

Thermo Xcalibur

Library Browser

User Guide

Creating and Searching Spectral Libraries

Software Version 4.5

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General Laboratory Equipment. Not intended for use in diagnostic procedures.

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Preface

The Thermo Xcalibur™ mass spectrometry data system includes all the software needed to create, search, and edit libraries. This guide describes the following:

- How to create and edit custom libraries for MS, MS/MS, or MSⁿ spectra
- How to manage multiple libraries
- How to search multiple libraries

Contents

- [Related Documentation](#)
- [Special Notices](#)
- [Contacting Us](#)

Related Documentation

Thermo Fisher Scientific provides these guides for the Xcalibur data system:

- *Xcalibur Quick Start Guide*
- *Xcalibur Getting Started Guide*
- *Xcalibur Data Acquisition and Processing User Guide*
- *Xcalibur Quan Browser User Guide*
- *Xcalibur Qual Browser User Guide*
- *Xcalibur Library Browser User Guide*
- *XReport User Guide*

Help is available from within the Xcalibur data system and the National Institute of Science and Technology (NIST™) Mass Spectral Search application.

❖ To view the product manuals

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

- To access the Xcalibur manual set, do one of the following:
 - From the computer taskbar, choose **Start > All Programs** (Windows 7) > **Thermo Scientific Xcalibur** (Windows 10 and Windows 7) > **Manuals** (Windows 7).
 - From the Xcalibur home page – Roadmap view, choose **Help > Manuals**.
- To access the manual set for the Thermo Scientific mass spectrometer from the computer taskbar, choose **Start > All Programs** (Windows 7) > **Thermo Instruments** (Windows 10 and Windows 7) > *mass spectrometer*.

❖ To view user documentation from the Thermo Fisher Scientific website

1. Go to thermofisher.com.
2. Point to **Services & Support** and click **Manuals** on the left.
3. In the Refine Your Search box, search by the product name.
4. 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.

❖ To view Help

- From the application window, choose **Help > *product-name* Help** or press the F1 key.
- In applications that have a Communicator bar, click a field or parameter to display definitions, required actions, ranges, defaults, and warnings.

Special Notices

Make sure you follow the precautionary statements presented in this guide. The special notices appear in boxes.

Special notices include the following:

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.		

Overview of Library Browser

This chapter gives a brief overview of the Library Browser window and a summary of the steps for creating, editing, and searching custom libraries and printing the library search reports.

Contents

- [Library Browser Process Overview](#)
- [About Library Browser](#)

Use the Xcalibur Library Browser window to do the following:

- Create spectral libraries, including MS/MS fragmentation libraries.
- Run automatic or manual, post-acquisition library searches on MS/MS fragmentation spectra.

Note Throughout this guide, the term *Library Browser* is used synonymously with the term *NIST MS Search* (National Institute of Standards and Technology Mass Spectral Search Program and Library System) to refer to the NIST MS Search desktop.

Library Browser Process Overview

Figure 1 provides a summary of the steps you perform to create, edit, and search libraries and to print reports using the Xcalibur data system.

When using the Library Browser, you can export a spectrum from the Qual Browser window to create a custom user library of MS/MS or MSⁿ spectra, one entry at a time. To include a spectrum in a library, open a raw data file¹ in Qual Browser. Enhance a spectrum by averaging several scans and by subtracting background scans. Then, export the spectrum to Library Browser. See [Exporting Spectrum Files to Library Browser](#) for more information about this process.

After exporting the spectrum to Library Browser, you can edit the spectrum information. For example, you can change the name of the entry or specify the molecular weight or the CAS (Chemical Abstract Service) registry number. You can even attach a chemical structure to the library entry or select which mass-to-charge ratios to include. See [Managing Libraries](#) for more information.

IMPORTANT For MS/MS and MSⁿ spectra, however, do not delete any of the masses that the data system detects because the presence of a particular mass-to-charge ratio, rather than its intensity, is essential to identifying a compound.

Finally, the Xcalibur data system provides three ways to search libraries and print custom reports:

- Automatically, by batch reprocessing data files in Sequence Setup with an appropriate processing method (See [Setting Up and Running Automated Library Searches](#) for more information.)
- Manually, by using a single spectrum in Qual Browser (See [Submitting a Spectrum to a Library Search in Qual Browser](#) for more information.)
- Manually, by exporting a spectrum to Library Browser (See [Exporting Spectrum Files to Library Browser](#) for more information.)

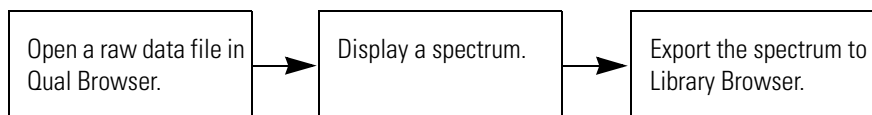
To print custom reports during sequence processing or batch reprocessing, you must select an appropriate report template in the processing method. In addition, you can set up the processing method to automatically export spectra to a user library in Library Browser during sequence processing or batch reprocessing.

To print a custom report following a manual library search in the Qual Browser or Library Browser window, choose **File > Print** from the Qual Browser menu bar or **File > Print Report** from the Library Browser menu bar.

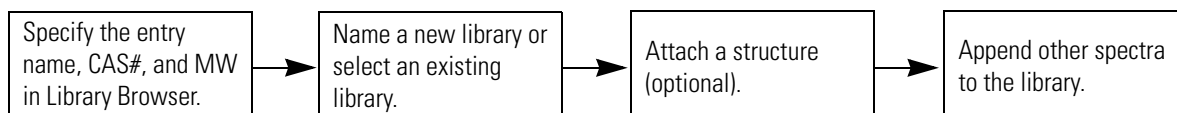
¹ A raw data file is an unprocessed data file acquired from a Thermo Scientific instrument controlled by the Xcalibur data system or equivalent application.

Figure 1. Library Browser process overview

Create a Library Spectrum

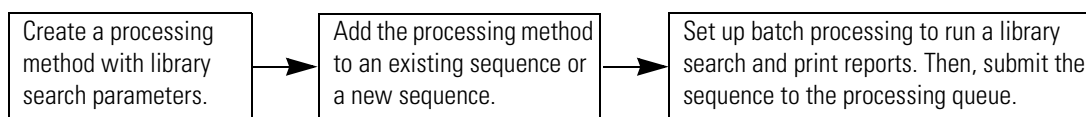


Create a Library or Add to an Existing Library

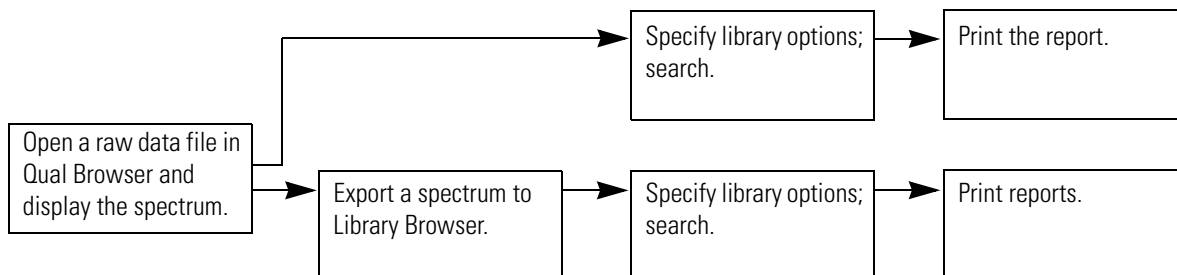


Search Libraries and Print Reports

Automatically, using RAW or RST files



Manually, using a single spectrum



About Library Browser

The Xcalibur data system uses the NIST Mass Spectral Search Program and Library System.

Note Thermo Fisher Scientific provides the NIST Mass Spectral Search Program (version 2.0f) with the Xcalibur data system.

The NIST libraries give access to the following:

- An extensive collection of chemical names
- Chemical Abstracts Service (CAS) registry numbers
- Molecular formulas and weights
- Chemical structures

You can create user libraries using spectra from the following sources:

- Exported from Qual Browser
- Exported automatically during sequence processing or batch reprocessing
- From other sources including text files

The program permits searches in many different ways:

- Find reference spectra that most closely match a submitted spectrum.
- Locate spectra or compounds that have certain specified characteristics (for example, the abundance of certain peaks).
- Display the mass spectra of selected molecules.

For information about the features of the NIST Mass Spectral Search application, see the Help system provided with the application.

Exporting Spectrum Files to Library Browser

The Xcalibur data system includes a subset of the NIST mass spectral library called nistdemo. The NIST/EPA/NIH Main Library contains more than 100 000 compounds with MS spectra obtained primarily in the electron ionization (EI) scan mode.

The following procedures show how to export a spectrum file to the Library Browser window using one of the steroid.raw data files in the following folder:

drive:\Xcalibur\examples\data

Follow these procedures to export spectrum files from Qual Browser to Library Browser or to add spectrum files to an existing library during sequence processing or batch reprocessing.

Contents

- [Opening a Raw Data File in Qual Browser](#)
- [Viewing a Spectrum in Qual Browser](#)
- [Subtracting Background Spectra](#)
- [Manually Exporting Spectrum Files from Qual Browser](#)
- [Exporting Spectrum Files Automatically During Sequence Processing](#)

Opening a Raw Data File in Qual Browser

This procedure describes how to open a raw data file in the Qual Browser window. Open the example raw data file, steroids14.raw, or a representative raw data file with a spectrum or spectra of interest.

❖ To open a raw data file in the Qual Browser window

1. Open the Qual Browser window by doing one of the following:

- On the Xcalibur Roadmap view, click the **Qual Browser** icon, .

—or—

- On the Xcalibur Roadmap menu bar, choose **GoTo > Qual Browser**.

2 Exporting Spectrum Files to Library Browser

Opening a Raw Data File in Qual Browser

2. Open a raw data file as follows:

- a. Choose **File > Open** from the menu bar or click the **Open** icon, , in the toolbar.

The Open Raw File dialog box opens.

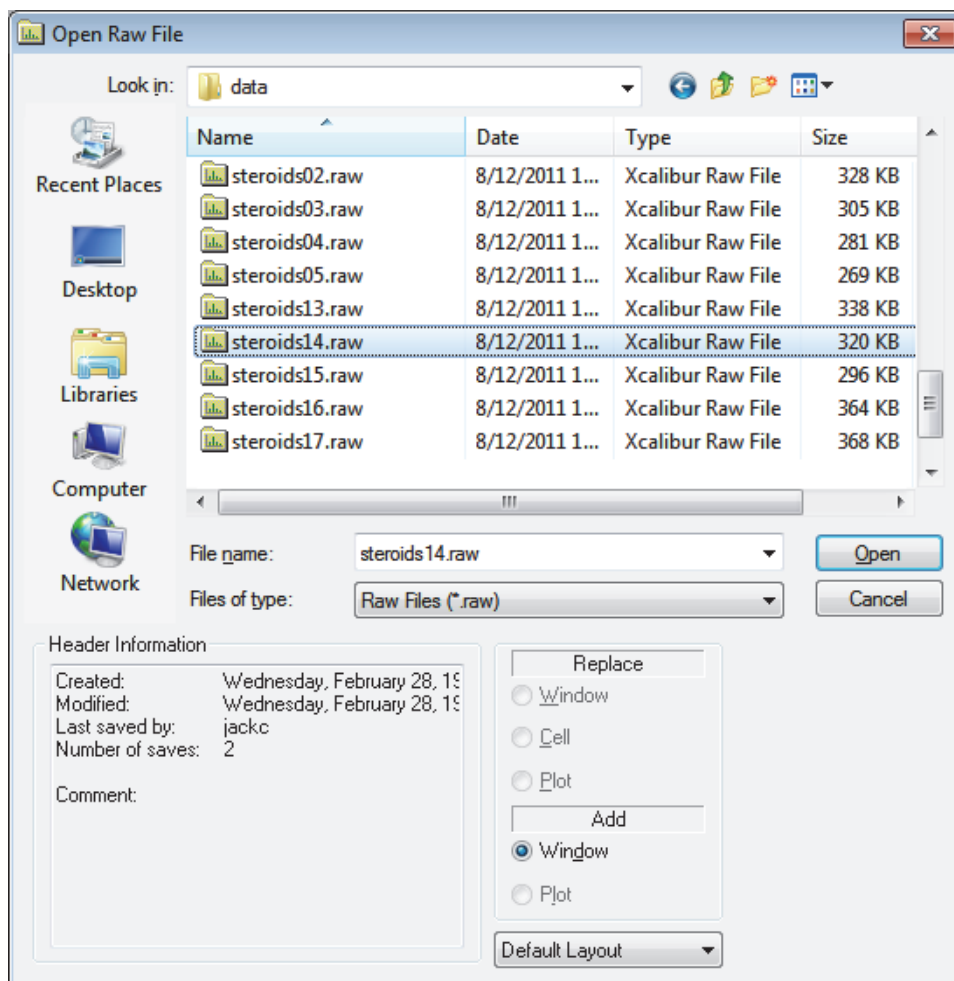
- b. Browse to the location of the raw data file (Figure 2):

drive:\Xcalibur\examples\data

- c. Select one of the steroids.raw files or a raw data file that you want to export a spectrum from.
- d. In the list at the bottom of the dialog box, select **Default Layout**.

The default layout provided with the Xcalibur data system displays a two-cell grid with a chromatogram view and a spectrum view. The chromatogram view displays the total ion chromatogram (TIC) and the spectrum view displays the spectrum from the initial time point (RT = 0.0 minutes).

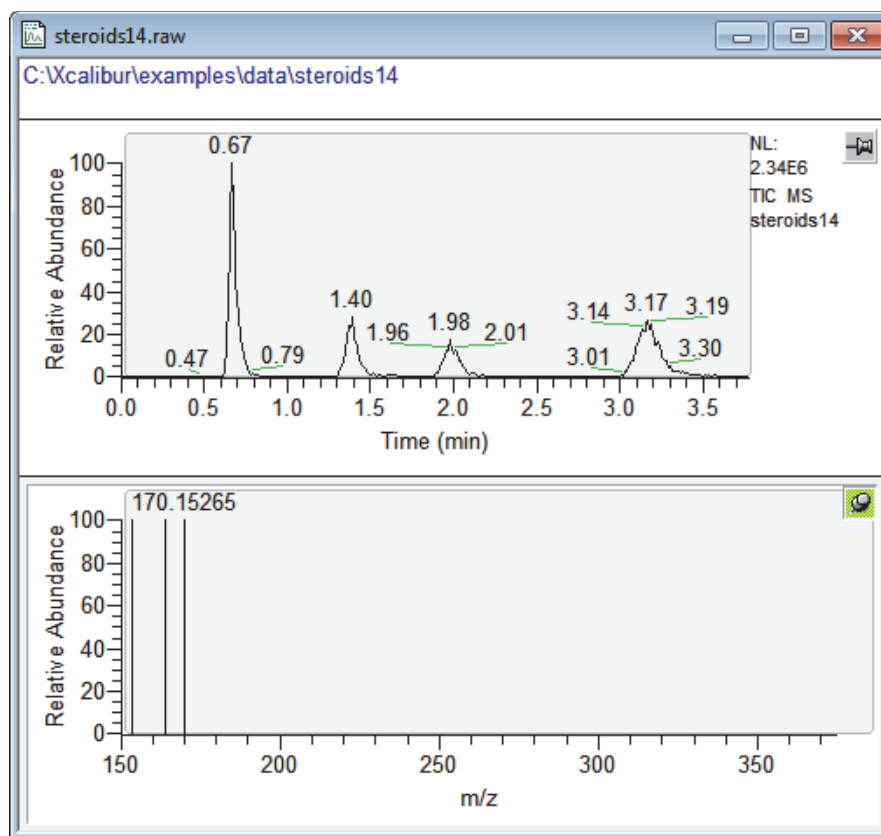
Figure 2. Open Raw File dialog box with the selection of steroid14.raw



- e. Click **Open**.

The TIC chromatogram and the first mass spectrum for this data file appear in the grid (Figure 3).

Figure 3. Default layout for a raw data file



Go to the next procedure, [Viewing a Spectrum in Qual Browser](#).

Viewing a Spectrum in Qual Browser

To view the mass spectrum of interest, use the interactive cells of the Qual Browser window. The following procedure describes how to set up a four cell layout with the following views: chromatogram, spectrum, scan filters, and averaged spectrum.

❖ To display the mass spectrum of interest

1. Beginning with the default layout of two cells in the grid, with the upper cell displaying a chromatogram view and the lower cell displaying a spectrum view, add two more cells to the grid:

- In the toolbar, click the **Insert Cells Left** icon, .

—or—

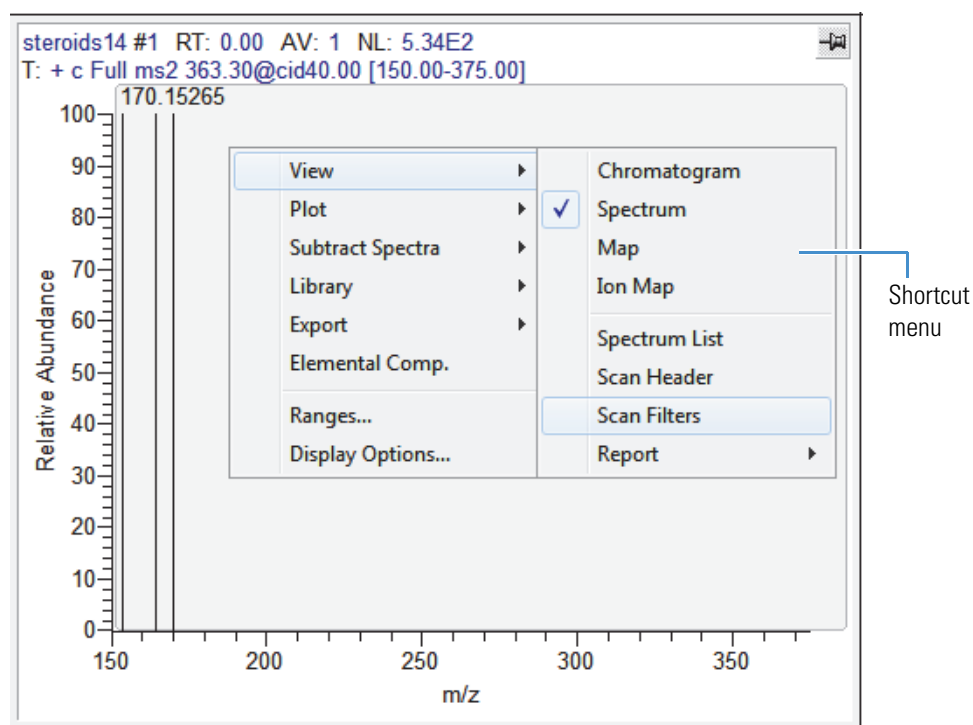
- On the menu bar, choose **Grid > Insert Cells > Left**.

All of the cells are inactive.

2. In the lower left cell, change the view to the scan filter view by right-clicking the cell and choosing **Scan Filters** from the shortcut menu ([Figure 4](#)).

Note When none of the cells in the grid are pinned, clicking a cell makes it the active cell. An active but unpinned cell has a gray border.

Figure 4. Choosing Scan Filters from the shortcut menu



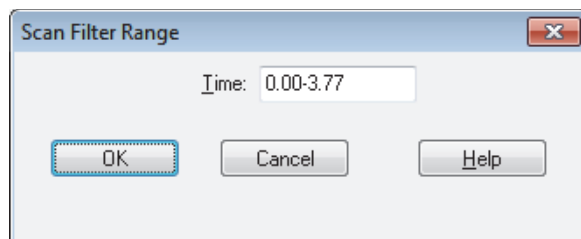
3. In the lower left cell, change the range of the scan filters view to the entire time range of the chromatogram as follows:

- a. Right-click the scan filter view and choose **Ranges** from the shortcut menu.

The Scan Filter Range dialog box opens.

- b. If the value in the Time box is 0.00, type a dash and the end time point for the chromatogram in the box (Figure 5). Otherwise, set the time range to the full time range of the chromatogram (*first time point–last time point*).

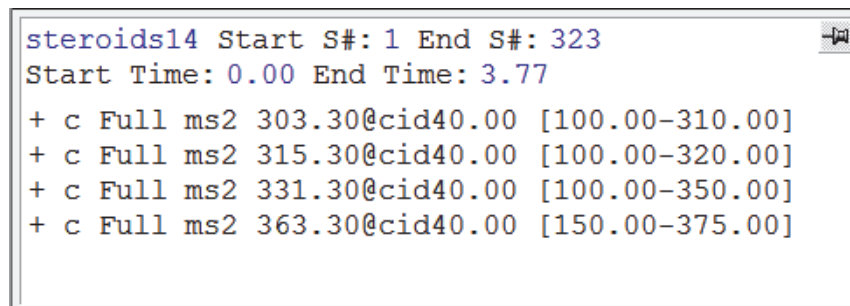
Figure 5. Scan Filter Range dialog box with a time range specified in the Time box



- c. Click **OK**.

The scan filters view lists all the scan filters in the raw data file (Figure 6).

Figure 6. Scan filters



4. In the upper left cell, change the TIC chromatogram to a mass range chromatogram for a selected scan filter as follows:

- a. Click the pin icon, , in the upper right corner of the cell (pin the cell) to make it the active and pinned cell .

The last entry in the scan filter list is for a mass range chromatogram of all ions between m/z 150 to 375.

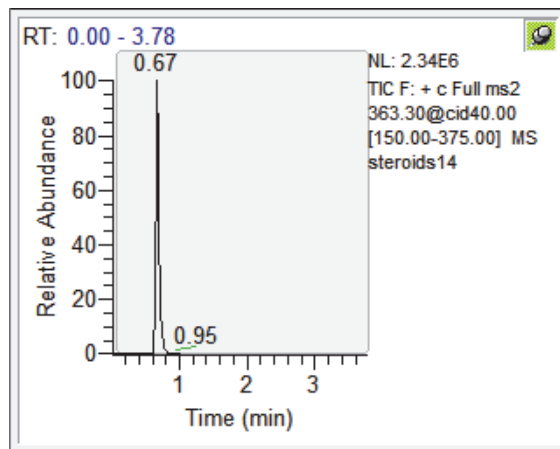
- b. Select the last entry in the scan filter list.

The last entry becomes surrounded with a box and the cursor becomes a page cursor.

- c. Drag the page cursor to the upper left cell.

When you release the page cursor, the upper left cell displays the mass range chromatogram for the selected scan filter (Figure 7).

Figure 7. Mass range chromatogram for the selected scan filter (full MS2 m/z)



5. In the upper right cell, change the display to an averaged spectrum as follows:
 - a. Pin the cell.
 - b. Right-click the pinned cell and choose **View > Spectrum** from the shortcut menu.
 - c. In the upper left cell (full range MS2 chromatogram), drag the cursor across the baseline width of the chromatographic peak.

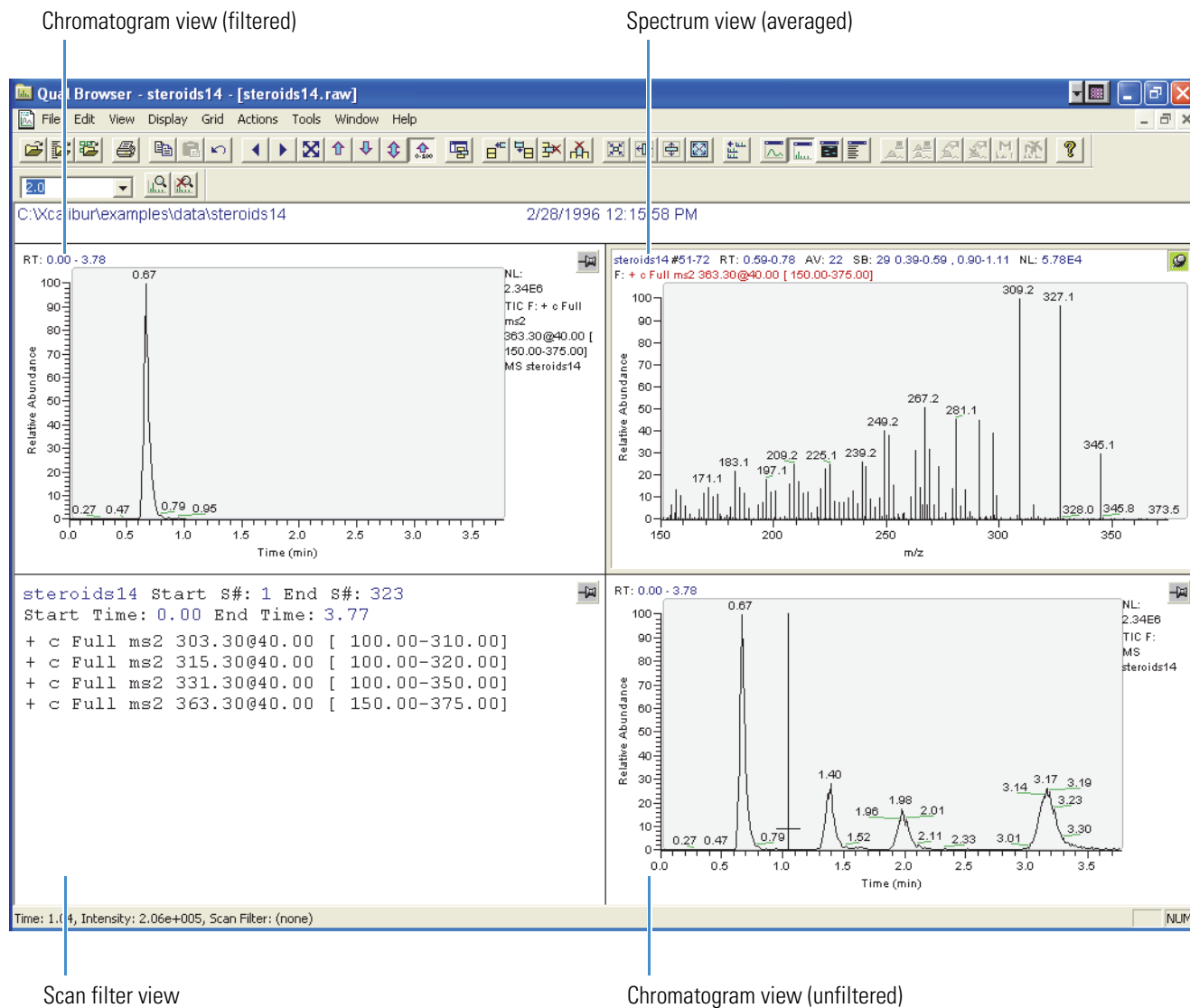
An averaged spectrum appears in the upper right cell.

6. Pin the lower right cell and choose **View > Chromatogram** from the shortcut menu.

An unfiltered TIC chromatogram appears in the cell. Confirm that the grid looks similar to the one in [Figure 8](#).

Figure 8 shows the following views (clockwise from lower left): scan filter view, (filtered) chromatogram view, (filtered) spectrum view (averaged, and chromatogram view (unfiltered).

Figure 8. Qual Browser window



Leave this layout open and go to the next procedure, [Subtracting Background Spectra](#).

Subtracting Background Spectra

You can subtract the background spectra in two ways: graphically by choosing **Actions > Subtract Spectra** from the Qual Browser menu bar or automatically by specifying a background file in the Subtract Background dialog box.

These procedures describe the two ways you can perform background subtraction:

- [Using the Subtract Background Tool](#)
- [Subtracting Background Spectra Graphically](#)

Using the Subtract Background Tool

Use the Subtract Background window to subtract a raw data file or a single scan from a raw data file from any other selected raw data file. You can use this utility to subtract a background spectrum from a raw data file or deconvolute merged or overlapping component peaks.

For more information, refer to the *Xcalibur Qual Browser User Guide*.

❖ To subtract the background from a raw data file

1. In the Qual Browser window, choose **Tools > Background Subtract**.

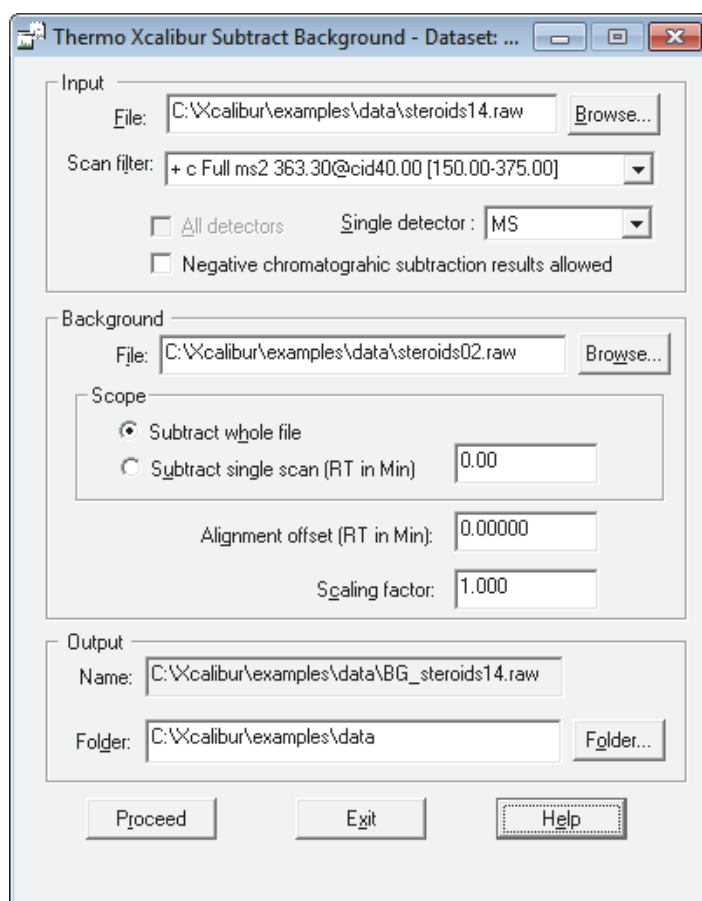
The Subtract Background window opens ([Figure 9](#)).

2. In the Input area, set up the data source information for the input file as follows:
 - a. In the File box, type the path name and file name of the input file, or click **Browse** and locate the file with the Open dialog box.
 - b. In the Single Detector list, select the detector used to acquire the data of interest. If the raw data file contains data from more than one detector, the All Detectors check box is available. To subtract the background for all the data sources in the raw data file, select the **All Detectors** check box.
 - c. In the Scan Filter list, select a scan filter from the list of scan filters that are stored in the RAW file.
3. In the Background area, do the following:
 - a. To select the background file, type the path name and file name of the background file in the File box or click **Browse** and locate the file using the Open dialog box.
 - b. Select the scope of the subtract background file operation as follows:
 - To subtract the entire background file from the input file, select the **Subtract Whole File** option.
 - To subtract a single scan from the background file from each scan of the input file, select the **Subtract Single Scan (RT in Min)** option and type the retention time for the scan in the associated box.

- c. Specify alignment and scaling as follows:
 - To offset the subtraction of the background file from the input file, type the required offset in the Alignment Offset (RT in Min) box.
 - To scale the subtraction of the background file from the input file, type the required factor in the Scaling Factor box.
4. In the Output area, specify the location of the output file by typing the full path location in the Folder box, or by clicking **Folder** and browsing to the required location.

The Name box displays the output file as BG_<Input File> (Figure 9).

Figure 9. Subtract Background dialog box



5. Do one of the following:
 - To abandon the file operation and close the dialog box, click **Exit**. The dialog box closes.
 - To start the subtract background file operation, click **Proceed**. When the background subtraction is complete, a message box appears. Click **OK** to close the message box. Click **Exit** to close the dialog box.

Subtracting Background Spectra Graphically

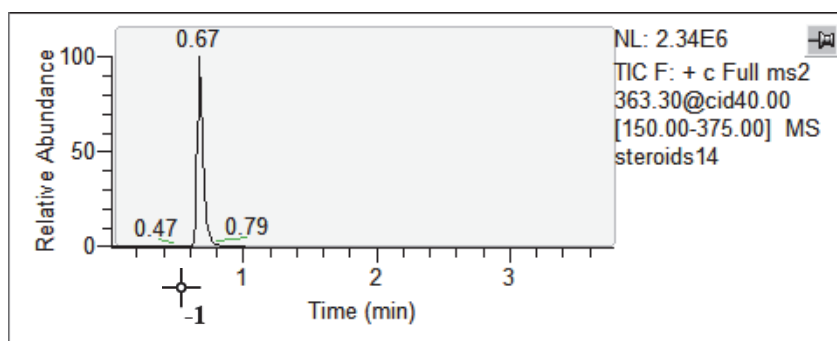
To subtract background spectra, eliminating background peaks from either one range (either side of the chromatogram peak of interest) or two ranges (both sides of the chromatogram peak of interest), pin the spectrum view and use the cursor in the chromatogram view.

❖ To select two scan ranges for background subtraction

1. Pin the spectrum view to work interactively in the chromatogram view.
2. Right-click the spectrum view and choose **Actions > Subtract Spectra > 2 Ranges** from the shortcut menu.

A crosshair cursor labeled -1 appears (Figure 10).

Figure 10. Crosshair cursor for background subtraction in the chromatogram view



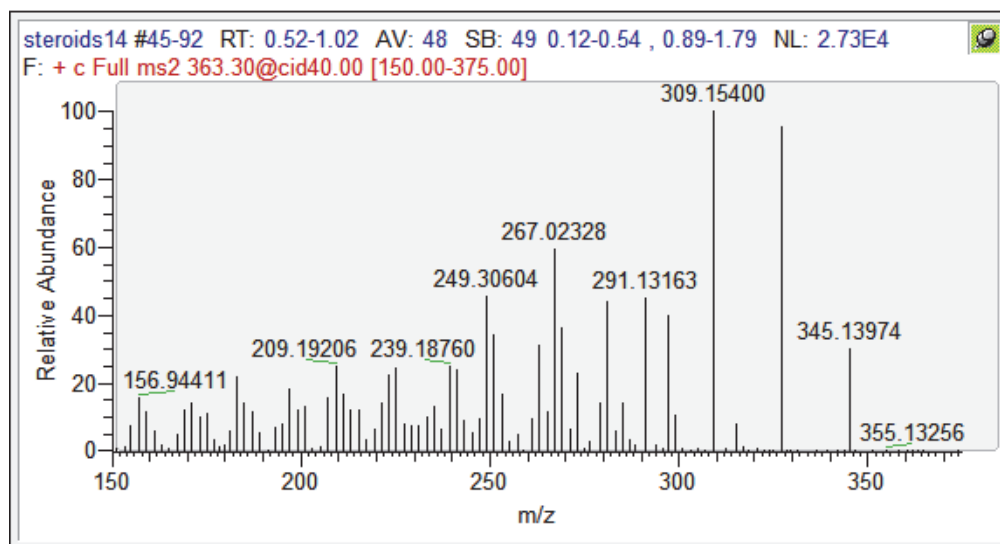
3. In the chromatogram view, select a baseline region that is close to the chromatographic peak of interest.
 4. Drag the cursor away from the peak of interest and across a few scans that are representative of the first scan range to subtract. Then, release the mouse button to define the first range.
- The cursor label changes to -2.
5. Select a baseline region on the other side of the peak of interest.
 6. Drag the cursor away from the peak of interest and across a few scans that are representative of the second scan range to subtract. Then, release the mouse button. to define the second range.

When you release the mouse button, the data system subtracts an average of the selected scans and redraws the spectrum view. The spectrum view header shows the number of subtracted scans (Figure 11).

For example, SB: 49 0.12–0.54, 0.89–1.99 indicates the following:

- Qual Browser has applied background subtraction to the spectrum by using a 49-scan average.
- Retention time ranges used in the subtraction are 0.12 to 0.54 min and 0.89 to 1.99 min.

Figure 11. Spectrum view after a 2-range background subtraction



❖ **To undo background subtraction**

Choose **Actions > Subtract Spectra > Clear** from the menu bar.

Manually Exporting Spectrum Files from Qual Browser

To create a library entry for a custom library, you can export a spectrum to the Library Browser window from either a spectrum view in the Qual Browser window or during processing or batch reprocessing of raw data files in the Sequence Setup view.

Note For best results, read the documentation that the National Institute of Science and Technology (NIST) provides with the NIST Mass Spectral Search application before you export a spectrum file to the application.

This topic describes how to export a spectrum file from the Qual Browser window.

❖ To export a spectrum from Qual Browser to Library Browser

1. Open a raw data file in the Qual Browser window.
2. In the spectrum view, select the spectrum that you want to export (see [Viewing a Spectrum in Qual Browser](#)).
3. Right-click the spectrum view and choose **Library > Export to Library Browser**.

The NIST Library Search window opens.

The data system converts the mass and intensity data of the spectrum to a text file and copies the file to the Spec List pane. The Qual Browser window stays open. The data system creates the following:

- A copy of the exported spectrum in the Xcalibur\Libspecs folder.
The file is given an (.msd) extension with the same file name as the original data file, although this is truncated to eight characters (8.3 file name format).
- An index file containing details about all exported spectra.

The data system places the exported spectrum into the Spec List (Spectrum List). For information about using the NIST Mass Spectral Search application, read the documentation that is supplied with the application.

Exporting Spectrum Files Automatically During Sequence Processing

You can set up automatic exporting of spectra to a user library in a processing method. When you run or batch reprocess a sequence that contains the processing method, you can turn on the spectrum exporting feature.

When an exported spectrum file does not match any of the spectrum files in the selected library, the data system appends the new spectrum file to the library.

❖ **To set up a processing method that exports spectra to a user library**

1. Choose **GoTo > Processing Setup** from the home page menu bar.

The Processing Setup window opens.

2. Choose **View > Qual**.

The Qual view of the Processing Setup window opens with the Identification page displayed.

3. Click the **Library Search Options** tab to display the Library Search Options page.

4. Check the libraries that are in use as follows:

- a. Click **Search List**.

The Search List dialog box opens.

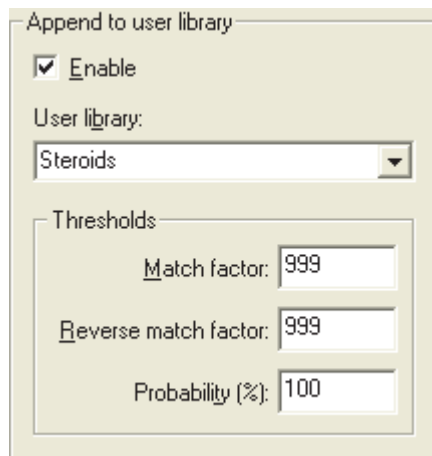
- b. Check the list of available libraries.

- c. Add or remove libraries from the Available Libraries area, and then click **OK** to save the changes and close the dialog box.

5. In the Append to User Library area, select the **Enable** check box.

Figure 12 shows the Append to User Library area on the Library Search Options page in the Processing Setup – Qual view.

Figure 12. Append to user library area



Append to user library

☒ **Enable**

User library:
Steroids

Thresholds

Match factor: 999

Reverse match factor: 999

Probability (%): 100

6. In the User Library list, select an existing library or type the name of a spectral library where you want to append the exported spectra.

If you type a new library name, the library is created only if a spectrum fails the matching criteria. To ensure that spectrum files are appended to the specified library, enter the highest possible values in the Thresholds boxes. The data system only appends spectrum files that fail the matching criteria.

7. Type threshold values for Match Factor, Reverse Match Factor, and Probability%. To confirm that all spectra are appended to the library, type **999**, **999**, and **100** respectively.

During processing and after any requested enhancement of a relevant chromatogram peak apex scan, the Xcalibur data system submits the spectrum to a library search:

- If the top hit from a library search exceeds (or is equal to) any one of the threshold values, the data system returns the hit list and the spectrum is not appended to the specified library.
- If the top hit fails to reach any of the threshold values, the data system discards the hit list (no search results are reported) and appends the searched spectrum to the specified library. Unless otherwise specified, the library is stored in the NIST\MSSearch folder.

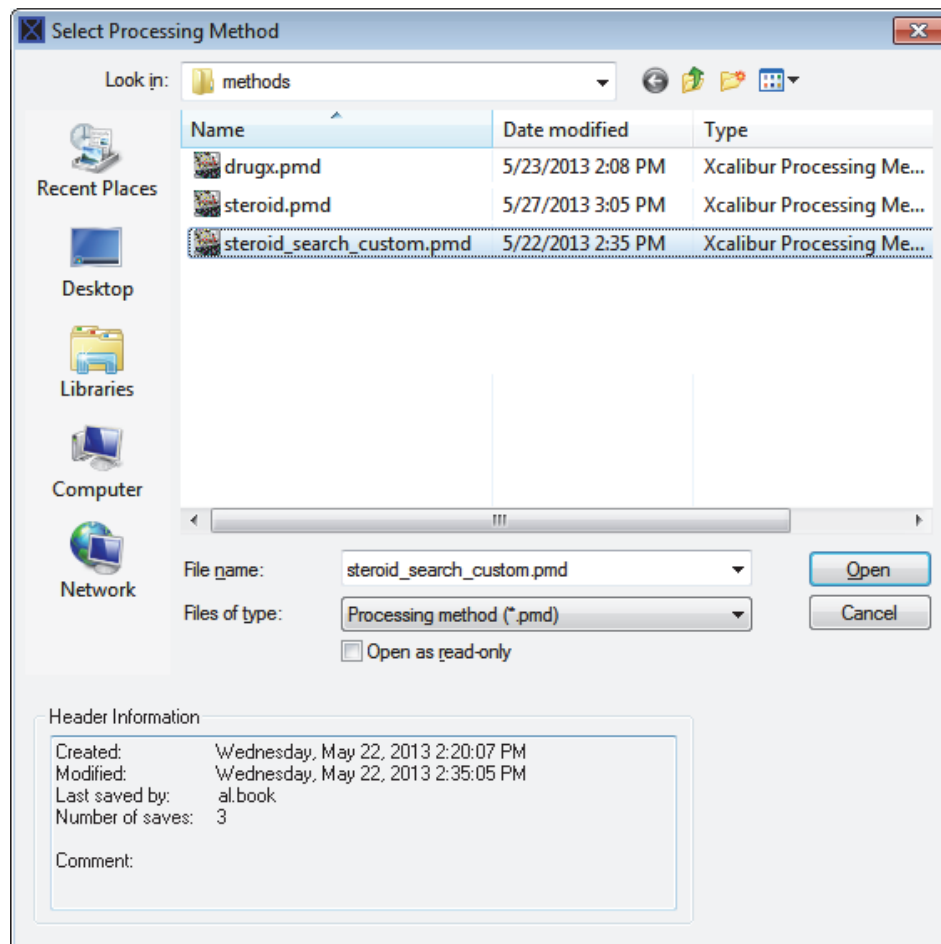
8. Save the processing method.

❖ To automatically export spectra to the designated library

1. From the Processing Setup window, open the Sequence Setup view by choosing **GoTo > Xcalibur Home Page** from the menu bar. If the Sequence Setup view is not displayed, open it by choosing **View > Sequence Setup View**.
2. Do one of the following:
 - If you have not already acquired a set of raw data files, create a new sequence as described in the *Xcalibur Data Acquisition and Processing User Guide*.
 - If the acquisition sequence that contains the raw data files you want to process is not open, choose **File > Open**. Then, in the Open dialog box, browse to the appropriate folder, select the sequence file (SLD) of interest, and click **Open**.
3. If you have not already added the processing method to the sequence, do the following:
 - a. Double-click the **Processing Method** column.

The Select Processing Method dialog box opens (Figure 13).

Figure 13. Select Processing Method dialog box



- b. Browse to the appropriate folder, select the processing method (PMD file) of interest, and click **Open**.
4. Do one of the following:
 - To export the spectra during data acquisition, in the Processing Actions area of the Run Sequence dialog box, select the **Qual** check box.
 - To export the spectra during batch reprocessing, in the Batch Reprocess dialog box, select the **Qual** check box. Then, select the **Peak Detection and Integration** check box and the **Library Search** check box.

If the library that is specified in the processing method does not exist, the Xcalibur data system creates it.

2 Exporting Spectrum Files to Library Browser

Exporting Spectrum Files Automatically During Sequence Processing

When a spectrum is added to a user library, it contains the following basic information:

- Complete mass/intensity list
- Name formatted as <filename>#<scannumber> RT: <rt> AV: <av> NL: <nl>, for example: steroids02#1 RT: 0.01 AV: 1 NL: 2.14E3
- Comment showing the scan filter, such as T: + c Full ms2 363.30 [150.00 – 375.00]
- Molecular weight (Mol Weight) and CAS number set to zero

You might want to modify the basic information or provide the following:

- Chemical formula
- List of synonyms
- Molecular weight
- CAS number
- Chemical structure (in MOL, SDF, or MDL file format)

When you attach a structure to the file, you can automatically add the chemical formula and molecular weight to the file by clicking From Structure as described in [Managing the NIST Libraries](#).

Managing Libraries

In the Library Browser window, you can create, manage, and search user libraries. Use these functions to create reference libraries from your own spectra.

Follow these procedures to add your spectrum files to a user library, to manage your library list, and to convert your libraries to another format.

The data system stores the spectral libraries in the following folder:

drive:\Program Files\NISTMS\MSSEARCH

Contents

- [Adding Spectrum Files to a User Library](#)
- [Managing the NIST Libraries](#)
- [Converting Libraries to Another Format](#)

Adding Spectrum Files to a User Library

You can add a spectrum file to a user library after you manually export the file from the Qual Browser window. Or you can automatically add spectrum files to a user library during sequence processing if you enable the Add to Library feature in the processing method and set the appropriate match threshold criteria (see [Exporting Spectrum Files Automatically During Sequence Processing](#)).

The following procedure describes how to add a spectrum that you manually exported from the Qual Browser window to a user library.

❖ To add an unedited spectrum file to a library

1. Export a spectrum from Qual Browser. See [Manually Exporting Spectrum Files from Qual Browser](#).

The Library Browser window opens.

2. Choose **Window > Librarian**.

The Librarian window opens.

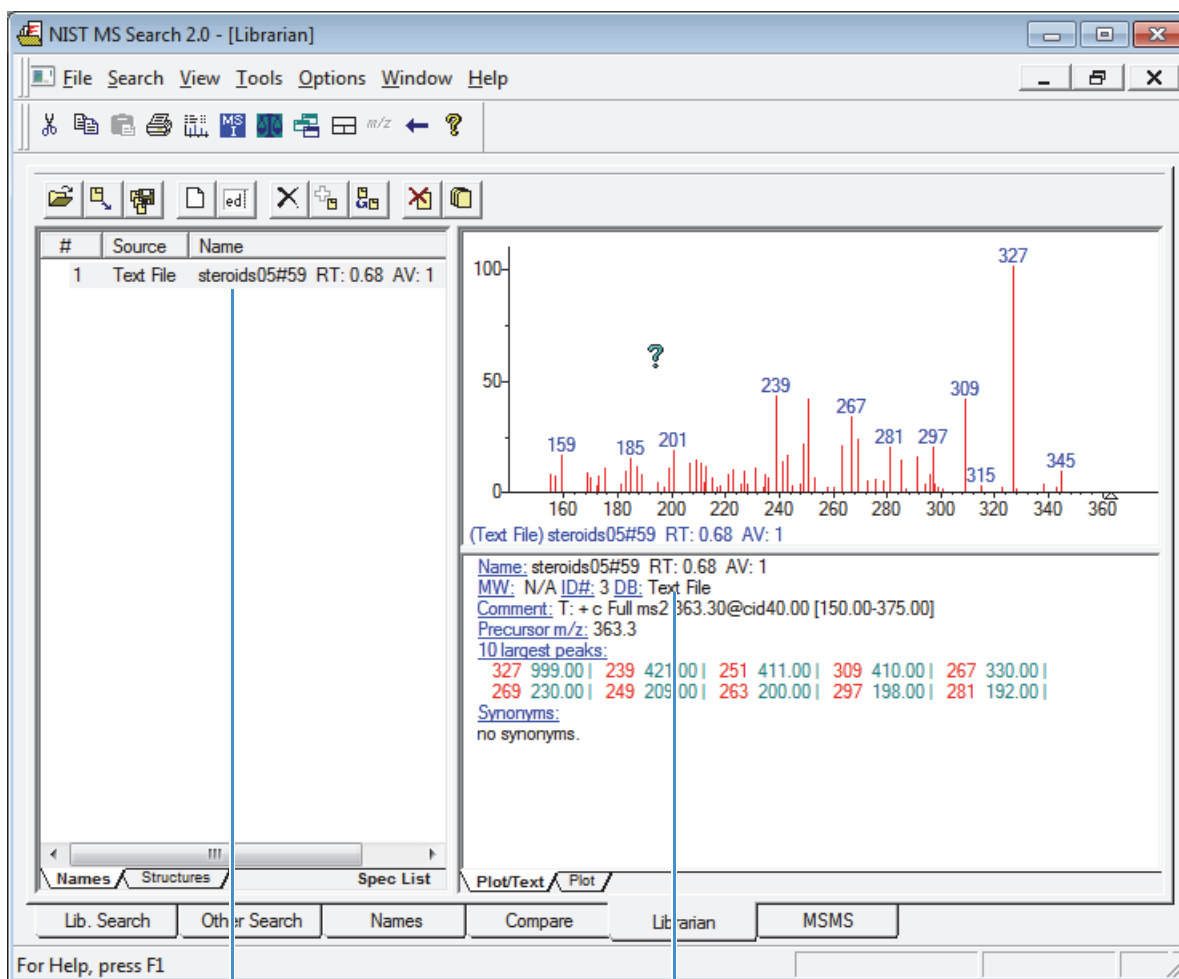
3 Managing Libraries

Adding Spectrum Files to a User Library

3. In the Spec. List, select the spectrum that you want to add to a library (Figure 1).

The Spec List contains one row for each spectrum. The Src column lists the source of the spectrum as one of the following: a text file (A), the Spectrum Editor (E), or a library. User libraries are coded with the first two letters of the library name. The Name column lists the spectrum name.

Figure 1. NIST MS Search 2.0 – Librarian window



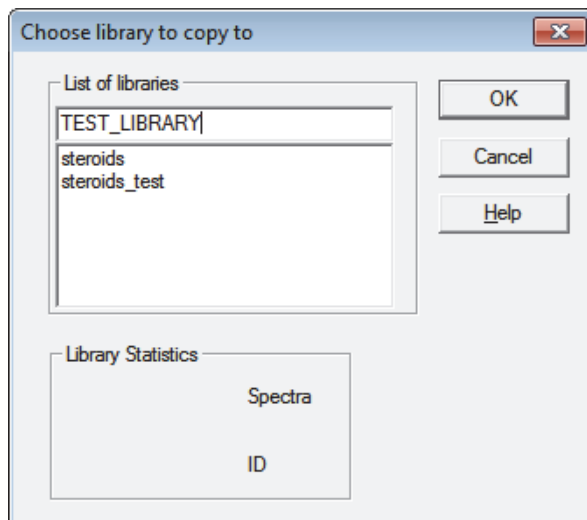
Exported spectrum from the peak at RT = 0.68 minutes in the steroids05.raw data file

Text File label

- Click the **Add to Library** icon, , in the Librarian window toolbar.

The Choose Library to Copy To dialog box opens (Figure 2).

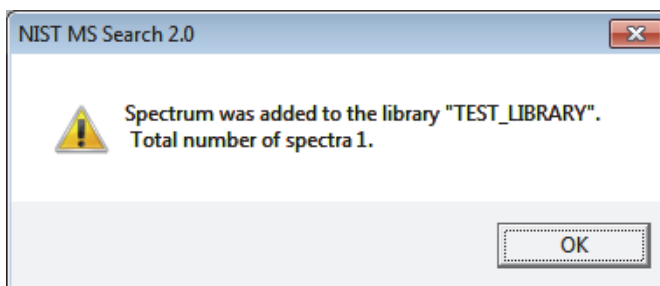
Figure 2. Choose Library to Copy To dialog box



- Choose the library that you want to add the spectrum file to or type the name of a new library in the box.
- Click **OK** to add the new spectrum file to an existing library or to a new library.

A message box that lists the name of the library and the number of spectra in the library appears (Figure 3).

Figure 3. Information about the library



- Click **OK** to add the spectrum to the library.

Managing the NIST Libraries

To add, delete, or move a library from the NIST libraries list, use the Manage Libraries page of the Library Manager application. This section shows you how to complete the following tasks:

- [Adding a Library](#)
- [Deleting a Library](#)
- [Copying a Library](#)

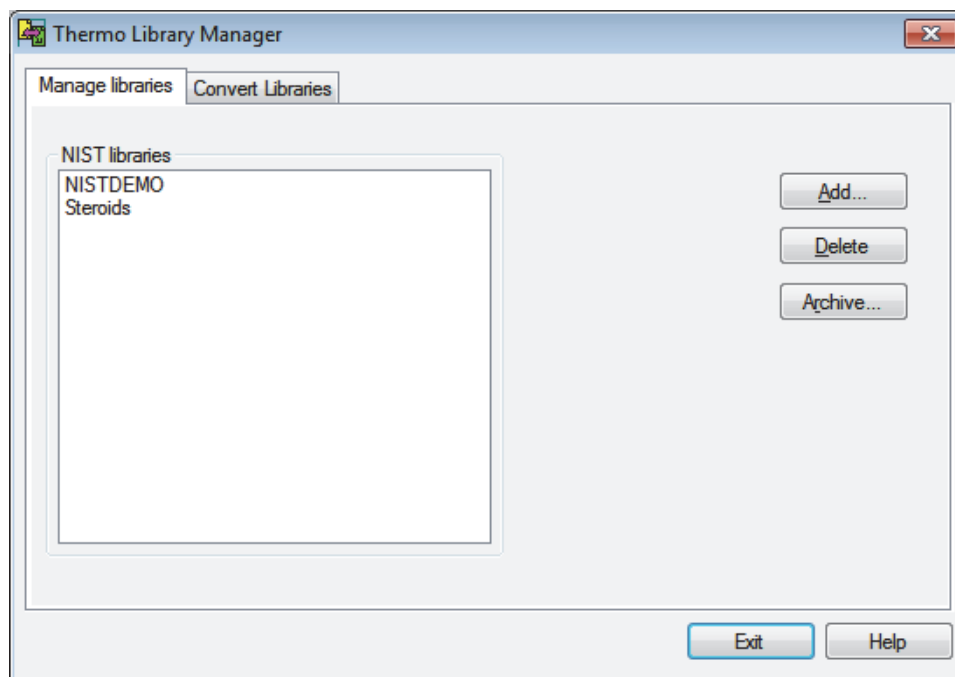
For more information about the Manage Libraries page of the Library Manager application, see [Library Manager Application](#).

❖ To open the Library Manager application

1. Open the Xcalibur home page – Roadmap view.
2. From the menu bar, choose **Tools > Library Manager**.

The Library Manager application opens with the Manage Libraries page displayed ([Figure 4](#)).

Figure 4. Thermo Library Manager dialog box



Adding a Library

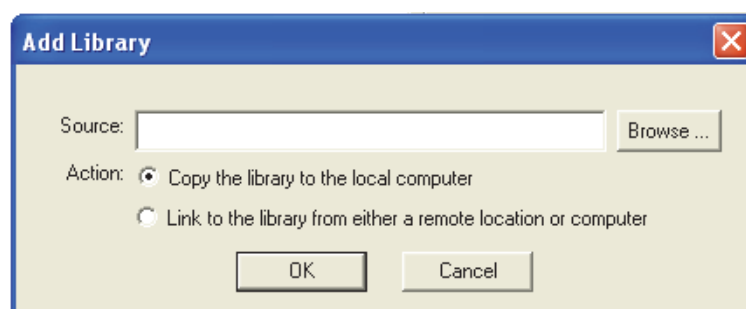
When you add a library to the NIST libraries list, either copy the library file to the local computer or link to the library at a remote location without copying files.

❖ To add a library

1. Open the Manage Libraries page of the Library Manager application as described in [Managing the NIST Libraries](#).
2. Click **Add**.

The Add Library dialog box opens ([Figure 5](#)).

Figure 5. Add Library dialog box



3. In the Add Library dialog box, type the path for the new library file in the Source box or click **Browse** to bring up the Browse for Folder dialog box and find the file of interest.
4. Select one of the two options:
 - Copy the library to the local computer.
 - Link to the library from either a remote location or computer.

Tip Because libraries can be large, you can often save time by selecting the Link option rather than the Copy option.

5. Click **OK**.

The data system adds the selected library to the NIST Libraries list in the Library Manager application.

6. If you have no more tasks to complete with the Library Manager, click **Exit**.

Deleting a Library

❖ To delete a selected library in the NIST Libraries list

1. Open the Manage Libraries page of the Library Manager application as described in [Managing the NIST Libraries](#).
2. Select a library to delete from the NIST Libraries list.
3. Click **Delete**.

The system prompts you to confirm the deletion.

4. To delete the selected library, click **Yes**.
5. If you have no more tasks to complete with the Library Manager, click **Exit**.

Copying a Library

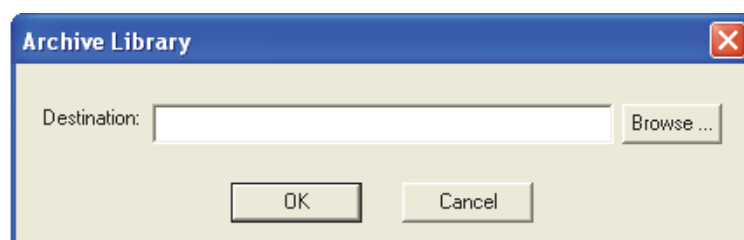
You can copy a selected library to another directory on the computer or network by using the Archive feature.

❖ To copy a library

1. Open the Manage Libraries page of the Library Manager application as described in [Managing the NIST Libraries](#).
2. Select a library to copy from the NIST Libraries list.
3. Click **Archive**.

The Archive Library dialog box opens (see [Figure 6](#)).

Figure 6. Archive Library dialog box



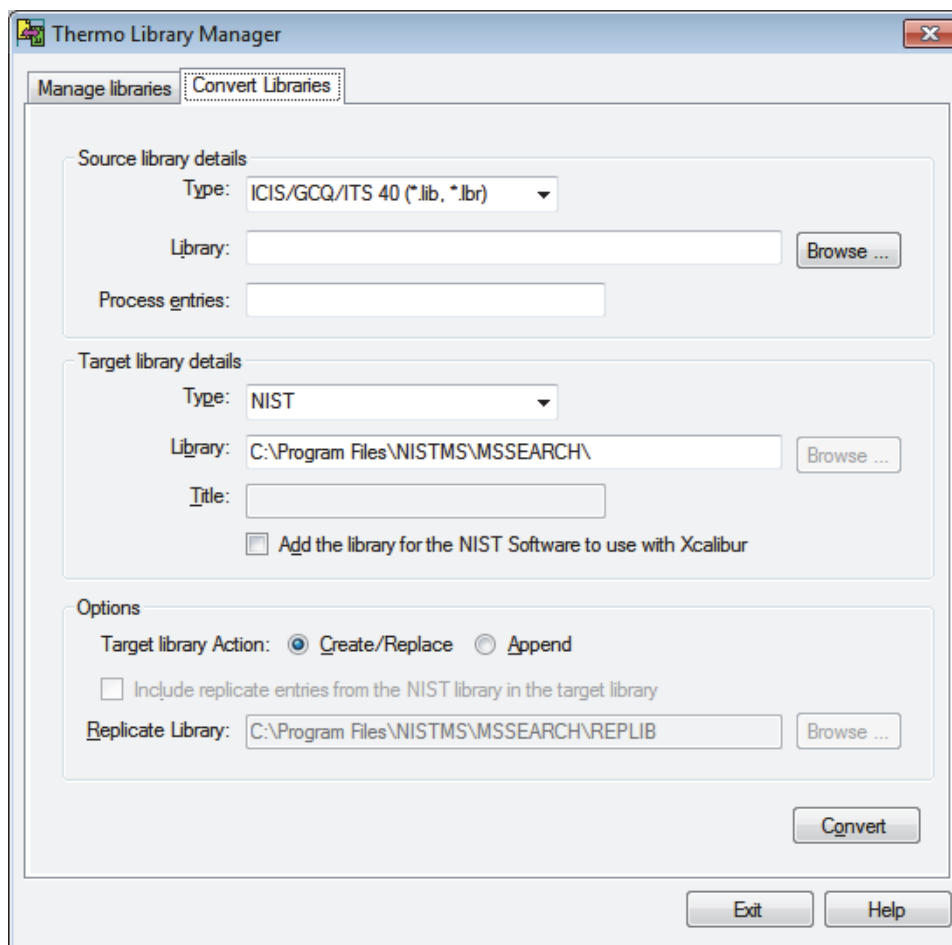
4. Type the path for the copied library file in the Destination box or click **Browse** to bring up the Browse for Folder dialog box and find the desired location.
5. To copy the selected library to the remote location, click **OK**.
6. If you have no more tasks to complete with the Library Manager, click **Exit**.

Converting Libraries to Another Format

To convert all or any portion of a library to another format, use the Convert Libraries page of the Library Manager application (Figure 7). Also, use this page to copy a library to another location.

For more information about the Convert Libraries page, see [Convert Libraries Page](#).

Figure 7. Convert libraries page



❖ To convert a library from one format to another

1. Open the Library Manager application as described in [Managing the NIST Libraries](#).
2. Click the **Convert Libraries** tab to open the Convert Libraries page.
3. In the Source Library Details area, do the following:
 - In the Type list, select the type of source library, based on the file name extension.
 - In the Library box, type the path to the source library or click **Browse** to open the Browse for Folder dialog box and find a file.

- In the Process Entries box, to convert only certain entries from the source library, type the number range of the entries to convert. For example, to convert only entries #100 to #200, type **100–200**.
4. In the Target Library Details area, do the following:
- In the Type list, select the type of target library based on the file name extension.
 - In the Library box, type the path to the target library or click **Browse** to open the Browse for Folder dialog box and find a folder.

Note When you select NIST as the target library type, the default target library is the library folder for the Xcalibur data system: C:\NIST02\MSSEARCH\.

When you select ICIS/GCQ/ITS 40 or MassLab as the target library type, the Title box becomes available.

- In the Title box, type the title for the converted library.
5. In the Options area, do the following:
- Select either the **Create/Replace** option or the **Append** option.
Create/Replace is selected by default.
When you select NIST as the source library type, the Include Replicate Entries from the NIST Library in the Target Library check box becomes available.
 - Click the **Include Replicate Entries from the NIST Library in the Target Library** check box to copy replicate entries.
When you select the Include Replicate Entries check box, the Replicate Library box becomes available. The data system stores the default replicate library, REPLIB, in the following folder:
drive:\NIST02\MSSEARCH
 - To use a different replicate library, type the path to the desired library in the Replicate Library box or click **Browse** to open the Browse for Folder dialog box and find a folder.
6. To begin the conversion process, click **Convert**.

The Conversion Status box displays sequential chronological (top to bottom) messages such as:

Started the conversion on SEP 3, 1999 at 10:01, please wait
Finished the conversion on SEP 3, 1999 at 10:02
Converted 570 entries

7. If you have no more tasks to complete with the Library Manager, click **Exit** to close the Library Manager application.

Searching Libraries

After you create a custom library, you can use it for library searches. You can search spectral libraries in three ways:

- Manually from within the Qual Browser window
- Manually from within the Library Browser window
- Automatically during sequence processing or batch reprocessing

Follow the procedures in this chapter to run library searches in the Qual Browser window or during batch processing.

Contents

- [Submitting a Spectrum to a Library Search in Qual Browser](#)
- [Setting Up and Running Automated Library Searches](#)

Submitting a Spectrum to a Library Search in Qual Browser

After you create a custom user library in the Library Browser window, you can submit a spectrum to a library search from the Qual Browser window. Qual Browser uses the library or libraries listed on the Search List page and the search parameters specified on the Search Parameters page of the Search Properties dialog box.

❖ To submit a spectrum in Qual Browser to a library search

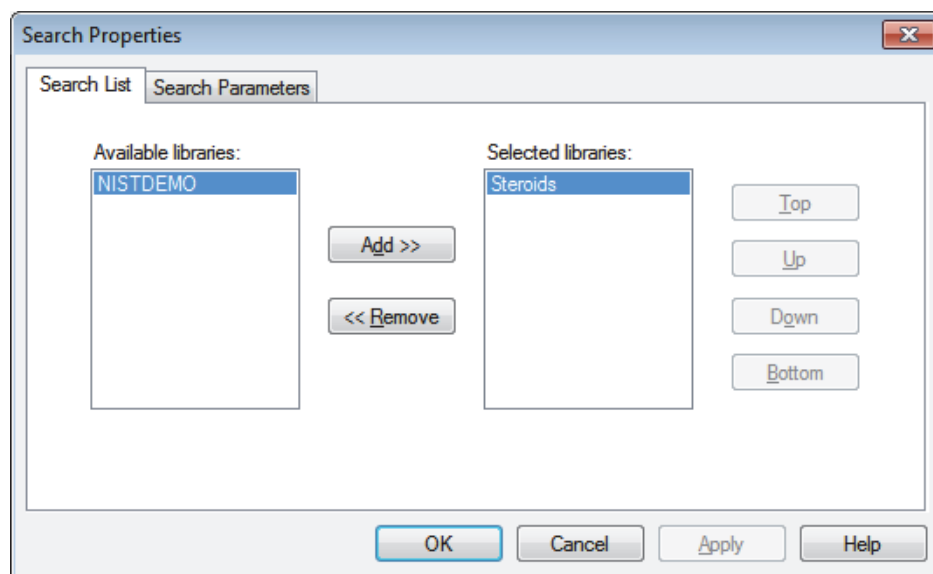
1. Open a raw data file in the Qual Browser window.
2. Open a chromatogram view as follows:
 - a. Click the pin icon, , in the upper right corner of the cell (pin the cell) where you want to open the chromatogram view.

The pin icon changes to the pinned state, , to indicate that the chromatogram view is the active and pinned cell.
 - b. Choose **View > Chromatogram** or click the **View Chromatogram** icon, , in the toolbar.
3. Open a spectrum view as follows:
 - a. Click the pin icon, , in the upper right corner of the cell (pin the cell) where you want to open the spectrum view.

The pin icon, , changes to the pinned state to indicate that the spectrum cell is the active and pinned cell.
 - b. Choose **View > Spectrum** or click the **View Spectrum** icon, , in the toolbar.
4. To display or enhance a spectrum, choose from these options:
 - With the spectrum cell pinned, click the chromatogram at the retention time of interest (a peak apex, for example).

The spectrum from this time point appears in the spectrum view.
 - To view a spectrum averaged across a peak, drag the cursor through the chromatogram peak of interest.
 - Enhance the spectrum, if necessary, by using background subtraction. For more information on this step, see [Subtracting Background Spectra](#).
5. Set up the library search options as follows:
 - a. Choose **Actions > Library > Options**.

The Search Properties dialog box opens with the Search List page displayed ([Figure 8](#)).

Figure 8. Search Properties dialog box

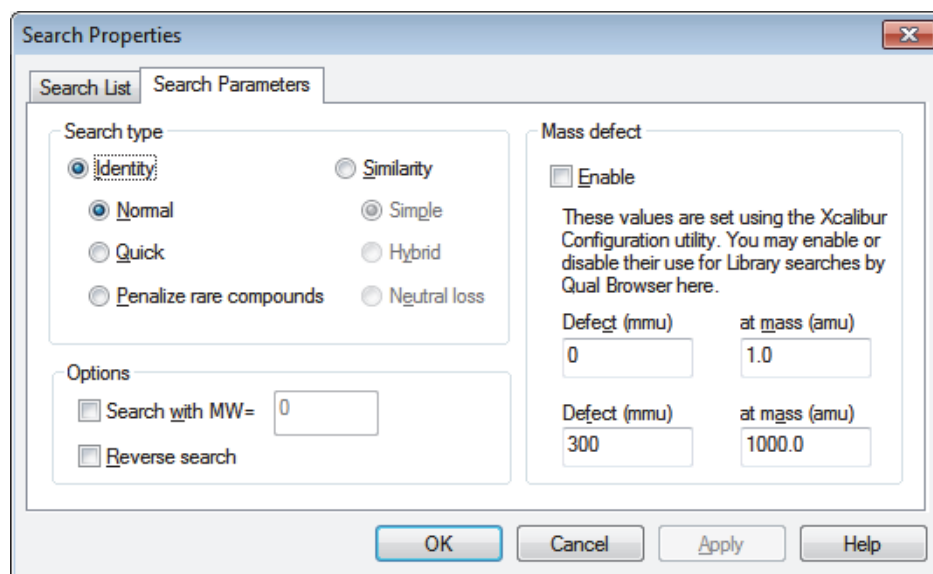
- b. Select the libraries that you want to search as follows:
- To move a library from the Available Libraries box to the Selected Libraries box, select the library and click **Add**.
 - To remove a library from the Selected Libraries box to the Available Libraries box, select the library and click **Remove**.
 - To change the search order of the selected libraries, select the library that you want to move. Then, click the appropriate button:
 - Click **Top** to move the library to the top of the list.
 - Click **Up** to move the library Up by one position.
 - Click **Down** to move the library down by one position.
 - Click **Bottom** to move the library to the bottom of the list.
- c. Click the **Search Parameters** tab.

The Search Parameters page opens (Figure 9).

4 Searching Libraries

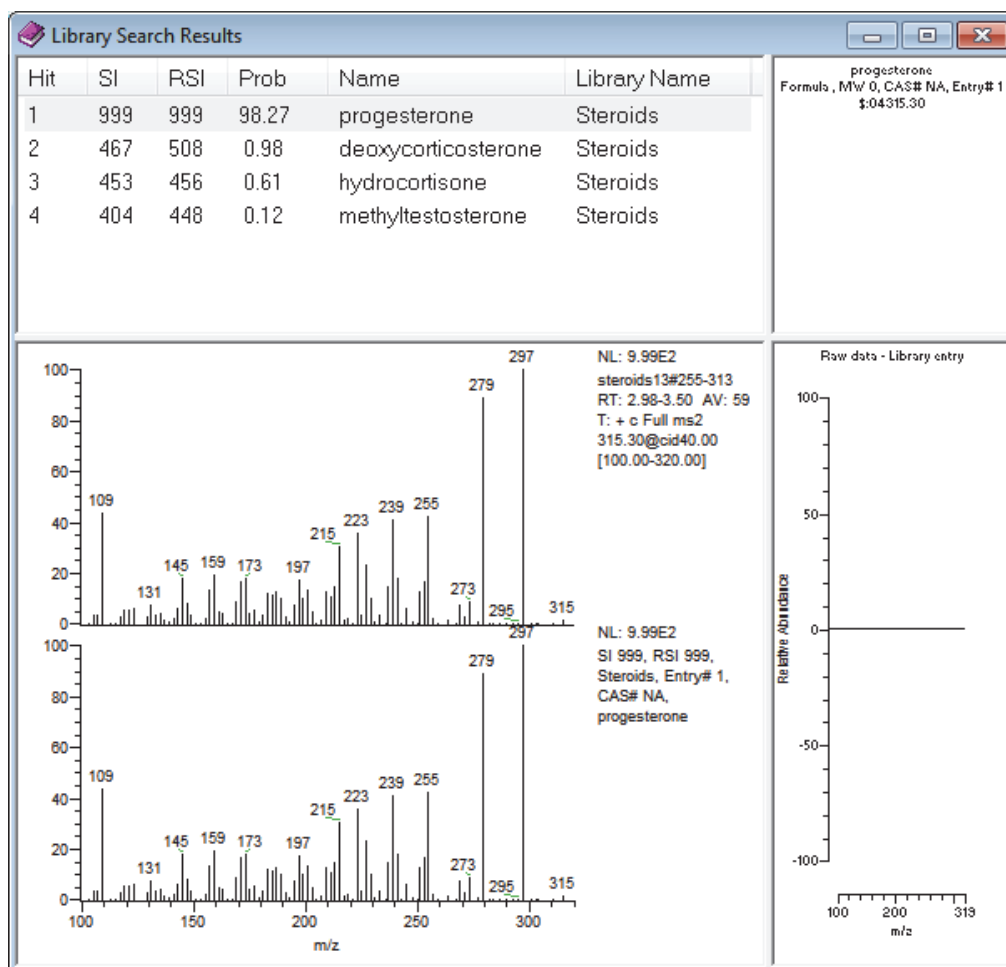
Submitting a Spectrum to a Library Search in Qual Browser

Figure 9. Search Parameters page



- d. Make the appropriate selections and entries.
 - e. Click **Apply** to save the settings.
 - f. Click **OK** to close the dialog box.
6. To start the library search, do one of the following:
- Choose **Actions > Library > Search** from the menu bar.
 - Click the **Library Search Spectrum** icon, , in the toolbar.
- or—
- Right-click the spectrum view and choose **Library > Search** from the shortcut menu.

Qual Browser displays the results of the library search in the Library Search Results window (Figure 10).

Figure 10. Library Search Results window in Qual Browser

The interactive cells of the Library Search Results window show the following library search results, displayed clockwise from the upper left quadrant:

- Hits list (a list of matching spectrum files)
- Molecular structure, including formula, molecular weight, name, and library index number
- Difference spectrum (*Raw Data minus Library Entry*)
 - Peaks above the x axis are relatively more intense in the spectrum than in the library entry.
 - Peaks below the x axis are relatively more intense in the library entry than in the sample spectrum.
- Comparison of the sample spectrum and the library entry

4 Searching Libraries

Submitting a Spectrum to a Library Search in Qual Browser

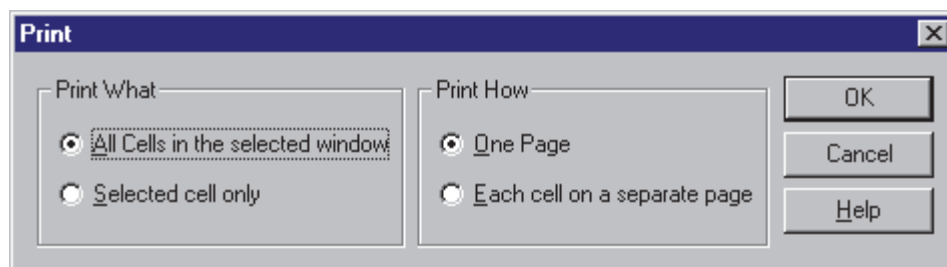
❖ To print the library search report

Note When you print a report from the Qual Browser window, the data system uses the default printer for the data system computer.

1. Choose **File > Print Preview**.

The Print dialog box opens ([Figure 11](#)).

Figure 11. Print dialog box



2. Select the options for your print display.
3. To close the dialog box and preview the results, click **OK**.
4. To display the Print dialog box again, click **Print** and click **OK**.
5. To print the results, click **OK** in the second Print dialog box.

See [Library Sample Reports](#) for an example of library search results initiated from Qual Browser.

For more information about this window, see [Library Search Results Window](#).

Setting Up and Running Automated Library Searches

You set up the parameters for a library search in a processing method. After you add the processing method to a sequence, you can automatically process the data during a sequence run or following data acquisition by batch reprocessing the sequence.

To run automated library searches and print reports, follow these procedures:

1. [Setting Up Library Searches in a Processing Method](#)
2. [Setting Up the Qualitative Processing Sequence](#)
3. [Batch Reprocessing the Sequence and Printing Library Search Reports](#)

Setting Up Library Searches in a Processing Method

To search libraries automatically, set up the qualitative parameters in the processing method. You set up the qualitative parameters for a processing method in the Qual view of the Processing Setup window.

Note Using the Library Search Constraints page requires specific knowledge about the compounds you are looking for. When you are running a qualitative analysis on a sample set, you might not know what compounds are in the samples, so it is not always possible to use the parameters on the Library Search Constraints page to refine automated processing.

❖ To open the Qual view of the Processing Setup window

1. Do one of the following:
 - On the Xcalibur Roadmap view, click the **Processing Setup** icon, .
 - or—
 - On the Xcalibur home page menu bar, choose **GoTo > Processing Setup**.
2. On the Processing Setup menu bar, choose **View > Qual**.

Follow these procedures to set up the library search parameters for a processing method:

1. [Setting Up the Identification Parameters for a Qualitative Processing Method](#)
2. [Setting Up the Library Search Options in a Processing Method](#)
3. [Specifying the Libraries for an Automated Search](#)
4. [Setting Up the Search Constraints for an Automated Library Search](#)
5. [Setting Up Reports for Automated Library Searches](#)

Setting Up the Identification Parameters for a Qualitative Processing Method

Use the Identification page of the Processing Setup – Qual view to select the peak integration algorithm and the scan filters.

❖ To set up the parameters on the Identification page of the Qual view

1. Open the Qual view of the Processing Setup window (see [To open the Qual view of the Processing Setup window](#)).

2. Open a representative raw data file as follows:

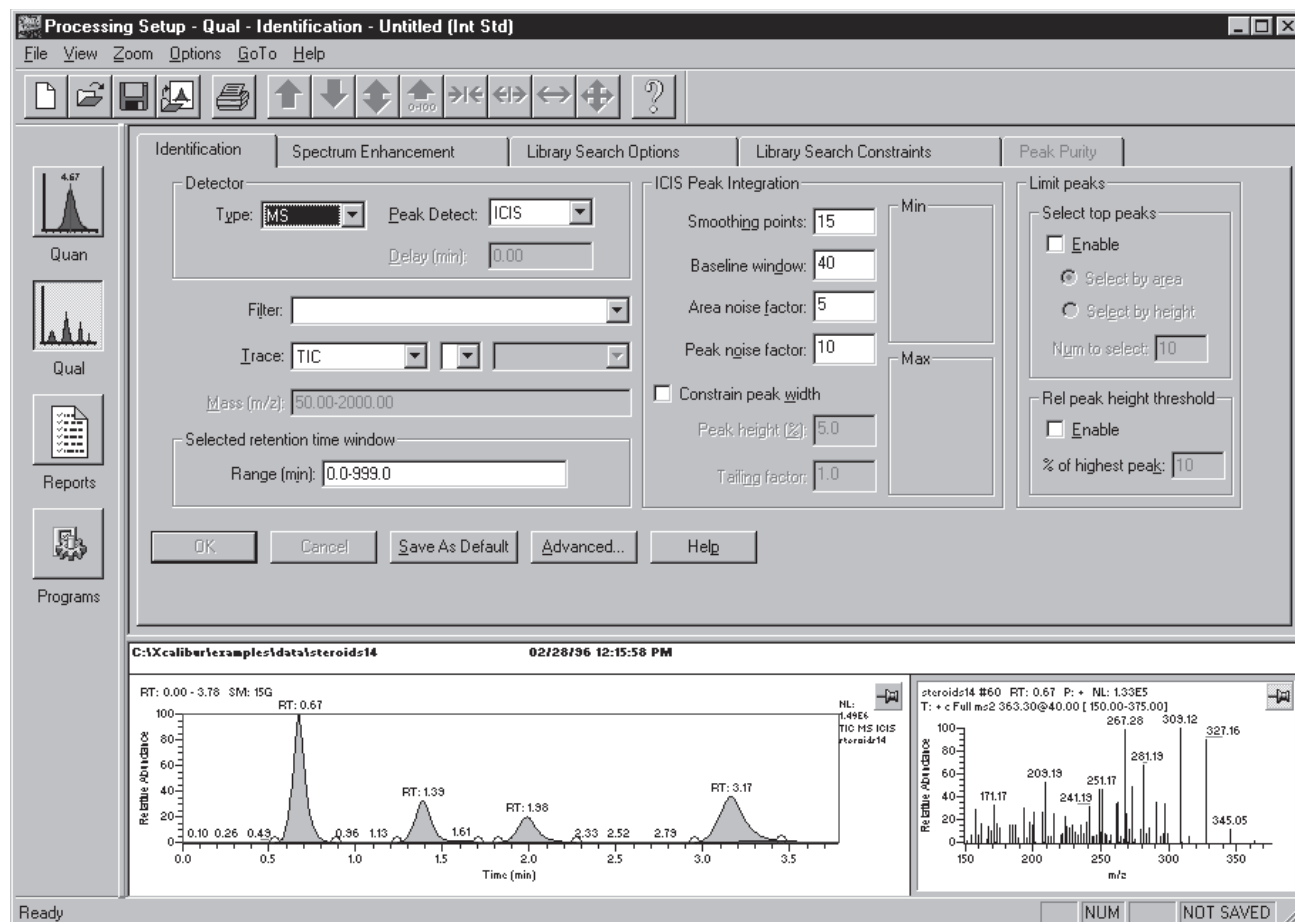
- a. From the menu bar, choose **File > Open Raw File**.

The Open Raw File dialog box opens.

- b. Browse to and select an appropriate raw data file. Then, click **Open**.

The chromatogram and spectrum views become populated with data from the raw data file ([Figure 12](#)).

Figure 12. Qual view of the Processing Setup window with an example raw data file



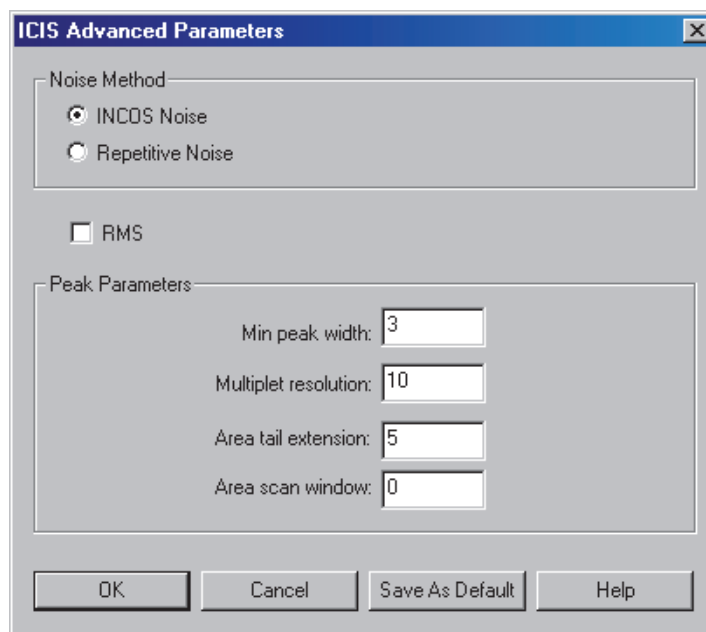
3. On the Identification page, do the following:
 - a. Select a detector type.
 - b. Select a peak detect algorithm in the Peak Detect list to specify how the data system finds and processes chromatogram peaks.

ICIS	This algorithm has been designed for MS data and has superior peak detection efficiency at low MS signal levels. This is the Xcalibur default peak detection algorithm.
Genesis	This algorithm is the original Xcalibur peak detection algorithm and has been provided for backward compatibility with Xcalibur 1.0 data system studies.
Avalon	This algorithm supports detectors other than MS and detects negative chromatographic peaks and shoulders more accurately than Genesis or ICIS.
 - c. In the Filter list, select a scan filter.
 - d. To accept current changes to the Identification page, click **OK**.
 - e. To set advanced parameters, click **Advanced** (Figure 13).

Note For the following procedure, the ICIS Advanced Parameters dialog box opens. If you choose another peak detection algorithm, a different Advanced Parameters dialog box opens. Fill in the values that are appropriate for the method.

- f. Confirm that the **INCOS Noise** option is selected in the Noise Method area.

Figure 13. ICIS Advanced Parameters dialog box



4 Searching Libraries

Setting Up and Running Automated Library Searches

- g. To close the dialog box and return to the Processing Setup window, click **OK**.
- h. To apply changes to the Identification page, click **OK**.

Go to the next procedure, [Setting Up the Library Search Options in a Processing Method](#), to set up the library search options.

Setting Up the Library Search Options in a Processing Method

Use the Library Search Options page (see [Figure 14](#)) in the Qual view of the Processing Setup window to set up the library search options in a processing method.

For more information about creating a processing method, refer to the *Xcalibur Data Processing and Acquisition User Guide*.

Note The Xcalibur data system uses the NIST Mass Spectral Search Program algorithms to perform its library searches. The algorithms and related software are distributed by the Standard Reference Data Program of the National Institute of Standards and Technology and are the copyright of the US Secretary of Commerce.

❖ To set up the library search option parameters for a processing method

1. Set up the identification parameters as described in [Setting Up the Identification Parameters for a Qualitative Processing Method](#), if you have not already done so.
2. Click the **Library Search Options** tab to open the Library Search Options page ([Figure 14](#)).

Figure 14. Library Search Options page in the Qual view of the Processing Setup window

Identification | Spectrum Enhancement | **Library Search Options** | Library Search Constraints | Peak Purity

Search type

☒ Identity ☐ Similarity

☒ Normal ☐ Simple

☐ Quick ☐ Hybrid

☐ Penalize rare compounds ☐ Neutral loss

Options

Maximum number of hits:

☐ Reverse search

☒ Search with MW =

Append to user library

☒ Enable

User library:

Thresholds

Match factor:

Reverse match factor:

Probability (%):

Mass Defect

☐ Enable

Defect (mmu) at mass (amu)

Defect (mmu) at mass (amu)

OK Cancel Save As Default Search List... Help

3. In the Search Type area, do one of the following:
 - To submit processed spectra to an identity search, select the **Identity** option. Then, select one of the three Identity search types:
 - Select the **Normal** option to use a normal identity search.
 - Select the **Quick** option to use a quick identity search.
 - Select the **Penalize Rare Compounds** option if you want a modified normal identity search.
 - To submit processed spectra to a similarity search, select the **Similarity** option. Then select one of the three Similarity search types:
 - Select the **Simple** option to use a Simple Similarity search.
 - Select the **Hybrid** option to use a Hybrid Similarity search.
 - Select the **Neutral Loss** option if you want a Neutral Loss Similarity search.

The difference between the two search types is primarily in the weightings of the spectrum as a function of mass.

4. In the Options area, do the following:
 - To limit the number of search results to be returned by a library search and reported in the result file, type a number in the Maximum Number of Hits box.
 - If you know the molecular weight of your target analyte and want to restrict the search to library compounds of the same molecular weight, select the **Search with MW =** check box and type the molecular weight in the associated box.

When you select the Search with MW= option, the Molecular Weight option on the Library Search Constraints page becomes unavailable.
 - To select the sorting method for hits, do one of the following:
 - To sort hits by Reverse Match Factor, select the **Reverse Search** check box.
 - To sort hits by the Forward Match Factor, clear the **Reverse Search** check box.
5. To include mass defect values for library searches, select the **Enable** check box in the Mass Defect area.
6. To add new spectra to a user library, do the following:
 - a. In the Append to User Library area, select the **Enable** check box.

The User Library list and the parameters in the Thresholds area become available.

- b. Select the user library and specify the spectrum thresholds as follows:
 - From the User Library list, select the target user library.
 - Type a threshold value in the Match Factor box.
 - Type a threshold value in the Reverse Match Factor box.
 - Type a threshold value in the Probability (%) box.
7. To save the settings on the Library Search Options page, click **OK**.

Leave the Library Search Options page open and go to the next procedure, [Specifying the Libraries for an Automated Search](#).

Specifying the Libraries for an Automated Search

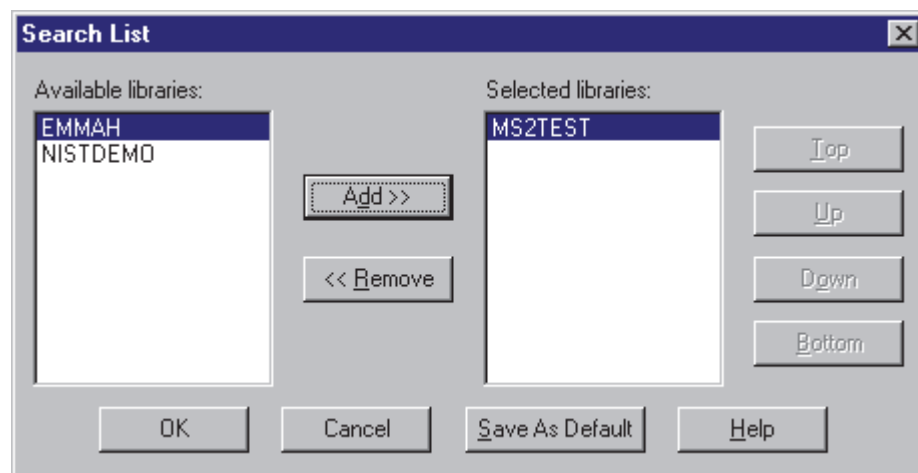
When you set up a processing method to automate library searches, you must specify the libraries to be searched.

❖ To specify the libraries to be searched

1. On the Library Search Options page of the Processing Setup – Qual view, click **Search List** ([Figure 14 on page 38](#)).

The Search List dialog box opens ([Figure 15](#)).

Figure 15. Search List dialog box



2. To select a library to search, select the library name in the Available Libraries list and click **Add** to move it to the Selected Libraries list.
3. Click **OK** to select that library and return to the Processing Setup – Qual view.

To set up search constraints for the automated library search, go to the next procedure, [Setting Up the Search Constraints for an Automated Library Search](#). Otherwise, go to [Setting Up Reports for Automated Library Searches](#) to add a library search report to the method.

Setting Up the Search Constraints for an Automated Library Search

For processing efficiency, constrain an automated library search using some of the options on the Library Search Constraints page of the Processing Setup – Qual view (these are all normally not active). For example, you can exclude certain high intensity ions that appear in many compounds or that are present in the spectrum background. You can target a search to a particular range of molecular weights or to compounds containing certain elements.

Setting up the options on the Library Search Constraints page requires specific knowledge about the target compounds in the chromatogram. Acquiring this knowledge is not always possible with a qualitative analysis.

The Library Search Constraints page contains five groups of options to constrain the library search (Figure 16). To display the Library Search Constraints page, from the Qual view of the Processing Setup window, click the **Library Search Constraints** tab.

See the following topics to set up the constraints:

- [Applying a Molecular Weight Constraint](#)
- [Applying the Other Databases Constraint](#)
- [Applying a Name Fragment Constraint](#)
- [Applying Element Constraints](#)
- [Applying Mass Spectral Peak Constraints](#)

Figure 16. Library Search Constraints page from Qual View

The screenshot shows the 'Library Search Constraints' tab selected. The interface includes the following sections:

- Molecular weight:** An 'Enable' checkbox and a 'Range' input field with the value '1-999999'.
- Other databases:** An 'Enable' checkbox and a list of checkboxes for 'Fine', 'TSCA', 'RTECS', 'EPA', 'USP', 'HODGC', 'NIH', 'EINECS', and 'IR'. A 'Clear All' button is at the bottom.
- Name fragment:** An 'Enable' checkbox and a 'Name' input field.
- Element constraints:** An 'Enable' checkbox, an 'Individual element' table, and an 'Elements in compound' section.

	Element	Condition	Value
*		>	0
- Mass spectral peak constraints:** An 'Enable' checkbox, a table, and radio buttons for 'Absolute' and 'Relative'.

	Type	m/z	From	To
*	<New>	0	1	1

Set parameters and save your settings by clicking **OK**. To save your settings for future searches, click **Save as Default**.

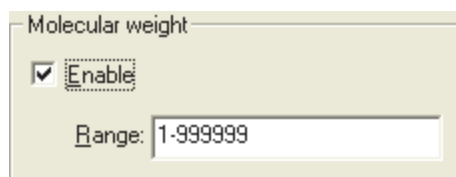
Applying a Molecular Weight Constraint

Follow this procedure to set up the parameters in the Molecular Weight area of the Processing Setup – Qual view.

❖ To limit the library search to compounds with a specific molecular weight or molecular weight range

1. Select the **Enable** check box in the Molecular Weight area (Figure 17).

Figure 17. Molecular weight area



Molecular weight

☒ Enable

Range: 1-999999

2. In the Range box, type a molecular weight or molecular weight range.

To specify a range, use the format *low mass–high mass*. The valid range is 1 to 999 999. All search results must satisfy the specified molecular weight range.

Note This constraint is not available if you have already selected the Search with MW= check box on the Library Search Options page of the Processing Setup – Qual view.

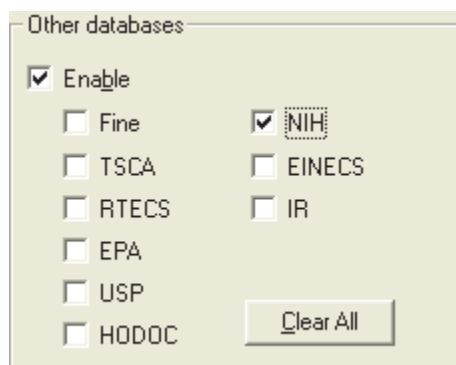
Applying the Other Databases Constraint

Follow this procedure to set up the parameters in the Other Databases area of the Processing Setup – Qual view.

❖ **To limit the library search to entries in the NIST library that are also featured in other databases**

1. Select the **Enable** check box in the Other Databases area (Figure 18). NIST library entries contain references to other commercial databases if they contain information about the compound.

Figure 18. Other databases area



2. Select one or more databases from the available list. To use a database constraint, select its check box. If you do not want to use a database constraint, make sure its check box is clear.

Fine	Commercially Available Fine Chemical Index
TSCA	Toxic Substances Control Act Inventory
RTECS	Registry of Toxic Effects of Chemical Substances
EPA	EPA Environmental Monitoring Methods Index
USP	US Pharmacopoeia/U.S.A.N.
HODOC	CRC Handbook of Data of Organic Compounds
NIH	NIH-NCI Inventory File
EINECS	European Index of Commercial Chemical Substances
IR	NIST/EPA Gas Phase IR Database

The data system only reports search results if they feature in one or more, but not necessarily all, of the selected databases.

Applying a Name Fragment Constraint

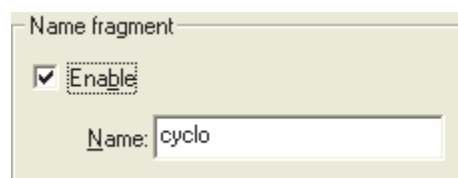
Follow this procedure to set up the parameters in the Name Fragment area of the Processing Setup – Qual view.

❖ To limit the search to compounds with a specific name or name fragment

1. Select the **Enable** check box in the Name Fragment area (Figure 19).

The Name box accepts a text string (up to 39 characters) to represent a fragment of a compound name, for example, “cyclo”. The library search filters the search results and only returns those containing the specified text in their names. The entry is not case sensitive; for example “CYCLO” returns compounds containing the fragments “cyclo”, “Cyclo”, “CYCLO”, and any other case permutations.

Figure 19. Name fragment area



2. Type a name fragment in the Name box.

Applying Element Constraints

Follow this procedure to set up the parameters in the Element Constraints area on the Library Search Constraints page of the Processing Setup – Qual view.

To constrain the library search to compounds with specific element profiles, follow one of these methods:

- [To use the Individual Elements constraints](#)
- [To use the Elements in Compound constraints](#)

❖ To use the Individual Elements constraints

1. In the Elements Constraints area, select the **Enable** check box.

Use the Individual Element area to set specific criteria about the elements required in a library search result (hit). For example, the entries shown in Figure 20 would only return search results for compounds that contain more than five fluorine atoms and exactly three chlorine atoms.

Figure 20. Element Constraints area

Element constraints

☒ Enable

Individual element

	Element	Condition	Value
1	F	>	5
2	Cl	=	3
*		>	3

Elements in compound

Elements:

F,Cl

☒ All ☐ Some

Clear

You do not need to provide a complete elemental profile. The library search returns compounds if they satisfy all the specified criteria regardless of any other elements present. Use this option to specify which elements you do **not** want to be in a library hit (spectrum match). For example, C = 0 confirms that no search results contain carbon.

When a contradiction occurs, for example, C < 2, and C > 4, the data system displays an error message. Correct the contradiction to proceed.

- In the Individual Element area, do the following for each element that you want to constrain:
 - In the Element column, type the required element abbreviation. You must use the IUPAC approved abbreviation for each element. For example, type capital F for fluorine or Cl for chlorine.
 - In the Condition column of the same row, select from the three available conditions: < (less than), > (greater than), or = (equal to).
 - In the Value column of the same row, type the required number of atoms for the element constraint condition.

❖ To use the Elements in Compound constraints

- In the Elements Constraints area, select the **Enable** check box.
- In the Elements in Compound area, in the **Elements** box, type the IUPAC approved abbreviation for each element (see [Figure 20](#)) that must be present in returned search results. Separate each element in the list (of up to 30 characters) by the character specified as the list separator character. Refer to “Changing the List Separator Character” in the *Xcalibur Data Acquisition and Processing User Guide* for more information.
- Select the **All** option to have the returned search results contain all, and only, the listed elements. For example “C, H, O” would return HCHO but not CO₂, CH₄, or CH₂Cl₂.

- Select the **Some** option to have the returned search results contain at least one of the specified elements and no elements other than those listed. For example “C, H, O” would return CO₂, CH₄, and HCHO but not CH₂Cl₂ (Cl not allowed).

If you leave the box blank, the data system does not apply the Elements in compound constraint function. If you type an invalid element, the data system reports an error when you click anywhere else on the page.

If there are no contradictions, you can use the two types of elemental constraints together. For example, if the Individual Element area contains “C=0” or “C<1” and the Elements In Compound box contains “C” when the All option has been selected, the data system displays an error message. Correct the contradiction to proceed.

Applying Mass Spectral Peak Constraints

Follow this procedure to set up the parameters in the Mass Spectral Peak Constraints area of the Processing Setup – Qual view.

The Mass spectral peak constraint feature builds a profile of ions and their abundances to be matched against library entries during the search.

For information about the parameters in the Mass Spectral Peak Constraints area, refer to the *Xcalibur Data Acquisition and Processing User Guide*.

❖ To apply and set up mass spectral peak constraints

- Select the **Enable** check box in the Mass Spectral Peak Constraints area (Figure 21).

The search algorithm only returns search results matching the specified constraints.

Figure 21. Example of a relative mass spectral peak constraint

Mass spectral peak constraints

☒ Enable

	Type	m/z	From	To
1	Normal	0	1	1
*	<New>	0	1	1

☒ Absolute
☐ Relative

- Select the Absolute or Relative option:
 - To evaluate all table entries as a percentage of the base (largest) ion in the spectrum, select the **Absolute** option.
 - To treat the first entry as an absolute Normal or Loss type, select the **Relative** option. The data system considers subsequent entries in the table relative to the first.

3. For each mass spectral peak that you want to constrain, do the following in the Mass Spectral Peak Constraints table:
 - In the Type list, do the following:
 - Select from the four available types for the Absolute option: **Normal**, **Loss**, **Rank** or **Maxmass**.
 - Select from the two available types for the Relative option: **Normal** or **Loss**.
 - In the *m/z* column of the same row, do the following:
 - For a Normal, Rank, or Maxmass type constraint, type the *m/z* value of the mass spectral peak to be constrained. The valid range is **0–2000**,
 - For a Loss type constraint, type the value of a neutral loss. The valid range is **0–64**.
 - In the From column of the same row, do the following:
 - For a Normal, Loss, or Maxmass type constraint, type the minimum abundance of the constrained mass spectral peak.
 - For a Rank type constraint, type the lowest position of the ion in an intensity ordered list of spectral peaks.

For the Rank type constraint, the From value cannot be greater than the To value. If the From value equals the To value, the designated ion must have that rank in the retrieved spectrum.
 - In the To column of the same row, do the following:
 - For a Normal, Loss, or Maxmass type constraint, type the maximum abundance of the constrained mass spectral peak.
 - For a Rank type constraint, type the highest position of the ion in an intensity ordered list of spectral peaks.

Note If you switch between Absolute and Relative modes, the Xcalibur data system prompts you with a warning message before clearing all rows in the grid.

Setting Up Reports for Automated Library Searches

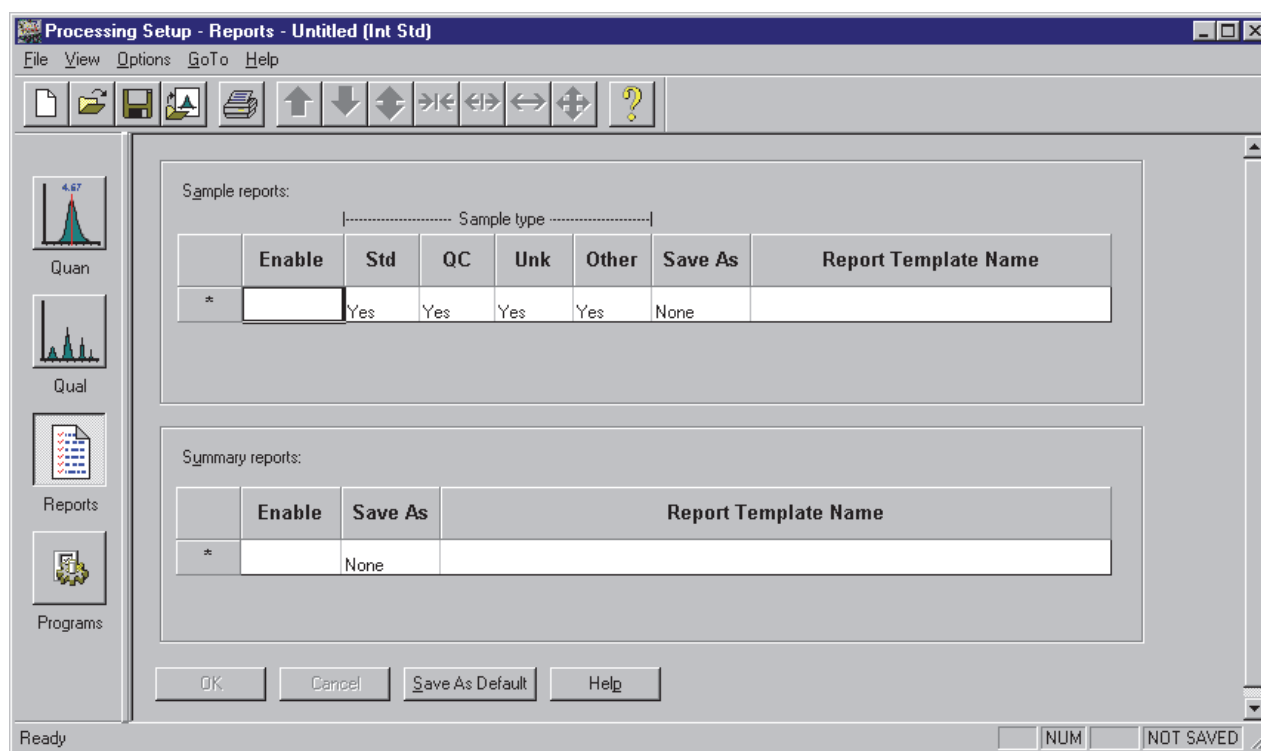
To produce and print reports automatically, specify report options from the Reports view of the Processing Setup window after setting up the library search parameters.

❖ To display the data in the format of a custom report template

1. In the Processing Setup window, choose **View > Reports**.

The Reports view opens (see Figure 22).

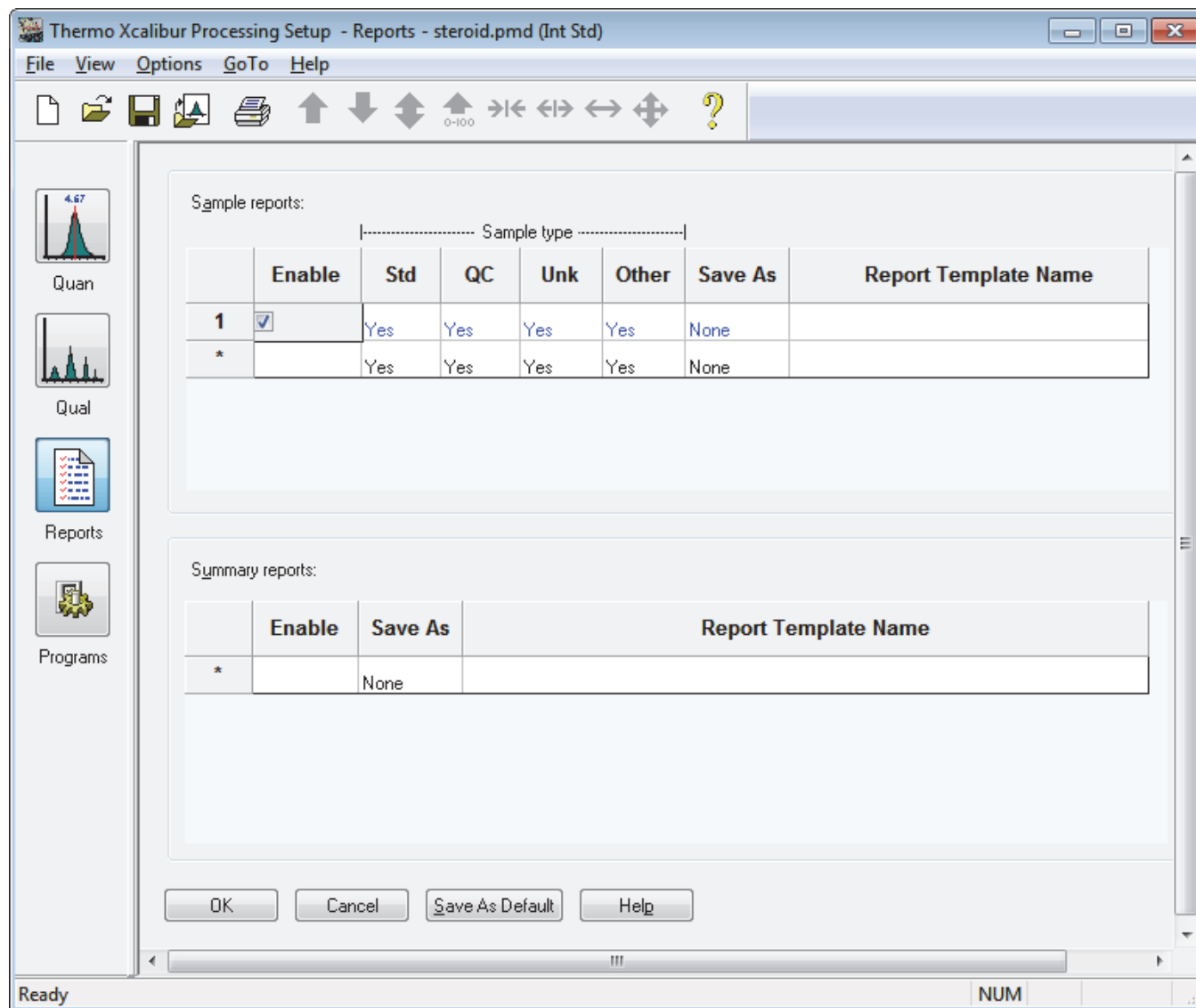
Figure 22. Reports view of the Processing Setup window



2. If the Apply Changes? dialog box opens, read the ⚠ message and click **Yes**.

3. Click the **Enable** cell in the Sample Reports area. When a check box appears, select the check box to make row 1 active (Figure 23).

Figure 23. Reports view with Row 1 active



4. Specify the sample types in row 1 as follows:
 - a. To exclude the standards from the report, click **Yes** in the Std column and clear the check box.
 - b. To exclude the quality control samples, click **Yes** in the QC column and clear the check box.
 - c. Click **Yes** in the Other column and clear the check box.

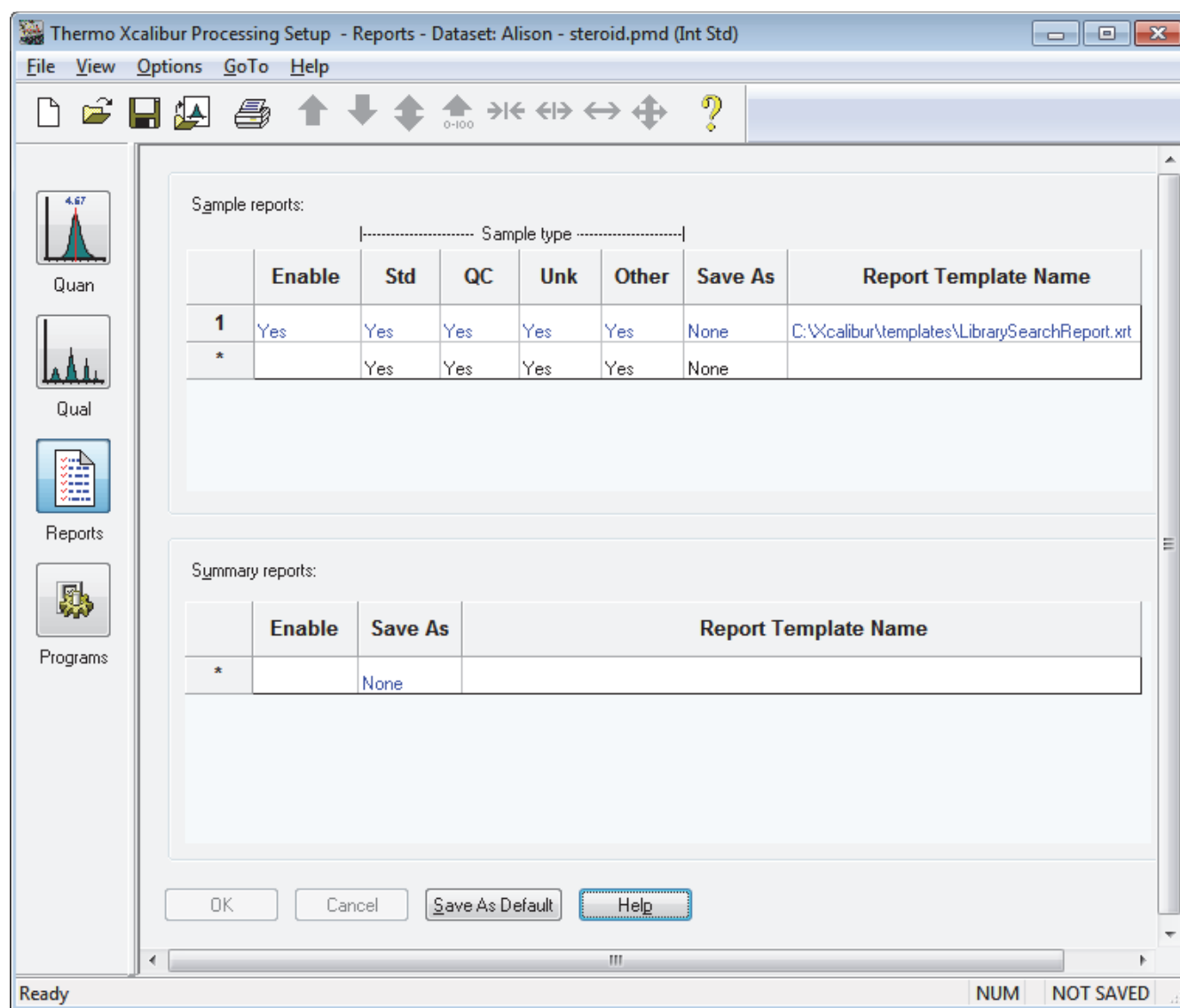
4 Searching Libraries

Setting Up and Running Automated Library Searches

5. Select a report template in row 1 as follows:
 - a. Double-click the Report Template Name column.
The Browse for Sample Report Template dialog box opens.
 - b. Select the **LibrarySearchReport.xrt** template or your own custom template for library reports. Then, click **Open**.
6. To apply changes to the Reports view, click **OK**.

Figure 24 shows the Reports view and a specified Report Template Name.

Figure 24. Reports view of the Processing Setup window

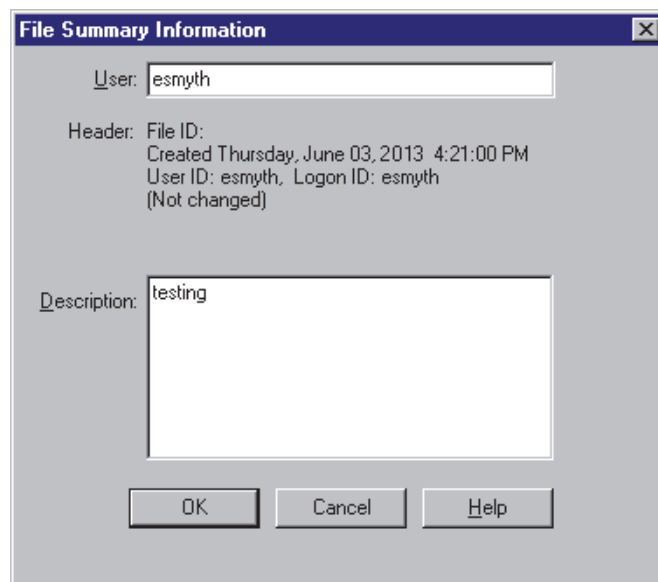


7. Save the processing method as follows:

- a. Choose **File > Save As**.

The File Summary Information dialog box opens (Figure 25).

Figure 25. File Summary Information dialog box

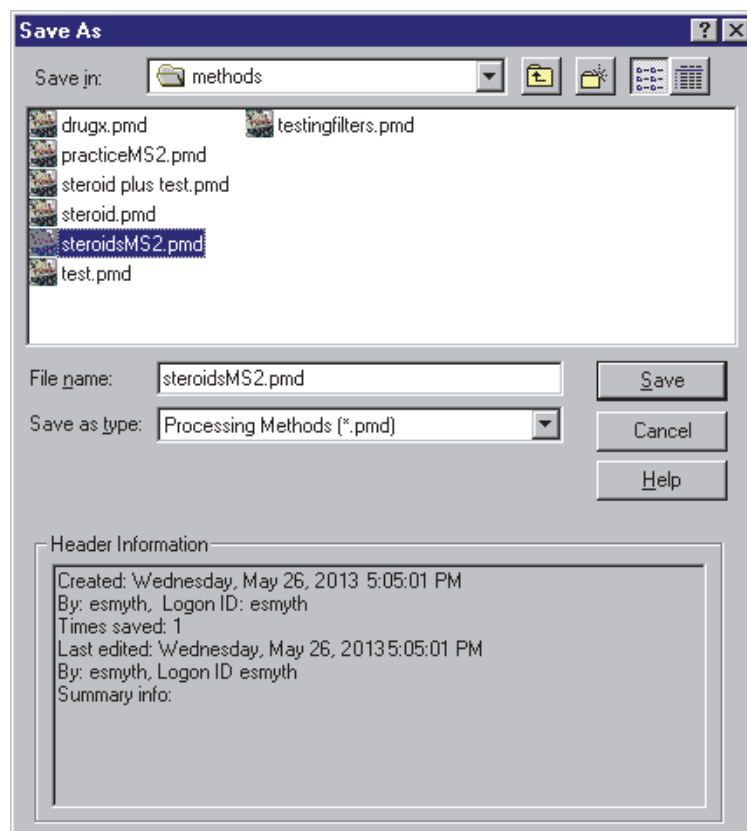


- b. Type file summary information in the Description box and click **OK**.

The Save As dialog box opens.

- c. Type a name for the processing method in the File Name box (Figure 26).

Figure 26. Save As dialog box



- d. To save the method and return to the Reports view, click **Save**.
8. To close the Processing Setup window and return to the Xcalibur home page, choose **File > Exit**.

Setting Up the Qualitative Processing Sequence

To search libraries and print reports automatically, set up a processing sequence that contains the raw data files to be processed and the processing method with the library search parameters.

For information about creating a processing method for automated library searches, see [Setting Up Library Searches in a Processing Method](#).

❖ To set up the processing sequence

1. Open the Sequence Setup view by doing one of the following:

- On the home page – Roadmap view, click the **Sequence Setup** icon, .

–or–

- On the Xcalibur home page, choose **View > Sequence Setup View** from the menu bar.

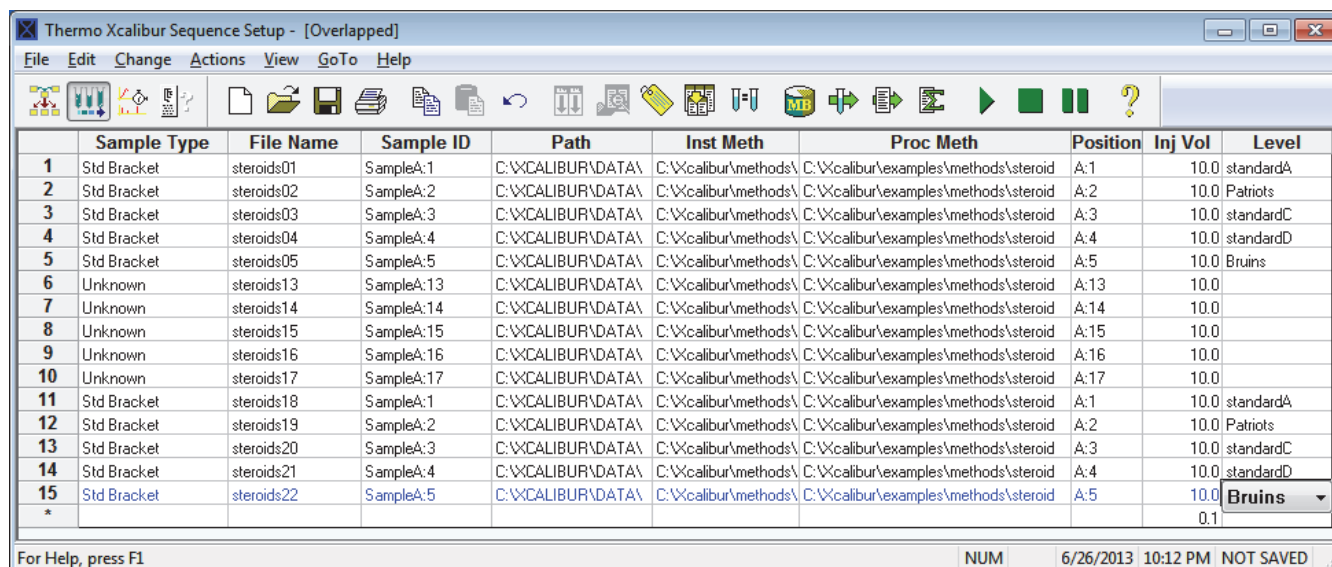
2. From the menu bar, choose **File > Open**.

The Open dialog box opens.

3. Select the sequence file (SLD) that contains the raw data files that you want to reprocess. Then, click **Open**.

The sample list appears in the Sequence Setup view ([Figure 27](#)).

Figure 27. Sequence Setup view



	Sample Type	File Name	Sample ID	Path	Inst Meth	Proc Meth	Position	Inj Vol	Level
1	Std Bracket	steroids01	SampleA:1	C:\XCALIBUR\DATA\	C:\Xcalibur\methods\	C:\Xcalibur\examples\methods\steroid	A:1	10.0	standardA
2	Std Bracket	steroids02	SampleA:2	C:\XCALIBUR\DATA\	C:\Xcalibur\methods\	C:\Xcalibur\examples\methods\steroid	A:2	10.0	Patriots
3	Std Bracket	steroids03	SampleA:3	C:\XCALIBUR\DATA\	C:\Xcalibur\methods\	C:\Xcalibur\examples\methods\steroid	A:3	10.0	standardC
4	Std Bracket	steroids04	SampleA:4	C:\XCALIBUR\DATA\	C:\Xcalibur\methods\	C:\Xcalibur\examples\methods\steroid	A:4	10.0	standardD
5	Std Bracket	steroids05	SampleA:5	C:\XCALIBUR\DATA\	C:\Xcalibur\methods\	C:\Xcalibur\examples\methods\steroid	A:5	10.0	Bruins
6	Unknown	steroids13	SampleA:13	C:\XCALIBUR\DATA\	C:\Xcalibur\methods\	C:\Xcalibur\examples\methods\steroid	A:13	10.0	
7	Unknown	steroids14	SampleA:14	C:\XCALIBUR\DATA\	C:\Xcalibur\methods\	C:\Xcalibur\examples\methods\steroid	A:14	10.0	
8	Unknown	steroids15	SampleA:15	C:\XCALIBUR\DATA\	C:\Xcalibur\methods\	C:\Xcalibur\examples\methods\steroid	A:15	10.0	
9	Unknown	steroids16	SampleA:16	C:\XCALIBUR\DATA\	C:\Xcalibur\methods\	C:\Xcalibur\examples\methods\steroid	A:16	10.0	
10	Unknown	steroids17	SampleA:17	C:\XCALIBUR\DATA\	C:\Xcalibur\methods\	C:\Xcalibur\examples\methods\steroid	A:17	10.0	
11	Std Bracket	steroids18	SampleA:1	C:\XCALIBUR\DATA\	C:\Xcalibur\methods\	C:\Xcalibur\examples\methods\steroid	A:1	10.0	standardA
12	Std Bracket	steroids19	SampleA:2	C:\XCALIBUR\DATA\	C:\Xcalibur\methods\	C:\Xcalibur\examples\methods\steroid	A:2	10.0	Patriots
13	Std Bracket	steroids20	SampleA:3	C:\XCALIBUR\DATA\	C:\Xcalibur\methods\	C:\Xcalibur\examples\methods\steroid	A:3	10.0	standardC
14	Std Bracket	steroids21	SampleA:4	C:\XCALIBUR\DATA\	C:\Xcalibur\methods\	C:\Xcalibur\examples\methods\steroid	A:4	10.0	standardD
15	Std Bracket	steroids22	SampleA:5	C:\XCALIBUR\DATA\	C:\Xcalibur\methods\	C:\Xcalibur\examples\methods\steroid	A:5	10.0	Bruins
*								0.1	

4. Modify the sample list as appropriate:
 - To exclude samples from the list, select rows to exclude and choose **Edit > Delete Row**. The data system displays a message box to confirm the Delete Row command. Click **Yes**.
 - To view the Sample Type column, click the left side of the horizontal scroll bar at the bottom of the workspace. Double-click the Row 1 cell in the Sample Type column to display a drop-down list. Then, scroll up to select **Unknown**.
 - Expand the width of the Path column to confirm that the directory is the one storing the raw data files. For example, raw data files containing steroids data are found in C:\Xcalibur\examples\data.
5. To select the processing method of interest, do the following:
 - a. Double-click in row 1 of the Processing Method column.

The Select Processing Method dialog box opens.
 - b. Select the processing method that you want to use to run an automated library search. Then, click **Open**.

The data system populates the Processing Method column with the selected processing method.
6. To save the sequence list file, choose **File > Save As**.

The File Summary Information dialog box opens.
7. Type a description in the Comment box and click **OK**.

The Save As dialog box opens.
8. Type a name in the File Name box to name the sequence.
9. Click **Save** to save the sequence list and return to the Sequence Setup view.

To batch reprocess the sequence and print reports, go to the next procedure, [Batch Reprocessing the Sequence and Printing Library Search Reports](#).

Batch Reprocessing the Sequence and Printing Library Search Reports

Follow this procedure to batch reprocess a sequence and print reports.

Tip During batch reprocessing, the data system sends the user-specified reports to the default printer for the data system computer. You can select the paper size and page orientation in the Page Setup dialog box. To open this dialog box, choose **File > Page Setup** from the menu bar.

❖ To batch reprocess a sequence and print library search reports

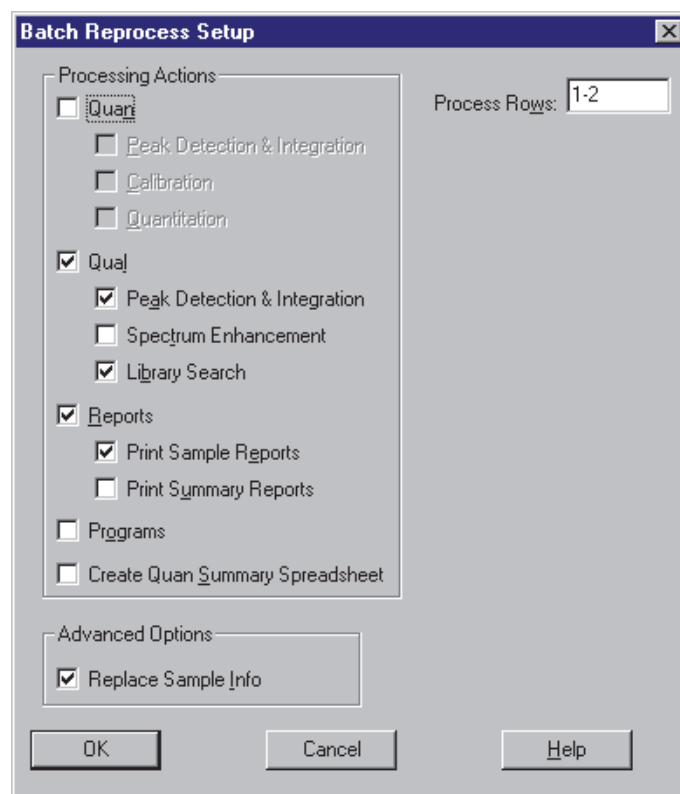
1. Set up the processing sequence as described in [Setting Up the Qualitative Processing Sequence](#).
2. If you closed the processing sequence, open it in the Sequence Setup view by choosing **File > Open** from the menu bar.
3. To select the rows in the current sequence to process, select the row number in the first row to process and drag the cursor to the bottom row.

The data system highlights the selected rows.

4. Do one of the following:
 - Click the **Batch Reprocess** icon, , in the toolbar.
- or—
- Choose **Actions > Batch Reprocess**.

The Batch Reprocess Setup dialog box opens ([Figure 28](#)).

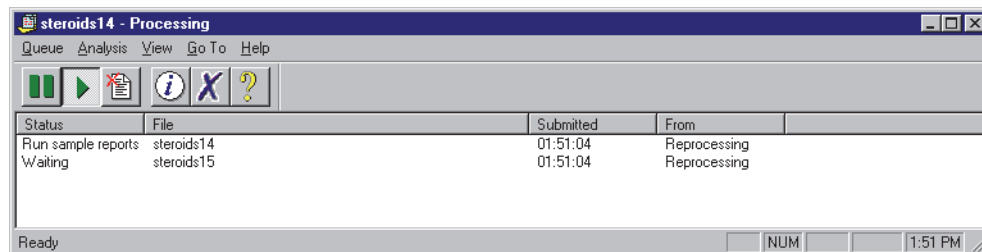
Figure 28. Batch Reprocess Setup dialog box



5. Confirm that the Process Rows box lists all row numbers (for example 1–2). If the numbers are missing, double-click the box and type the row numbers.
6. To perform a library search, select the **Qual** check box. Then, select the **Peak Detection & Integration** check box, the (optional) **Spectrum Enhancement** check box, and the **Library Search** check box.
7. To print the library search sample report, select the **Reports** check box. Then, select the **Print Sample Reports** check box.
8. To initiate batch processing of the selected samples, click **OK**. If the data system prompts you to save your changes, click **Yes** in the confirmation box.

- To display the Processing Status window (Figure 29), click the **Queue Manager** task in your computer task bar.

Figure 29. Processing Status window



Two beeps signal the end of batch processing.

- Check your printed reports to see that they provide the information you wanted.

4 Searching Libraries

Setting Up and Running Automated Library Searches

Library Sample Reports

This appendix contains samples of possible library search reports printed during batch reprocessing of a sequence or from within the Qual Browser window.

Contents

- [Report from a Library Search During Batch Reprocessing](#)
- [Report from a Library Search Using Qual Browser](#)

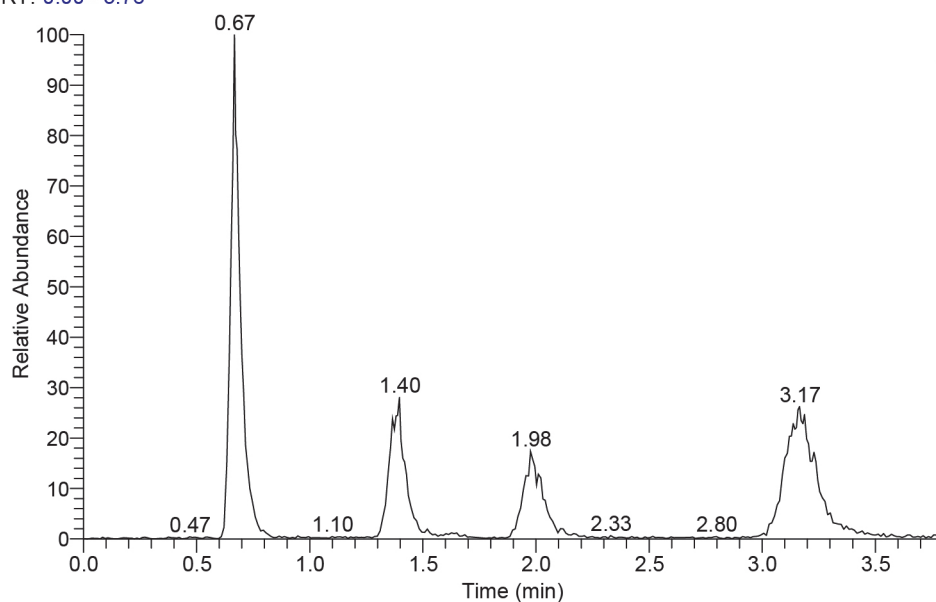
Report from a Library Search During Batch Reprocessing

The Xcalibur data system prints library search reports automatically when you process or batch reprocess a sequence. This library search report was generated with the LibrarySearchReport.xrt template. For more information, see [Setting Up and Running Automated Library Searches](#).

Library Search Report

Data File:	steroids14	Original Data Path:	C:\pitcon\trial2
Current Data Path:	C:\Xcalibur\examples\data	Sample Type:	Unknown
Sample ID:	Sample14	Sample Name:	
Operator:	jackc	Acquisition Date:	02/28/96 12:15:58 PM
Run Time (min)	378	Comments:	
Vial:	2	Scans:	323
Low Mass (m/z)	100.00000	High Mass (m/z)	375.00000
Sample Weight:	0.00	ISTD Amount	0.000
Calibration Level:		Dilution Factor	100
Instrument Method: C:\pitcon\trial2\steroidMSMSis			
Original Processing Method: C:\pitcon\trial2\steroidmsmsIS			
Current Processing Method: N/A			

RT: 0.00 - 3.78

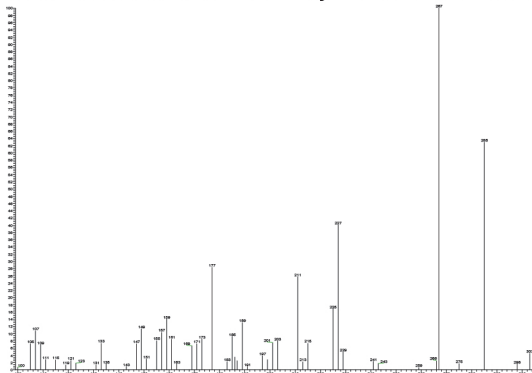


NL:
2.34E6
TIC MS
steroids14

Library Search Report

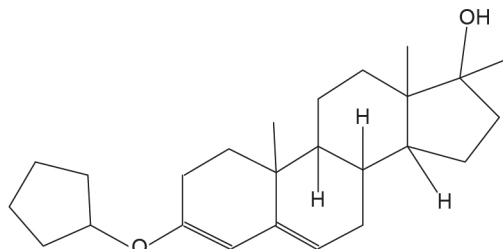
Hit Spectrum

SI 999, RSI 999, steroids2, Entry# 2, CAS# NA, methyltestosterone



Compound Structure

methyltestosterone
Formula C₂₅H₃₈O₂, MW 370, CAS# NA, Entry# 2
\$:04303.30



RT	Scan#	Probability
1.98	167	98.25

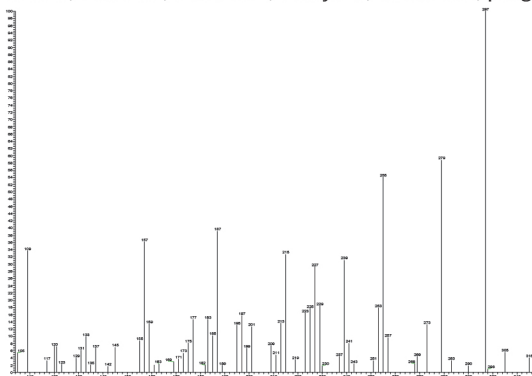
Compound Name	SI	RSI	Cas #
methyltestosterone	999	999	NA

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Library Search Report

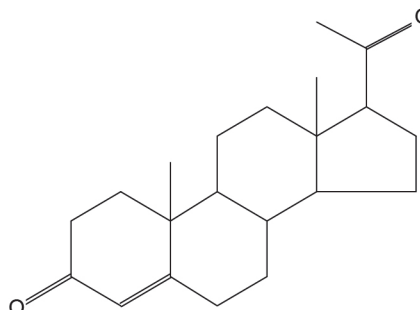
Hit Spectrum

SI 999, RSI 999, steroids2, Entry# 3, CAS# NA, progesterone



Compound Structure

progesterone
Formula C₂₁H₃₀O₂, MW 314, CAS# NA, Entry# 3
\$:04315.30



RT	Scan#	Probability
3.17	268	98.51

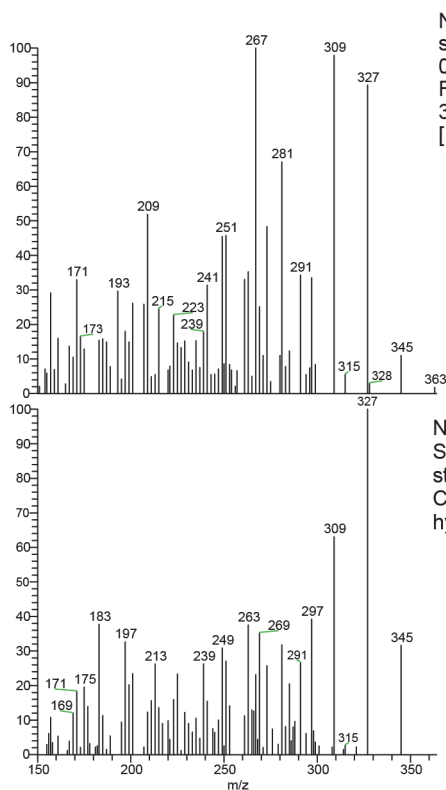
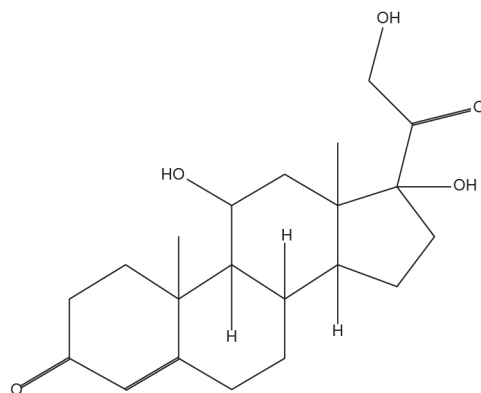
Compound Name	SI	RSI	Cas #
progesterone	999	999	NA

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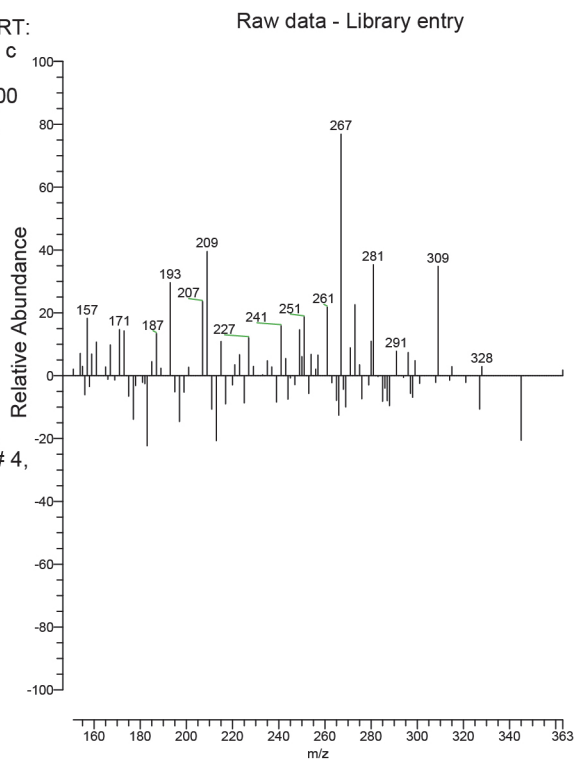
Report from a Library Search Using Qual Browser

The following is an example of a library search report that you can print from the Qual Browser window. For more information, see [Submitting a Spectrum to a Library Search in Qual Browser](#).

Hit	SI	RSI	Prob	Name	Library Name	
1	706	735	98.63	hydrocortisone	steroids2	hydrocortisone
2	382	595	0.98	progesterone	steroids2	Formula C ₂₁ H ₃₀ O ₅ , MW 362, CAS# NA, Entry# 4
3	357	519	0.30	deoxyhydrocorticosterone	steroids2	\$:04363.30
4	323	638	0.07	methyltestosterone	steroids2	



NL: 9.99E2
SI 706, RSI 735,
steroids2, Entry# 4,
CAS# NA,
hydrocortisone



A Library Sample Reports

Report from a Library Search Using Qual Browser

Library Browser

This chapter describes the Library Manager application that you can access from the Tools menu on the Xcalibur home page and the Library Search Results window that opens when you submit a library search from the spectrum view of the Qual Browser application.

Contents

- [Library Manager Application](#)
- [Library Search Results Window](#)

For more information about the NIST MS Search application, refer to the Help provided with the application.

Library Manager Application

Use the Library Manager application to manage NIST libraries used with the NIST search software and to convert libraries between the ICIS/GCQ/ITS 40, MassLab, NIST, and ANDI-MS formats.

Xcalibur Library Manager supports the following conversions.

From \ To	ICIS/GCQ/ITS 40	MassLab	ANDI-MS	NIST
ICIS/GCQ/ITS 40		✓	✓	✓
MassLab	✓		✓	✓
ANDI-MS	✓	✓		✓
NIST	✓	✓	✓	

Note The Xcalibur data system does not directly support INCOS, LAB-BASE, or JCAMP library conversions. However, MassLab data system users have a conversion program to convert from a LAB-BASE user library to a MassLab user library. In addition, a conversion tool exists in ICIS (a UNIX system) that can convert a LAB-BASE user library to a MassLab user library.

The Library Manager application has the following pages:

- [Convert Libraries Page](#)
- [Manage Libraries Page](#)

Convert Libraries Page

Use the Library Manager – Convert Libraries page to convert one type of source library to another type of library at a target location and to copy a library to another location. This table describes the parameters on the Convert Libraries page.

Table 1. Convert Libraries page parameters (Sheet 1 of 3)

Parameter	Description
Source Library Details	
Type [Source]	Specifies the source library file type that you want to convert to another file type. Type or select any of the following file types: ICIS/GCQ/ITS 40 (LIB or LBR), MassLab (IDB), ANDI-MS (CDF), NIST, or AutoMass (SPR, PRS, NAM, or HDR).
Library/Browse [Source]	Specifies the source library that you want to convert. To change the library, click Browse and select the path to the source library on your computer or network.
Process Entries [Source]	Specifies the number range of the library entries that you want to convert from the source library. If you leave the box empty, the Xcalibur data system converts all entries. The format is <i>First Entry–Last Entry</i> . For example, to convert library entry #100 through library entry #200, type 100–200 in the Process Entries box.
Target library details	
Type [Target]	Specifies the target library file type when converting the source library. If you select source library file type ICIS/GCQ/ITS 40, MassLab, ANDI-MS, or NIST, you can select from the following target library file types: ICIS/GCQ/ITS 40 [(LIB) or (LBR)], MassLab (IDB), NIST, or ANDI-MS (CDF). If you select source library file type AutoMass, you can only select the NIST target library file type. If you select the library type NIST, the Xcalibur data system displays the path to the NIST library folder in the Library box. You specified this location when you installed NIST.

Table 1. Convert Libraries page parameters (Sheet 2 of 3)

Parameter	Description
Library/Browse [Target]	Specifies the file folder to store the converted library file. To change the folder, click Browse and select the target folder on your computer or network.
Title [Target]	Type in a title for the ICIS/GCQ/ITS 40 library or for the Mass Lab library that you create during the conversion. You can add a title to the new library using any format. Note This box in the Target library details area only becomes active when you select an ICIS/GCQ/ITS 40 or MassLab library.
Add the library to the NIST software for use with Xcalibur	Selecting this check box adds the converted library to the NIST software for use with the data system.
Options	
Target library action: Create/Replace	Select this option to create a new library in the target directory or to replace an existing library. You can also append (add) the new (converted) entries to a previously created target library.
Target library action: Append	Select this option to append (adds) the new (converted) entries to a previously created target library. You can also create a new library in the target directory or to replace an existing library.
Include replicate entries from the NIST library in the target library	Selecting this check box includes replicate entries in the target library. Note This check box is only available if you are converting from a NIST library to another format.
Replicate library/browse	Specifies the location of a replicate library. To change the replicate library, click Browse and select the folder for the replicate library on your computer or network. If you specify a replicate library, the Xcalibur data system adds replicate entries into the appropriate replicate library. If you select the library type NIST, the Xcalibur data system displays the path to the NIST replicate library folder in the Library box. You specify this location when you install NIST software.

Table 1. Convert Libraries page parameters (Sheet 3 of 3)

Parameter	Description
Button	
Convert	Starts the library conversion you have specified using the Convert Libraries page. The data system opens the Library Conversion Status dialog box and displays the Conversion Status progress bar and the Conversion Status box. The Status bar displays messages such as the following: Processed 100% of the entries, continuing on The Conversion Status box displays sequential chronological (top to bottom) messages such as the following: • Started the conversion on SEP 3, 1999 at 10:01, please wait • Finished the conversion on SEP 3, 1999 at 10:02 • Converted 570 entries

Manage Libraries Page

Use the Library Manager – Manage Libraries page to add a library to the NIST libraries list or to delete a library from the NIST libraries list. You can also copy a library to another location. This table describes the parameters on the Manage Libraries page.

Table 2. Manage Libraries page parameters (Sheet 1 of 2)

Parameter	Description
NIST Libraries	
NIST Libraries list	Lists all of the NIST libraries currently available on your computer or network. You can add libraries to this list, delete libraries from this list, and copy libraries on the list to another location.
Buttons	
Add	Adds a library to the NIST Libraries list. The Add Library dialog box opens. The Add Library dialog box has the following parameters: • Source: Specifies the name and location of the library that you want to add. • Action options: – Copy the library to the local computer: Select this option to copy the selected library to your computer. – Link to the library from either a remote location or computer: Select this option to access the library remotely. Because libraries can be large, you might save time by using the Link option rather than the Copy option. Click OK when you have selected the library you want to add and selected Action options.

Table 2. Manage Libraries page parameters (Sheet 2 of 2)

Parameter	Description
Delete	Deletes the library that you have previously selected in the NIST Libraries list. Select the library that you want to delete from the NIST Libraries list. Click Delete. The Delete Library message box opens with the following message: Are you sure you want to delete the selected NIST library? Click Yes. The Xcalibur data system removes the library from the list.
Archive	Copies a selected library to another directory on your computer or network. Select the library that you want to copy to another directory. Click Archive. The Archive Library dialog box opens. The Archive Library dialog box has the following parameters: • Parameter • Description • Destination: Specify the location for the selected library. Use Browse to select a destination for the selected file. Click OK. The data system makes a copy of the selected NIST library and stores it in the selected directory.

Library Search Results Window

Qual Browser displays this window in its workspace when you submit a spectrum in a spectrum view to a library search or when you open a result file containing library search results from qualitative processing.

The Library Search Results window displays matching library spectra (hits) in a four-pane arrangement. Clockwise from the top left, the four panes are Hit List, Molecular Structure, Difference Spectrum, and Comparison.

Hit List

The Hit List lists the best matches found during the library search. Three factors describe the accuracy of the match to your spectrum:

SI	A direct matching factor for the unknown and the library spectrum.
RSI	A reverse search matching factor ignoring any peaks in the unknown that are not in the library spectrum.
Prob	A probability factor based on the differences between adjacent hits in an SI ordered list.

With the SI and RSI matching factors, a perfect match results in a value of 1000. As a general guide 900 or greater is an excellent match; 800–900, a good match; and 700–800, a fair match. A matching factor less than 600 is a poor match. Unknown spectra with many peaks tend to yield lower match factors than otherwise similar spectra with fewer peaks.

The probability factor is a complex parameter based on the SI matching factor and the difference between adjacent matches. If a hit has an SI match factor > 900 and the next best hit has a match factor of 300, the probability of the compound being correctly identified is high. Conversely, if several hits are returned with very similar SI matching factors, the probability of a correct assignment is low.

Molecular Structure

Shows the formula, structure, molecular weight, name and library index number of the currently selected hit in the Hit List.

Difference Spectrum

Compares the submitted spectrum with the currently selected library spectrum in the Hit List. Peaks above the *x* axis are relatively more intense in the sample than the library entry. Negative peaks are relatively more intense in the library entry than in the sample spectrum.

Comparison

Displays the submitted spectrum above the currently selected library spectrum in the Hit List pane (list of matching spectrum files).

Note Avoid making positive assignments based solely on the statistical result of a library search. The Xcalibur data system might identify a compound with an unusual structure (or, more importantly, an unusual mass spectrum) in a definitive way. More usually, your unknown might be a member of a class of compounds with very similar mass spectra. The ability of Qual Browser or any search system to distinguish between them is limited. In many cases, the best that the search algorithm can do is identify a class of compounds that have similar mass spectra — and usually similar structure. In most cases, you should seek confirmation by other analysis techniques.

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