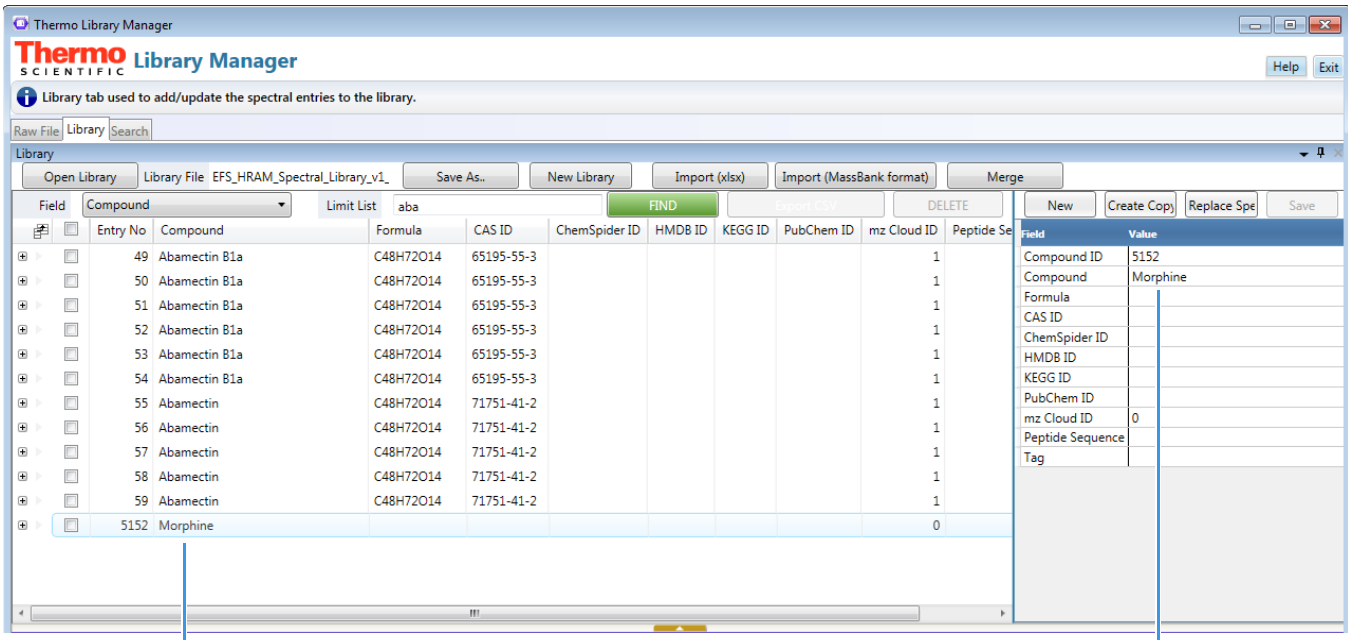
6. Double-click **Compound1** in the Value column or backspace over it and type the new name, **Morphine**. Press ENTER.

   The Save button now becomes available.

7. Save the new record by clicking **Save**.

   The Morphine record replaces Compound1 at the bottom of the table on the Library page, as shown in Figure 15.

Figure 15. Morphine record added to the database

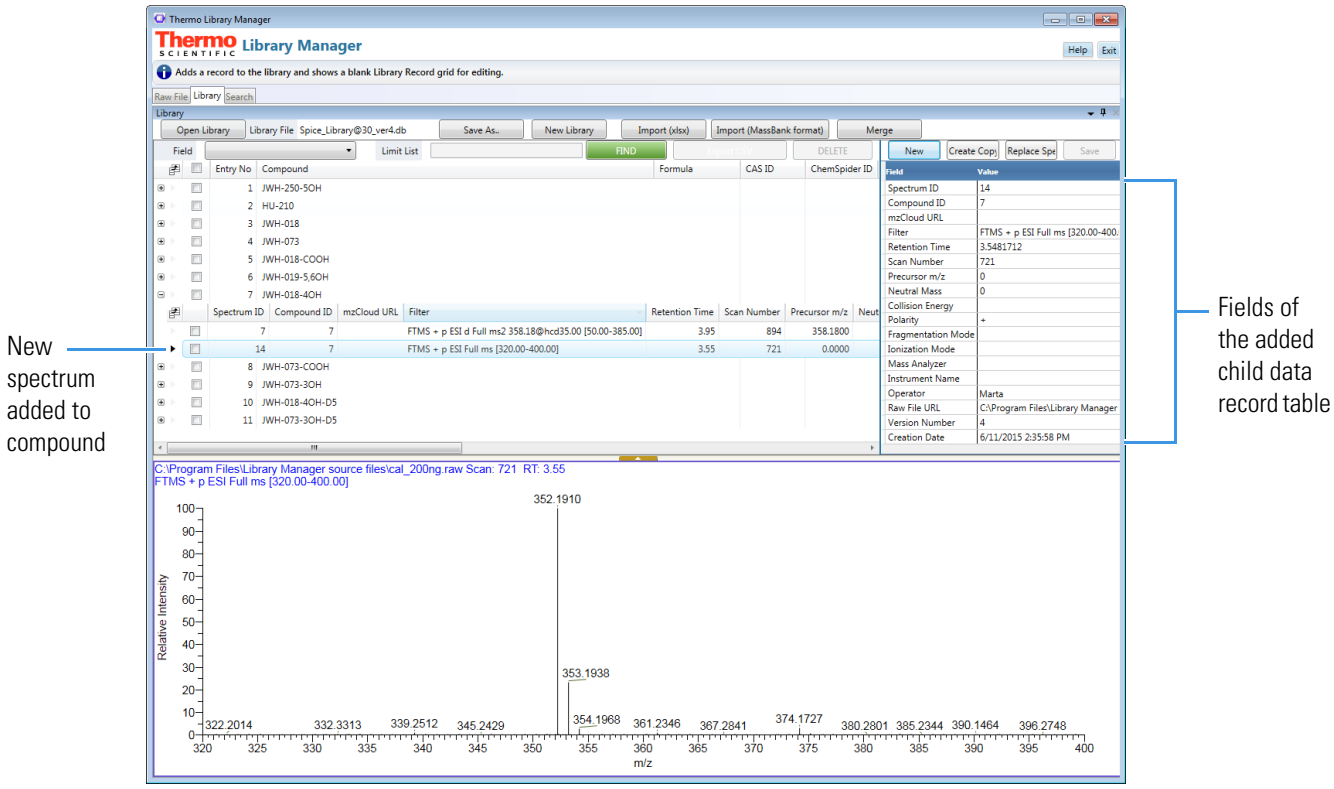


❖ To add a spectrum to an existing compound

1. On the Library page, select the check box to the left of the compound to add the data record to.
2. (Optional) Click the Expand icon (+) to the left of the compound to display the child data records of the compound.
3. Click **New**.

   The Library Manager application adds a new data record containing the currently selected mass spectrum to the list of child data records of the selected compound and assigns it a number, as shown in Figure 16. It also adds the fields of the new child data record table to the Field and Value columns on the right side of the page.

Figure 16. New spectrum added to a compound



Importing Data Records from Excel Files into a Library

You can import data records from a Microsoft Excel™ (.xlsx) file. Importing a number of data records at once is useful after you have created a library.

The Excel file that you import must reside in the same folder as the raw data file.

The Excel file that you import must be in a specific format with the following required columns:

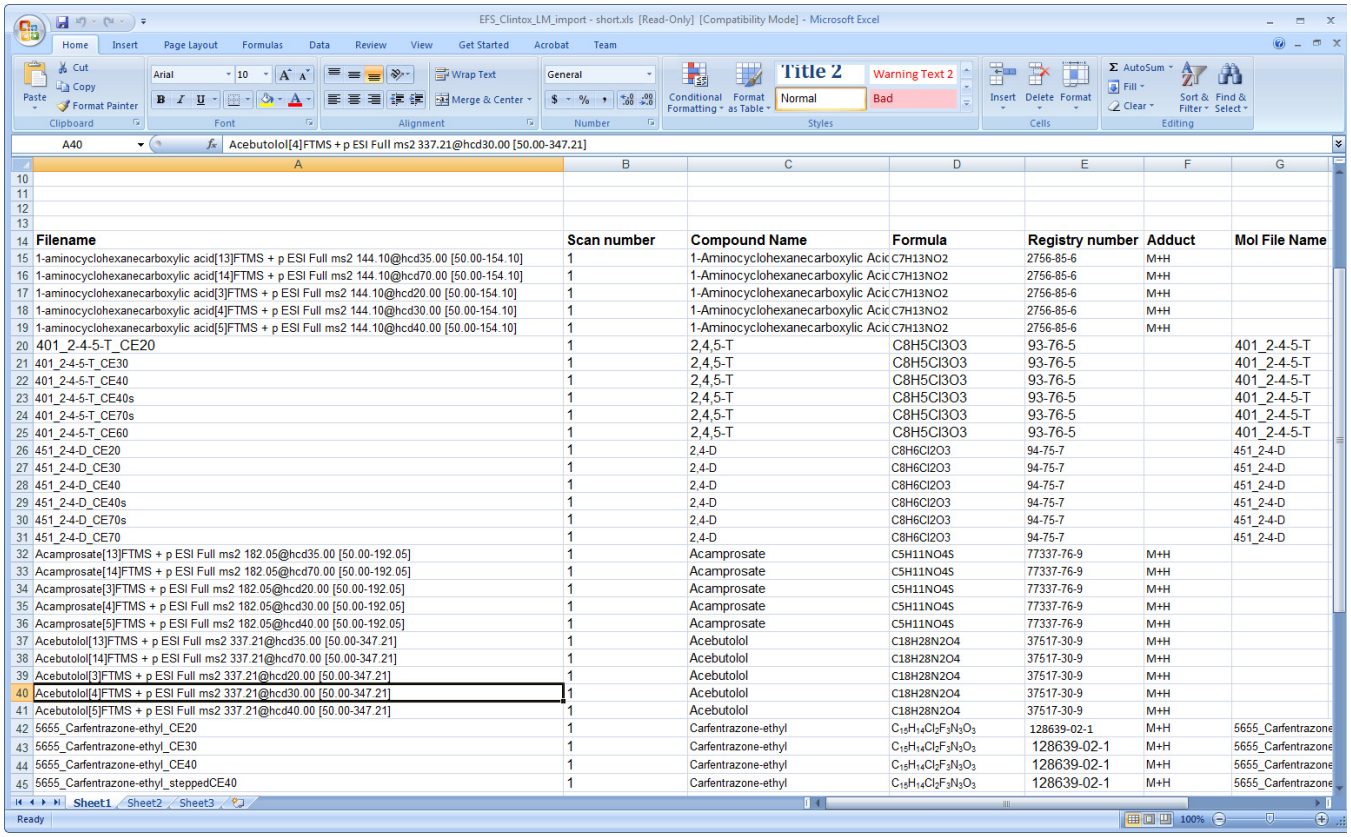
- Filename: Specifies the name of the raw data file.
- Scan Number: Specifies which scan from the raw data file is to be added to the library.
- Compound Name: Specifies the name of the substance associated with the spectrum.
- Formula: Specifies the chemical formula of the substance associated with the spectrum.
- Registry Number: Specifies the Chemical Abstracts Service (CAS) ID number of the substance associated with the spectrum, which is the unique chemical registry number that CAS assigns to the substance associated with the spectrum.

- Adduct: Specifies the name of the chemical compound that might fragment to give the same spectrum as the compound and therefore alter the compound's mass-to-charge ratio (*m/z*).
- Mol File Name: Specifies the name of the molecular structure file.

The Excel file cannot contain optional columns.

Figure 17 shows a sample Excel file in the correct format for importation.

Figure 17. Sample Excel file correctly formatted



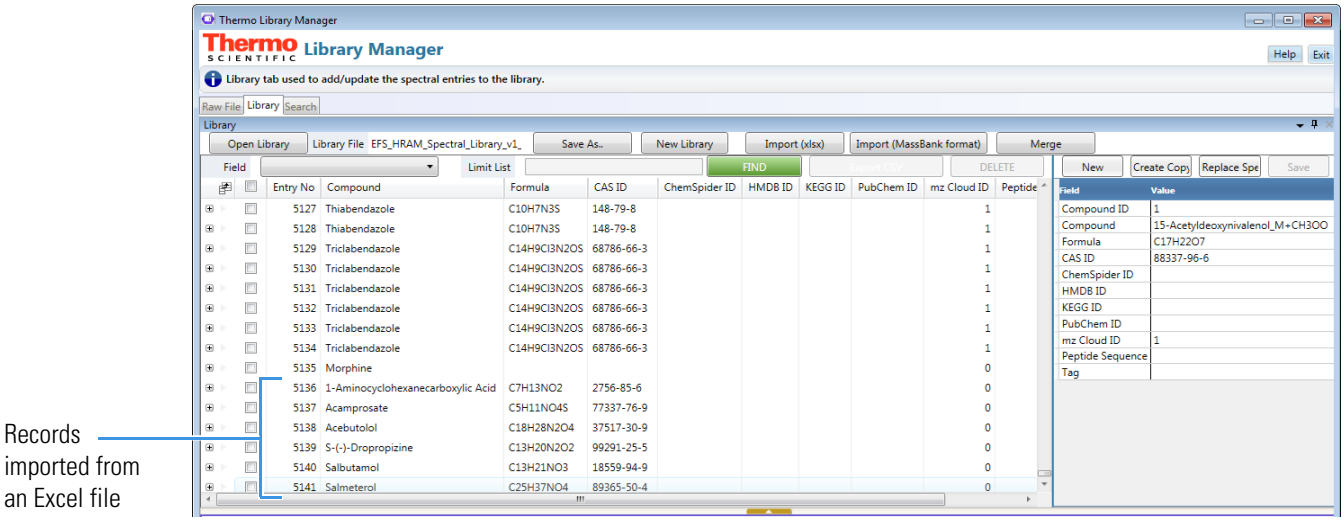
Filename	Scan number	Compound Name	Formula	Registry number	Adduct	Mol File Name
1-aminocyclohexanecarboxylic acid[13]FTMS + p ESI Full ms2 144.10@hcd35.00 [50.00-154.10]	1	1-Aminocyclohexanecarboxylic Acic	C7H13NO2	2756-85-6	M+H	
1-aminocyclohexanecarboxylic acid[14]FTMS + p ESI Full ms2 144.10@hcd70.00 [50.00-154.10]	1	1-Aminocyclohexanecarboxylic Acic	C7H13NO2	2756-85-6	M+H	
1-aminocyclohexanecarboxylic acid[3]FTMS + p ESI Full ms2 144.10@hcd20.00 [50.00-154.10]	1	1-Aminocyclohexanecarboxylic Acic	C7H13NO2	2756-85-6	M+H	
1-aminocyclohexanecarboxylic acid[4]FTMS + p ESI Full ms2 144.10@hcd30.00 [50.00-154.10]	1	1-Aminocyclohexanecarboxylic Acic	C7H13NO2	2756-85-6	M+H	
1-aminocyclohexanecarboxylic acid[5]FTMS + p ESI Full ms2 144.10@hcd40.00 [50.00-154.10]	1	1-Aminocyclohexanecarboxylic Acic	C7H13NO2	2756-85-6	M+H	
401_2-4-5-T_CE20	1	2,4,5-T	C8H5Cl3O3	93-76-5		401_2-4-5-T
401_2-4-5-T_CE30	1	2,4,5-T	C8H5Cl3O3	93-76-5		401_2-4-5-T
401_2-4-5-T_CE40	1	2,4,5-T	C8H5Cl3O3	93-76-5		401_2-4-5-T
401_2-4-5-T_CE40s	1	2,4,5-T	C8H5Cl3O3	93-76-5		401_2-4-5-T
401_2-4-5-T_CE70s	1	2,4,5-T	C8H5Cl3O3	93-76-5		401_2-4-5-T
401_2-4-5-T_CE60	1	2,4,5-T	C8H5Cl3O3	93-76-5		401_2-4-5-T
451_2-4-D_CE20	1	2,4-D	C8H6Cl2O3	94-75-7		451_2-4-D
451_2-4-D_CE30	1	2,4-D	C8H6Cl2O3	94-75-7		451_2-4-D
451_2-4-D_CE40	1	2,4-D	C8H6Cl2O3	94-75-7		451_2-4-D
451_2-4-D_CE40s	1	2,4-D	C8H6Cl2O3	94-75-7		451_2-4-D
451_2-4-D_CE70s	1	2,4-D	C8H6Cl2O3	94-75-7		451_2-4-D
451_2-4-D_CE70	1	2,4-D	C8H6Cl2O3	94-75-7		451_2-4-D
Acamprosate[13]FTMS + p ESI Full ms2 182.05@hcd35.00 [50.00-192.05]	1	Acamprosate	C5H11NO4S	77337-76-9	M+H	
Acamprosate[14]FTMS + p ESI Full ms2 182.05@hcd70.00 [50.00-192.05]	1	Acamprosate	C5H11NO4S	77337-76-9	M+H	
Acamprosate[3]FTMS + p ESI Full ms2 182.05@hcd20.00 [50.00-192.05]	1	Acamprosate	C5H11NO4S	77337-76-9	M+H	
Acamprosate[4]FTMS + p ESI Full ms2 182.05@hcd30.00 [50.00-192.05]	1	Acamprosate	C5H11NO4S	77337-76-9	M+H	
Acamprosate[5]FTMS + p ESI Full ms2 182.05@hcd40.00 [50.00-192.05]	1	Acamprosate	C5H11NO4S	77337-76-9	M+H	
Acebutolol[13]FTMS + p ESI Full ms2 337.21@hcd35.00 [50.00-347.21]	1	Acebutolol	C18H28N2O4	37517-30-9	M+H	
Acebutolol[14]FTMS + p ESI Full ms2 337.21@hcd70.00 [50.00-347.21]	1	Acebutolol	C18H28N2O4	37517-30-9	M+H	
Acebutolol[3]FTMS + p ESI Full ms2 337.21@hcd20.00 [50.00-347.21]	1	Acebutolol	C18H28N2O4	37517-30-9	M+H	
Acebutolol[4]FTMS + p ESI Full ms2 337.21@hcd30.00 [50.00-347.21]	1	Acebutolol	C18H28N2O4	37517-30-9	M+H	
Acebutolol[5]FTMS + p ESI Full ms2 337.21@hcd40.00 [50.00-347.21]	1	Acebutolol	C18H28N2O4	37517-30-9	M+H	
5655_Carfentrazone-ethyl_CE20	1	Carfentrazone-ethyl	$C_{15}H_{14}Cl_2F_3N_3O_3$	128639-02-1	M+H	5655_Carfentrazone
5655_Carfentrazone-ethyl_CE30	1	Carfentrazone-ethyl	$C_{15}H_{14}Cl_2F_3N_3O_3$	128639-02-1	M+H	5655_Carfentrazone
5655_Carfentrazone-ethyl_CE40	1	Carfentrazone-ethyl	$C_{15}H_{14}Cl_2F_3N_3O_3$	128639-02-1	M+H	5655_Carfentrazone
5655_Carfentrazone-ethyl_steppedCE40	1	Carfentrazone-ethyl	$C_{15}H_{14}Cl_2F_3N_3O_3$	128639-02-1	M+H	5655_Carfentrazone

❖ To import data records into a library

1. Click the **Library** tab if the Library page is not already selected.
2. Click **Import (xlsx)**.
3. In the Open dialog box, browse to the Excel file and select it or type its path and name in the File Name box, and click **Open**.

   The Library Manager application appends the imported data records to the bottom of the data records table on the Library page, as shown in Figure 18.

Figure 18. Records imported from an Excel file appended to the bottom of the data records table



Importing Data Records from MassBank into a Library

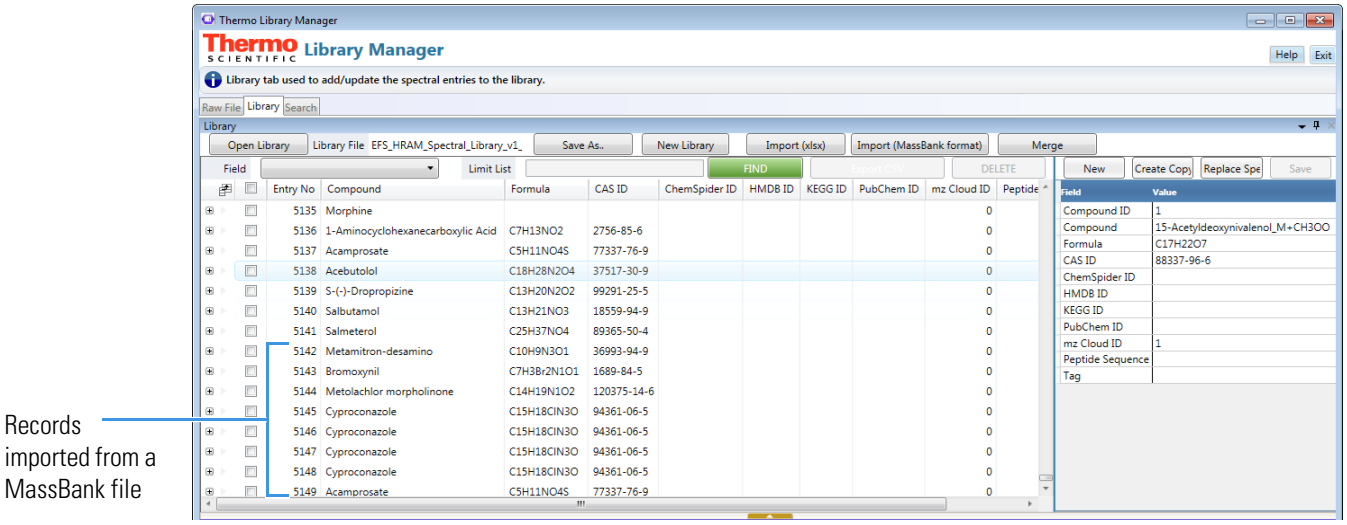
You can import data records from the spectral libraries of MassBank, a public repository of mass spectral data.

❖ To import data records from MassBank

1. Click the **Library** tab if the Library page is not already selected.
2. On the Library page, click **Import (MassBank format)**.
3. In the Open dialog box, browse to the TXT files and select them, or type the path and file name in the File Name box, and click **Open**.

   The application appends the imported data records to the bottom of the data records table on the Library page, as shown in Figure 18.

Figure 19. Records imported from a MassBank file appended to the bottom of the data records table



Exporting a Spectrum from a Library to a CSV File

You can export a spectrum from a library to a comma-separated values (CSV) file for importation into TraceFinder.

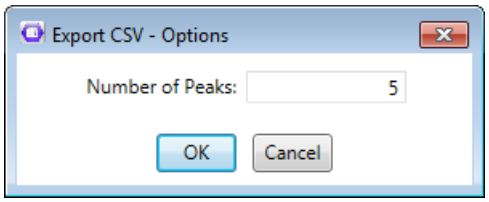
❖ To export a library

1. Click the **Library** tab if the Library page is not already selected.
2. Select the check box to the left of the compound or spectrum that you want to export.

   The Export CSV button becomes available.
3. Click **Export CSV**.
4. In the Save As dialog box, browse to the location of the file where you want to save the exported library or type the path and the name of the file in the File Name box, and click **Save**.

   The Export CSV - Options dialog box opens, as shown in Figure 20.

Figure 20. Export CSV - Options dialog box



5. In the Number of Peaks box, type the number of peaks that will be exported to the CSV file.

   Valid range: 1–10

   Default: 5

6. Click **OK**.

   The Library Manager application saves the library in a file with a .csv suffix.

Adding Metadata to a Library or Changing Metadata in a Library

Metadata is the data associated with a spectrum that is included in a data record. You can add metadata to a library that might not originally have been associated with the spectrum, and you can also change the existing metadata in a library.

❖ To add metadata to a library or to change metadata in a library

1. Manually add the desired data to the table of data records on the Library page, or change the existing data in the table.

   For information about the columns in the data table on the Library page, see "Library records" on page 33.

2. On the Library page, click **Save**.

   The Library Manager application saves the currently displayed record in the library.

Copying a Data Record

You can create a data record that is a copy of the currently selected data record on the Library page. You can then alter information in the copied record.

❖ To copy a data record

1. Click the **Library** tab if the Library page is not already selected.
2. Select the entry number of the data record that you want to copy in the Entry No. column of the Library page.
3. Click **Create Copy**.

   The Library Manager application adds a duplicate of the data record that you copied to the end of the table of data records. It has the next available entry number.

Replacing a Spectrum

You can replace a spectrum in a library data record. You might find a record with an associated spectrum that is erroneous. You can replace this spectrum with the correct spectrum from the raw data file.

❖ To replace a spectrum

1. Follow the instructions in "Selecting the Spectrum" on page 7 to find the correct spectrum on the Raw File page.
2. Click the **Library** tab.
3. Click **Replace Spectrum**.

   The Library Manager application replaces the spectrum associated with the data record with the selected spectrum from the raw data file.

Saving a Library

You can save a library under a new name that you specify.

❖ To save a library with a new name

1. Click the **Library** tab if the Library page is not already selected.
2. Click **Save As**.
3. In the Save As dialog box, browse to the location of the library to save, or enter its path and name in the File Name box and select **Database File** (***.db**) in the Save as Type box.
4. Click **Save**.

Merging Libraries

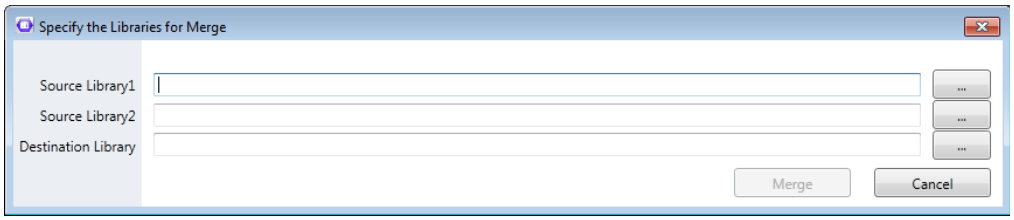
You can merge two libraries into one library. You might want to merge libraries to expand the range of data available for comparison. For example, you could join a library containing pesticide information to a library containing personal care product information.

❖ To merge two libraries into one

1. Click the **Library** tab if the Library page is not already selected.
2. Click **Merge**.

   The Specify the Libraries for Merge dialog box appears, as shown in Figure 21.

Figure 21. Specify the Libraries for Merge dialog box



3. In the Source Library1 box, specify the path and name of the first library to merge, or click the **Browse** button (...) to browse to the location.
4. In the Source Library2 box, specify the path and name of the second library to merge, or click the **Browse** button (...) to browse to the location.
5. In the Destination Library box, specify the path and name of the merged library, or click the **Browse** button (...) to browse to the location.
6. Click **Merge**.

Specify the Libraries for Merge Dialog Box Parameters

Table 2 describes the parameters in the Specify the Libraries for Merge dialog box.

Table 2. Specify the Libraries for Merge dialog box parameters

Parameter	Description
Source Library1	Specifies the path and name of the first library to merge.
Source Library2	Specifies the path and name of the second library to merge.
Destination Library	Specifies the path and name of the merged library.
Merge	Merges the two specified libraries.
Cancel	Closes the dialog box without merging any libraries.

Library Manager Parameters

This topic describes the parameters on each page of the Library Manager.

- Raw File Page Parameters
- Library Page Parameters
- Search Page Parameters

Raw File Page Parameters

The Raw File page displays the data in the loaded raw data file and provides a means of filtering it.

Table 3 describes the parameters on the Raw File page.

Table 3. Raw File page Parameters (Sheet 1 of 2)

Parameter	Description
Raw File	Displays the name and path of the loaded raw data file.
Open Raw File	Opens the Open dialog box so that you can select the raw data file to load.
Scan Number	Displays the scan number of the currently displayed mass spectrum. You can move among the scans with the forward and back buttons.
Show Filters	Determines whether the Filter Parameters pane, shown in Figure 4 on page 7, appears in the upper left area of the Library Manager window.
Filter Parameters pane	
Filter	Specifies the criterion to filter by. The information in the raw data file determines what filters appear in the Filter list.
Time Range	Specifies the range of data to filter by. The first box specifies the beginning of the range of data to use, and the second box specifies the end of the range to use.
Trace Type	Specifies the type of chromatogram to filter by: • (Default) TIC: Displays a total ion current (TIC) chromatogram, which displays a point for every spectrum in the chromatogram, where the *x* axis displays the retention time of the spectrum, and the *y* axis displays the summed intensity of all peaks (TIC) in the spectrum. • Base Peak: Displays a base peak ion chromatogram. A base peak chromatogram is very similar to a total ion current chromatogram, but instead of the summed intensity of all peaks (TIC), it displays the intensity of the largest peak (base peak) in the spectrum on the *y* axis. The *x* axis displays the analysis data from the beginning of the analysis. The base peak chromatogram lists the detected peaks and the retention time associated with each peak. • Target Mass: Displays a subset of a mass chromatogram. When you select this type of chromatogram, the Filter Mass boxes become available.

Table 3. Raw File page Parameters (Sheet 2 of 2)

Parameter	Description

Filter Mass	Specifies the mass, tolerance, and unit to use for filtering a target mass chromatogram:
	• First box: Specifies the mass to use for filtering the chromatogram.
	• Second box: Specifies the mass tolerance window for the filter mass to use for filtering the chromatogram.
	• Third box: Specifies the unit to display the mass and tolerance in:
	  • mmu: Millimass units (one thousandth of a mass unit)
	  • (Default) ppm: Parts per million (one millionth of the filter mass)
	The Filter Mass boxes become available when you select Target Mass in the Trace Type list.

Chromatogram	Displays the chromatogram of the data in the raw data file. • Relative Intensity (*y* axis): Displays the ratio of the intensity of a specific peak to the intensity of the peak with the highest intensity. • RT(min) (*x* axis): Displays the retention time of the spectrum, which is the time after injection at which a compound elutes. Retention time can also refer to the total time that the compound is retained on the chromatograph column.
Mass spectrum	Displays the mass spectrum associated with the selected scan number. • Relative Intensity (*y* axis): Displays the ratio of the intensity of a specific peak to the intensity of the peak with the highest intensity. • *m/z* (*x* axis)*:* Displays the mass-to-charge ratio of ions formed from molecules. This ratio is the quantity formed by dividing the mass of an ion, in daltons, by the number of charges carried by the ion.

Library Page Parameters

The Library page displays information about the currently selected spectrum.

Table 4 describes the parameters on the Library page.

Table 4. Library page parameters (Sheet 1 of 5)

Parameter	Description
Open Library	Opens the Open Existing Library dialog box so that you can select the library to open.
Library File	Displays the name of the open library.
Save As	Opens the Save As dialog box so that you can save a library under a new name.
New Library	Opens the New Library dialog box so that you can assign a new name and location to a library that you created.
Import (xlsx)	Opens the Open dialog box so that you can import data records from a Microsoft Excel (.xlsx) file.
Import (MassBank Format)	Imports data records (spectra) from MassBank, which is a public repository of mass spectral data.
Merge	Merges two libraries together.
Field	Lists all the fields in the library to use with the Find function so that the Library Manager application searches the correct field for the search term. • Compound: Specifies the name of the substance associated with the spectrum. • Formula: Specifies the chemical formula of the substance associated with the spectrum. • CASIDnumber: Specifies the unique chemical registry number assigned by the Chemical Abstracts Service to the substance associated with the spectrum. • Filter: Specifies the scan filter from the original raw data file. • PeptideSequence: Specifies the amino acid sequence of a peptide or protein associated with the spectrum.
Limit List	Specifies the terms to use to filter the selection you made in the Field list. This box becomes available when you specify a category in the Field list.
Find	Searches the library for the data that meets the filtering criteria given in the Limit List box and Field list.

Table 4. Library page parameters (Sheet 2 of 5)

Parameter	Description
Export CSV	Opens the Save As dialog box so that you can select the CSV file to export the selected library databases to.
Delete	Deletes any selected records in the data records table.
New	Adds a new record to the library.
Create Copy	Creates a new record that is a copy of the currently selected library record.
Replace Spectrum	Replaces the spectrum associated with the currently displayed record with the spectrum from the raw data file.
Save	Saves the currently displayed record to the library. This button is inactive if the current record is not different from the library entry.
Library records	Displays the data records in the library in several columns.
Entry No.	Assigns a sequential record number to a spectrum.
Compound	Displays the name of the substance associated with the entry number in the library.
Formula	Displays the chemical formula of the substance associated with the entry number in the library.
CAS ID	Displays the unique chemical registry number that the Chemical Abstracts Service assigns to the substance associated with the spectrum to search for in the library.
ChemSpider ID	Displays the identification of the compound in the ChemSpider™ online data repository (http://www.chemspider.com).
HMDB ID	Displays the identification of the compound in the Human Metabolome Database (HMDB) online data repository (http://www.hmdb.ca).
KEGG ID	Displays the identification of the compound in the Kyoto Encyclopedia of Genes and Genomes (KEGG™) online data repository (http://www.genome.jp/kegg).
PubChem ID	Displays the identification of the compound in the PubChem℠ online data repository.
mz Cloud ID	Displays the identification of the compound in the mzCloud™ database, which is an online database provided by HighChem (http://www.mzCloud.org).
Peptide Sequence	Displays the amino acid sequence of a peptide or protein that corresponds to the spectrum in the library.

Table 4. Library page parameters (Sheet 3 of 5)

Parameter	Description
Tag	Has no functionality at this time.
Child records	Displays the spectra belonging to a specific compound when you click the Expand icon (+) to the left of the compound name.
Spectrum ID	Specifies the identification of the spectrum in the database.
Compound ID	Displays the sequential number assigned to the selected item in the Entry No column.
mzCloud URL	Displays the URL of the mzCloud online database provided by HighChem (http://www.mzCloud.org).
Filter	Displays the conditions under which the data in the raw data file was collected from the instrument, for example, the type of mass spectrometer used, ionization mode, scan dependency, scan type, scan mode, precursor *m/z*, fragmentation mode, and scan range.
Retention Time	Displays the time after injection at which a compound elutes. The total time that the compound is retained on the chromatograph column.
Scan Number	Displays the scan number in the raw data file that the spectrum is associated with.
Precursor m/z	Specifies the mass of the precursor ion associated with the spectrum to search for in the library.
Neutral Mass	Specifies the mass of the molecule.
Collision Energy	Displays the amount of energy used when the ions collided with the gas during fragmentation.
Polarity	Displays the polarity of the spectrum, either positive or negative.
Fragmentation Mode	Displays the fragmentation technique used to fragment the precursor ion, for example, CID or HCD.
Ionization Mode	Displays the type of process used to produce the precursor ion from a neutral atom or molecule, for example, ESI or MALDI.
Mass Analyzer	Displays the name of the mass analyzer used to collect the sample.
Instrument Name	Displays the name of the instrument used to collect the data in the raw data file.
Operator	Displays the name of the person who collected the data in the raw data file.
Raw File URL	Displays the URL of the raw data file.

Table 4. Library page parameters (Sheet 4 of 5)

Parameter	Description
Version Number	Displays the version number assigned to the spectrum in the mzCloud online database provided by HighChem (http://www.mzCloud.org).
Creation Date	Displays the date that the raw data file was created.
Field/Value	Displays categories of information about the selected spectrum—for example, the formula of the substance associated with the spectrum—and information about the specific instance selected—for example, a formula of C17H13CIN4 for the substance associated with the spectrum.
Compound ID	Displays the sequential number assigned to the selected item in the Entry No column.
Compound	Displays the formula of the selected item as shown in the Compound column.
Formula	Displays the formula of the selected item as shown in the Formula column.
CAS ID	Displays the unique chemical registry number that the Chemical Abstracts Service assigns to the substance associated with the spectrum as shown in the CAS ID column.
ChemSpider ID	Displays the identification of the compound in the ChemSpider online data repository as shown in the ChemSpider ID column.
HMDB ID	Displays the identification of the compound in the Human Metabolome Database (HMDB) online data repository as shown in the HMDB ID column.
KEGG ID	Displays the identification of the compound in the Kyoto Encyclopedia of Genes and Genomes (KEGG) online data repository as shown in the KEGG ID column.
PubChem ID	Displays the identification of the compound in the PubChem online data repository as shown in the PubChem ID column.
mz Cloud ID	Displays the identification of the compound in the mzCloud database, an online database provided by HighChem.
Peptide Sequence	Displays the amino acid sequence of a peptide or protein that corresponds to the spectrum in the library as shown in the Peptide Sequence column.
Tag	Has no functionality at this time.

Table 4. Library page parameters (Sheet 5 of 5)

Parameter	Description
	Note For a description of other fields that appear in the Field/Value table, see "Child records" on page 34.
Mass spectrum	Displays the mass spectrum associated with the selected scan number. • Relative Intensity (*y* axis): Displays the ratio of the intensity of a specific peak to the intensity of the peak with the highest intensity. • *m/z* (*x* axis)*:* Displays the mass-to-charge ratio of ions formed from molecules. This ratio is the quantity formed by dividing the mass of an ion, in daltons, by the number of charges carried by the ion.

Search Page Parameters

The Search page specifies the criteria to search for a spectrum in the library and displays the search results.

Table 5 describes the parameters on the Search page.

Table 5. Search page parameters (Sheet 1 of 3)

Parameter	Description
Field	Specifies the search criterion. You can select from the following criteria: • Compound: Specifies the name of the substance associated with the spectrum to search for in the library. • Formula: Specifies the chemical formula of the substance associated with the spectrum to search for in the library. • Precursor m/z: Specifies the mass of the precursor ion of the substance associated with the spectrum to search for in the library. When you select this option, the Precursor m/z box becomes available. • CASIDnumber: Specifies the unique chemical registry number that the Chemical Abstracts Service assigns to the substance associated with the spectrum to search for in the library.
Precursor m/z	Specifies the value used to match individual peaks between the mass spectrum being searched and the library entries. This box becomes available only when you select Precursor m/z in the Field list. You can specify up to four decimal places. For spectra that arise from MS/MS experiments, setting the Precursor m/z parameter limits the returned spectra according to the MS1 set point.
Precursor Tolerance (ppm)	Specifies the maximum difference in mass allowed for retrieved spectra relative to the query spectrum, in parts per million. You can use values with one decimal place from 0.1 to 1000. The default is 5.0.
Fragment Tolerance	Specifies the tolerance that determines whether comparing an observed fragment ion mass to a theoretical fragment ion mass is considered a match.
Limit Search	Specifies the terms to use to filter the selection you made in the Field list.
Percent Cut-off (%)	Filters out results below a percentage of the highest score. For example, if the highest score is 0.900 and the setting in the Percent Cut-off (%) box is 60%, the results will include scores between 0.900 and 0.540 (0.9 × 60% = 0.540).

Table 5. Search page parameters (Sheet 2 of 3)

Parameter	Description
Search Type	Specifies the search algorithm to use: • Forward: Searches a number of peaks in the unknown spectrum against the peaks in a spectrum from the spectral library. A forward search uses the raw data file mass spectrum to examine the library. If the unknown spectrum includes a peak that is not in a given library spectrum, the score for the match is negatively affected. Use a forward search when the unknown spectra are of high quality—that is, when they have good fragmentation and few low-intensity background peaks. • Reverse: Searches the top few peaks in the library spectrum against the unknown spectrum. A reverse search uses the library spectra to examine the raw data file mass spectrum. If the unknown spectrum does not contain any peaks from a library, the score for the match is negatively affected, but the presence of additional peaks in the unknown spectrum has no effect on the score. Use a reverse search if the unknown spectrum includes peaks from several components or has a lot of background noise.
Remove Precursor Ion	Determines whether the Library Manager application removes from the spectra any mass or intensity data that is within 2.2 Da of the precursor ion. In an MS/MS experiment, the precursor ion normally does not appear in the spectrum, but sometimes it can appear and interfere with the scoring of the algorithm. This option corrects this problem. • (Default) Selected: Removes from the spectra any mass or intensity data that is within 2.2 Da of the precursor ion. • Clear: Retains in the spectra any mass or intensity data that is within 2.2 Da of the precursor ion.
Search	Performs the requested search.
Compound	Specifies the name of the substance associated with the spectrum to search for in the library.
Spectrum ID	Specifies the identification of the spectrum in the database.
Formula	Specifies the chemical formula of the substance associated with the spectrum to search for in the library.
Precursor m/z	Specifies the mass of the precursor ion associated with the spectrum to search for in the library.
Neutral Mass	Specifies the mass of the molecule.

Table 5. Search page parameters (Sheet 3 of 3)

Parameter	Description
CAS ID Number	Specifies the unique chemical registry number that the Chemical Abstracts Service assigns to the substance associated with the spectrum to search for in the library.
Classic Score	Displays a ratio of the unknown spectra against the spectra in the library. The score does not reside in the library.
NIST Score	Displays the score from HighChem's implementation of the NIST™ library search algorithm.
High Res Score	Displays the score calculated by HighChem's search algorithm.
Filter	Specifies the scan filter from the original raw data file.
Library pane	Displays the library spectrum searched for.
Difference pane	Displays the difference between the query spectrum selected in the raw data file and the library spectrum.
Query pane	Displays the spectrum selected in the raw data file.

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