thermoscientific

Thermo

mzVault

User Guide

Software Version 2.1

XCALI-97970 Revision A • May 2018

ThermoFisher SCIENTIFIC

mzVault, Compound Discoverer, and TraceFinder are trademarks; and Orbitrap and Thermo Scientific are registered trademarks of Thermo Fisher Scientific Inc. in the United States.

The following are registered trademarks in the United States and other countries: Microsoft, Windows, and Excel are registered trademarks of Microsoft Corporation. Adobe, Acrobat, and Reader are registered trademarks of Adobe Systems Inc.

The following are registered trademarks or service marks in the United States: Chemical Abstracts Service is a registered trademark of the American Chemical Society Federally Chartered Corp. ChemSpider is a registered trademark of ChemZoo Inc. KEGG is a registered trademark of Minoru Kanehisa (Individual). NIST is a registered trademark of the National Institute of Standards and Technology. PubChem is a registered service mark of the U.S. National Library of Medicine.

mzCloud is a registered trademark of HighChem, Ltd. in Slovakia.

All other trademarks are the property of Thermo Fisher Scientific Inc. and its subsidiaries.

Release history: Revision A May 2018

Software version: mzVault 2.1

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

C

Contents

Preface . . . . . **vii**
Accessing Documentation vii
Special Notices viii
Contacting Us ix

Chapter 1 Introduction **1**
Features 1
Workflows for Browsing, Building, and Searching Libraries 1
Default Search and Recalibration Parameter Settings 2
Curated Spectra 2
Inputs and Output File Types 3
Input Files 3
Output Files 3
What's New in This Release 3

Chapter 2 Getting Started **5**
Opening and Closing the mzVault Application 5
Opening the mzVault Application 5
Closing the mzVault Application 7
Starting from the Landing Page or the Search Tab 7
Starting a Browse or Build Workflow from the Landing Page 8
Starting a Search Workflow from the Landing Page 8
Starting a Search Workflow from the Search Tab 9
Navigation Between the Application Tabs 10
Displaying the Compound Tab and Its Toolbar 11
Displaying the Compound List Tab and Its Toolbar 11
Controlling the Visibility of the Toolbars 12
Opening and Modifying the Layout of Tabbed Pages 12
Scaling and Copying Graphical Plots 13
Changing the Zoom Level of a Graphical Plot 14
Copying a Graphical Plot to the Clipboard 14
Displaying or Hiding Table Columns 14

Chapter 3 Browsing Libraries 15
Opening a Library for Browsing 15
Closing a Library 16
Reviewing the Library Entries 17
Displaying a Subset of Records to Browse 18
Browse Tab 20
Browse Toolbar 20
Library Page Panes 21

Chapter 4 Building and Editing Libraries 23
Build Workflow Overview 24
Opening a Library for Editing 24
Opening a New Library for Editing 24
Opening an Existing Library for Editing 25
Importing NIST or MassBank Records into an mzVault Library 25
Merging mzVault Libraries 26
Deleting Compound Records or Spectra from a Library 27
Deleting Compound Records from a Library 27
Deleting Spectra from a Library 27
Adding Individual Records to a Library 28
Manually Adding a New Compound to a Library 28
Manually Adding Spectra and a Structure to a Compound Entry 31
Creating, Saving, and Opening Compound List Files 36
Creating a Compound List 36
Specifying a Compound's Formula and Precursor Mass 38
Saving a Compound List as an XML File 40
Opening a Compound List File 40
Adding Multiple Records to a Library by Processing a Compound List 40
Setting Up the Spectrum Selection Parameters 40
Processing a Compound List 42
Exporting Compounds or Spectra from a Library to a CSV File 44
Copying a Record or a Compound in a Compound List 44
Copying a Record in an Editable Library 45
Copying a Compound in a Compound List File 45
Saving a Library 45
Build Tab 45
Compound Tab 47
Compound List Pane of a Library Page 49
Compound List Tab 51
Compound List Toolbar 52
Compound List Page 53
Spectrum Selection Parameters Dialog Box 54
Processing Parameters Dialog Box 55

Chapter 5 Searching Libraries 57
Performing a Library Search 57
Selecting the Libraries for the Search 58
Opening a Raw Data File 59
Selecting the Query Spectrum 61
Setting the Search and Query Spectrum Parameters 62
Starting the Library Search 64
Reviewing and Exporting the Search Results 64
Reviewing the Search Results 64
Exporting the Search Results 66
Starting a New Search for Comparison 67
Limiting the Library Entries to Search 68
Search Tab 70
Search Toolbar 71
Library Search Page 72

Chapter 6 Application Options 79
Setting the Default Library Search Parameters 79
Setting the Default Recalibration Parameters 80
Setting Up and Managing Write Access to Libraries 81
Restricting Write Access to a Library 82
Unlocking a Restricted Library for Editing 83
Changing the Password or Removing the Password Security 83
mzVault Options Dialog Box 84
Default Library Search Parameters Page 84
Parameters on the Default Recalibration Parameters Page 88

Index 95

Preface

This guide describes how to use the Thermo mzVault™ application to create and modify mass spectral libraries of accurate mass data.

Contents

- Accessing Documentation
- Special Notices
- Contacting Us

❖ **To suggest changes to the documentation or to the Help**

Complete a brief survey about this document by clicking the button below. Thank you in advance for your help.

Accessing Documentation

The mzVault application includes complete documentation. For system requirements, refer to the Release Notes on the software DVD for the host application.

❖ **To view the mzVault User Guide and mzVault Quick Start Guide**

- From the Microsoft™ Windows™ taskbar, choose **Start > All Programs > Thermo mzVault > Manuals > Thermo mzVault User Guide** or **Thermo mzVault Quick Start Guide**.
- From the application window, choose **Menu > mzVault User Guide** or **mzVault Quick Start Guide**.

❖ **To view the mzVault Help**

From the application window, choose **Menu > mzVault Help** or click  .

❖ **To view user documentation from the Thermo Fisher Scientific website**

1. Go to thermofisher.com.
2. Click **Services & Support**.
3. Under Product Documentation, click **Manuals**.
4. In the Refine Your Search box, search by the product name.
5. From the results list, click the title to open the document in your web browser, save it, or print it.

   To return to the document list, click the browser **Back** button.

Special Notices

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

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

Contact	Email	Telephone	QR Code*
U.S. Technical Support	us.techsupport.analyze@thermofisher.com	(U.S.) 1 (800) 532-4752	
U.S. Customer Service and Sales	us.customer-support.analyze@thermofisher.com	(U.S.) 1 (800) 532-4752	
Global Support	❖ **To find global contact information or customize your request** 1. Go to thermofisher.com. 2. Click **Contact Us**, select the country, and then select the type of support you need. 3. At the prompt, type the product name. 4. Use the phone number or complete the online form. ❖ **To find product support, knowledge bases, and resources** Go to thermofisher.com/us/en/home/technical-resources. ❖ **To find product information** Go to thermofisher.com/us/en/home/brands/thermo-scientific.		

Note To provide feedback for this document, go to surveymonkey.com/s/PQM6P62 or send an email message to Technical Publications (techpubs-lcms@thermofisher.com).

* You can use your smartphone to scan a QR Code, which opens your email application or browser.

1

Introduction

These topics briefly describe the features available in the mzVault application and the application's inputs and outputs.

Contents

- Features
- Inputs and Output File Types
- What's New in This Release

Features

The mzVault application offers the following features and workflows:

- Workflows for Browsing, Building, and Searching Libraries
- Default Search and Recalibration Parameter Settings
- Curated Spectra

Workflows for Browsing, Building, and Searching Libraries

The mzVault application includes three workflows.

Browse Workflow

Use the Browse workflow to review the contents of an mzVault library. When you open a library from the Browse tab, you can view its compound entries, and the spectra and two-dimensional structures associated with each entry. To modify the open library, you can click the Build tab, and then unlock the library if it is restricted to read-access only.

Build Workflow

Use the Build workflow to create and modify mzVault libraries. You can open the library that you want to modify from the Browse tab or the Build tab.

There are three ways to add records to an mzVault library that is open for editing:

- Add individual compound entries from the Build tab by clicking New (in the Compound area), and then adding spectra to the new compound entry from the Compound tab (see "Adding Individual Records to a Library" on page 28).
- Add multiple compound entries by creating and processing a list of compounds from the Compound List tab (see "Adding Multiple Records to a Library by Processing a Compound List" on page 40).
- Import compounds from a MassBank or NIST™ file (see "Importing NIST or MassBank Records into an mzVault Library" on page 25).

There are two ways to add records to an unrestricted mzVault library without opening it for editing:

- Merge records from two unrestricted libraries into it.
- Import records from MassBank or NIST files into it.

Note After merging libraries or importing files into a destination library, the application automatically opens the library for editing.

Search Workflow

Use the Search workflow to search up to five mzVault libraries for mass spectra that match a selected query spectrum. You select the libraries that you want to search and the query spectrum that you want to match from the Search tab.

For best results, use the search workflow to validate your mzVault libraries.

Default Search and Recalibration Parameter Settings

You can set up the default parameter values for a library search or spectrum recalibration.

Curated Spectra

You can curate spectra by thresholding, which removes noise; averaging, which averages the masses of spectra over a user-selectable time range; or recalibration, which corrects the spectra for known or possible measurement errors.

You can curate a spectrum manually from the Compound tab before you add it to a compound entry, or you can set up automated curation from the Compound List tab before you process a compound list file.

Inputs and Output File Types

The following topics describe the file types that the mzVault application processes and generates:

- Input Files
- Output Files

Input Files

The mzVault application accepts the following files as input:

- Raw data files (RAW), which contain mass spectra from a Thermo Scientific™ mass spectrometer
- Library database (DB) files, which contain compound records
- XML files, which contain lists of compounds
- MassBank text (TXT) files, which are libraries of spectra from MassBank, a public repository of mass spectral data
- NIST files (MSP), which are libraries of spectra from the National Institute of Science and Technology

Output Files

The mzVault application generates the following files as output:

- (Optional) Excel™ (XLSX) files, which contain the search results
- XML files, which contain lists of compounds
- CSV files, which contain the compounds or spectra exported from a library
- Library database (DB) files

What's New in This Release

In this release of the mzVault application, you can do the following:

- Set up multiple filters for browsing or searching mzVault libraries.
- Import MassBank files or NIST files.

> **Note** The application merges entries with the same compound name or chemical formula. The merged library entry includes all the spectral data from the merged entries.

- Password-protect your mzVault libraries.
- Add retention time information to the library records.

2

Getting Started

If you are familiar with a previous version of the mzVault application, use the *mzVault 2.1 Quick Start Guide* to get started with the current release.

These topics describe how to open and close the application, start a workflow from the landing page, modify the arrangement and visibility of some of the user-interface elements, and resize or copy the spectrum and chromatogram plots.

Contents

- Opening and Closing the mzVault Application
- Starting from the Landing Page or the Search Tab
- Navigation Between the Application Tabs
- Controlling the Visibility of the Toolbars
- Opening and Modifying the Layout of Tabbed Pages
- Scaling and Copying Graphical Plots
- Displaying or Hiding Table Columns

Opening and Closing the mzVault Application

To open and close the mzVault application, see these topics:

- Opening the mzVault Application
- Closing the mzVault Application

Opening the mzVault Application

You can open the mzVault application by clicking its corresponding desktop icon or by choosing the appropriate Start menu command. Initially, the application opens to the Browse tab. You can change this start-up behavior by specifying a default search library (see "Setting the Default Library Search Parameters" on page 79).

❖ To open the mzVault application

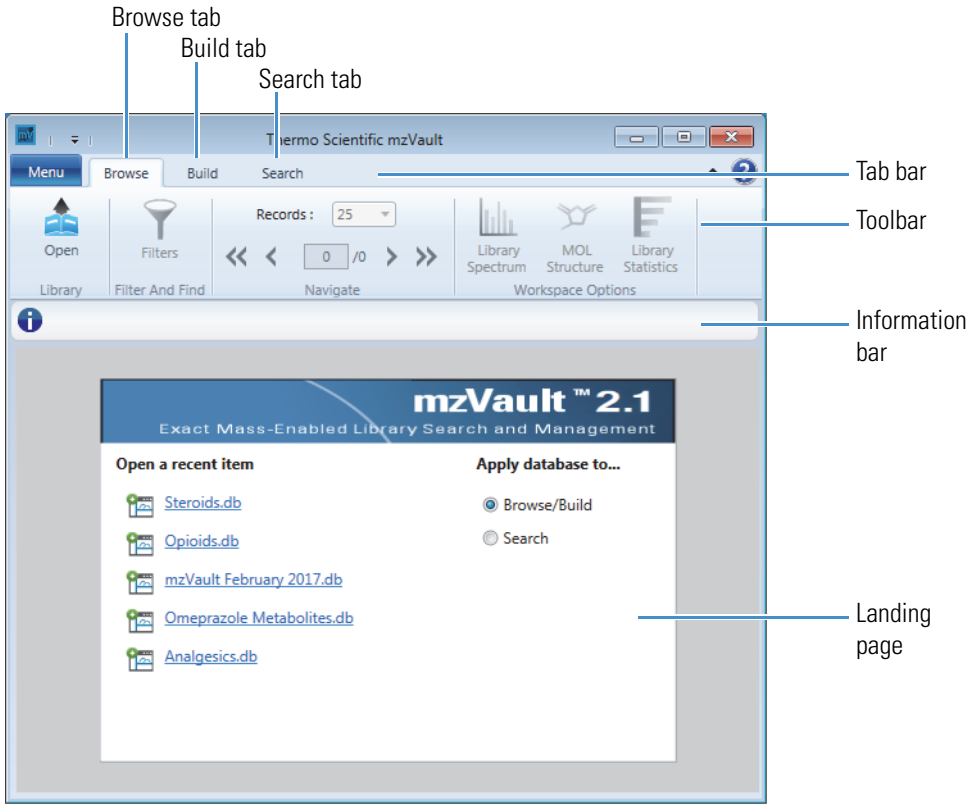
- From the Start menu, choose **All Programs > Thermo mzVault > Thermo mzVault**.
- From the taskbar, click the **mzVault** icon,  .

–or–

- From the desktop, double-click the **mzVault** shortcut icon,  .

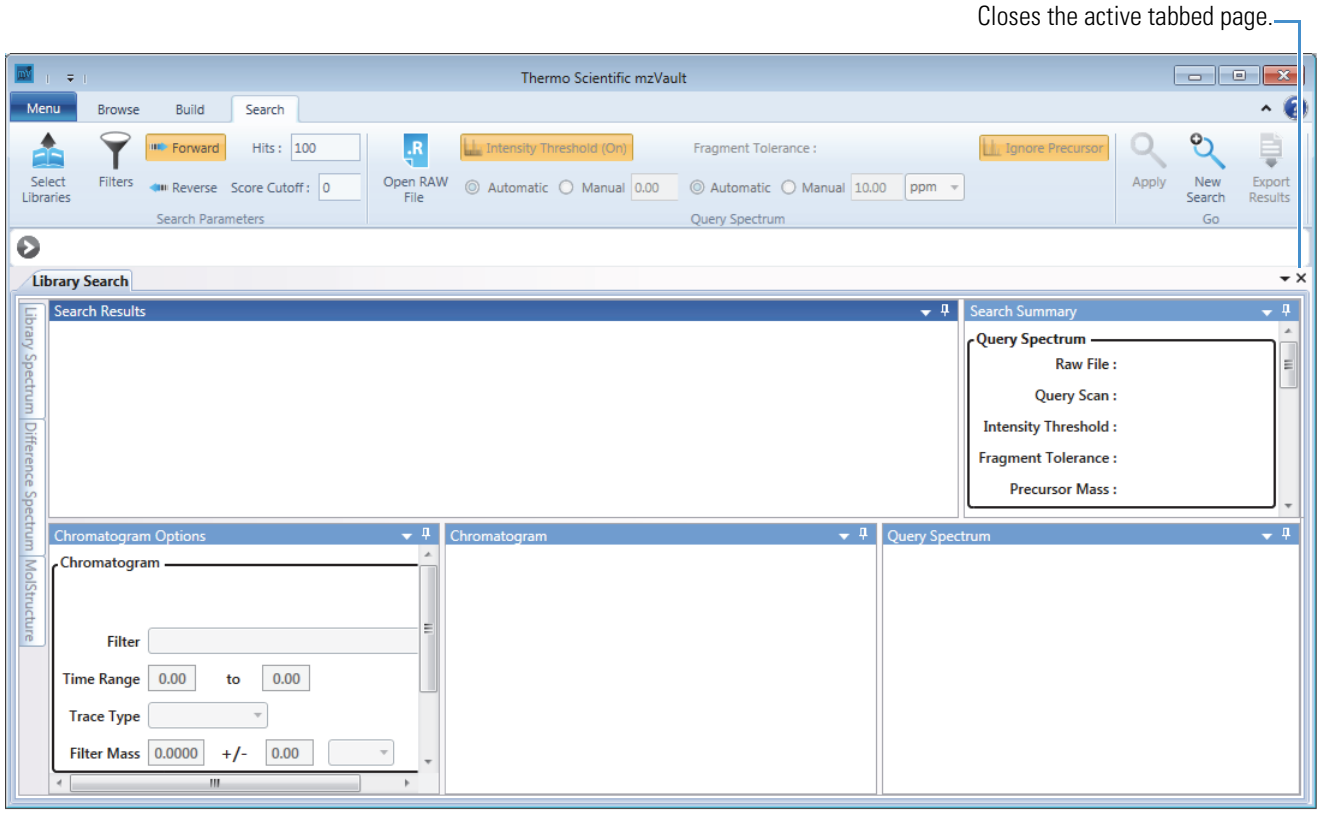
Without a specified library, the mzVault window opens to the Browse tab and the landing page (Figure 1).

Figure 1. mzVault window opened to the landing page



With a specified library (or libraries), the application opens to the Search tab and displays the Library Search page (or the Multi-Search page) below the toolbar (Figure 2). Clicking the close icon (×) on the far right of the page tab closes the search page and displays the landing page.

Figure 2. mzVault window opened to the Search tab with a Library Search page



Closing the mzVault Application

❖ **To save changes and close the application**

1. Either choose **Menu > Exit** or click the **Exit** icon,  .
2. At the confirmation message, click **Yes**.

Starting from the Landing Page or the Search Tab

To start a browse/build workflow from the landing page or a search workflow from the landing page or the Library Search page, see these topics:

- Starting a Browse or Build Workflow from the Landing Page
- Starting a Search Workflow from the Landing Page
- Starting a Search Workflow from the Search Tab

Starting a Browse or Build Workflow from the Landing Page

❖ **To start a browse/build workflow from the landing page**

1. If the landing page is not displayed, close all the tabbed pages below the toolbar.
2. Under Apply Database To, select the **Browse/Build** option.

   The Browse tab opens.
3. Do one of the following:
   - Under Open a Recent Item, click a hyperlink.
   - In the toolbar, click **Open**, locate the library, and click **Open**.

   The selected library opens as a tabbed page below the toolbar.
4. Use the navigation tools in the toolbar to browse through the library entries.
5. To modify the opened library, click the **Build** tab.
6. If the library is password-secured, click the **Lock** icon,  . Then, in the Restricted Access Dialog box, enter the password and click **OK**.
7. Do any of the following:
   - To add individual compound entries, see "Adding Individual Records to a Library."
   - To semi-automatically add multiple compound entries, see "Adding Multiple Records to a Library by Processing a Compound List."
   - To delete compound entries or spectra, see "Deleting Compound Records or Spectra from a Library."
   - To import compound entries, see"Importing NIST or MassBank Records into an mzVault Library."

Starting a Search Workflow from the Landing Page

❖ **To start a library search workflow from the landing page**

1. If the landing page is not displayed, close all the tabbed pages below the toolbar.
2. On the landing page, under Apply Database To, select the **Search** option.

   The Search tab opens.
3. Do one of the following:
   - Under Open a Recent Item, click a hyperlink (Figure 3).

Figure 3. Landing page with hyperlinks to recently opened libraries

–or–

- In the toolbar, click **Select Libraries** and select up to five libraries.

The library search page opens below the toolbar.

4. In the toolbar, click **Open RAW File**, locate the raw data file of interest, and click **Open**.
5. On the library search page, select the query spectrum to search against.
6. In the toolbar, set up the search parameters and the query spectrum options, and then click **Apply**.

For complete instructions, see "Performing a Library Search" on page 57.

Starting a Search Workflow from the Search Tab

If you frequently identify compounds by using specific libraries, select these libraries when you set up the default library search parameters (see "Setting the Default Library Search Parameters" on page 79).

❖ To start a search workflow from the Search tab

1. If the application currently opens to the landing page, set it to open to the Search tab as follows:
   a. Choose **Menu > Options**.
   b. Click the **Search Parameters** tab on the left if it is not already selected (by default).
   c. In the mzVault Search area, locate the libraries of interest and click **Open**.

      Note The libraries must be in the same directory folder.

   d. Click **Save**.

e. Close and reopen the application.

The mzVault window opens to the Search tab and displays the Library Search page or the Multi-Search page below the toolbar.

2. Do one of the following:
   - To use only the default libraries, go to step 4.
   - To select a different library, in the toolbar, click **Select Libraries** and select up to five libraries.
3. In the toolbar, click **Open RAW File**, locate a the raw data file of interest, and click **Open**.
4. On the search page, select the query spectrum to search against.
5. In the toolbar, set up the search parameters and the query spectrum options, and then click **Apply**.

For complete instructions, see "Performing a Library Search" on page 57.

Navigation Between the Application Tabs

Besides the three core tabs—Browse, Build, and Search—the application has two contextual tabs—Compound and Compound List.

These topics describe the navigation from the Build tab to the Compound and Compound List tabs:

- Displaying the Compound Tab and Its Toolbar
- Displaying the Compound List Tab and Its Toolbar

Table 1 describes the function of the core and contextual application tabs.

Table 1. Application tabs and toolbars (Sheet 1 of 2)

Tab	Function	Availability
Browse	Open a library and browse its pages.	Always available
Build	Add, copy, or delete compound entries in a library. Also import NIST or MassBank records into a library or merge two mzVault libraries into a third mzVault library.	Always available
Search	Search mzVault libraries for spectra that match a selected query spectrum.	Always available

Table 1. Application tabs and toolbars (Sheet 2 of 2)

Tab	Function	Availability
Compound	Edit individual compound entries.	See Displaying the Compound Tab and Its Toolbar.
Compound List	Create and batch-process a compound list.	See Displaying the Compound List Tab and Its Toolbar.

Displaying the Compound Tab and Its Toolbar

You can add the Compound tab to the tab bar in two ways: add a new compound to an opened, editable mzVault library, or select a compound (its check box) in an opened, editable library. The Build tab stays active, however, while the Compound tab remains closed.

❖ To display the Compound tab and its toolbar

1. Open a library for editing (see "Opening a Library for Editing" on page 24).
2. If the library has restricted access, unlock it (see "Unlocking a Restricted Library for Editing" on page 83).
3. To display the Compound tab in the tab bar, do one of the following:
   - In the Compound area of the Build toolbar, click **New**.

     The application adds a placeholder row to the Compound List table and selects the check box to the left of the compound.

   –or–

   - In the Compound List pane of the tabbed library, select the check box for at least one compound.
4. To display the Compound toolbar, click the **Compound** tab.

Displaying the Compound List Tab and Its Toolbar

❖ To display the Compound List tab and its toolbar

1. Click the **Build** tab.
2. In the Build toolbar, click **New Compound List** or **Open Compound List**.

   The Compound List tab and the Compound List toolbar appear. In addition, the following tabbed page appears below the toolbar:

   - If you clicked New Compound List, the New_Compound List page appears.
   - If you clicked Open Compound List, the *Named Compound List* page appears.

Controlling the Visibility of the Toolbars

You can show or hide any of the five application tabs.

❖ **To hide or show a toolbar**

- To hide a toolbar, click the up arrow (^) in the upper right corner of the application.
- To show a hidden toolbar, click the down arrow (v) in the upper right corner of the application.

Opening and Modifying the Layout of Tabbed Pages

Table 2 lists the tabbed pages that you can display in the mzVault application. It also describes how to open these pages.

Each of the tabbed pages contains one or more docked panes. You can close panes that have a Close icon (), change any pane to floating a window, hide any pane as a vertical bar, and reposition the docked panes.

Table 2. Tabbed pages in the mzVault application (Sheet 1 of 2)

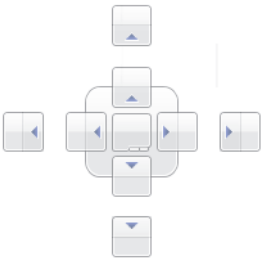
Page name	To display ...
Library Name	Open a library from the Build or Browse tab. The *Library Name* page appears below the respective toolbar.
New_Compound List	In the Build toolbar, click **New Compound List**. The New_Compound List page opens below the Compound List toolbar.
Compound List Name	In the Build toolbar, click **Open Compound List**. The selected file opens below the Compound List toolbar.
Library Search	In the Search toolbar, click **Select Libraries** and select a single library. The Library Search page opens below the Search toolbar.
Multi-Search	In the Search toolbar, click **Select Libraries** and select multiple libraries. The Multi-Search page opens below the Search toolbar.

Table 2. Tabbed pages in the mzVault application (Sheet 2 of 2)

Page name	To display ...
Library Name-Integer	Search a single library for matching spectra. The *Library Name-Integer* page, which displays the search results, opens below the Search toolbar.
Multi-Search_*Integer*	Search multiple libraries for matching spectra. The Multi-Search_*Integer* page, which displays the search results, opens below the Search toolbar.

Table 3 describes the tasks for modifying the page layout.

Table 3. Tasks for modifying the layout of a tabbed page

Task	Action
Close a pane.	Click the **Close** icon, .
Hide a pane as a vertical tab.	Click the **Auto Hide** icon, .
Float a pane.	Drag and release the pane.
Change the position of a docked pane.	1. Drag the pane by its title bar. A positioning tool appears along the vertical median of the window. The tool consists of four directional arrows in a diamond pattern around a central rounded rectangle. In addition to the tool, directional arrows appear on all four sides.  2. Drag the pointer until it aligns with the appropriate directional arrow.

Scaling and Copying Graphical Plots

You can view chromatogram and spectrum plots after you open a raw data file on the Compound page and the Search page.

To scale a plot or copy it to the Clipboard, follow these topics as needed:

- Changing the Zoom Level of a Graphical Plot
- Copying a Graphical Plot to the Clipboard

Changing the Zoom Level of a Graphical Plot

To change the zoom level of the chromatogram and spectrum plots, see Table 4.

Table 4. Changing the scaling of a plot

Task	Action
Zoom in on a region of a plot.	Drag the cross-shaped pointer over the area of the plot that you want to enlarge.
Undo the last zoom.	Right-click the plot and choose **Undo Zoom**.
Return the scaling to the last zoom level after undoing a zoom level.	Right-click the plot and choose **Redo Zoom**.
Return the plot to its original scale.	Right-click the plot and choose **Reset Scaling**.

Copying a Graphical Plot to the Clipboard

You can copy a graphical plot to the Clipboard as a raster image.

❖ **To copy a plot**

Right-click the plot, and choose **Copy to Clipboard**.

Displaying or Hiding Table Columns

You can choose whether to display or hide columns in the Search Results table and Compound List table for a library.

Note You cannot change the columns in the Compound List table for a compound list.

❖ **To display or hide a table column**

1. Click the **Field Chooser** icon,  , in the upper left corner of the table.

   The Field Chooser dialog box opens.

2. Do one of the following:

   - To display a column, select its check box.
   - To hide a column, clear its check box.

Browsing Libraries

These topics explain how to browse the records in an existing mzVault library.

Contents

- Opening a Library for Browsing
- Closing a Library
- Reviewing the Library Entries
- Displaying a Subset of Records to Browse
- Browse Tab

Opening a Library for Browsing

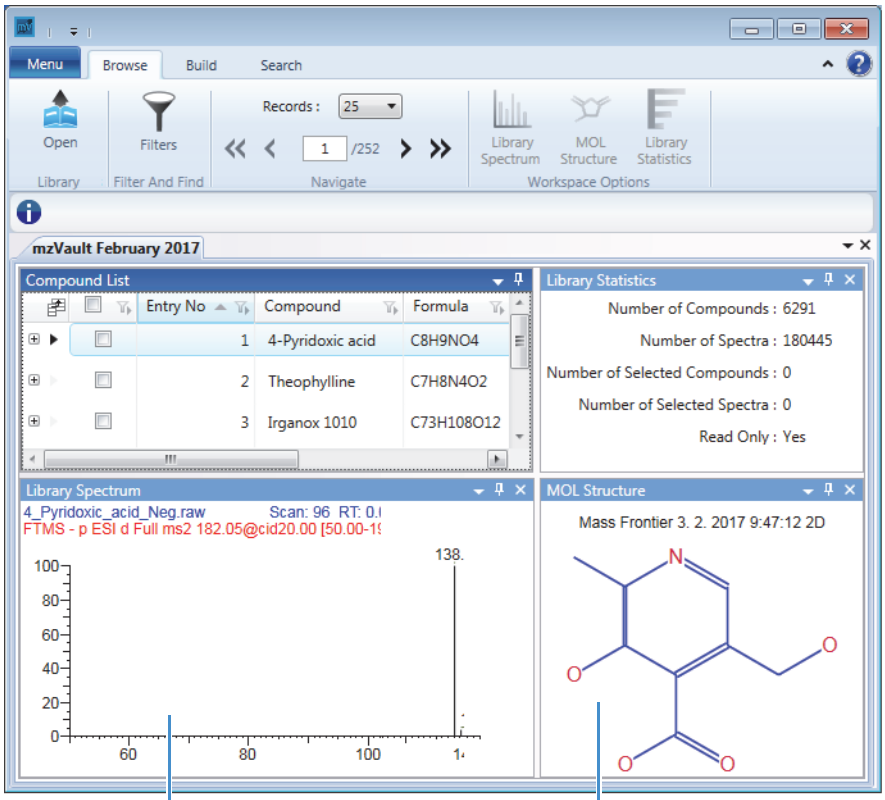
You can open an existing library and examine its records by using the Browse tab. You can open only one library at a time.

❖ **To open an existing library**

1. Click the **Browse** tab.
2. In the Browse toolbar, click **Open** and select the library.

   The tabbed *Library Name* page opens and displays the first library entry. Figure 4 shows the Browse toolbar and the tabbed page for an mzVault library named mzVaultFebruary2017.

Figure 4. *Library Name* page below the Browse toolbar



Displays the selected library spectrum. Initially, the application selects the first spectrum for the first entry.

Displays the molecular structure (MOL) file of the selected compound.

3. If any of these panes are closed—Library Spectrum, MOL Structure, or Library Statistics—open the pane by clicking its icon in the toolbar.

With the factory default layout, a *Library Name* page contains four panes. The Compound List pane is on the upper left, the Library Statistics pane is on the upper right, the Library Spectrum pane is on the lower left, and the MOL Structure pane is on the lower right. You can close the Library Statistics, Library Spectrum, and MOL Structure panes, but you cannot close the Compound List pane. For more information about page layouts, see "Opening and Modifying the Layout of Tabbed Pages" on page 12.

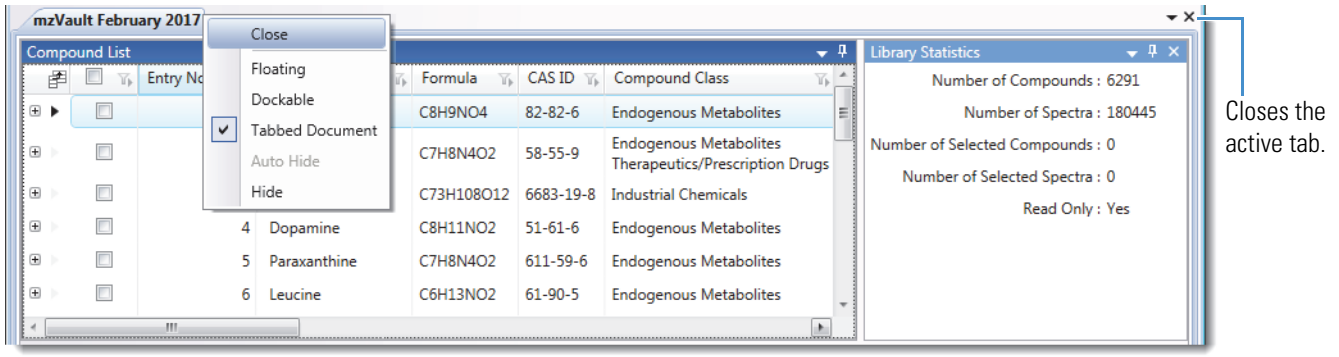
Closing a Library

After you open a *Library Name* page as a tabbed page, you can leave the library open as you open the Build, Search, or Compound List pages.

❖ **To close a single *Library Name* page**

Right-click the *Library Name* tab and choose **Close** (Figure 5). Or, select the tab if multiple tabs are available, and then click the **Close** icon, ⊠.

Figure 5. Close command and close icon



Reviewing the Library Entries

Use the Browse tab to review the records in an mzVault library.

Note To review MassBank or NIST files, you must first import their compound entries into an mzVault library.

❖ **To review the compounds of interest in an mzVault library**

1. From the application window, click the **Browse** tab.
2. In Browse toolbar, click **Open**.
3. Locate the library and click **Open**.
4. To browse a subset of the compound records, apply the appropriate filters (see "Displaying a Subset of Records to Browse" on page 18).
5. To navigate through the library pages, do the following in the Navigate area of the Browse toolbar:
   a. Select the number of data records to display on a page from the Records list. You can select to display 25 (the default), 50, 100, 500, 1000, or All records per page.
   b. To move through the pages, use the first (<<), previous (<), next (>), and last page (>>) icons. Or, to go to a specific page, type the number of the page in the box and press ENTER.
6. To review all the compound information, scroll to the right.
7. To review the scan data for a compound entry, click the expand (+) icon to the left of the entry.

Displaying a Subset of Records to Browse

By filtering, you can display a subset of the records in the Compound List pane for the library that you are browsing.

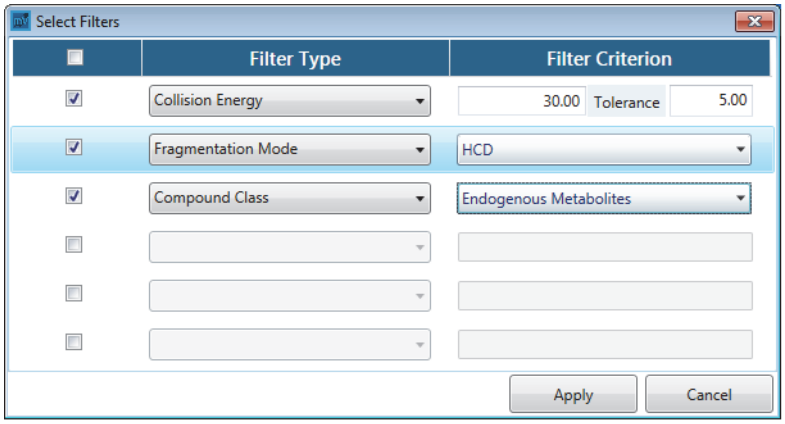
❖ To filter the library entries for browsing

1. Open the library from the Browse tab.
2. In the Browse toolbar, click **Filters**.

   The Select Filters dialog box opens.
3. For up to six filters, do the following:
   a. Select the check box on the left to make the filter selections available.
   b. Select a filter type.
   c. Set up the filter criterion for the selected filter.

   Figure 6 shows three filters.

Figure 6. Select Filters dialog box with three filters



4. Click **Apply**.

   The application applies the filters and displays only the entries that fit the filter criteria.

Table 5 describes the effect of the available filter types.

Table 5. Filters for limiting the library entries to browse (Sheet 1 of 2)

Filter Type	Effect
Collision Energy and Tolerance	Displays entries with scan data acquired at the specified collision energy within the specified tolerance. Valid entries: Numeric values > 0.00
Compound	Displays entries that contain the specified text string. Valid entries: Alphanumeric and special characters
Compound Class	Displays the entries for the selected compound class. **Note** The Compound Class list only includes compound classes found in the selected library.
Curation Type	Displays the entries that include entries with the selected type of curated spectra. **Note** The Curation Type list only includes the curation types in the selected library.
Formula	Displays the entries that include the specified formula or partial formula. Valid entries: Alphanumeric and special characters.
Fragmentation Mode	Displays the entries that include scan data for the specified fragmentation mode. **Note** The Fragmentation Mode list only includes the fragmentation modes in the selected library.
Peptide Sequence	Displays the entries that include the specified peptide sequence.
Precursor m/z and Tolerance	Displays the entries that include scans for the specified precursor *m/z* value within the specified tolerance. • Valid entries for m/z value: Numeric values > 10.0000 • Valid entries for tolerance: 5 ppm, 5 mmu, or 0.05 amu (default); range: 0.0001 to 1000
Precursor Mass Range	Displays the entries that include scans for the specified range of precursor *m/z* values. Valid entries: $m/z_{(max)} - m/z_{(min)} > 0.1$ amu
Retention Time	Displays the entries that include scans for the specified retention time within a tolerance of 0.05 min. Valid entries: Positive numeric values

Table 5. Filters for limiting the library entries to browse (Sheet 2 of 2)

Filter Type	Effect
Retention Time Range	Displays the entries that include scans for the specified retention time range. Valid entries: $RT_{(max)} - RT_{(min)} > 0.1$
Scan Filter	Displays the entries that include scans for the specified scan filter. Valid entries: All or part of a valid scan filter

Browse Tab

These topics describe the parameters in the Browse toolbar and the panes on the tabbed library page:

- Browse Toolbar
- Library Page Panes

Browse Toolbar

The Browse toolbar (Figure 7) contains options for browsing a library's records.

Figure 7. Browse toolbar

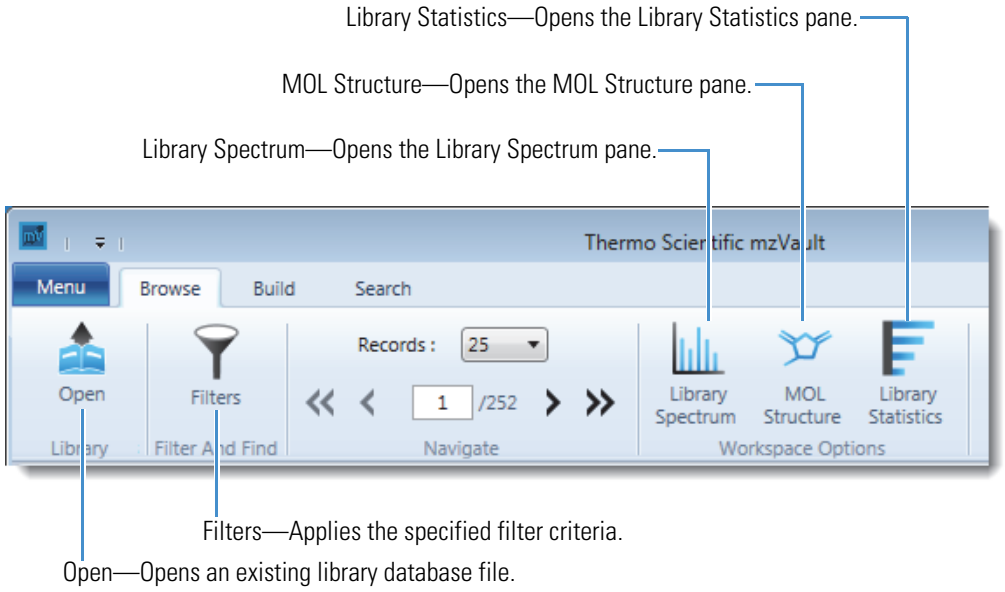


Table 6 describes the parameters in the Browse toolbar.

Table 6. Browse toolbar parameter descriptions

Button/Icon/Pane	Description
Library	
Open	Opens the Open dialog box for selecting a library file.
Filter and Find	
Filters	Opens the Select Filters dialog box where you can select up to six filters.
Navigate	
Records	Specifies the number of records displayed at a time. Default: 25; selections: 25, 50, 100, 500, 1000, or All
<< (First Page)	Displays the first page of the data records table.
< (Previous)	Displays the previous page of the data records table.
> (Next)	Displays the next page of the data records table.
>> (Last)	Displays the last page of the data records table.
Workspace Options	
Library Spectrum	Displays the Library Spectrum pane along the bottom of the *Library Name* page.
MOL Structure	Displays the MOL Structure pane in the bottom right corner of the *Library Name* page.
Library Statistics	Displays the Library Statistics pane on the right side of the *Library Name* page.

Library Page Panes

Table 7 describes the panes on the tabbed *Library Name* page.

Table 7. *Library Name* page panes (Sheet 1 of 2)

Pane	Description
Compound List pane	See "Compound List Pane of a Library Page" on page 49.
	Note The compound information is read-only from the Build tab and editable from the Browse tab.
Library Spectrum pane	Displays the spectrum selected in the Compound List pane.

Table 7. *Library Name* page panes (Sheet 2 of 2)

Pane	Description
Library Statistics pane	Displays the number of compounds in the loaded library, the number of spectra, the number of selected compounds, the number of selected spectra, and whether the library is read-only.
MOL Structure pane	Displays the molecular structure file for the compound selected in the Compound List pane. It displays the molecular structure file containing the Kekulé diagram of the selected compound if the library record contains the necessary MOL data.

4

Building and Editing Libraries

To create and edit libraries in the mzVault application, see these topics.

Contents

- Build Workflow Overview
- Opening a Library for Editing
- Importing NIST or MassBank Records into an mzVault Library
- Merging mzVault Libraries
- Deleting Compound Records or Spectra from a Library
- Adding Individual Records to a Library
- Creating, Saving, and Opening Compound List Files
- Adding Multiple Records to a Library by Processing a Compound List
- Exporting Compounds or Spectra from a Library to a CSV File
- Copying a Record or a Compound in a Compound List
- Saving a Library
- Build Tab
- Compound Tab
- Compound List Pane of a Library Page
- Compound List Tab

Build Workflow Overview

To modify an editable mzVault library, you can add or delete compounds, add or delete spectra, import compounds from NIST or MassBank files, or merge it with other mzVault libraries.

To open an editable mzVault library for editing, follow any of these topics:

- Opening a Library for Editing
- Importing NIST or MassBank Records into an mzVault Library
- Merging mzVault Libraries

To add records to an editable mzVault library, follow any of these topics:

- Importing NIST or MassBank Records into an mzVault Library
- Merging mzVault Libraries
- Adding Individual Records to a Library
- Adding Multiple Records to a Library by Processing a Compound List

To delete compound entries or only their associated spectra from an editable library, follow these topics:

- Deleting Compound Records from a Library
- Deleting Spectra from a Library

Opening a Library for Editing

To open a new library or an existing library from the Build tab, see these topics:

- Opening a New Library for Editing
- Opening an Existing Library for Editing

Opening a New Library for Editing

You can open a new library from the Build tab.

❖ **To open a new library for editing**

1. Click the **Build** tab.
2. In the Select Libraries area, click **New**.

3. In the New Library dialog box, name the library file, select its directory folder, and click **Save**.

   The new library opens as a tabbed page below the toolbar. The library's compound list is empty.

Opening an Existing Library for Editing

You can open a library for browsing, and then click the Build tab. Or, you can open the library from the Build tab.

❖ **To open an existing library for editing from the Build tab**

1. Click the **Build** tab.
2. In the Select Libraries area, click **New**.
3. In the New Library dialog box, select a library and click **Save**.
4. At the prompt, click **Yes**.

   The library opens as a tabbed page below the toolbar.
5. If the library has restricted access ( ), unlock it (see "Unlocking a Restricted Library for Editing" on page 83).

Importing NIST or MassBank Records into an mzVault Library

You can import NIST or MassBank records into an mzVault Library that is open for editing or an unopened mzVault library that is not password-secured.

For information about opening a library for editing, see "Build Workflow Overview" on page 24).

❖ **To import NIST or MassBank records into an mzVault Library**

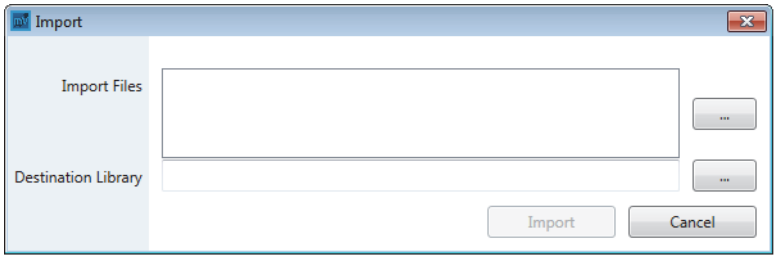
1. Open a library for editing.
2. In the toolbar, click **Import**.
3. In the Open dialog box, select the file type to import (TXT for MassBank or MSP for NIST), locate the files, and click **Open**.

–or–

1. Click the **Build** tab, but do not open a library.
2. In the toolbar, click **Import**.

   The Import dialog box opens (Figure 8).

Figure 8. Import dialog box



3. Click the browse icon next to Import Files. Then, select the file type (TXT for MassBank or MSP for NIST), locate the files to import, and click **Open**.
4. Click the browse icon next to Destination Library. Then, locate an mzVault destination library that is not password-secured and click **Import**.

   The selected destination library opens as a tabbed page below the toolbar.

Merging mzVault Libraries

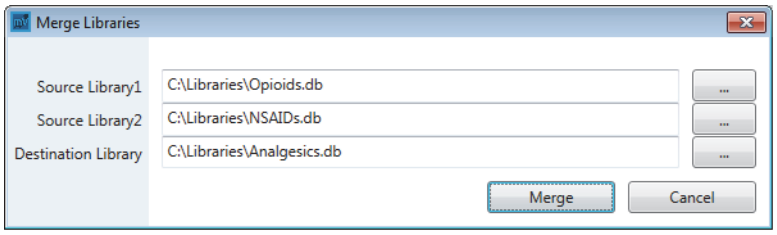
You can merge two editable mzVault libraries into a third editable mzVault library.

❖ To merge mzVault libraries

1. Click the **Build** tab.
2. In the toolbar, click **Merge**.

   The Merge Libraries dialog box opens (Figure 9).

   Figure 9. Merge Libraries dialog box



3. Do the following:
   a. Locate the source libraries.
   b. Locate the destination library or type a new file name in the Open dialog box.

      Note You must select two source libraries and a destination library. The source libraries must be existing libraries. The destination library, existing or new, must have a different name than the source libraries.

   c. Click **Merge**.

      The destination library opens as tabbed page below the toolbar.

Deleting Compound Records or Spectra from a Library

You can delete compound records or individual spectra from an editable library.

Follow these topics as needed:

- Deleting Compound Records from a Library
- Deleting Spectra from a Library

Deleting Compound Records from a Library

After you open a library and unlock it if it is read-only, you can delete compound records.

❖ **To delete compound records from a library**

1. Open a library for editing (see "Build Workflow Overview" on page 24).
2. Select the check boxes to the left of the compounds that you want to delete.
3. In the Build toolbar, click **Delete**.

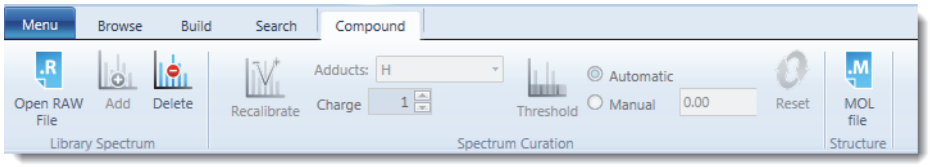
   The Delete Records from Library dialog box opens.
4. Confirm the compounds to delete. Clear the check boxes for any compounds that you want to retain.
5. Click **OK**.
6. To save the modified library, click **Save** in the toolbar.

Deleting Spectra from a Library

You can delete individual spectra from the compound entries in a library.

❖ **To delete spectra**

1. Open a library for editing (see "Build Workflow Overview" on page 24).
2. Click the expand icon (**+**) to the left of each compound where you want to delete spectra.
3. Select the check box for each spectrum that you want to delete.
4. Click the **Compound** tab.
5. In the Compound toolbar, click **Delete**.

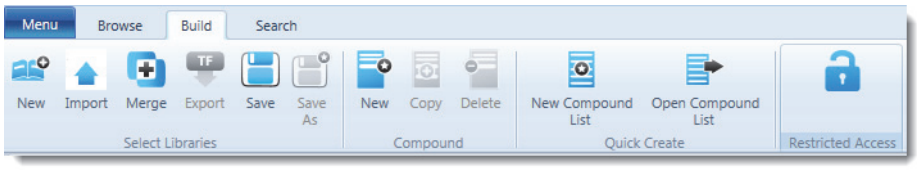


The Delete Records from Library dialog box opens and displays the spectra for each compound where you selected at least one spectrum for deletion.

6. Verify the selections, and then click **OK**.

Note If you delete all the spectra associated with a compound, the application deletes the compound from the library.

7. To save the changes, click the **Build** tab, and click **Save** in the toolbar.



Adding Individual Records to a Library

You can add a new compound to a library from the Build tab, and then add spectra and a MOL structure to the compound entry from the Compound tab.

Follow these topics in order:

1. Manually Adding a New Compound to a Library
2. Manually Adding Spectra and a Structure to a Compound Entry

Manually Adding a New Compound to a Library

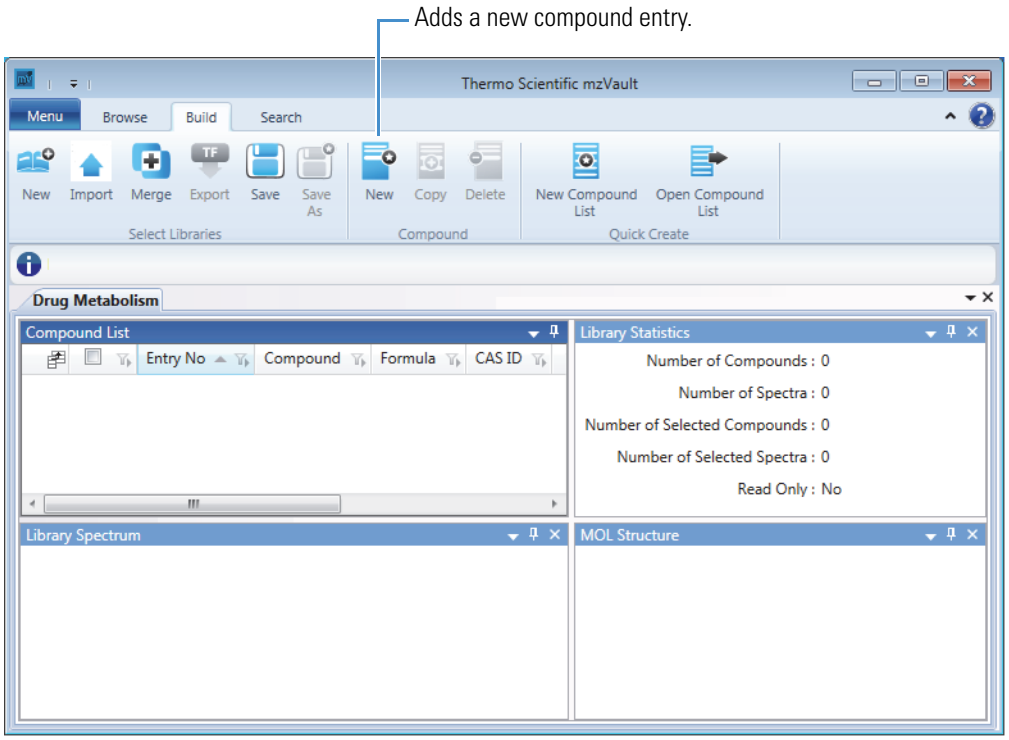
You can add compounds individually to a library with read/write privileges.

❖ To add a new compound to a library

1. Create a new library or open an existing library for editing (see "Opening a Library for Editing" on page 24).

   Figure 10 shows a new library.

Figure 10. New library



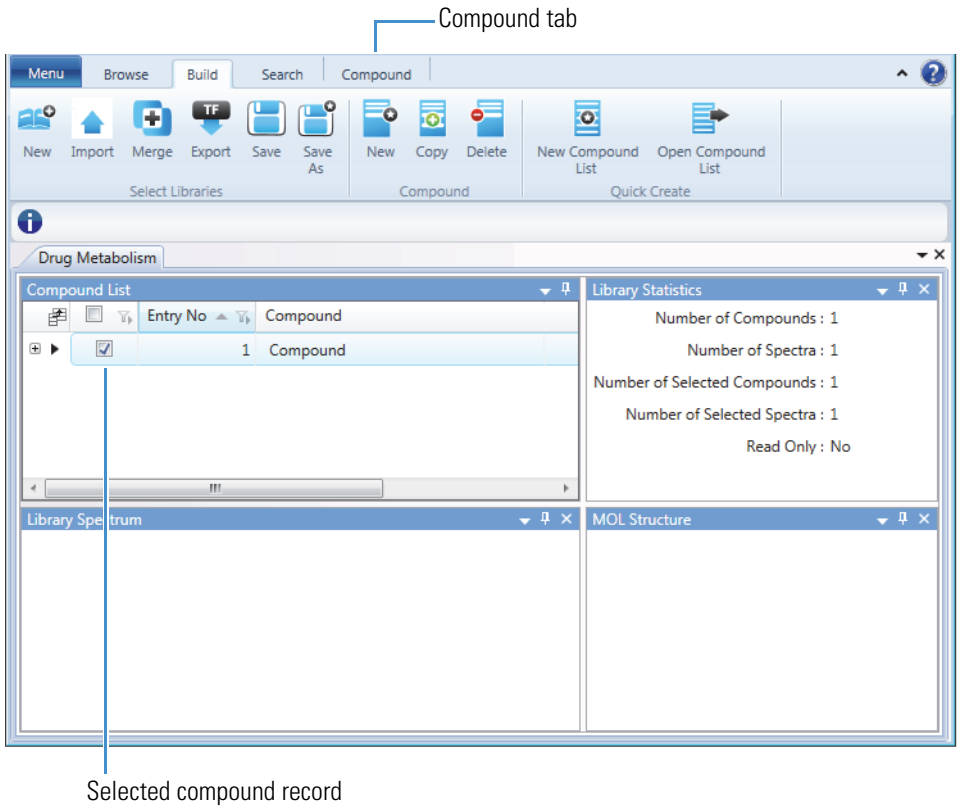
2. In the Compound area of the Build toolbar, click **New**.

   The application adds a record to the table in the Compound List pane. It also selects the record's check box, which adds the Compound tab to the tab bar (Figure 11). The application uses "Compound" as a placeholder for the compound name.

   Note To add compounds with similar features, use the Copy button (see "Copying a Record or a Compound in a Compound List" on page 44).

   Except for the Entry No column, you can edit all of the table cells. To access all of the table cells, scroll to the right.

Figure 11. New record added to a library



Note In the following steps, scroll right if a column is not visible.

3. To enter information in a table cell, double-click the cell, and then type or paste the appropriate text.

   For a chemical formula, use each element's symbol in the periodic table and its count. For example, for caffeine, enter C8H10N4O2. For details about each column, see "Compound List Pane of a Library Page" on page 49.

4. To save changes to the library, click **Save** in the Build toolbar.

To add spectra to the new compound entry, go to step 1c in the next procedure "Manually Adding Spectra and a Structure to a Compound Entry."

Manually Adding Spectra and a Structure to a Compound Entry

Use the Compound tab to manually add spectra and a MOL structure to a compound entry.

Follow these topics as needed:

- Manually Adding a Spectrum to a Compound Entry
- Creating an Averaged Spectrum
- Adding a MOL Structure to a Compound Entry

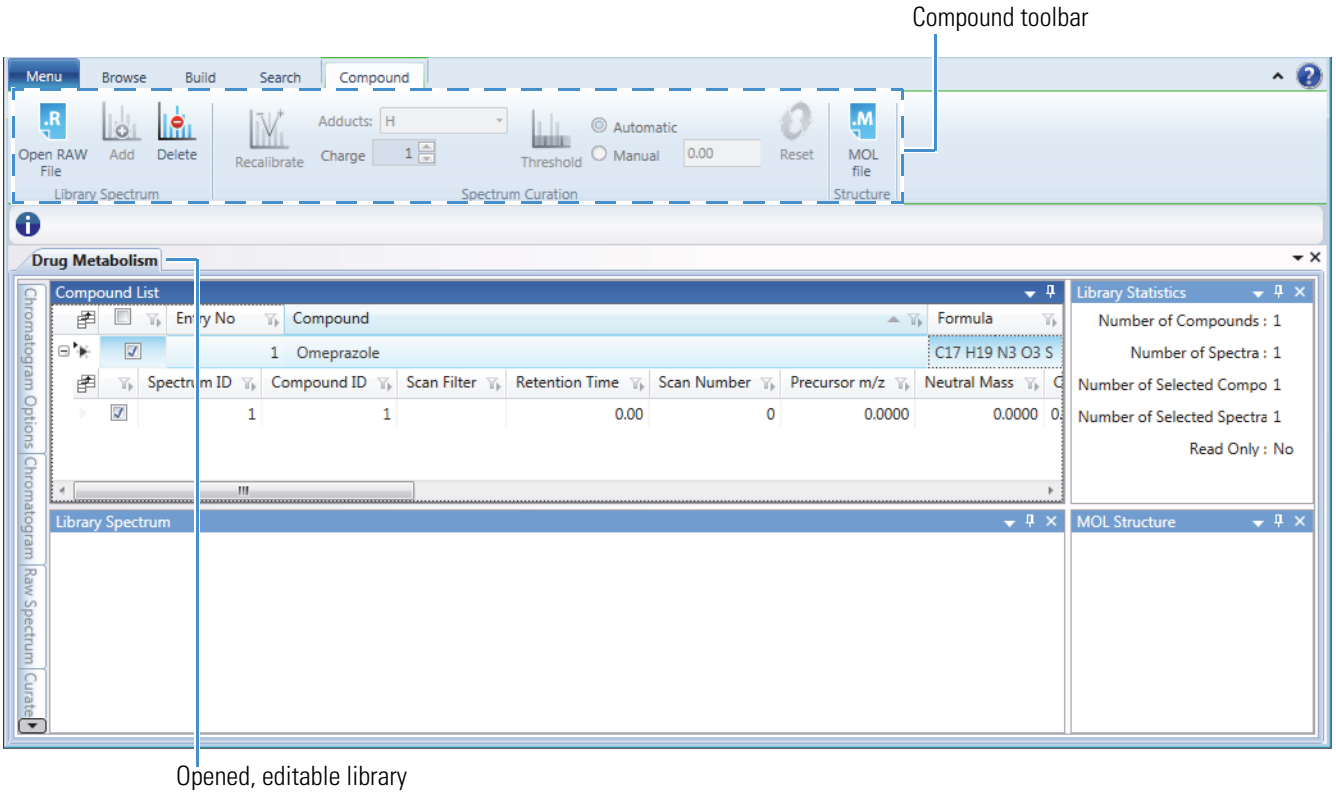
Manually Adding a Spectrum to a Compound Entry

❖ To add a spectrum to a compound record

1. If the Compound tab is not active, make it active as follows:
   a. If the library of interest is not open, open it for editing (see "Build Workflow Overview" on page 24).
   b. Select the check box to the left of the compound of interest.

      The Compound tab appears in the tab bar.
   c. To display the Compound toolbar (Figure 12), click the **Compound** tab.

Figure 12. Compound toolbar and tabbed library page



2. In the Compound toolbar, click **Open Raw File**, browse to the location of the raw data file containing the spectrum you want to add to the compound, and click **Open**.

   The Chromatogram Options, Chromatogram, Raw Spectrum, and Curated Spectrum panes appear below the Compound List pane.

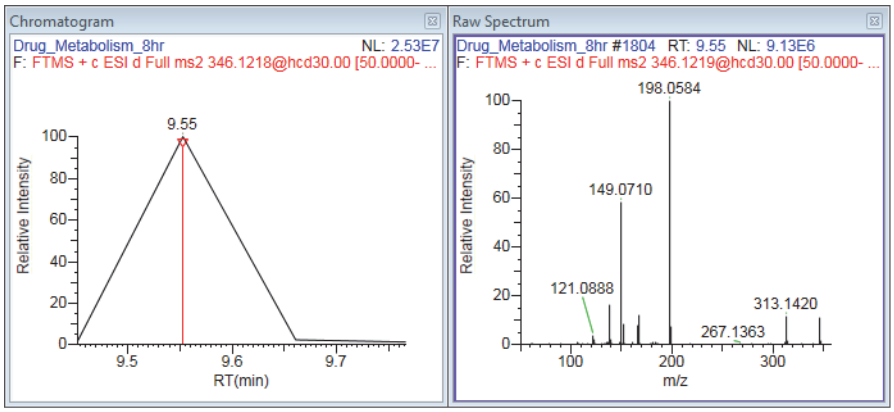
3. In the Chromatogram Options pane, make the appropriate selections and entries to display the filtered chromatogram of interest in the Chromatogram pane.

4. Select the spectrum as follows:

   - To select the spectrum for a single time point, click the time point in the Chromatogram pane.

     The selected spectrum appears in the Raw Spectrum pane (Figure 13).

     Figure 13. Spectrum from a single time point

   - To select an averaged spectrum, go to "Creating an Averaged Spectrum" on page 34.

IMPORTANT The curation order makes a difference when applying a manual threshold level to a thresholded and recalibrated spectrum. To retain the manual threshold level, recalibrate the spectrum first, and then apply the manual threshold level.

5. (Optional) To recalibrate a single spectrum, do the following:

   a. Verify the chemical formula in the Formula column of the compound entry.

   b. In the Compound toolbar, modify the adduct selection and charge, if necessary. Then, click **Recalibrate**.

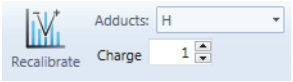
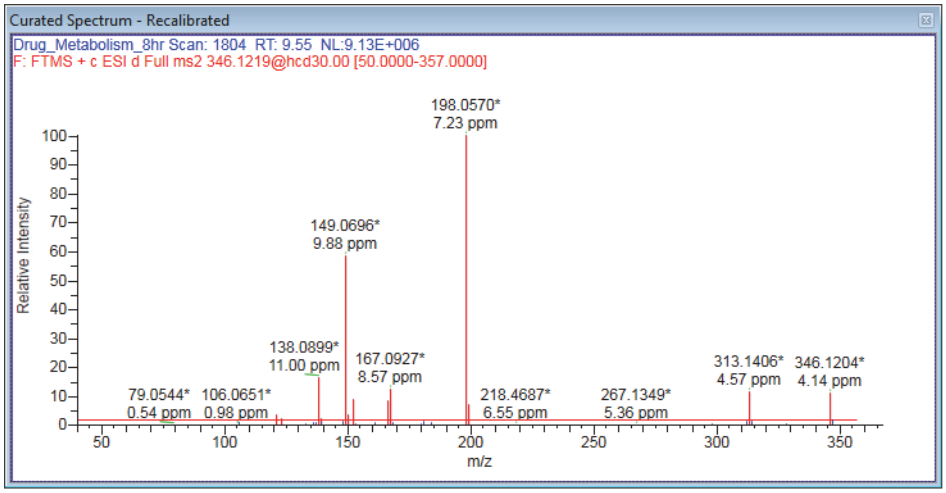
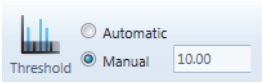
   

   Figure 14 shows a recalibrated spectrum.

Figure 14. Recalibrated spectrum



6. (Optional) To threshold a spectrum, do the following in the Compound toolbar:
   a. Select the **Automatic** option or the **Manual** option.
   b. If you select the Manual option, enter an intensity level from **0** to **100**% of the base peak intensity.

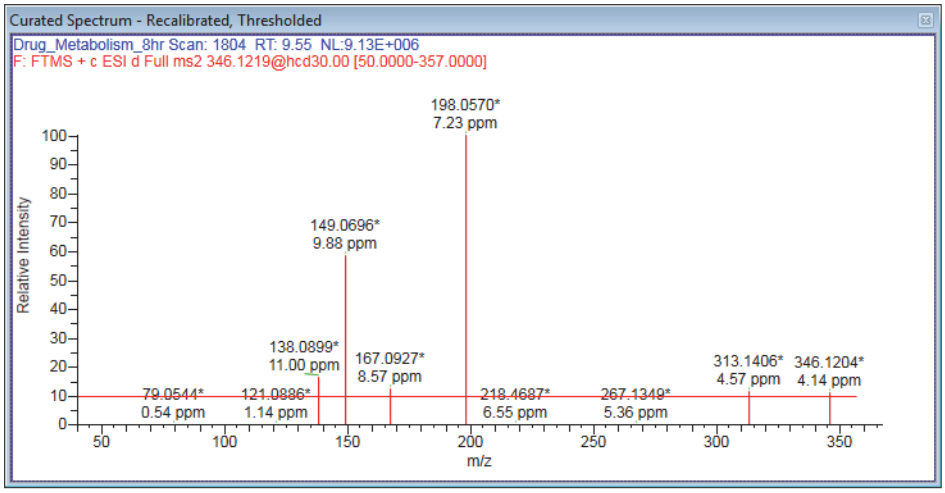


   c. Click **Threshold**.

      The application removes the mass peaks with intensities below the specified threshold.

Figure 15 shows a recalibrated and manually thresholded spectrum.

Figure 15. Recalibrated and manually thresholded spectrum

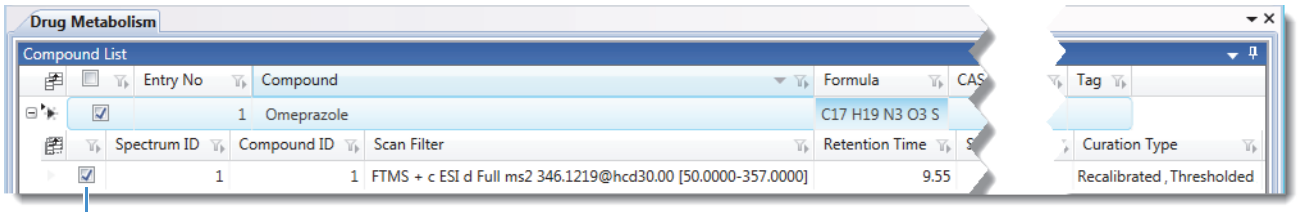


Tip To undo the curation, click **Reset**.

7. To add the spectrum of interest to the compound entry, do the following:
   a. Click the Raw Spectrum pane or the Curated Spectrum pane to make it active.
   b. In the Compound toolbar, click **Add**.

   The application adds a new data record containing the currently selected mass spectrum to the list of existing spectral data records of the selected compound and assigns it a number in the Spectrum ID column (Figure 16).

Figure 16. New spectrum added to a compound



Creating an Averaged Spectrum

To minimize the effect of "spectral tilting," which can occur when the amount of an analyte entering the mass spectrometer changes during a scan, create an averaged spectrum.

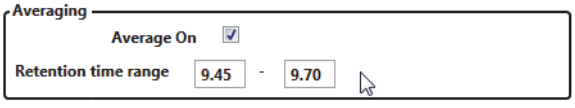
Note To create an averaged spectrum, the application averages scans with similar scan filters across the selected time range. If you do not select a scan filter, the application uses the scan filter for the highest-intensity scan across the selected time range.

❖ To create an averaged spectrum

1. Open a library for editing and select the compound that you want to edit. Then, from the Compound tab, open a raw data file and select the chromatogram of interest (see step 1 through step 3 of the previous procedure "Manually Adding a Spectrum to a Compound Entry" on page 31).
2. In the Chromatogram Options pane, select the **Average On** check box.
3. To select the time range to average, do one of the following:
   - In the Chromatogram pane, drag the pointer horizontally across the time range of interest.

   –or–

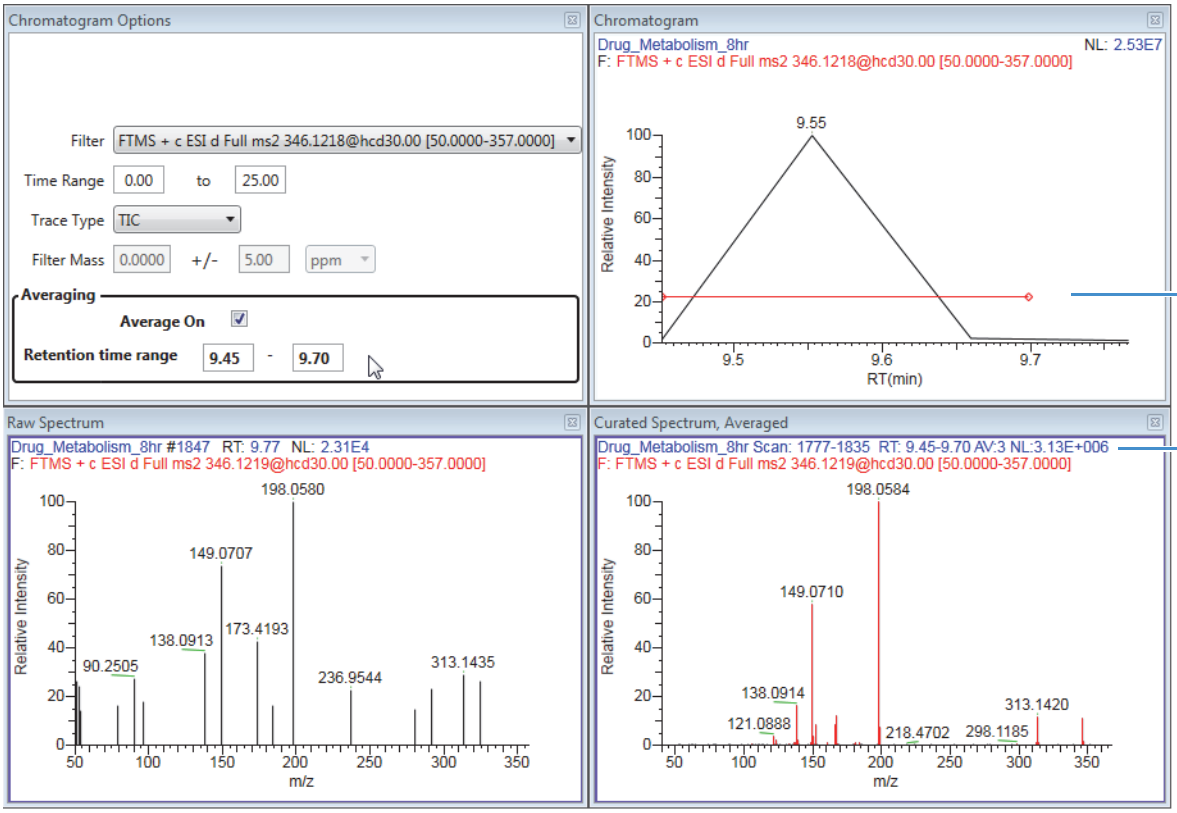
   - In the Chromatogram Options pane, type the start and end times in the Retention Time Range boxes. Then, click outside the time boxes or press the ENTER key to activate averaging.



In the Chromatogram pane, a horizontal red line with start and end markers indicates the time range to average.

Figure 17 shows the creation of an averaged spectrum for the time range of 9.45 to 9.70 min in a filtered chromatogram.

Figure 17. Creating an averaged spectrum



To threshold the spectrum and add it to the compound entry, go to step 6 of the previous procedure "Manually Adding a Spectrum to a Compound Entry" on page 31.

Note The application does not currently support recalibrating an averaged spectrum.

Adding a MOL Structure to a Compound Entry

Use the Compound tab to add a MOL structure to a compound entry. You do not need to open a raw data file to add a MOL structure.

❖ To add a MOL structure to a compound entry

1. Open a library for editing (see "Build Workflow Overview" on page 24).

2. Display the Compound toolbar (see "Displaying the Compound Tab and Its Toolbar" on page 11).
3. In the Compound List table, select the check box for the compound that you want to edit.
4. In the Compound toolbar, click **MOL File**.
5. In the Open dialog box, select the MOL file for the selected compound and click **Open**.
6. Save the modified library (see "Saving a Library" on page 45).

Creating, Saving, and Opening Compound List Files

Follow these topics to create, save, and open compound list (XML) files:

- Creating a Compound List
- Specifying a Compound's Formula and Precursor Mass
- Saving a Compound List as an XML File
- Opening a Compound List File

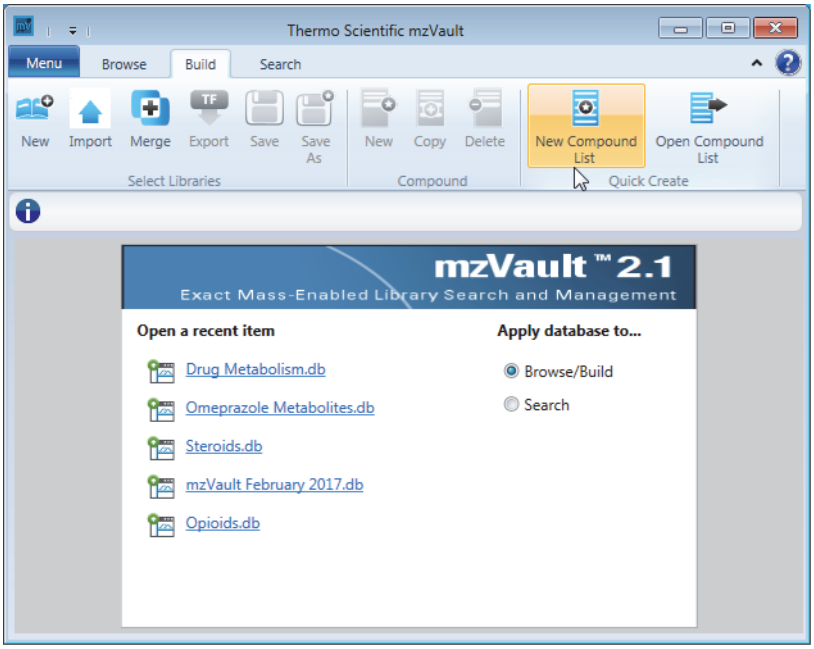
Creating a Compound List

The following procedure describes how to add compounds to a compound list and enter the compound information for each entry.

❖ To create a compound list

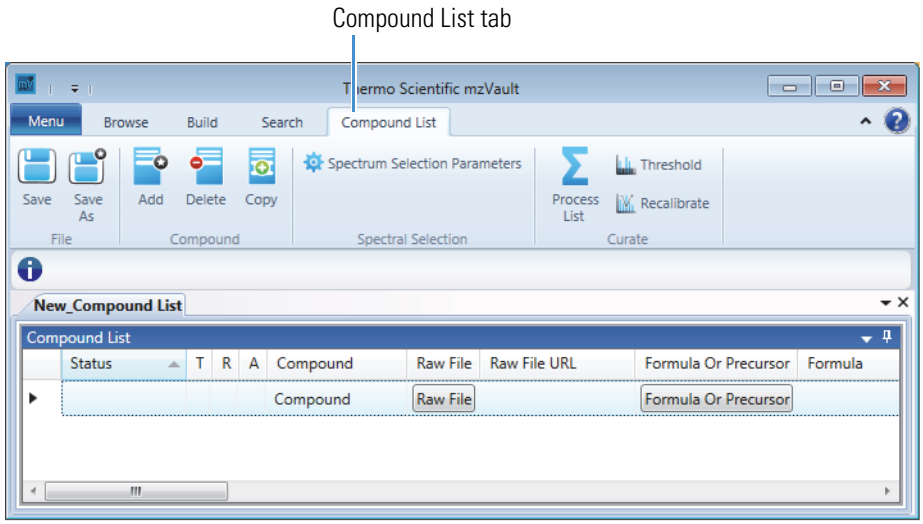
1. Click the **Build** tab.
2. In the toolbar, click **New Compound List** (Figure 18).

Figure 18. Build toolbar with New Compound List button



The New_Compound List page opens on the Compound List page, and a placeholder compound appears in the compound list (Figure 19).

Figure 19. New Compound list on the Compound List page



Note In the following steps, scroll right if a column is not visible.

3. For each compound that you want to add, do one of the following in the Compound List toolbar:

   - Click **Add** for each additional entry.
   - Click **Copy** for each additional entry that is similar to the currently selected entry.

4. Edit each entry as follows:

   a. In the Compound column, double-click the **Compound** or **Compound_Copy** placeholder name and type the name of the compound that you want to add.

   > **Note** After you enter data into any columns that do not contain a button in the following steps, press ENTER or click outside the table cell.

   b. To select the raw data file that contains spectral data for the compound, in the Raw File column, click **Raw File**. Then, in the Open dialog box, select the appropriate raw data file and click **Open**.

   The path and name of the raw data file appear in the Raw File URL column.

   c. To set up the entry's precursor *m/z* value, chemical formula, or both, in the Formula Or Precursor column, follow the instructions in the next topic "Specifying a Compound's Formula and Precursor Mass."

   > **IMPORTANT** To add recalibrated spectra to the compound list, you must enter a formula for the compound entry. This formula and the adduct ion information determine the precursor *m/z* value for the entry.

   d. In the Polarity column, select a polarity.

   e. (Optional) In the MOL File column, click **MOL File**. Then, in the Open dialog box, locate a MOL file and click **Open**.

   The path and name of the MOL file appear in the MOL File URL column.

   For details about the remaining optional text entries, see "Compound List Tab" on page 51.

5. (Optional) To save the compound list for later use, go to the next topic "Saving a Compound List as an XML File."

Specifying a Compound's Formula and Precursor Mass

When you set up the information for a compound in a compound list (XML) file, you use the Processing Parameters dialog box to set up these two processing parameters:

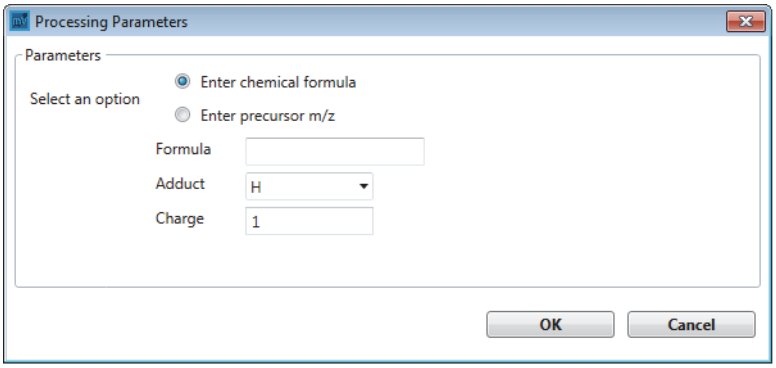
- The precursor *m/z* value for extracting spectra from the raw data
- (Optional) The chemical formula for recalibrating the extracted spectra

❖ To specify the precursor *m/z* value for a compound

1. If you have not already opened a compound list file for editing, open one from the Build toolbar (see the previous topic "Creating a Compound List" on page 36).
2. In the Compound List table, click **Formula or Precursor** in the Formula or Precursor column for a compound.

The Processing Parameters dialog box opens (Figure 20).

Figure 20. Processing Parameters dialog box with the default selections



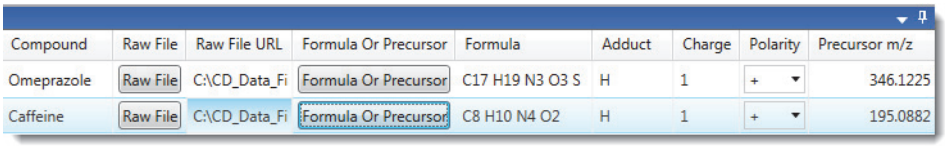
3. To specify the precursor *m/z* value, do one of the following:

   a. To enter a chemical formula, select the **Enter Chemical Formula** option.

   b. Type the chemical formula in the Formula box, select the adduct ion from the Adduct list, and type the ion's charge in the Charge box.

   c. Click **OK**.

   In the Compound List table, the chemical formula appears in the Formula column, and the calculated precursor *m/z* value appears in the Precursor m/z column. If you select the Recalibrate option when you process the compound list, the application uses the chemical formula.



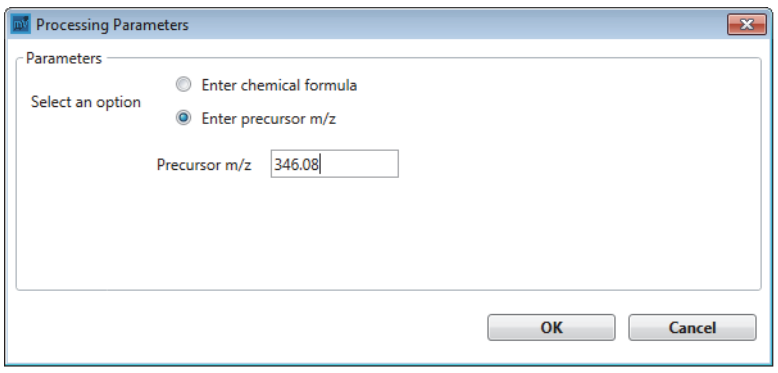
Compound	Raw File	Raw File URL	Formula Or Precursor	Formula	Adduct	Charge	Polarity	Precursor m/z
Omeprazole	Raw File	C:\CD_Data_Fi	Formula Or Precursor	C17 H19 N3 O3 S	H	1	+	346.1225
Caffeine	Raw File	C:\CD_Data_Fi	Formula Or Precursor	C8 H10 N4 O2	H	1	+	195.0882

–or–

   a. To enter a precursor *m/z* value, select the **Enter Precursor m/z** option.

   b. Type the precursor *m/z* value in the Precursor m/z box (Figure 21).

Figure 21. Processing Parameters dialog box with the Enter Precursor m/z option selected



c. Click **OK**.

The precursor *m/z* value appears in the Precursor m/z column.

Saving a Compound List as an XML File

You can save the compound list on the New_Compound List page for later use.

1. Create a compound list (see "Creating a Compound List" on page 36).
2. To save the new compound list as an XML file, click **Save** in the Compound List toolbar.
3. In the Save As dialog box, name the file, select its directory folder, and click **Save**.

Note You cannot save a compound list until you select a raw data file for each entry.

Opening a Compound List File

You can open a saved compound list (XML file) to view it or edit it.

❖ **To open a compound list**

1. Click the **Build** tab.
2. In the toolbar, click **Open Compound List**.
3. Locate the XML file and click **Open**.

Adding Multiple Records to a Library by Processing a Compound List

You can create a list of compounds that you can then process and add to a library. You must manually enter each compound name and the information pertaining to it, but the mzVault application automatically adds the specified spectra to each compound entry and the new compound entries to an open mzVault library.

To add records to an mzVault library by processing a compound list, follow these steps:

1. Setting Up the Spectrum Selection Parameters
2. Processing a Compound List

Setting Up the Spectrum Selection Parameters

For processing a compound, the application uses the parameters that you set up in the Spectrum Selection Parameters dialog box.

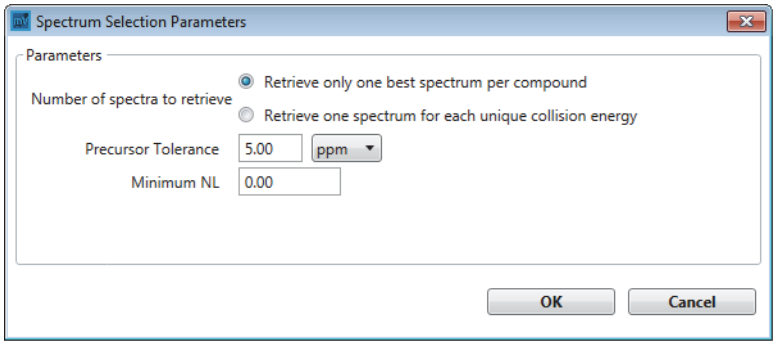
❖ To set up the spectrum selection parameters

1. Create a compound list and add the compounds of interest (see "Creating, Saving, and Opening Compound List Files" on page 36).
2. If you saved and closed the compound list, open it (see "Opening a Compound List File" on page 40).

   Opening a compound list opens the Compound List page.
3. In the Compound List toolbar, click **Spectrum Selection Parameters**.

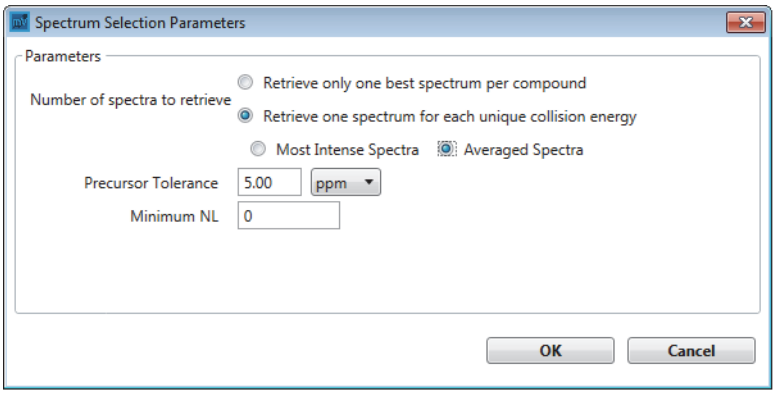
   The Spectrum Selection Parameters dialog box opens (Figure 22).

   Figure 22. Spectrum Selection Parameters dialog box with the default settings



4. Select the number of spectra to retrieve as follows:
   - To retrieve one best spectrum per compound, select the **Retrieve Only One Best Spectrum Per Compound** option.
   - To retrieve the most intense spectrum for each unique collision energy, select the **Retrieve One Spectrum for Each Unique Collision Energy** option. Then, select the **Most Intense Spectra** option.
   - To retrieve an averaged spectrum for each unique collision energy, select the **Retrieve One Spectrum for Each Unique Collision Energy** option. Then, select the **Averaged Spectra** option (Figure 23).

Figure 23. Spectrum Selection Parameters dialog box with the Averaged Spectra option selected



5. To set up the tolerance for the precursor *m/z* value, select the units, and then type a value in the Precursor Tolerance box.
6. (Optional) In the Minimum NL box, type an appropriate intensity threshold—for example, the noise level recorded in the raw data file—for the selected spectra.

   The application ignores spectra with NL values below this threshold and does not retrieve them.

   Note The Minimum NL box accepts entries in standard form or scientific notation.

7. Click **OK**.

Processing a Compound List

You can automatically add compound entries to an mzVault library by processing a compound list.

❖ To process a compound list

1. Open a library for editing (see "Build Workflow Overview" on page 24).
2. Create a new compound list or open an existing compound list (see "Opening a Compound List File" on page 40).

   Note Opening an existing or creating a new compound list opens the Compound List tab.

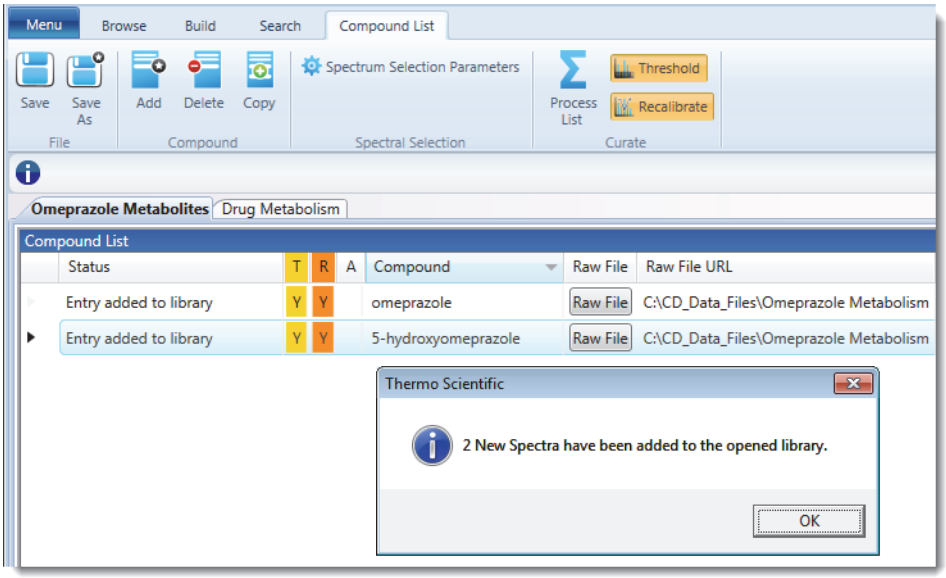
3. (Optional) To curate the spectra, do one or both of the following:
   - To remove noise peaks, click **Threshold**.
   - To recalibrate the spectra, click **Recalibrate**.

4. Click **Process List**.

   The application searches for the spectra in the raw data files, and adds the compound entries and their found spectra to the library. When processing finishes, a confirmation message appears.

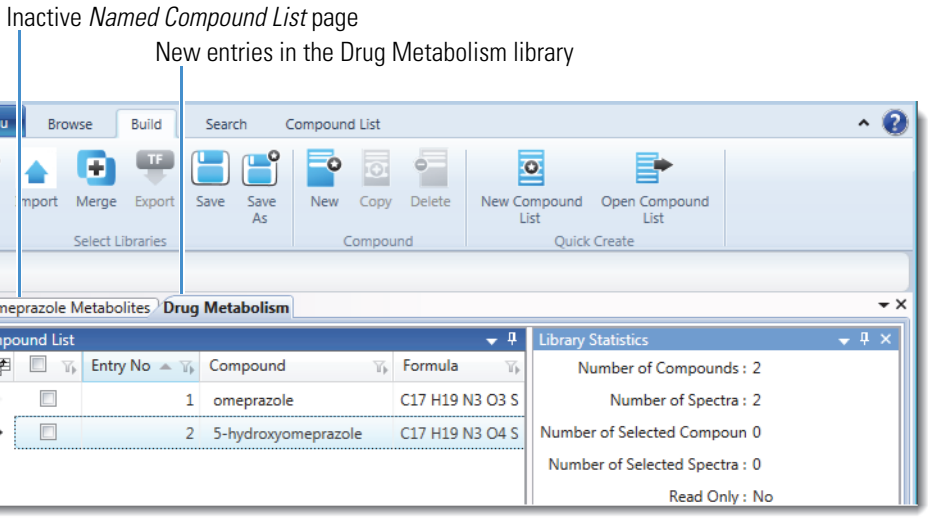
   Figure 24 shows a processed compound list and the confirmation message.

   Figure 24. Compound List page with an open library and a named compound list



5. Click **OK**.
6. (Optional) Click the **Save** icon or the **Save As** icon to save the compound list.
7. Click the **Build** tab and review the newly added compound entries (Figure 25).

   Figure 25. Drug Metabolism library with two compounds



8. Click **Save** to save the changes to the library.

Exporting Compounds or Spectra from a Library to a CSV File

You can export compounds or spectra from a library to a comma-separated values (CSV) file for importing into the TraceFinder application.

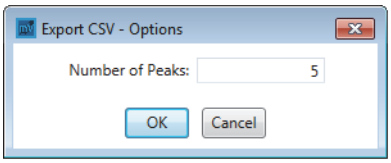
❖ **To export compound or spectra from a library to a CSV file**

1. Click the **Build** tab.
2. Select the check boxes to the left of the compounds or spectra that you want to export.

   The Export button becomes available.
3. Click **Export**.
4. In the Save As dialog box, select a file directory, name the file, and click **Save**.

   The Export CSV - Options dialog box opens (Figure 26).

   Figure 26. Export CSV - Options dialog box

5. Type the number of peaks that will be exported to the CSV file.

   Valid range: 1–10; default: 5
6. Click **OK**.

   The application saves the selected entries in a file with a .csv suffix.

Copying a Record or a Compound in a Compound List

You can copy a selected data record in an editable library or the currently selected row in a compound list (XML) file. You can then alter some or all of the information in the copied record or row.

Follows these topics as needed:

- Copying a Record in an Editable Library
- Copying a Compound in a Compound List File

Copying a Record in an Editable Library

❖ **To copy a data record in an editable library**

1. Click the **Build** tab.
2. If the library is restricted, unlock it (see "Unlocking a Restricted Library for Editing" on page 83).
3. Select the check box to the left of the compound that you want to copy.
4. In the Build toolbar, click **Copy**.

   The application adds a copy of the data record to the end of the table of data records, assigns it the next available entry number, and appends "_Copy" to the name.

Copying a Compound in a Compound List File

❖ **To copy a row in the Compound List pane of a compound list file**

1. Open the compound list (XML file).
2. Select a row in the Compound List pane.
3. In the Compound List toolbar, click **Copy**.

   The application adds a copy of the row to the end of the table and appends "_Copy" to the name.

Saving a Library

Use the Build tab to save a modified library under its current name or a new name.

❖ **To save a modified library**

1. Click the **Build** tab.
2. To retain the same name for a library or rename it, click **Save** or **Save As**, respectively.

Build Tab

The Build tab is made up of the Build toolbar and the opened, editable library. For information about the library page that opens below the toolbar, see "Library Page Panes" on page 21.

Use the Build toolbar to create a new library, open an existing library, merge libraries, import files into an existing library, open a new or existing compound list, or add compounds to or delete compounds from a library.

Note When you open a library file from the Build tab, it opens as a tabbed page below the toolbar. You can add compounds, edit the compound information, and delete compounds from the Build tab, but you cannot add spectra or MOL files from this tab.

This figure shows the Build toolbar.

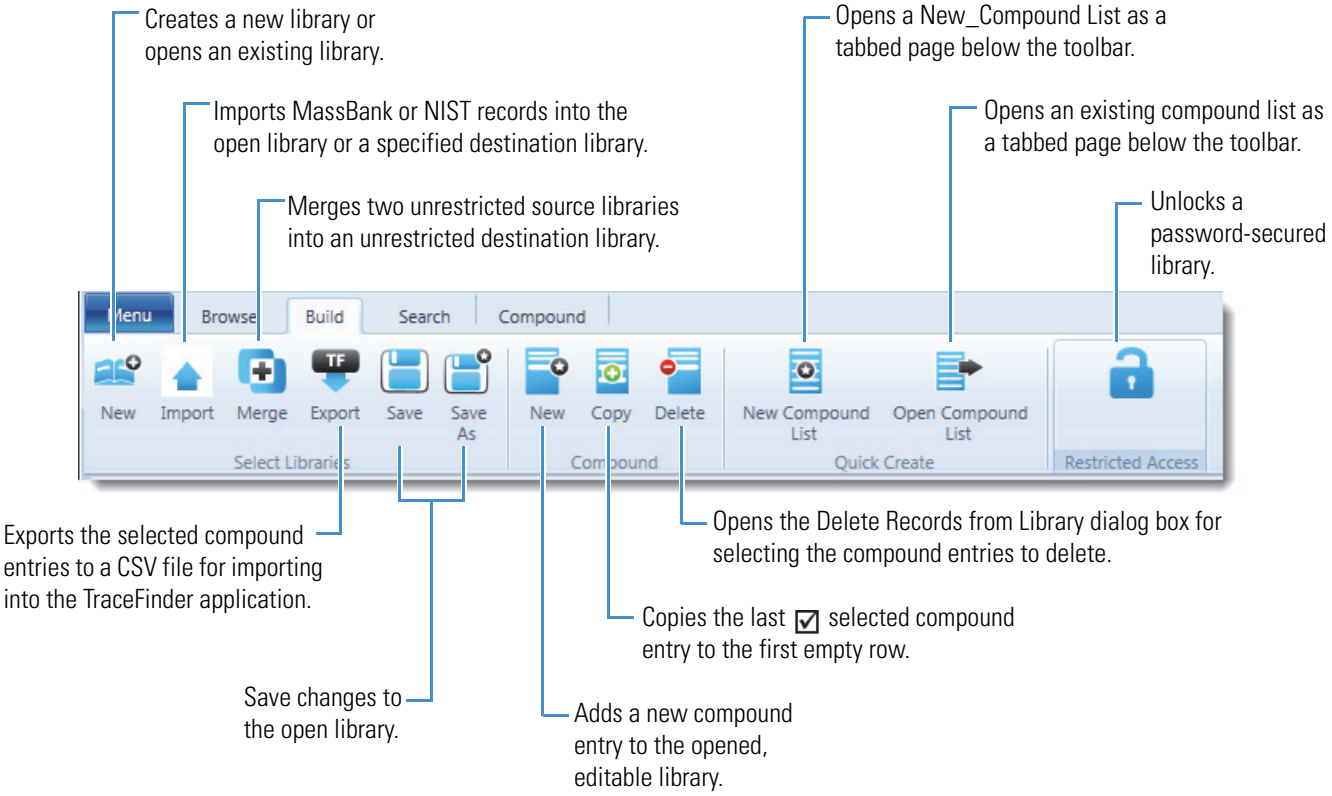


Table 8 describes the parameters in the Build toolbar.

Table 8. Build toolbar parameter descriptions (Sheet 1 of 2)

Parameters	Description
Select Library	
New	Opens the Save As dialog box so that you can specify the location and name of a new library.
Import	Imports compound entries with associated spectra from MassBank or NIST files (public repositories of mass spectral data) into an opened, editable library or a specified, unrestricted destination library.
Merge	Combines the data from two unrestricted libraries into a third unrestricted library.

Table 8. Build toolbar parameter descriptions (Sheet 2 of 2)

Parameters	Description
Export	Exports selected compound entries to a comma-separated values (CSV) file for importing into the TraceFinder application. Available when you select the check boxes of compound entries that have associated spectra.
Save	Saves the currently displayed record to the library. Remains inactive if no changes have been made to the library since the last save.
Save As	Opens the Save As dialog box so that you can browse to the location where you want to save a new library, or save the selected entries of an editable library under a new name.
Compound	
New	Adds a new compound to the library.
Copy	Copies the selected compound. To select a compound for copying, select its associated check box.
Delete	Deletes the selected compounds from the library. To select a compound for deletion, select its associated check box.
Quick Create	
New Compound List	Opens the Compound List tab and toolbar, the New Compound List tabbed page containing a Compound List pane, and adds a placeholder entry to the Compound List pane.
Open Compound List	Opens the Compound List tab and toolbar and the selected XML file.
Restricted Access	
This area appears in the toolbar when you open a restricted library.	
Lock icon ( )	Opens the Restricted Access dialog box for entering the password that unlocks the library.

Compound Tab

The Compound tab is made up of the Compound toolbar and the opened, editable library. Until you open a raw data file for selecting a spectrum, the tabbed library page contains the same panes as it does from the Browse or Build tabs. Opening a raw data file adds the following panes —Chromatogram Options, Chromatogram, Raw Spectrum, Curated Spectrum, and MOL Structure. For information about these panes, see "Library Search Page" on page 72.

This figure shows the Compound toolbar.

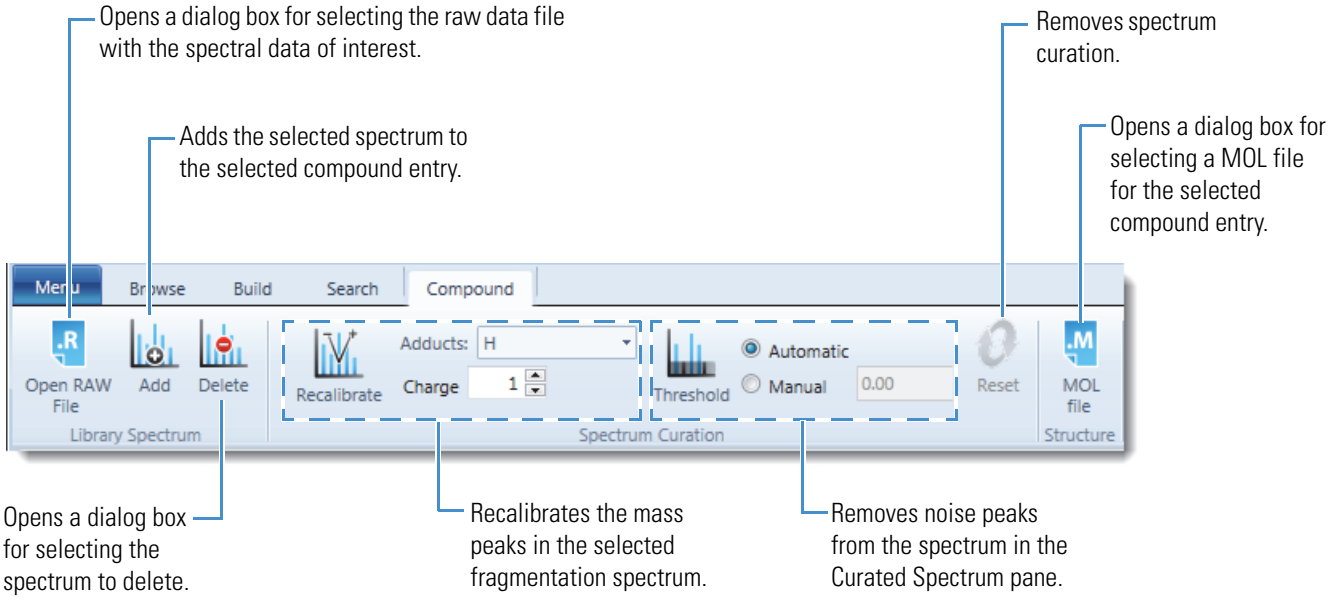


Table 9 describes the parameters in the Compound toolbar.

Table 9. Compound toolbar parameter descriptions (Sheet 1 of 2)

Parameter	Description
Library Spectrum	
Open Raw File	Opens the Open dialog box so that you can select a raw data file.
Add	Adds the selected spectrum to the compound after it has been recalibrated or thresholded.
Delete	Deletes the selected spectrum from the compound.
Spectrum Curation	
Recalibrate	Recalibrates the spectrum.
Adducts	Specifies the adduct.
Charge	Specifies the charge of the precursor ion.
Threshold	Thresholds the spectrum.
Automatic	Determines whether to threshold a spectrum automatically.
Manual	Determines whether to threshold a spectrum manually.

Table 9. Compound toolbar parameter descriptions (Sheet 2 of 2)

Parameter	Description
Reset	Restores a spectrum to its original state before recalibration or thresholding. Available when the Curated Spectrum view contains a thresholded or recalibrated spectrum.
Structure	
MOL File	Opens the Open dialog box for locating a MOL structure file.

Compound List Pane of a Library Page

The Compound List pane of a library page lists the compound and spectral data records in the library. It displays the same columns on all three tabs: Browse, Build, and Compound. The compound level columns are read-only on the Browse tab and editable on the Build and Compound tabs.

Table 10 describes the parameters in the Compound List pane.

Table 10. Compound List pane of the Browse, Build, and Compound tabs (Sheet 1 of 3)

Columns	Description
Compound columns Displays information about the library compounds.	
Entry No.	Assigns a sequential record number to a compound or spectrum.
Compound	Specifies the name of the compound.
Formula	Specifies the chemical formula of the compound. Format for each element: *PeriodicTableSymbolCount* For example: C8H10N4O2 or C8 H10 N4 O2 represents the chemical formula for caffeine.
	IMPORTANT If you add a space between each element in a chemical formula, remember to include spaces when you search for chemical formulas in the library.
CAS ID	Specifies the unique Chemical Abstracts Service™ registry number assigned to the compound.
Compound Class	Specifies the classification of the compound, for example, Endogenous Metabolites, Therapeutic/Prescription Drugs, or Pesticides.

Table 10. Compound List pane of the Browse, Build, and Compound tabs (Sheet 2 of 3)

Columns	Description
ChemSpider ID	Specifies the identification number of the compound in the ChemSpider™ online data repository (www.chemspider.com).
HMDB ID	Specifies the identification number of the compound in the Human Metabolome Database (HMDB) online data repository (www.hmdb.ca).
KEGG ID	Specifies the identification number of the compound in the Kyoto Encyclopedia of Genes and Genomes (KEGG™) online data repository (www.genome.jp/kegg).
PubChem ID	Specifies the identification number of the compound in the PubChem^{SM} online data repository (https://pubchem.ncbi.nlm.nih.gov/).
mzCloud ID	Specifies the identification number of the compound in the mzCloud™ database (www.mzCloud.org).
PeptideSequence	Displays the amino acid sequence of the peptide.
Tag	Displays text that you can later use to sort and filter the data.
Spectrum columns	
Displays the spectra belonging to a specific compound when you click the expand icon (+) to the left of the compound name.	
Spectrum ID	Displays the identification number 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 (www.mzCloud.org).
Filter	Displays the scan filter from the raw data file.
Retention Time	Displays the retention time for the library spectrum.
Scan Number	Displays the scan number in the original raw data file for the library spectrum.
Precursor m/z	Displays the mass-to-charge ratio of the precursor ion associated with the spectrum.
Neutral Mass	Displays the uncharged, neutral 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, either positive or negative.

Table 10. Compound List pane of the Browse, Build, and Compound tabs (Sheet 3 of 3)

Columns	Description
Fragmentation Mode	Displays the fragmentation technique used to fragment the precursor ion, for example, CID or HCD.
Ionization Mode	Displays the ionization mode used, for example, ESI or MALDI.
Mass Analyzer	Displays the type of mass analyzer.
Instrument Name	Displays the name of the Thermo Scientific mass spectrometer used to acquire the raw data file.
Contributor	Identifies the person who added the compound to the library.
Raw File URL	Displays the URL of the raw data file.
Version Number	Displays the version number of the mzCloud online database (www.mzCloud.org).
Creation Date	Displays the creation date of the raw data file.
Curator	Displays the name of the person who added the curated spectrum to the library.

Compound List Tab

The Compound List tab appears when you click either of these buttons in the Build toolbar—New Compound List or Open Compound List.

The Compound List tab includes its toolbar and either a New_Compound List page or a *Named Compound List* page. Each of these tabbed pages displays a compound list that you can process to add records to the opened, editable library.

For information about the Compound List toolbar, the tabbed pages that open below the toolbar, and the dialog boxes that you can access from the tab, see these topics:

- Compound List Toolbar
- Compound List Page
- Spectrum Selection Parameters Dialog Box
- Processing Parameters Dialog Box

Compound List Toolbar

This figure shows the Compound List toolbar.

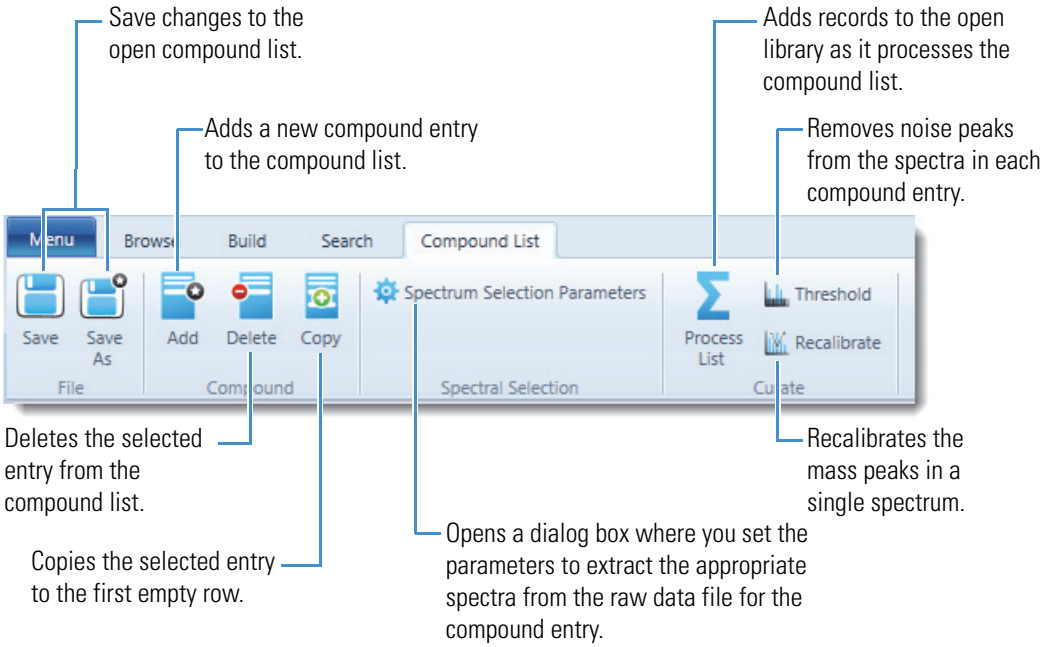


Table 11 describes the parameters in the Compound List toolbar. For information about the tabbed compound list page, see "Compound List Page" on page 53.

Table 11. Compound List toolbar parameter descriptions (Sheet 1 of 2)

Parameters	Description
File	
Save	Opens the Save As dialog box so that you can save the compound list to an XML file.
Save As	Opens the Save As dialog box so that you can save the compound list to an XML file with a different name.
Compound	
Add	Adds a new compound entry to the compound list.
Delete	Deletes a compound from the compound list.
Copy	Copies a compound entry to the next row in the compound list.
Spectral Selection	
Spectrum Selection Parameters	Opens the Spectrum Selection Parameters dialog box ("Spectrum Selection Parameters Dialog Box" on page 54).

Table 11. Compound List toolbar parameter descriptions (Sheet 2 of 2)

Parameters	Description
Curate	
Process List	Searches for spectra in the raw data file and adds the found spectra to the library.
Threshold	Thresholds spectra.
Recalibrate	Recalibrates spectra.

Compound List Page

Table 12 describes the parameters on the Compound List page below the Compound List toolbar.

Table 12. Compound List page parameter descriptions (Sheet 1 of 2)

Parameter	Description
Status	Displays the status of each compound in the compound list as the application processes the list, for example, `No Spectrum Found`.
T	Displays a yellow color to indicate that the spectra are thresholded.
R	Displays an orange color to indicate that the spectra are recalibrated.
A	Displays a blue color to indicate that the spectra are averaged.
Compound	Displays the name of the substance associated with the entry number in the library.
Raw File	Opens the Open dialog box so that you can locate the raw data file where the compound can be found.
Raw File URL	Displays the URL of the raw data file where the compound can be found.
Formula or Precursor	Opens the Processing Parameters dialog box for entering a chemical formula or the precursor *m/z*.
Formula	Displays the chemical formula of the substance associated with the entry number in the library.
Adduct	Displays the adduct specified in the Processing Parameters dialog box.
Charge	Displays the charge of the precursor ion specified in the Processing Parameters dialog box.

Table 12. Compound List page parameter descriptions (Sheet 2 of 2)

Parameter	Description
Polarity	Specifies the polarity of the adduct ion, either positive or negative.
Precursor m/z	Specifies the mass-to-charge ratio of the precursor ion associated with the spectrum.
MOL File	Opens the Open dialog box for locating a MOL file for the compound.
MOL File URL	Displays the URL of the MOL file.
See "Compound List Pane of a Library Page" on page 49 for information about the following columns: Compound Class, CAS ID, ChemSpider ID, HMDB ID, PubChem ID, KEGG ID, PeptideSequence, and Tag.	

Spectrum Selection Parameters Dialog Box

Table 13 describes the parameters in the Spectrum Selection Parameters dialog box (Figure 22 on page 41).

Table 13. Spectrum Selection Parameters dialog box parameter descriptions (Sheet 1 of 2)

Parameter	Description
Retrieve Only One Best Spectrum Per Compound	Retrieves from the raw data file the best MS/MS spectrum for the precursor *m/z*. The resulting library entry contains only one spectrum for that compound. This option is selected by default.
Retrieve One Spectrum for Each Unique Collision Energy	Retrieves from the raw data file one MS/MS spectrum for each unique collision energy for the precursor *m/z*. The spectrum is either the most intense—that is, the highest NL value—or the average of all spectra collected at each collision energy. The resulting library entry contains one spectrum for each unique collision energy acquired.
Most Intense Spectra	Retrieves the spectra with the highest NL values. Available for the Retrieve One Spectrum for Each Unique Collision Energy option.
Averaged Spectra	Retrieves averaged spectra, which are the average of the masses of spectra over an entire time range. Available for the select Retrieve One Spectrum for Each Unique Collision Energy option.

Table 13. Spectrum Selection Parameters dialog box parameter descriptions (Sheet 2 of 2)

Parameter	Description
Precursor Tolerance/unit	Specifies the precursor tolerance and the unit of tolerance.
Minimum NL	Specifies the threshold NL value of the best MS/MS spectrum in intensity counts. The application ignores the spectra with NL values below this threshold and does not retrieve them. You can enter the NL value in standard form or scientific notation: Valid range: 0 or 1 to 10 000 000 000 ($1e^{10}$); default: 0 (no minimum threshold)

Processing Parameters Dialog Box

Use the Processing Parameters dialog box to enter either a chemical formula for a neutral compound and the adduct species and charge for its ionized form or the precursor mass for the adduct ion.

Clicking Formula or Precursor in the Formula or Precursor column of the Compound List table on the New Compound List page opens this dialog box.

Table 14 describes the parameters in the Processing Parameters dialog box (Figure 20).

Table 14. Processing Parameters dialog box parameter descriptions

Parameter	Description
Enter Chemical Formula	Uses a chemical formula, adduct, and charge to determine the precursor mass-to-charge value to search for in the scan filter for a spectrum. The recalibration algorithm uses the chemical formula.
Formula	Specifies the chemical formula of the selected compound. Available for the Enter Chemical Formula option.
Adduct	Specifies the adduct of the selected compound. Available for the Enter Chemical Formula option.
Charge	Specifies the charge of the precursor ion. Available for the Enter Chemical Formula option.
Enter Precursor m/z	Uses the precursor *m/z* to determine the mass to search for.
Precursor m/z	Specifies the mass-to-charge ratio of the precursor ion of the selected compound. Available for the Enter Precursor m/z option.

5

Searching Libraries

Follow these topics as needed.

Contents

- Performing a Library Search
- Reviewing and Exporting the Search Results
- Starting a New Search for Comparison
- Limiting the Library Entries to Search
- Search Tab

For information about specifying the default parameter settings for library searches, see "Setting the Default Library Search Parameters" on page 79.

Performing a Library Search

To search mass spectral libraries for matching spectra, do the following:

1. Select one or more libraries (database files) (see the next topic Selecting the Libraries for the Search).
2. Open the raw data file that contains the mass spectra you want to search for (see "Opening a Raw Data File" on page 59).
3. Select the query spectrum (see "Selecting the Query Spectrum" on page 61).
4. (Optional) Set up the search parameters (see "Setting the Search and Query Spectrum Parameters" on page 62).
5. Start the search (see "Starting the Library Search" on page 64).

Selecting the Libraries for the Search

The first step in searching a library for a spectrum is to select the libraries to search.

Note You can select up to five libraries for the search, but the libraries must reside in the same directory folder.

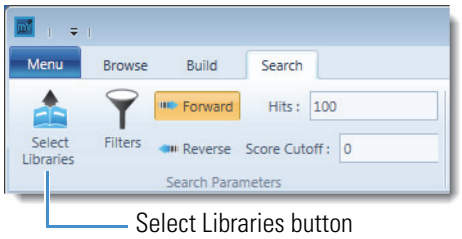
There are three ways to select the libraries to search:

- Specify a default library (see "Starting a Search Workflow from the Search Tab" on page 9).
- Select a library from the landing page ("Starting a Search Workflow from the Landing Page" on page 8).
- Select up to five libraries from a directory folder (see the following procedure).

❖ To select up to five libraries from a directory folder

1. Click the **Search** tab.
2. In the Search toolbar, click **Select Libraries** (Figure 27).

   Figure 27. Search Parameters area of the Search toolbar

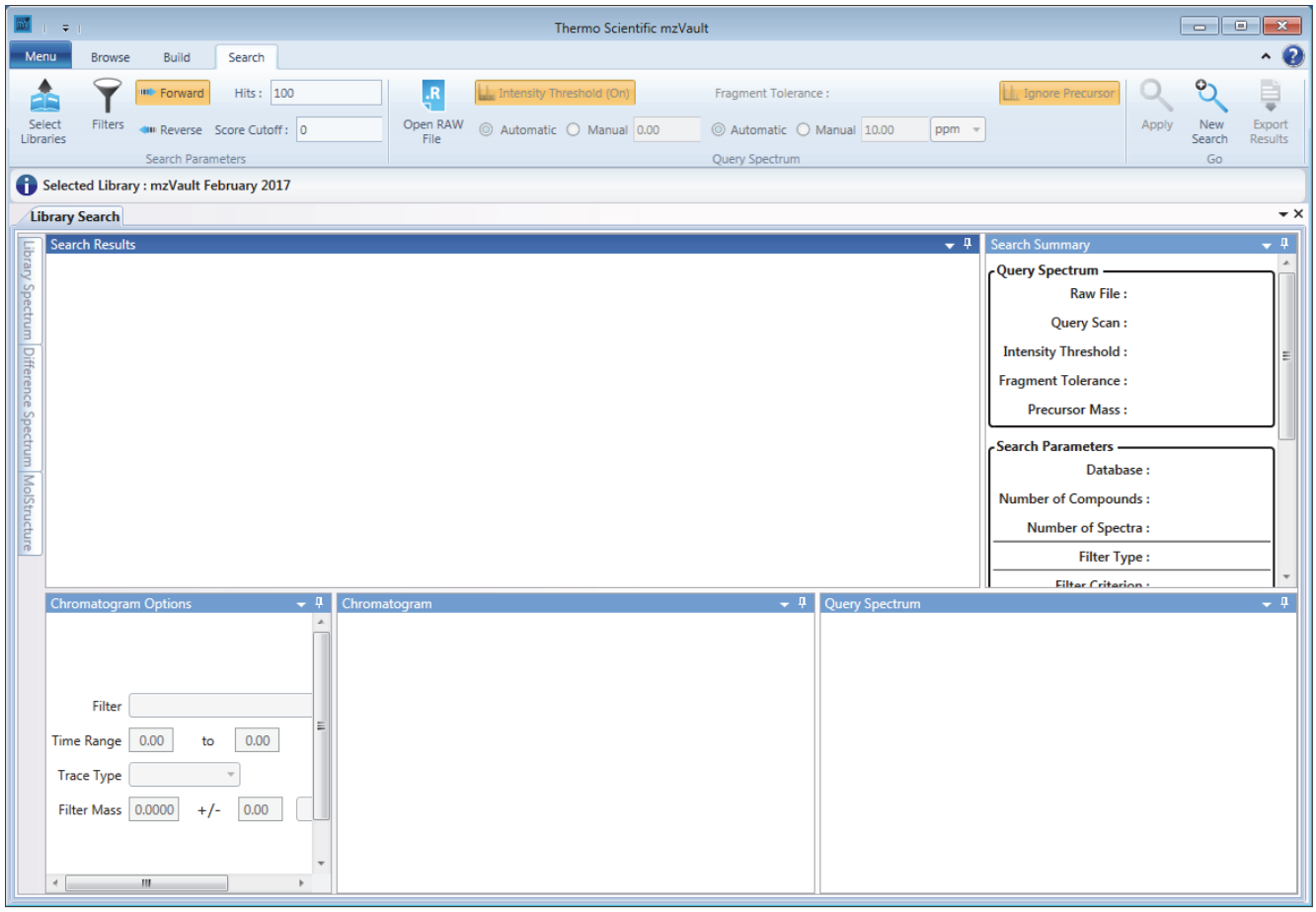
3. In the Open dialog box, do the following:
   a. Browse to the folder that contains the library files (DB).
   b. Select up to five library files by using the SHIFT key (for contiguous files) or the CTRL key (for noncontiguous files).
   c. Click **Open**.

      The following page appears below the Search toolbar:

      - For a single library search, the Library Search page appears.
      - For a search of multiple libraries, the Multi-Search *Integer* page appears.

The Library Search page and the Multi-Search *Integer* page contain the same five panes (Figure 28). The bottom three panes are empty until you open a raw data file for selecting the query spectrum. The top two panes are empty until you run a library search.

Figure 28. Library Search page (before setting up a query spectrum)



Go to the next topic "Opening a Raw Data File."

Opening a Raw Data File

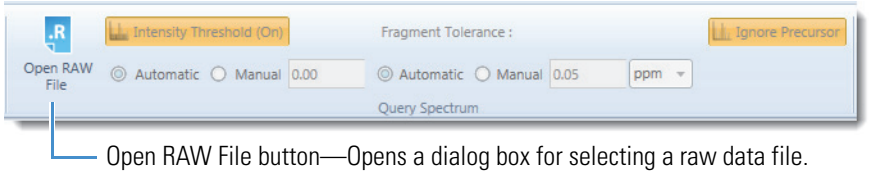
The second step in searching a library for a spectrum is to open the raw data file that contains the mass spectral data of interest. This file must contain mass spectral data acquired with a Thermo Scientific mass spectrometer that generates high-resolution accurate-mass data.

❖ To open a raw data file

1. Select the libraries that you want to search, if you have not already done so (see "Selecting the Libraries for the Search" on page 58).
2. In the Query Spectrum area of the Search toolbar, click **Open Raw File** (Figure 29).

> **IMPORTANT** The Open RAW button is always available—however, to open a raw data file, you must first select a library.

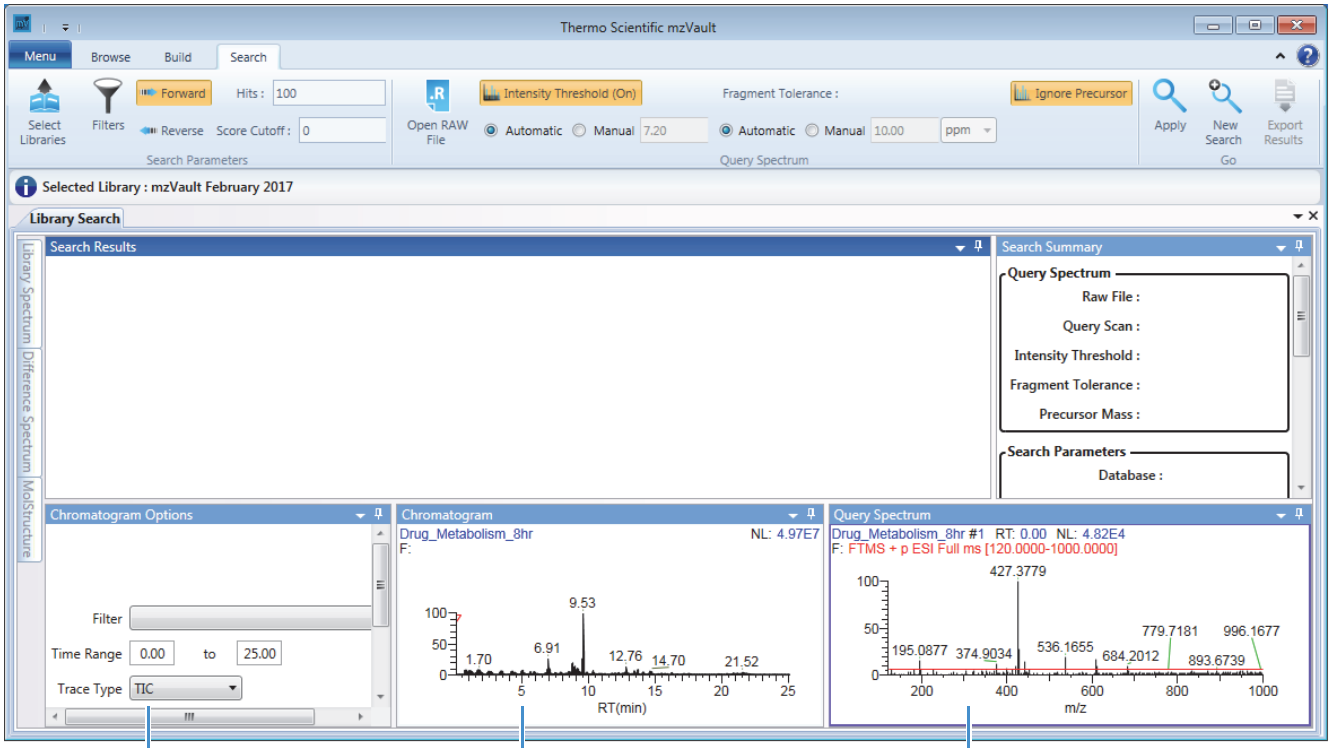
Figure 29. Query Spectrum area of the Search toolbar



3. In the Open dialog box, locate the raw data file and click **Open**.

   Figure 30 reflects information from the raw data file in the Chromatogram Options, Chromatogram, and Query Spectrum panes. By default, the Chromatogram pane displays the TIC chromatogram and the Query Spectrum pane displays scan 1.

Figure 30. Data from the raw data file displayed on the Library Search page



For information about the search parameters, see "Search Tab" on page 70.

Go to the next topic "Selecting the Query Spectrum."

Selecting the Query Spectrum

After you select the mass spectral libraries and the raw data file that contains your experimental data, the next step in searching a library is to select the query spectrum (the spectrum to search for).

❖ To select the query spectrum

1. In the Chromatogram Options pane, specify the filtered chromatogram to display in the Chromatogram pane:
   - (Optional) In the Filter list in the Chromatogram Options pane, select a scan filter to apply. The default selection is “none”.

     The scan filters in this list come from the experimental data in the raw data file.
   - (Optional) In the Time Range boxes, specify the retention time range to display. (This is another way to zoom.)
   - (Optional) From the Trace Type list, select the type of chromatogram to filter by:
     - (Default) **TIC**: Displays a total ion current chromatogram.
     - **Base Peak**: Displays a base peak ion chromatogram.
     - **Target Mass**: Displays an extracted ion chromatogram (XIC).

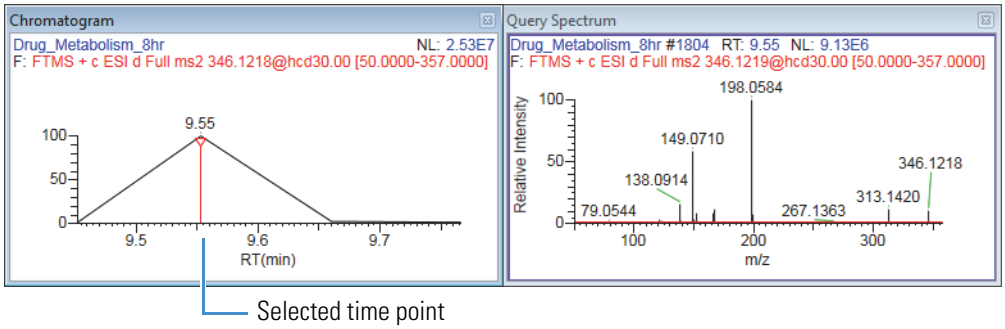
       The Filter Mass option becomes available when you select Target Mass in the Trace Type list.
2. If you selected Target Mass in the Trace Type list, specify the mass, tolerance, and unit to use for filtering the chromatogram in the Filter Mass boxes.
   a. In the first box, specify the mass to use for filtering the chromatogram.
   b. In the second box, specify the mass tolerance for the filter mass.
   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)
3. In the Chromatogram pane, do one of the following to select the spectrum of interest:
   - Click a specific time point in the chromatogram.

   –or–

   - Use the left and right arrow keys on the keyboard to select the spectrum.

   In the Chromatogram pane, the cursor changes to a red vertical line at the selected time point. In the Query Spectrum pane, the scan number in the header changes to reflect the selected scan, and the application updates the spectrum to that of the selected scan (Figure 31).

Figure 31. Selected time point and associated query spectrum



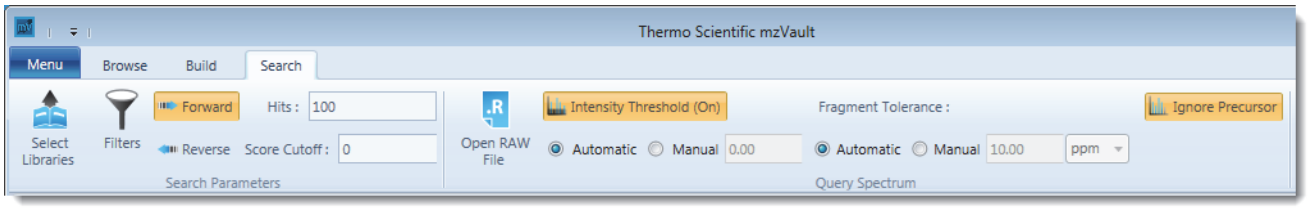
Go to the next topic "Setting the Search and Query Spectrum Parameters."

Setting the Search and Query Spectrum Parameters

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

To change the default settings for the library search parameters, see "Setting the Default Library Search Parameters" on page 79. Figure 32 shows the factory default settings for the Search toolbar.

Figure 32. Factory default settings for the Search toolbar



❖ To set up the search and query spectrum parameters

Note For details about the library search parameters, see "Default Library Search Parameters Page" on page 84.

1. Open the libraries to search.
2. Select the query spectrum.
3. In the Search Parameters area of the Search toolbar, set the search type and its limits as follows:
   - (Optional) To limit the search to a subset of the library entries, click **Filters**. Then, in the Select Filters dialog box, set up one or more filters and click **OK** (see "Limiting the Library Entries to Search" on page 68).

     Note The application uses the information in the selected libraries to populate the Filter Criterion lists.

- To run a forward search, click **Forward** if the button is not already selected (orange). Or, to run a reverse search, click **Reverse** (the button's background turns orange).
- (Optional) In the Hits box, type the number of the top-matching results to display in the Search Results pane of the Search page.

  If you select multiple libraries, the number of hits means the number of results per library. For example, if you select two libraries and set the number of Hits to 10, the search returns a maximum of 10 hits for each library, for a maximum total of 20 hits sorted by score.
- (Optional) In the Score Cutoff box, type a score, from **0** to **100**%, below which to filter out results.

4. Set the intensity threshold for the query spectrum peaks as follows:
   a. Click **Intensity Threshold (On)** or **(Off)** in the Query Spectrum area of the toolbar.

      This parameter specifies whether to ignore any peaks in the query spectrum that are less than the value specified by the Automatic or Manual threshold.
   b. If you chose Intensity Threshold (On), select the Automatic or Manual option.
      – (Default) **Automatic**: Uses an internal algorithm to calculate the threshold value.
      – **Manual**: Enables you to specify the threshold value to use for filtering spectrum peaks. Specify the threshold value in the adjacent box.
5. Set the fragment tolerance as follows:
   a. Under Fragment Tolerance in the Query Spectrum area of the toolbar, select the Automatic or Manual option to indicate how to specify the fragment tolerance.
      – (Default) **Automatic**: Uses the native instrument precision to determine the tolerance.
      – **Manual**: Enables you to specify the mass value for the tolerance in parts per million (**ppm**), millimass units (**mmu**), or atomic mass units (**amu**).
   b. For the Manual option, enter the tolerance value in the adjoining box. The fragment tolerance is a mass value, either absolute (mmu or amu) or relative (ppm), that determines whether a peak in the query spectrum matches a peak in a library spectrum.
6. In the Query Spectrum area of the toolbar, click **Ignore Precursor** to have the application ignore (remove from consideration), for the purpose of calculating scores, any mass that is within 2.2 Da of the precursor ion.

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

Go to the next topic "Starting the Library Search."

Starting the Library Search

Now you are ready to search the library for the spectrum that you are interested in. After you perform the first search, you can perform another search using a different library, a different raw data file, or different search parameters.

❖ To start a library search

1. If you have not already done so, select the libraries to be searched, select the query spectrum, and set up the search parameters (see "Performing a Library Search" on page 57).
2. In the Go area of the Search toolbar, click **Apply**.

   The search results appear in the Search Results pane of the library search page. They are sorted in descending order in the High Res Score column according to score (see "Reviewing the Search Results" on page 64).

Tip If you modify the search parameters and click Apply, the application overwrites the results displayed for the initial search. If you want to retain the current results and display the results of an additional search for comparison, start the next search by clicking New Search.

Reviewing and Exporting the Search Results

You can customize the data in the Search Results pane to display only the information you need. You can also export the customized results to a spreadsheet file.

Follow these topics to review the results of a library search and export the results to a spreadsheet file:

- Reviewing the Search Results
- Exporting the Search Results

Reviewing the Search Results

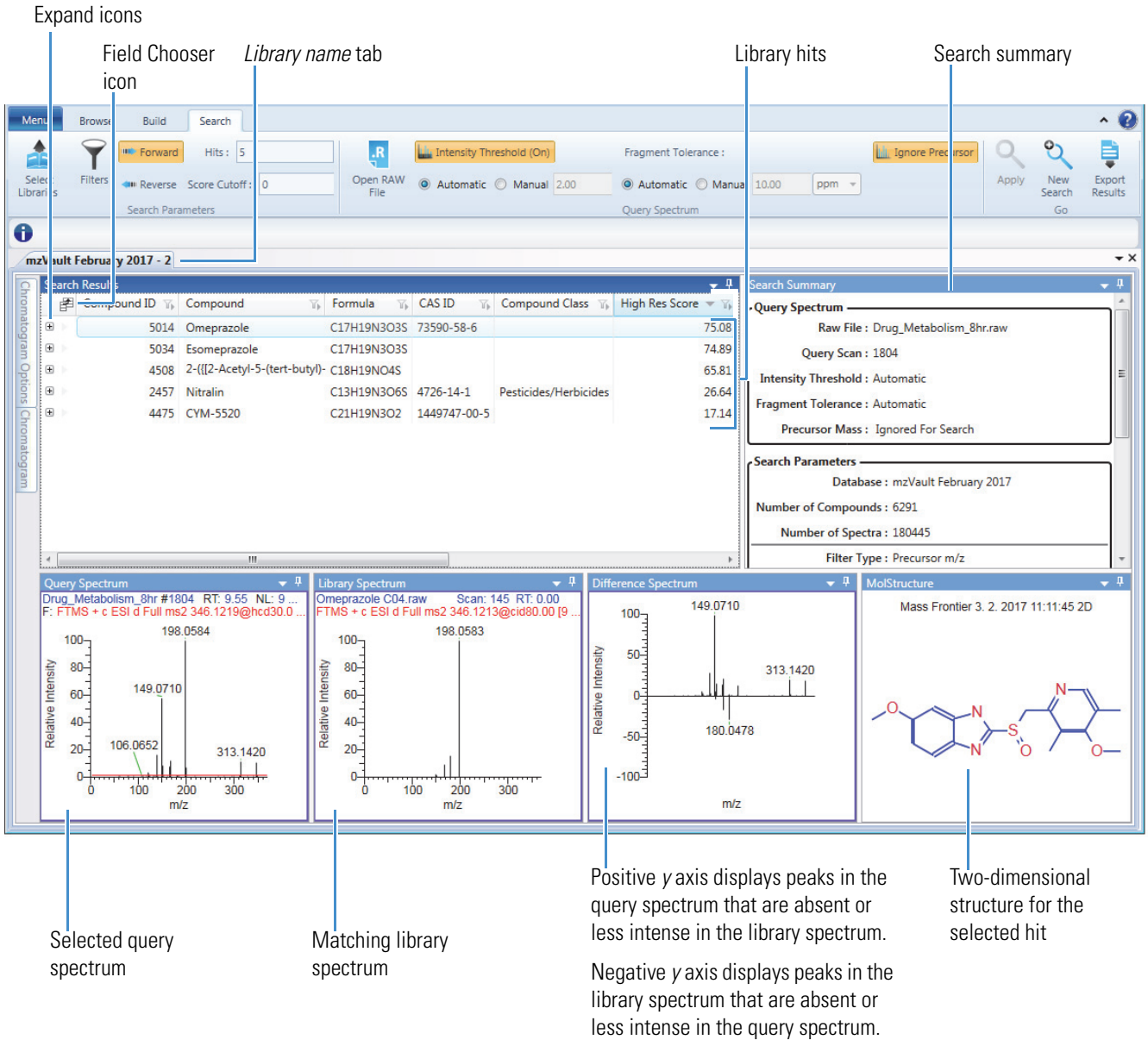
Use the Search Results pane to review the matching spectra found in the selected libraries.

❖ To review the search results

1. To sort the hits by a specific column, click its heading.
2. To view the list of spectra for a library match, click the expand icon (+) in the leftmost column.
3. To hide or display compound or spectrum columns, use the Field Chooser dialog boxes (see "Displaying or Hiding Table Columns" on page 14).

Figure 33 shows the results of a search that was limited to five hits for a specific precursor mass in the mzVaultFebruary 2017 library.

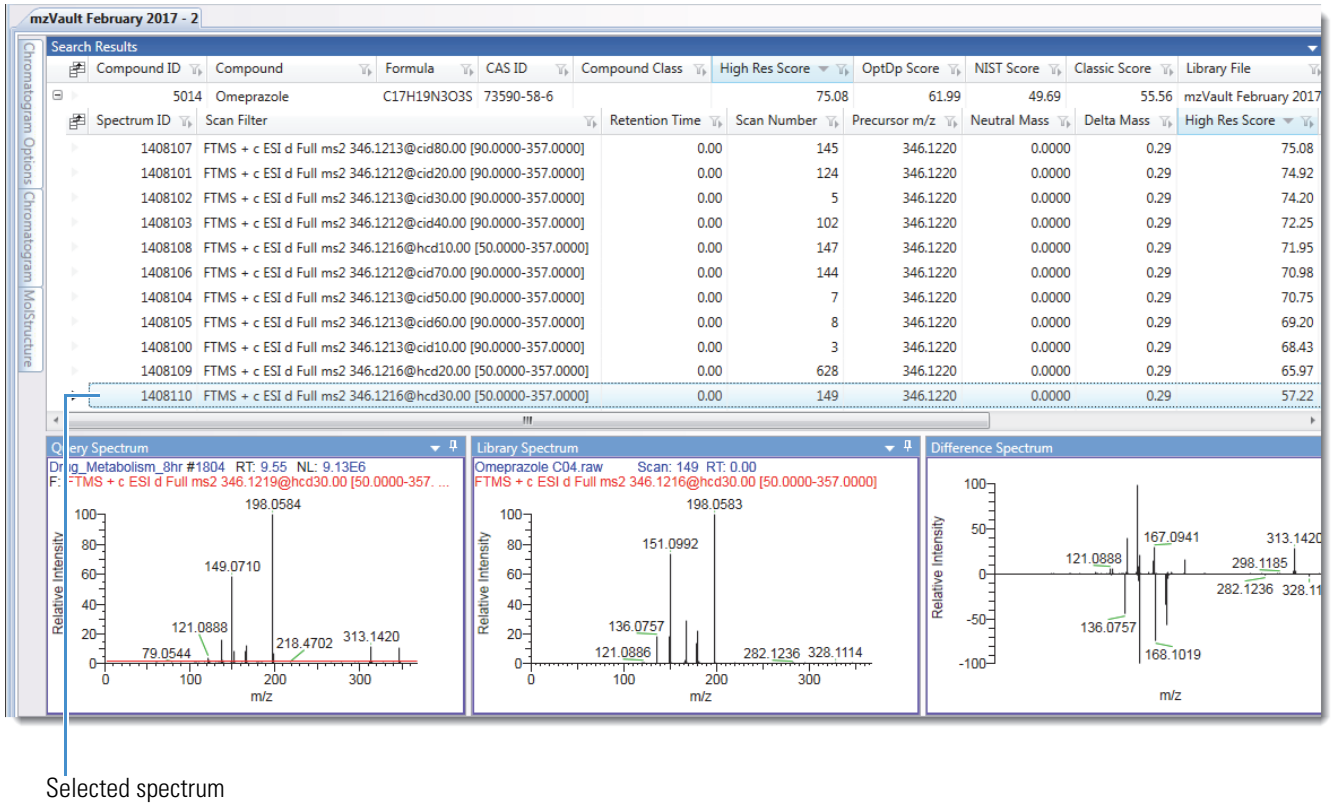
Figure 33. Library search results



4. To view a selected spectrum in the Library Spectrum pane, click the spectrum row in the expanded spectrum list.

   Figure 34 shows the selection of a spectrum in the expanded spectrum list for a specific hit.

Figure 34. Selection of a spectrum from an expanded spectrum list



Selected spectrum

Exporting the Search Results

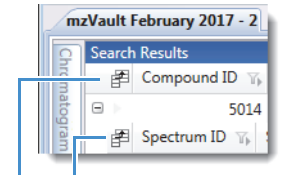
After you run a library search, you can export the results to a spreadsheet file.

❖ To export the results of a library search

1. To select the compound and spectrum information that you want to export, select the appropriate columns to display from the Field Chooser dialog boxes for the compound table and the spectrum subtable.

   Figure 35 shows the location of the Field Chooser icons for opening the Field Chooser dialog boxes for the compound table and spectrum subtable. The application exports only the displayed columns.

Figure 35. Location of the Field Chooser icons in the Search Results pane



Click to display the column selections for the spectrum subtable.

Click to display the column selections for the compound table.

2. In the Search toolbar, click **Export Results**.
3. In the Save As dialog box, browse to the location where you want to save the search results, name the file, and click **Save**.

   If you leave the file name blank, the application assigns a default name as follows:

   Search Results_*year_month_day_time*[*AM*|*PM*].xlsx

   Here is an example:

   Search Results_2018-04-20_10-42-10-AM.xlsx

Starting a New Search for Comparison

❖ **To perform another search and display the results on a new Search Results page**

1. In the Search toolbar, click **New Search**.

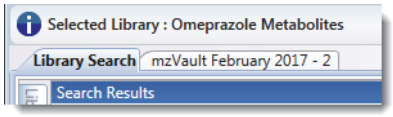
   Note Clicking the New Search icon loads the default search parameter settings (see "Setting the Default Library Search Parameters" on page 79).

   If the default search parameters include a default library, the application automatically selects it for the new search. Otherwise, the Open dialog box appears.

2. Depending on whether the default search settings include a library, do the following:

   - Use the default library or click **Select Libraries** and select a different library.
   - If the Open dialog box appears, select a new library or the library that you previously searched, and click **Open**.

   A new Library Search page appears as the active tab, and the previous *Library Name* tab becomes inactive.

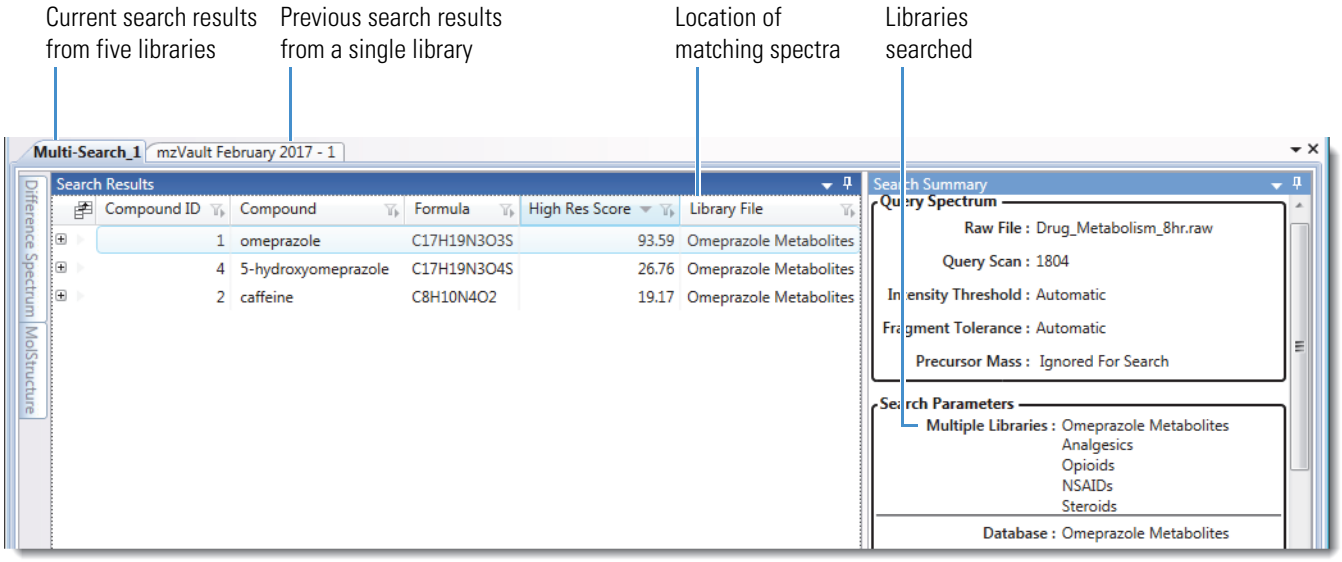


3. In the Search toolbar, click **Open Raw File**, and load or reload a raw data file.

   For information on selecting a raw data file, see "Opening a Raw Data File" on page 59.

4. Select the query spectrum (see "Selecting the Query Spectrum" on page 61).
5. (Optional) Change any parameters in the Search Parameters or the Query Spectrum area (see "Setting the Search and Query Spectrum Parameters" on page 62).
6. In the Search toolbar, click **Apply**.

The results of this search are displayed on a new search results page. The Search Parameters area of the Search Summary pane displays the names of the selected libraries. The hits in the Search Results pane specify the library file where the matching spectra were found.



Limiting the Library Entries to Search

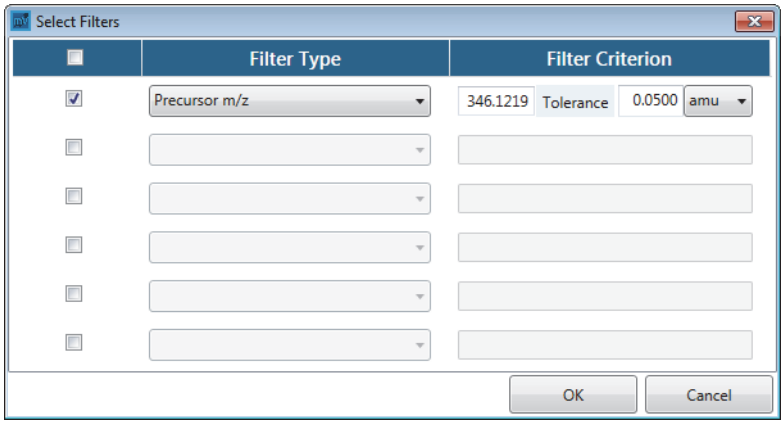
❖ **To filter the library entries for a library search**

1. From the Search tab, open the libraries that you want to search.
2. In the toolbar, click **Filters**.

   The Select Filters dialog box opens.
3. For each filter, do the following:
   a. Select the check box on the left to make the filter selections available.
   b. From the Filter Type list, select a filter type (see Table 15). Then, specify the filter criterion for the selected filter.

   Figure 36 shows the selection of the Precursor m/z filter.

Figure 36. Select Filters dialog box for a library search



4. Click **OK**.
5. From the toolbar, set up the other search parameters, and then click **Apply**.

Table 15. Filters for limiting the library entries to search (Sheet 1 of 2)

Filter Type	Effect
Collision Energy and Tolerance	Limits the search to entries with scan data acquired at the specified collision energy within the specified tolerance. Valid entries: Numeric values > 0
Compound	Limits the search to entries that contain the specified text string in the Compound column. Valid entries: Alphanumeric and special characters
Compound Class	Limits the search to entries for the selected compound class. **Note** The Compound Class list only includes compound classes found in the selected library.
Curation Type	Limits the search to library spectra for the selected curation type. **Note** The Curation Type list only includes the curation types in the selected library.
Formula	Limits the search to the entries that include the specified formula or partial formula. Valid entries: Alphanumeric and special characters
Fragmentation Mode	Limits the search to library spectra from the same fragmentation mode as the query spectrum.
Peptide Sequence	Limits the search to library entries that include the specified peptide sequence.

Table 15. Filters for limiting the library entries to search (Sheet 2 of 2)

Filter Type	Effect
Precursor m/z and Tolerance	Limits the search to library spectra for the specified precursor *m/z* value within the specified tolerance. Valid entries: Numeric values > 10
Precursor Mass Range	Limits the search to library spectra for the specified range of precursor *m/z* values. Valid entries: Numeric values > 10
Retention Time	Limits the search to library spectra from the specified retention time within a tolerance of 0.05 min. Default: Retention time of the query scan; valid entries: Positive or negative numeric values
Retention Time Range	Limits the search to library spectra from the specified retention time range. Valid entries: The maximum value must be greater than the minimum value by 0.1 min.
Scan Filter	Limits the search to library spectra for the specified scan filter. Valid entries: All or part of a valid scan filter

Search Tab

The Search tab is made up of the Search toolbar and the library search page.

The Search toolbar specifies the criteria to search for a spectrum in the library. The Library Search (or Multi-Search_*Integer*) page specifies the query spectrum. After you run a library search, a Library Search page changes to a *Library Name - Integer* page, and the application populates the following panes: Search Summary, Search Results, Library Spectrum, Difference Spectrum, and MOL Structure.

For information about the search parameters, see these topics:

- Search Toolbar
- Library Search Page

Search Toolbar

This figure shows the Search toolbar.

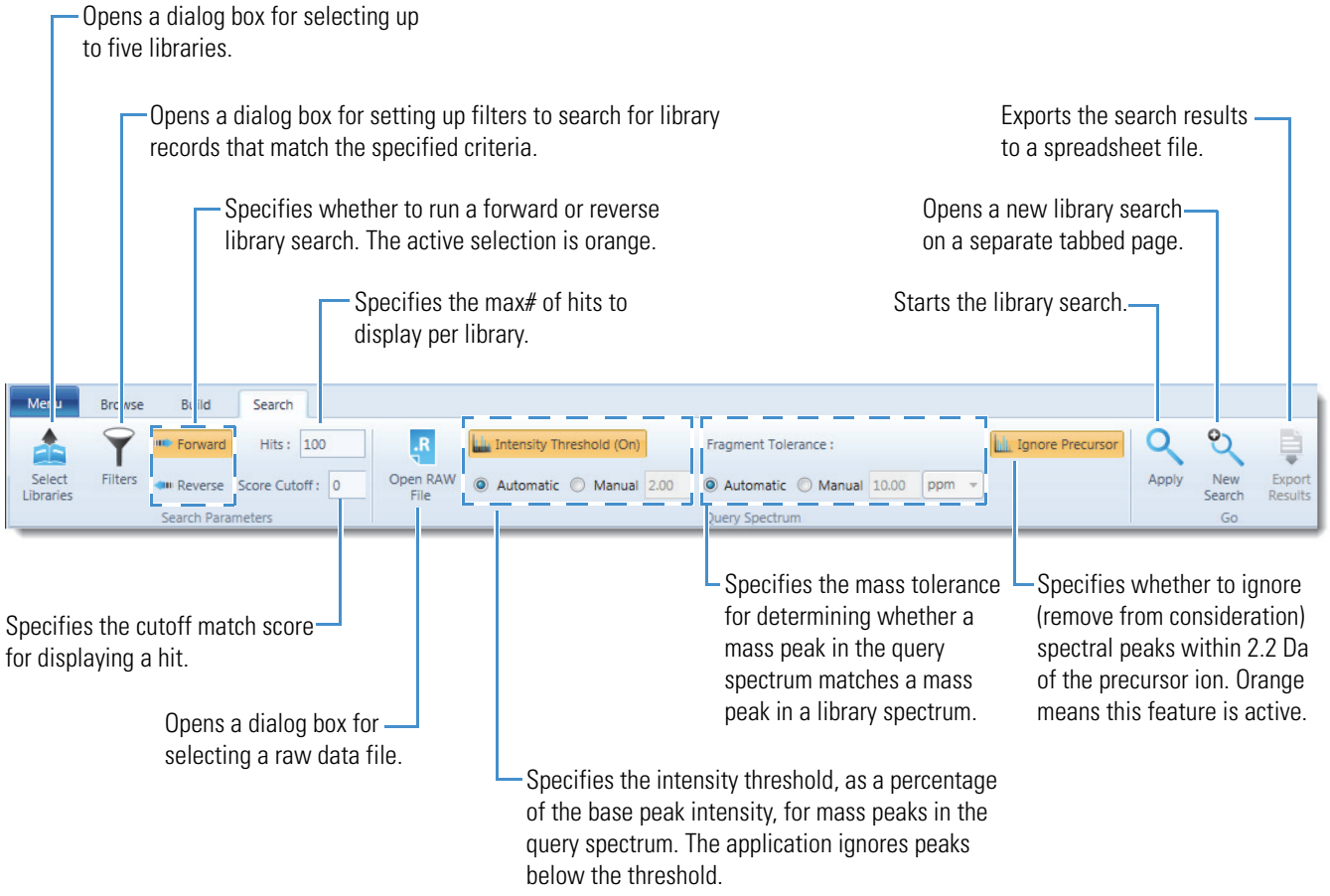


Table 16 describes the parameters in the Search toolbar.

Table 16. Search toolbar parameter descriptions (Sheet 1 of 2)

Parameter	Description
Search Parameters	
Select Libraries	Opens the Open dialog box for selecting the mzVault libraries to search. You can select up to five libraries.
Filters	Opens the Select Filters dialog box for setting up one to six filters that limit the library search to a subset of the library records (see "Limiting the Library Entries to Search" on page 68).
Note See "Default Library Search Parameters Page" on page 84 for information about the following parameters: Forward, Reverse, Hits, and Score Cutoff.	
Query Spectrum	

Table 16. Search toolbar parameter descriptions (Sheet 2 of 2)

Parameter	Description
Open Raw File	Opens the Open dialog box so that you can select a raw data file.
Note See "Default Library Search Parameters Page" on page 84 for information about the following parameters: Intensity Threshold, Fragment Tolerance, and Ignore Precursor.	
Go	
Apply icon	Performs the requested search.
New Search	Opens a new Library Search page with the default search parameters.
Export Results	Exports the search results as an Excel (XLSX) spreadsheet.

Library Search Page

The library search page (Library Search or the Multi-Search_*Integer*) appears after you select the libraries to search from the Search toolbar. Opening a raw data file populates the Chromatogram Options, Chromatogram, and Query Spectrum panes with data from the first scan in the file. Running a library search populates the Search Summary, Library Spectrum, Difference Spectrum, MOL Structure, and Search Results panes.

You use the Chromatogram Options pane, the Chromatogram pane, and the parameters in the Query Spectrum area of the Search toolbar to set up the query spectrum in the Query Spectrum pane.

Table 17 describes the parameters on a library search page.

Table 17. Library search page parameter descriptions (Sheet 1 of 6)

Parameter	Description
Search Results pane (post-search)	
Entry No.	Assigns a sequential record number to a compound or spectrum.
Compound ID	Displays the assigned database in the Entry No. column.
Compound	Specifies the name of the substance associated with the spectrum to search for in the library.
Formula	Specifies the chemical formula for the library entry.
CAS ID	Specifies the unique Chemical Abstracts Service registry number.
Compound Class	Displays the classification of the compounds in the mzCloud database, for example, Endogenous Metabolites, Therapeutic/Prescription Drugs, and Pesticides.
High Res Score	Displays a score calculated by a proprietary algorithm that indicates how well the library spectrum and the query spectrum match.

Table 17. Library search page parameter descriptions (Sheet 2 of 6)

Parameter	Description
OptDp Score	Displays a score calculated by an optimized dot product algorithm that indicates how well the library spectrum and the query spectrum match.
NIST Score	Displays a score calculated by a National Institute of Standards and Technology algorithm that indicates how well the library spectrum and the query spectrum match.
Classic Score	Displays a ratio of the unknown spectra to the spectra in the library.
PeptideSequence	Displays the amino acid sequence of a peptide associated with the spectrum.
Library File	Displays the name of the library database (DB) file.
Search Results pane (expanded table column)	
Spectrum ID	Specifies the identification of the spectrum in the database.
Filter	Specifies the scan filter from the raw data file.
Retention Time	Specifies the retention time from the raw data file.
Scan Number	Specifies the scan number from the raw data file.
Precursor m/z	Specifies the mass-to-charge ratio of the precursor ion associated with the spectrum to search for in the library.
Neutral Mass	Specifies the uncharged, neutral mass of the molecule.
Delta Mass	Specifies the difference in mass between the mass of a specific compound and the mass of a found component.
High Res Score	Displays the score calculated by a proprietary algorithm that indicates how well the library spectrum and the query spectrum match.
OptDp Score	Displays a score calculated by an optimized dot product algorithm that indicates how well the library spectrum and the query spectrum match.
NIST Score	Displays a score calculated by a National Institute of Standards and Technology-like algorithm that indicates how well the library spectrum and the query spectrum match.
Classic Score	Displays a ratio of the unknown spectrum to the library spectrum.
Raw File URL	Displays the name and path of the raw data file used in the search.

Table 17. Library search page parameter descriptions (Sheet 3 of 6)

Parameter	Description
Search Summary pane (post-search)	
Query Spectrum	Displays a summary of the parameter settings in the Query Spectrum area of the tab bar: • Raw File: Displays the name of the raw data file used. • Query Scan: Displays the scan number of the selected spectrum. • Intensity Threshold: Displays the setting of the Intensity Threshold (On/Off) parameter. • Fragment Tolerance: Displays the setting of the Fragment Tolerance (Automatic/Manual) parameter. • Precursor Mass: Indicates whether the Ignore Precursor parameter was chosen for the search.

Table 17. Library search page parameter descriptions (Sheet 4 of 6)

Parameter	Description
Search Parameters	Displays a summary of the parameter settings in the Search Parameters area. • Multiple Libraries: Displays the names of the selected library files. –or– • Database: Displays the name of the selected library file. • Number of Compounds: Displays the number of compounds in the library. • Number of Spectra: Displays the number of spectra in the selected library. • Filter: Displays the setting of the Filter parameter. • Filter Text: Displays the filtering criterion that you entered in the box beneath the Filter list when you selected any type of filter other than None or Precursor m/z from the Filter list. • Precursor m/z: Displays the setting of the Precursor m/z parameter in the Search Parameters pane. • Precursor Tolerance: Displays the setting of the Precursor Tolerance option in the Search Parameters pane. This setting is only available when you select the Precursor m/z filter from the Filter list. • Search Type: Displays the type of search selected, either forward or reverse. • Hits: Displays the setting of the Hits parameter. • Score Cutoff: Displays the setting of the Score Cutoff parameter.
Search Results	Displays a summary of the number of matching compounds and spectra found in the searched library. • Compound Matches: Displays the number of matching compounds found in the searched library. • Spectrum Matches: Displays the number of matching spectra found in the searched library.
Chromatogram Options pane	Displays the chromatogram filter options. This pane appears after you load a raw data file.
Filter	Lists the scans available.

Table 17. Library search page parameter descriptions (Sheet 5 of 6)

Parameter	Description
Time Range	Specifies the retention-time range to display. The first box specifies the start time, and the second box specifies the end time.
Trace Type	Specifies the type of chromatogram to filter by: • (Default) TIC: Displays a total ion current (TIC) chromatogram, where the *x* axis displays the retention time, 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 displays the intensity of the largest peak (base peak) in the spectrum on the *y* axis. The *x* axis displays the retention time. • Target Mass: Displays an extracted ion current chromatogram. When you select this type of chromatogram, the Filter Mass boxes become available.

Filter Mass	Specifies the mass, tolerance, and unit to use for filtering a target 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 mass tolerance unit:
	  • mmu: Millimass units (one thousandth of a mass unit)
	  • (Default) ppm: Parts per million (one millionth of the filter mass)

Chromatogram pane	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, in percent.
RT (min) (*x* axis)	Displays the retention time of the spectrum.

Table 17. Library search page parameter descriptions (Sheet 6 of 6)

Parameter	Description
Query Spectrum pane	Displays the spectrum to search for in the library database.
Header	Displays information about the selected spectrum. • *raw_file_name*: Displays the name of the raw data file, for example, cal200_ng. • # *number*: Displays the scan number of the query spectrum—for example, #853—or the range of scan numbers of the selected spectra. • RT: Displays the retention time. • NL: Displays the intensity of the most intense peak in the query spectrum. • F: Displays the scan filter used, for example, FTMS + p ESI Full ms [300.00–2000.00]. The scan filter indicates the type of mass analyzer used to acquire the data in the raw data file and the ionization technique used.
Relative Intensity (*y* axis)	Displays the ratio of the intensity of a specific peak to the intensity of the peak with the highest intensity, in percent.
m/z (*x* axis)	Displays the mass-to-charge ratio of ions. This ratio is calculated by dividing the mass of an ion, in daltons, by the number of charges carried by the ion.
Library Spectrum pane (post-search)	Displays the spectrum of the selected library match.
Relative Intensity (*y* axis)	Displays the ratio of the intensity of a specific peak to the intensity of the peak with the highest intensity, in percent.
m/z (*x* axis)	Displays the mass-to-charge ratio. This ratio is calculated by dividing the mass of an ion, in daltons, by the number of charges carried by the ion.
Difference Spectrum pane (post-search)	Displays the difference between the query spectrum and the matching library spectrum that you can select from the Spectrum subtable for a compound hit in the Search Results table.
Relative Intensity (*y* axis)	Displays the ratio of the intensity of a specific peak to the intensity of the peak with the highest intensity, in percent.
m/z (*x* axis)	Displays the mass-to-charge ratio. This ratio is calculated by dividing the mass of an ion, in daltons, by the number of charges carried by the ion.
MOL Structure pane (post-search)	Displays a compound's molecular structure.

6

Application Options

Follow these topics to set up the default parameters for searching libraries and recalibrating mass spectra and for adding password security to your libraries.

Contents

- Setting the Default Library Search Parameters
- Setting the Default Recalibration Parameters
- Setting Up and Managing Write Access to Libraries
- mzVault Options Dialog Box

Setting the Default Library Search Parameters

You can specify the default parameter settings for library searches.

❖ **To set the default parameters for a library search**

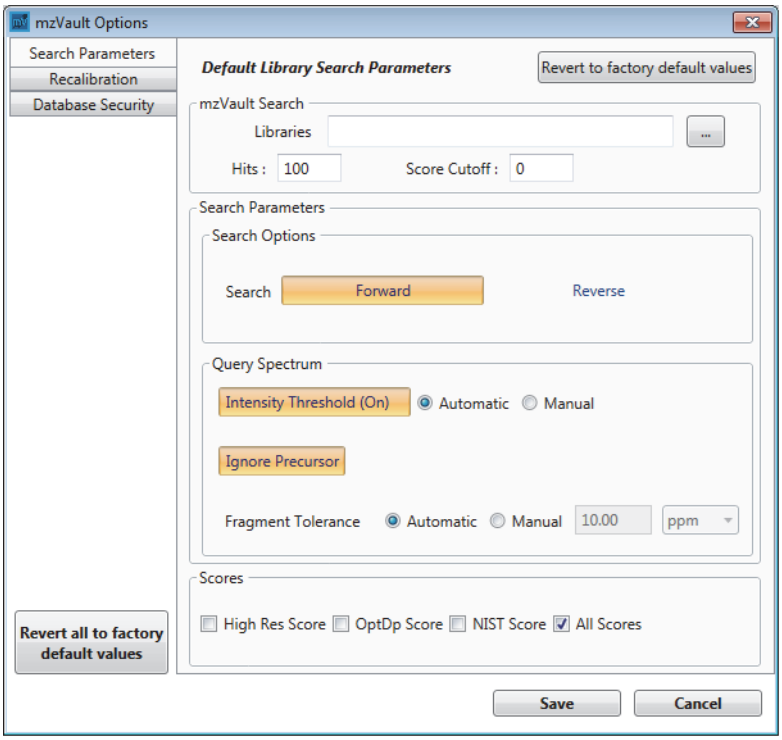
1. Open the Default Library Search Parameters page as follows:
   a. Choose **Menu > Options**.

      The mzVault Options dialog box opens.

   b. Click the **Search Parameters** tab on the left if it is not already selected (by default).

   Figure 37 shows the Default Library Search Parameters page.

Figure 37. Default Library Search Parameters page of the mzVault Options dialog box



2. Make the appropriate selections and entries. If you want to begin with the factory default values, click **Revert to Factory Default Values** before modifying the settings.

   For detailed information about the parameters, see "Default Library Search Parameters Page" on page 84.

3. Click **Save**.

Setting the Default Recalibration Parameters

Recalibration is the process of automatically correcting spectra for known or possible measurement errors.

❖ To set the parameters for recalibration

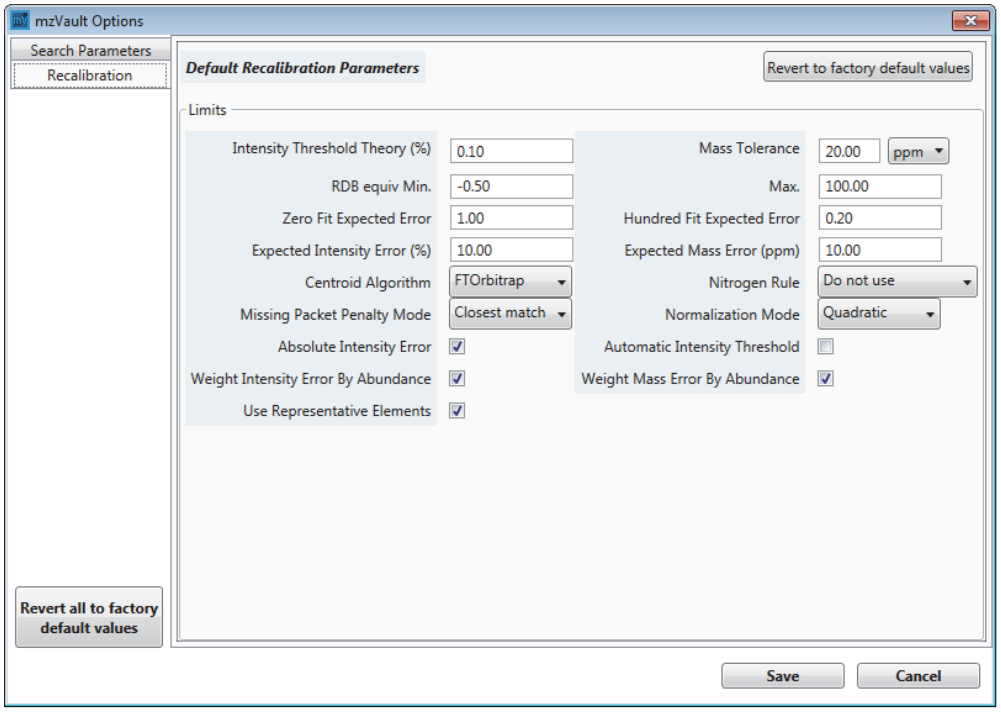
1. Choose **Menu > Options**.

   The mzVault Options dialog box opens (Figure 38).

2. Click the **Recalibration** tab on the left, if it is not already selected.

   Figure 38 shows the Default Recalibration Parameters page.

Figure 38. Default Recalibration Parameters page of the mzVault Options dialog box



3. Make the appropriate selections and entries. If you want to begin with the factory default values, click Revert to Factory Default Values before modifying the settings.

   For detailed information about the parameters on the Default Recalibration Parameters page, see "Parameters on the Default Recalibration Parameters Page" on page 88.

4. Click **Save**.

Setting Up and Managing Write Access to Libraries

You can restrict write access to your mzVault libraries. When you open a restricted library for editing, the Lock icon on the Build toolbar indicates that the library is locked.

Locked **Unlocked**

Note You cannot merge password-secured libraries. You also cannot select a password-secured library as the destination library when importing NIST or MassBank records.

To manage the password security feature, see these topics:

- Restricting Write Access to a Library
- Unlocking a Restricted Library for Editing
- Changing the Password or Removing the Password Security

Restricting Write Access to a Library

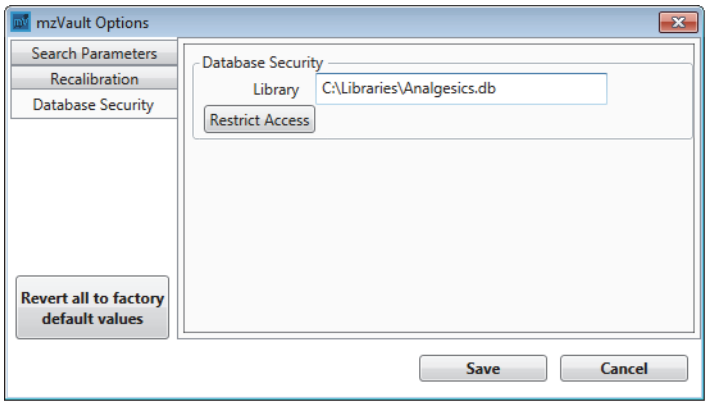
❖ **To restrict write access to an mzVault library**

1. Open a library with read/write access.
2. From the application window, choose **Menu > Options**.

   The mzVault Options dialog box opens.
3. In the left pane, select **Database Security** to display the Database Security page.

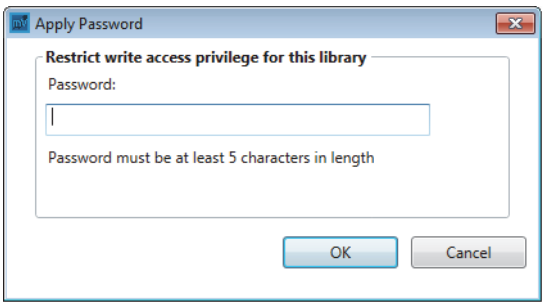
   The Library box displays the name and location of the open library.

   Figure 39. Database Security page of the mzVault Options dialog box



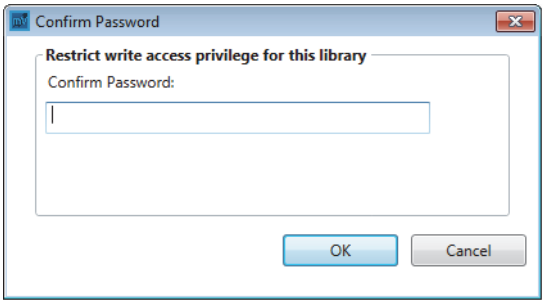
4. Click **Restrict Access**.
5. In the Apply Password dialog box, enter a password from 5 to 15 characters in length, and then click **OK**.

   Figure 40. Apply Password dialog box



6. In the Confirm Password dialog box, reenter the same password, and then click **OK**.

Figure 41. Confirm Password dialog box



7. At the bottom of the mzVault Options dialog box, click **Save**.

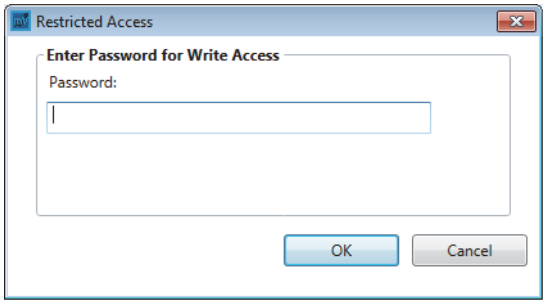
Unlocking a Restricted Library for Editing

To edit a library with restricted access, you must unlock it or remove its password security.

❖ To unlock a restricted library

1. In the Build toolbar, click the **Lock** icon,  .
2. In the Restricted Access dialog box, enter the password and click **OK**.

Figure 42. Restricted Access dialog box



Changing the Password or Removing the Password Security

If you know the password to open a library with restricted access, you can change the password or remove the password security.

❖ To change the password or remove the password security for a restricted library

1. In the Build toolbar, click the **Lock** icon to unlock the library.
2. From the application window, choose **Menu > Options**.

   The mzVault Options dialog box opens.

3. In the left pane, select **Database Security**.

   The Library box displays the name and location of the open library.

4. In the Database Security area, click **Manage Access**.
5. In the Change Password dialog box, do one of the following:

   - To change the password, type a different password and click **OK**. Then, in the Confirm Password dialog box, reenter the new password and click **OK**.

   –or–

   - To remove the password security and grant read/write access to all users, delete the password, and then click **OK**. At the prompt, click **Yes**.

6. At the bottom of the mzVault Options dialog box, click **Save**.

mzVault Options Dialog Box

These topics describe the parameters on the two pages of the mzVault Options dialog box:

- Default Library Search Parameters Page
- Parameters on the Default Recalibration Parameters Page

Default Library Search Parameters Page

Table 18 describes the parameters on the Default Library Search Parameters page of the mzVault Options dialog box. The default values for these parameters are the factory default values.

For information about opening this page and setting up the default parameter values, see "Setting the Default Library Search Parameters" on page 79.

Table 18. Default Library Search Parameters page parameter descriptions (Sheet 1 of 4)

Parameter	Description
mzVault Search	
Libraries	Specifies the default libraries to search (see "Starting a Search Workflow from the Search Tab" on page 9). You can select up to five libraries.

Table 18. Default Library Search Parameters page parameter descriptions (Sheet 2 of 4)

Parameter	Description
Hits	Specifies the number of top-matching results to display in the Search Results pane of the Search page. If you select multiple libraries, the number of hits means the number of results per library. For example, if you select two libraries and the search returns 200 results for each of them, and the Hits option is set to 50, the total results displayed is 100 (50 from the first library and 50 from the second library). Default: 100
Score Cutoff	Specifies the score below which to filter out results.
Search Options	
Search	• Forward: Conducts a forward search. The application searches the query spectrum against each library spectrum. If the query spectrum includes a peak that is not in a given library spectrum, the match score is negatively affected. Use a forward search when the query spectrum is of high quality—that is, when it has good fragmentation and few low-intensity background peaks. • Reverse: Conducts a reverse search, which searches each library spectrum against the query spectrum. If the query spectrum does not include peaks that are in the library spectrum, the match score is negatively affected, but the presence of additional peaks in the query spectrum has no effect on the score. Use a reverse search if the query spectrum includes peaks from several components or has a lot of background noise.

Table 18. Default Library Search Parameters page parameter descriptions (Sheet 3 of 4)

Parameter	Description
Query Spectrum	
Intensity Threshold On/Off	Determines whether the mzVault application ignores peaks in the query spectrum that are below the specified intensity threshold. • (Default) On: Ignores peaks in the query spectrum that are below the specified value. • Off: Does not ignore any peaks in the query spectrum. If you turn on the intensity threshold feature, the following options appear: • (Default) Automatic: Uses a proprietary algorithm to calculate the threshold value. • Manual: Select to manually specify the threshold value in the Query Spectrum area of the Search toolbar.
Ignore Precursor	When selected (orange), the search ignores (removes from consideration) mass peaks within 2.2 Da of the precursor ion's *m/z* value in the query spectrum; that is, the match score is not negatively affected if the library spectrum does not include a mass peak within 2.2 Da of the *m/z* value for the precursor ion.
Fragment Tolerance	Indicates how to specify the fragment tolerance. If you select Manual, enter the tolerance value in the adjoining box. The fragment tolerance is a mass value, either absolute (mmu or amu) or relative (ppm), that determines whether a mass peak in the query spectrum has the same mass within the specified tolerance as a mass peak in a library spectrum. • (Default) Automatic: Uses the native instrument precision to determine the tolerance. • Manual: Select to specify the mass value of the tolerance in parts per million (ppm), millimass units (mmu), or atomic mass units (amu). Default: 10.0 ppm, 10.0 mmu, or 0.05 amu

Table 18. Default Library Search Parameters page parameter descriptions (Sheet 4 of 4)

Parameter	Description
Scores	
High Res Score	Determines whether the application computes the score calculated by a proprietary algorithm that indicates how well the library spectrum and the query spectrum match. • (Default) Selected: Displays the score calculated by a proprietary algorithm. • Cleared: Does not display the score calculated by a proprietary algorithm.
OptDp Score	Determines whether the application displays the score calculated by an optimized dot product algorithm that indicates how well the library spectrum and the query spectrum match. • Selected: Displays the optimized dot product score. • (Default) Cleared: Does not display the optimized dot product score.
NIST Score	Determines whether the application computes the score calculated by a National Institute of Standards and Technology algorithm that indicates how well the library spectrum and the query spectrum match. • Selected: Displays the NIST score. • (Default) Cleared: Does not display the NIST score.
All Scores	Determines whether the application computes the scores calculated by all algorithms. • Selected: Displays all scores. • (Default) Cleared: Does not display all scores.
Revert All to Factory Default Values	Resets all the parameters on both the Default Library Search Parameters page and the Default Recalibration Parameters page to the values in place when the mzVault software was installed.
Revert to Factory Default Values	Resets all the parameters on the Default Library Search Parameters page to the values in place when the mzVault software was installed.

Parameters on the Default Recalibration Parameters Page

Table 19 describes the parameters on the Default Recalibration Parameters page of the mzVault Options dialog box. The default values for these parameters are the values in place when the mzVault software was installed.

Table 19. Parameters on the Recalibration page of the mzVault Options dialog box (Sheet 1 of 7)

Parameter	Description
Intensity Threshold Theory (%)	Specifies a threshold (as a percentage) to define which peaks of the isotope pattern to use in determining the spectral distance. The recalibration algorithm uses only the peaks with relative intensity higher than the set threshold for the spectral distance calculation. This threshold value applies only when you clear the Automatic Intensity Threshold option. Valid range: 0.00–10 000.00 Default: 0.10

Table 19. Parameters on the Recalibration page of the mzVault Options dialog box (Sheet 2 of 7)

Parameter	Description
RDB Equiv Min. and Max.	Specifies a range of values for double bonds and ring equivalents—a measure of the number of unsaturated bonds in a compound—that limits the calculated formulas to only those that make sense chemically. Limits range: –1000.0 to 1000.0 Default minimum value: –0.5, corresponding to a protonated, saturated compound Default maximum value: 100.00 The value is calculated by the following formula: $$D = 1 + \frac{\left[\sum_{i}^{i\max} Ni\,(Vi - 2)\right]}{2}$$ where: • D is the value for the RDB equivalents • $i$max is the total number of different elements in the composition • Ni is the number of atoms of element i • Vi is the valence of atom i The calculation produces an integer such as 3, which indicates an odd-electron ion, or a number with a remainder of 0.5, which indicates an even-electron ion.

Table 19. Parameters on the Recalibration page of the mzVault Options dialog box (Sheet 3 of 7)

Parameter	Description
Zero Fit Expected Error	Specifies a value to calibrate the conversion from the measured distance to a 0 percent spectral fit. The elemental composition algorithm computes the difference between isotopic patterns as a distance value. Usually, the algorithm converts the distance of one or higher to a 0 percent spectral fit (the patterns are completely different). You can set this parameter to a different value to calibrate the conversion. If the distance is higher than your set value, the algorithm determines that the spectral fit is 0 percent. Valid range: 0.00–10 000.00 Default: 1.00
Expected Intensity Error (%)	Specifies a value for the allowed intensity deviation of an isotope peak as a percentage of its theoretical intensity, relative to the monoisotopic ion. The elemental composition algorithm considers an isotope peak as not found if its relative intensity deviates by more than this percentage. Valid range: 0.00–10 000.00 Default: 10.00 **Tip** For best results, set this value to a number that causes up to 98 percent of all intensity deviations to be smaller than the allowed intensity deviation value.
Centroid Algorithm	Select the algorithm to use to generate the centroid spectrum. Select from these options: • (Default) FTOrbitrap • TSQ • GCQ • MAT

Table 19. Parameters on the Recalibration page of the mzVault Options dialog box (Sheet 4 of 7)

Parameter	Description
Missing Packet Penalty Mode	Select a penalty for each missing peak. A missing peak means that the elemental composition algorithm found no measured packet within the mass and intensity window, when the algorithm compares the theoretical isotope pattern of a candidate to the measured isotope pattern. Select from these options: • 1 Std Dev: Low penalty • 4 Std Dev: Medium penalty • 16 Std Dev: High penalty • (Default) Closest Match: The penalty is the distance between the theoretical packet and the closest measured packet outside the mass and intensity window. • Automatic: For Orbitrap™ or Fourier Transform (FT) spectra, the algorithm automatically applies a penalty depending upon the S/N ratio of the missing peak. – For a peak slightly above noise, it applies the low penalty. – For a peak highly above noise, it applies the high penalty. – For all other peaks, it applies the medium penalty. For other types of spectra, the algorithm automatically applies the medium penalty.
Absolute Intensity Error	Determines whether the intensity error is absolute. The error value is the difference between the theoretical and measured intensities of a peak. • (Default) Selected: Specifies that the intensity error is absolute. • Cleared: Specifies that the intensity error is relative.

Table 19. Parameters on the Recalibration page of the mzVault Options dialog box (Sheet 5 of 7)

Parameter	Description
Weight Intensity Error by Abundance	Select the check box to specify whether the observed intensity error on an isotope peak depends on its abundance. • (Default) Selected: An observed intensity error on a 10 percent BPI (base peak intensity) peak counts only a tenth of the same error on the base peak. • Cleared: An observed intensity error on a 10 percent BPI peak is equal to the same error on the base peak.
Use Representative Elements	Determines whether the application uses the Representative Elements table or the Protein Elements table for the recalibration calculations. • (Default) Selected: Uses the Representative Elements table. • Cleared: Uses the Protein Elements table. Currently the recalibration algorithm supports two types of element tables, differing mainly in their carbon (C) abundances. • The Representative Elements table has the following C abundances: – 12C: 0.9893 – 13C: 0.0107 • The Protein Elements table has the following C abundances: – 12C: 0.989136445 – 13C: 0.010863555
Mass Tolerance	Specifies a mass tolerance to restrict the number of possible elemental compositions. The recalibration algorithm returns recalculated *m/z* values for each peak (labeled with an asterisk *) only if the calculated mass matches the experimental mass within the specified mass tolerance. Valid range: 0.00–1000.00 ppm, 0–10.00 amu Default: 20.00 ppm

Table 19. Parameters on the Recalibration page of the mzVault Options dialog box (Sheet 6 of 7)

Parameter	Description
Hundred Fit Expected Error	Specify a value to calibrate the conversion from the measured distance to a 100 percent spectral fit. The elemental composition algorithm computes the difference between isotopic patterns as a distance value. Usually, the algorithm converts the distance of zero to a 100 percent spectral fit (the patterns are identical). You can set this parameter to a different value to calibrate the conversion. If the distance is between zero and your set value, the algorithm determines that the spectral fit is 100 percent. Valid range: 0.00–10 000.00 Default: 0.20
Expected Mass Error (ppm)	Specify a value (in ppm) to define the allowed mass deviation in the spectrum data. The elemental composition algorithm considers an isotope peak as found if its measured *m/z* is less than this amount away from the theoretical *m/z* for that isotope. Range: 0.00–10 000.00 Default: 10.00 ppm **Tip** For best results, set this value to a number that causes up to 98 percent of all mass deviations to be smaller than the allowed mass deviation value.
Nitrogen Rule	Determines whether and how to use the Nitrogen Rule. • (Default) Do Not Use: Do not use the Nitrogen Rule. • Even Electron Ions: Choose for even-electron ions, such as protonated species. • Odd Electron Ions: Choose for odd-electron ions, such as radical cations.

Table 19. Parameters on the Recalibration page of the mzVault Options dialog box (Sheet 7 of 7)

Parameter	Description
Normalization Mode	Select a normalization mode from the following options: • Base peak: Specifies the most common normalization mode. Its disadvantage is the propagation of the intensity error of the base peak to all isotope intensities. • Linear: Normalizes the theoretical and measured patterns so that the sum of all isotopic pattern intensities is the same. • (Default) Quadratic: Normalizes the theoretical and measured patterns so that the error squares (intensity differences) are minimized.
Automatic Intensity Threshold	Select the check box if the data for analysis is from an Orbitrap or Fourier Transform (FT) instrument and contains noise values. • Selected: The recalibration algorithm automatically sets the intensity threshold for the spectral distance calculation to use only the peaks from the theoretical pattern with a S/N ratio > 3. • (Default) Cleared: Does not set an intensity threshold.
Weight Mass Error by Abundance	Specifies whether the observed mass error on an isotope peak depends on its abundance. • (Default) Selected: An observed mass error on a 10% BPI (base peak intensity) peak is weighted a tenth of the same error on the base peak. • Cleared: An observed mass error on a 10% BPI peak is weighted equally as the same error on the base peak.
Revert to Factory Default Values	Resets all the parameters on the Default Recalibration Parameters page to the values in place when the mzVault software was installed.

Index

A

A column 53
Absolute Intensity Error parameter 91
Add button, Compound List toolbar 52
Add button, Compound toolbar 48
Adduct column 53
Adduct parameter 55
adducts 48, 53, 55
Adducts parameter 48
All Scores parameter 87
Apply button, Search toolbar 64, 67, 72
Apply Database To options 8
Apply Password dialog box 82
arranging windows, tool for 13
arrows, directional 13
Automatic Intensity Threshold parameter 94
Automatic parameter 48
Automatic setting 63, 86
Averaged Spectra parameter 54
averaging spectra 2, 34

B

base peak chromatograms 61, 76
Browse tab
  Library Spectrum pane 21
  Library Statistics pane 21–22
  MOL Structure pane 22
  purpose 1
Browse toolbar 20
  displaying subset of data records 18
  Library Spectrum button 21
  MOL Structure button 21
  parameters 20
browse/build workflow, starting 8
Build tab
  exporting spectra to CSV files 44
  parameters 45
  purpose 2
  saving libraries 45
Build toolbar 46–47
Build workflow 2

C

CAS ID column 49, 72
Centroid Algorithm parameter 90
centroid spectrum 90
Change Password dialog box 84
Charge column 53
charge of the precursor ion 48, 53, 55
Charge parameter 55
Charge parameter, Compound toolbar 48
ChemSpider ID column 50
ChemSpider online data repository 50
Chromatogram Options pane 32, 60, 75
Chromatogram pane 32, 60–61
Chromatogram parameter 76
chromatograms
  base peak 61, 76
  copying 14
  target mass 61, 76
  total ion current (TIC) 61, 76
Classic Score column 73
Clipboard 14
Collision Energy column 50
Compound Class column 49, 72
Compound column 49, 53, 72
Compound ID column 50, 72
compound list 36, 40
Compound List pane 21
  columns on 29, 49
  displaying subsets of data 18
Compound List tab
  New_Compound List page 37
  parameters 51

Compound List toolbar 11, 52
Compound Matches setting 75
Compound tab 47
Compound toolbar 11, 48
compounds
  adding spectra to 48
  adding to compound list 52
  adding to libraries 47
  copying 47
  copying to compound list 52
  deleting from compound list 52
  deleting from libraries 47
  deleting spectra from 48
Confirm Password dialog box 83
contacting us ix
Contributor column 51
Copy button, Build toolbar 45, 47
Copy button, Compound List 52
copying a selected data record 44
creating a compound list file 36
Creation Date column 51
CSV files 3, 44, 47
curated spectra 2
Curated Spectrum pane, location 32
curation order 32
Curator column 51

D

data records
  adding 28
  deleting 27
  displaying subset of 18
Database setting 75
default library search parameters 2
Default Library Search Parameters page 79, 84
default recalibration parameters 2, 80
Default Recalibration Parameters page 80, 88
Delete button, Build toolbar 47
Delete button, Compound List 52
Delete button, Compound toolbar 48
Delta Mass column 73
diamond pattern tool 13
Difference Spectrum pane 77
directional arrows 13
displaying or hiding table columns 14
documentation
  accessing vii
  additional vii
double bonds 89
downloading documents viii
dragging panes 13

E

Enter Chemical Formula parameter 55
Enter Precursor m/z parameter 55
Entry No. Name column 49, 72
Excel (XLSX) files 3, 72
Exit icon 7
Expected Intensity Error (%) parameter 90
Expected Mass Error (ppm) parameter 93
Export button, Build toolbar 44, 47
Export CSV - Options dialog box 44
Export Results button, Search toolbar 67, 72
exported search results file 67
exporting search results 66
exporting spectra to CSV files 44

F

F parameter 77
Field Chooser dialog box 14
file name, exported spreadsheet file 67
file types 3
Filter button, Browse toolbar 21
Filter column 50, 73
Filter Mass parameter 61, 76
Filter parameter 61, 71, 75
Filter setting 75
Filter Text setting 75
First Page icon 21
Formula column 49, 53, 72
Formula or Precursor column 38, 53
Formula parameter 55
forward search 85
Fourier Transform (FT) mass spectrometers 94
Fragment Tolerance parameter 63, 86
Fragment Tolerance setting 74
Fragmentation Mode column 51

G

getting started 5, 7
guide tool 13

H

header of Query Spectrum pane 77
High Res Score column 72–73
High Res Score parameter 87
HighChem 50
Hits parameter 63, 85

Hits setting 75
HMDB ID column 50
Human Metabolome Database (HMDB) online data repository 50
Hundred Fit Expected Error parameter 93

I

Ignore Precursor parameter 63, 86
Import button, Build toolbar 46
Import dialog box 26
importing files 25
input files, file types 3
Instrument Name column 51
Intensity Threshold parameter 63, 86
Intensity Threshold setting 74
Intensity Threshold Theory (%) parameter 88
Ionization Mode column 51

K

KEGG ID column 50
Kekulé diagram 22
Kyoto Encyclopedia of Genes and Genomes (KEGG) online data repository 50

L

landing page 6–8
Last icon 21
libraries
  adding a spectrum to an existing compound 31
  adding compounds to 47
  closing 17
  copying chromatograms or spectra 14
  copying compounds 47
  creating automatically from a compound list 36
  default parameters for searching 79
  deleting compounds from 47
  displaying subset of data records 18
  exporting data records from 47
  exporting spectra to CSV files 44
  importing files 25
  manually adding data records 28
  merging 46
  opening existing 15
  saving 47
  saving under a new name 45
  searching for a spectrum 64
  searching multiple at the same time 58
  selecting a spectrum 61
  selecting to search 58
library database (DB) files 3, 58, 73
Library File column 73
Library parameter 71, 84
Library Search page 64
Library Spectrum button, Browse toolbar 21
Library Spectrum pane 21, 77
Library Statistics button, Browse toolbar 21
Library Statistics pane 21–22
Library_name page 15, 17
Library_name Search Results page 68

M

m/z parameter 77
Manage Access button, Database Security page 84
Manual parameter 48
Manual setting 63, 86
Mass Analyzer column 51
Mass Tolerance parameter 92
MassBank 46
MassBank text (TXT) files 3
Merge button, Build toolbar 46
Merge Libraries dialog box 26
merging libraries 26
Minimum NL parameter 42, 55
Missing Packet Penalty Mode parameter 91
MOL File button, Compound toolbar 49
MOL File column 38, 54
MOL File URL column 38, 54
MOL files 38, 49, 54
MOL Structure button, Browse toolbar 21
MOL Structure pane 21–22, 77
MOL structure, adding 35
Most Intense Spectra parameter 54
multiple libraries 85
Multi-Search page 64
Multi-Search_number page 58
mzCloud database 50, 72
mzCloud ID column 50
mzCloud URL column 50
mzVault application
  automatically creating a library 36
  browsing a library 15
  closing libraries 17
  creating a compound list 36
  curating spectra 2
  displaying a subset of records in the Compound List pane 18
  exporting compounds or spectra to a CSV file 44
  exporting search results 66
  features 1
  inputs 3

managing libraries 23
manually adding data records to a library 28
opening a compound list 40
opening existing libraries 15
outputs 3
saving libraries 45
searching for a spectrum in a library 57, 64
selecting a spectrum 61
selecting libraries to search 58
setting default library search and recalibration parameters 2
setting default library search parameters 79
setting default recalibration parameters 80
setting the search parameters 62
viewing the search results 64
workflows available 1
mzVault icon 6
mzVault Options dialog box 79–80, 84
mzVault window 6

N

Neutral Mass column 50, 73
New button, Build toolbar 29, 46–47
New Compound List button, Build toolbar 36, 47
New Search icon 67, 72
New_Compound List button 47
New_Compound List page 37
Next icon 21
NIST Score column 73
NIST Score parameter 87
Nitrogen Rule 93
Nitrogen Rule parameter 93
NL parameter 77
Normalization Mode parameter 94
Number of Compounds setting 75
Number of Spectra setting 75

O

Open button, Browse toolbar 15, 21
Open Compound List button, Build toolbar 47
Open dialog box 60
Open Raw File button, Compound toolbar 32, 48
Open Raw File icon 59, 67, 72
OptDp Score column 73
OptDp Score parameter 87
Orbitrap mass spectrometers 94
order for curation 32
output files 3

P

password
changing 84
entering 83
password security
adding 82
removing 84
peptides 73
PeptideSequence column 50, 73
polarity 38, 50, 54
Polarity column 38, 50, 54
Precursor m/z column 50, 54, 73
Precursor m/z parameter 55
Precursor m/z setting 75
Precursor Mass setting 74
Precursor Tolerance parameter, Spectrum Selection Parameters dialog box 42, 55
Precursor Tolerance setting 75
Previous icon 21
Process List button, Compound List toolbar 43, 53
Processing Parameters dialog box 55
Protein Elements table 92
PubChem ID column 50
PubChem online data repository 50

Q

Query Scan parameter 74
Query Spectrum pane 60–61, 63
Query Spectrum parameter 74
Quick Create pane 40

R

R column 53
raw data files 38
displaying chromatogram of data in 76
displaying information in panes of the Search page 60
displaying name 74
displaying name and URL 73
displaying name of 77
inputs to mzVault application 3
opening on the Compound List pane 38
opening on the Compound tab 32, 48
opening on the Search tab 67
retention time 73
scan filter in 73
scan number 73
searching for spectra in 53
Raw File column 38, 53
Raw File parameter 74
Raw File URL column 38, 51, 53, 73

Raw Spectrum pane 32
RDB Equiv Min. and Max. parameters 89
Recalibrate button, Compound List toolbar 42, 48, 53
recalibrating spectra 2, 48, 53
Records list 17
Records parameter 21
Redo Zoom command 14
Relative Intensity parameter 76–77
Representative Elements table 92
Reset button, Compound toolbar 49
resetting chromatogram scaling 14
retention time 73
Retention Time column 50, 73
Retention Time Range boxes 34
Retrieve One Spectrum for Each Unique Collision Energy option 41
Retrieve One Spectrum for Each Unique Collision Energy parameter 54
Retrieve Only One Best Spectrum Per Compound option 41
Retrieve Only One Best Spectrum Per Compound parameter 54
reverse search 85
Revert All to Factory Default Values parameter 87
Revert to Factory Default Values parameter 87, 94
ring equivalents 89
RT (min) parameter 76
RT parameter 77

S

Save As button, Build toolbar 47
Save As button, Compound List toolbar 52
Save As dialog box 46–47
Save button, Build toolbar 47
Save button, Compound List 52
saving libraries 45
scan filter 73
scan number 73, 77
Scan Number column 50, 73
Score Cutoff parameter 63, 85
Score Cutoff setting 75
Search page
  Chromatogram Options pane 60
  Chromatogram pane 60
  copying a chromatogram or spectrum 14
  Query Spectrum pane 60
  searching for a spectrum 64
  selecting a spectrum 61
Search parameter 85
Search Parameters parameter 75
Search Results page 67
Search Results pane 64
Search Results parameter 75
Search Summary pane 74
Search tab
  parameters 70
  purpose 2
Search Type setting 75
Search workflow 2
Select Libraries button, Search toolbar 58
spectra
  adding to compounds 31
  copying 14
  displaying for a compound 64
  exporting to a CSV files 44
  recalibrating 48, 53
  searching for 53, 64
  selecting 61
  thresholding 48, 53
spectra, averaging 34
Spectrum ID column 50, 73
Spectrum Matches setting 75
Spectrum Selection Parameters button 52
Spectrum Selection Parameters dialog box 52, 54
start-up behavior 5
Status column 53

T

T column 53
table columns, displaying or hiding 14
Tag column 50
target mass chromatograms 61, 76
Thermo Scientific website, user documents viii
Threshold button, Compound List toolbar 42, 53
Threshold button, Compound page 48
thresholding
  automatically 48
  manually 48
thresholding spectra 2, 48, 53
Time Range parameter 61, 76
tool, guide or position 13
toolbars
  Browse toolbar 20
  Build toolbar 46
  Compound List toolbar 52
  Compound toolbar 48
  Search toolbar 71
total ion current (TIC) chromatograms 61, 76
Trace Type parameter 61, 76
two-dimensional structure, adding 35

U

Use Representative Elements parameter 92

V

Version Number column 51

W

Weight Intensity Error by Abundance parameter 92
Weight Mass Error by Abundance parameter 94
window position tool 13
write access, restricting 82

X

XML files 3, 40, 47, 52

Z

Zero Fit Expected Error parameter 90