

Thermo Xcalibur

Qual Browser

User Guide

Software Version 4.4

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Preface

This user guide for qualitative analysis describes how to use the Thermo Xcalibur™ mass spectrometry data system to identify unknown compounds or carry out a trace analysis. Before reading this manual, read the Getting Started manual for the Xcalibur data system and the getting started manual for your Thermo Scientific mass spectrometer so that you are familiar with the basic features of the Xcalibur data system, such as the Home Page and the Instrument Setup view.

Contents

- [About This Guide](#)
- [Related Documentation](#)
- [Safety and Special Notices](#)
- [Contacting Us](#)

About This Guide

This guide describes how to do the following:

- Use the Qual Browser window of the Xcalibur data system to review raw data.
- Submit spectra to library searches.

For information about acquiring data with the Xcalibur data system, refer to the *Xcalibur Data Acquisition and Processing User Guide*. For information about setting up personal user libraries of reference spectra, refer to the *Xcalibur Library Browser User Guide*.

Related Documentation

Thermo Fisher Scientific provides the following documentation 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 from within the data system

❖ To view the product manuals

- 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.

Safety and Special Notices

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

Safety and 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

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Introduction

This introduction provides a basic understanding of mass spectra and explains how to use Xcalibur, the Thermo Scientific™ mass spectrometry data system for qualitative analysis. Qualitative analysis focuses on solving two analysis problems:

- Identifying unknown compounds
- Confirming the presence of target compounds

Contents

- [Understanding Mass Spectra](#)
- [Analysis Modes for the Mass Spectrometer](#)

Understanding Mass Spectra

There are many different types of mass spectrometry (MS) detectors but the basic principles are the same in all cases: the MS ionizes the sample, separates the ions according to their mass¹, and moves the separated ions towards a detector where they are counted. The data system compiles a spectrum showing the mass distribution of the ions produced from the sample—a snapshot of ion intensities plotted against their mass-to-charge (m/z) ratios.

Ionization initially produces molecular ions, but complex secondary processes can cause the molecular ions to fragment. Together with molecular ions, these fragment ions make up the mass spectrum. For individual chemical substances, a mass spectrum can be a characteristic molecular fingerprint.

These topics describe some common features of mass spectra:

- [Base Peak](#)
- [Neutral Losses](#)
- [Effect of Ionization Modes](#)
- [Adduct Formation](#)
- [Effect of Isotopes](#)

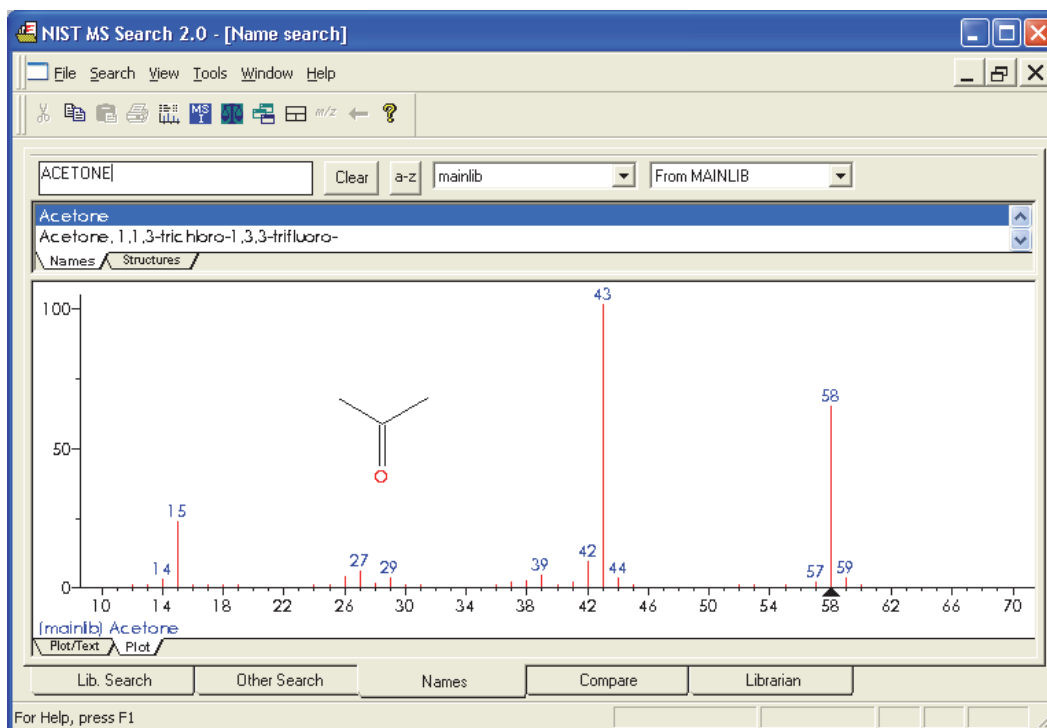
¹ In the majority of cases $z=1$ and the x axis becomes equivalent to mass, m .

Base Peak

In standard practice, the most abundant ion, called the base peak, is given an arbitrary abundance or intensity of 100. The Xcalibur data system reports all other peaks as a percentage of the size of the base peak. After this normalization, the data system can compare spectra directly.

Figure 1 is an example of a simple library spectrum showing the fragmentation of acetone C_3H_6O (molecular weight = 58 Da) in an electron ionization (EI) ion source. The most abundant ions have been labeled with their mass-to-charge ratios. In this example, the molecular ion (58 Da) is not the most abundant. The base peak is actually 43 Da because of the acetyl ion.

Figure 1. 70 eV electron ionization (EI) mass spectrum of acetone



Neutral Losses

You can use fragmentation patterns like the pattern in Figure 1 to determine molecular structure. For example, the neutral loss of 15 Da from the molecular ion of acetone indicates the presence of a methyl group in the original molecule. A subsequent loss of 28 Da corresponds to the loss of CO. Table 1 lists commonly observed neutral losses, measured by the molecular weight of the compound. Assign such losses to help deduce the structure of an unknown compound. A full structural analysis generally relies on the presence of a molecular ion and the measurement of the molecular weight of the compound.

Table 1. Common neutral losses

Loss	Fragment
15	CH ₃
18	H ₂ O
19	F
28	CO
29	C ₂ H ₅ or CHO
35	Cl
46	NO ₂
59	C ₃ H ₇ O, COOCH ₃ or CH ₂ COOH
77	C ₆ H ₅

In some cases, fragmentation is extensive, leaving little or no trace of a molecular ion. With no molecular ion, determining either the molecular weight or the structure is difficult.

Effect of Ionization Modes

The ionization mode affects the spectrum characteristics of a compound. These topics describe the common ionization modes for LC/MS (liquid chromatograph/mass spectrometer) and GC/MS (gas chromatograph/mass spectrometer) instruments:

- [Ionization Modes for LC/MS Instruments](#)
- [Ionization Modes for GC/MS Instruments](#)

Ionization Modes for LC/MS Instruments

LC/MS instruments use a variety of techniques, collectively called atmospheric pressure ionization (API). Detectors of this type can be configured to detect positive or negative ions.

API techniques offer soft ionization, usually with little or no fragmentation. An API spectrum typically contains only the protonated or deprotonated molecular ion. Compounds with basic sites (such as amines) can form protonated molecules $[M+H]^+$. These can be analyzed in positive ion detection mode (polarity +), giving an ion peak at the m/z value $M+1$ (where M represents the molecular weight of the compound).

Compounds with acidic sites (sulphonic acids, for example) can form deprotonated molecules $[M-H]^-$. These can be analyzed in negative ion mode (polarity -) as ion peaks at the m/z value $M-1$.

Ionization Modes for GC/MS Instruments

GC/MS instruments offer two techniques: electron ionization (EI) and chemical ionization (CI).

EI is very commonly used because it is simple and reproducible. The fragmentation pattern is effectively determined by the energy of the impacting electrons alone (electron energy, measured in eV). Very different types of mass spectrometers that use EI can produce virtually identical spectra as long as the electron energy is the same.

This reproducibility has led to an extensive library compilation for 70 eV EI spectra. With the Xcalibur Library Browser, you can access the NIST/EPA/NIH Mass Spectral Library with over 108 000 reference EI spectra. You can use library data to select confirmatory ions for your target compounds.

Note You can purchase the NIST Mass Spectral Search application from the National Institute of Science and Technology. Thermo Fisher Scientific provides this application with the Xcalibur data system.

Chemical ionization (CI) offers a softer method of forming ions. In CI, a controlled flow of a reagent gas, commonly ammonia, methane, or isobutane, is introduced into the area where ionization occurs (the ion source). Energetic electrons that pass through the source ionize the reagent gas, as in EI. These ions can then collide with neutral molecules, causing hydrogen transfer. This process is repeated when the reagent gas ions collide with analyte molecules.

CI usually produces protonated molecules, generally at a mass one unit greater than the molecular mass of the compound. Significantly less fragmentation occurs than in comparable EI spectra. Depending on the choice of reagent gas, adduct ions can form. For example, $M+NH_4$ is a typical adduct ion when ammonia is used as the reagent gas.

Under certain conditions, CI produces negative molecular ions formed by electron capture. The sensitivity of negative ion CI for certain classes of compounds (those containing double bonds, sulfur, phosphorus, chlorine, or bromine) can be orders of magnitude greater than positive CI or EI modes for those compounds.

For more information about the ionization modes available on your instrument, read the hardware manual and the instrument manual on how to get started.

Adduct Formation

If ionization takes place in the presence of contaminants or additives such as ammonium or sodium ions, some compounds are susceptible to adduct formation. These spectra show other ions in addition to, or instead of, the molecular ion (see Figure 2).

Figure 2. Mass spectrum showing sodium and acetonitrile adducts

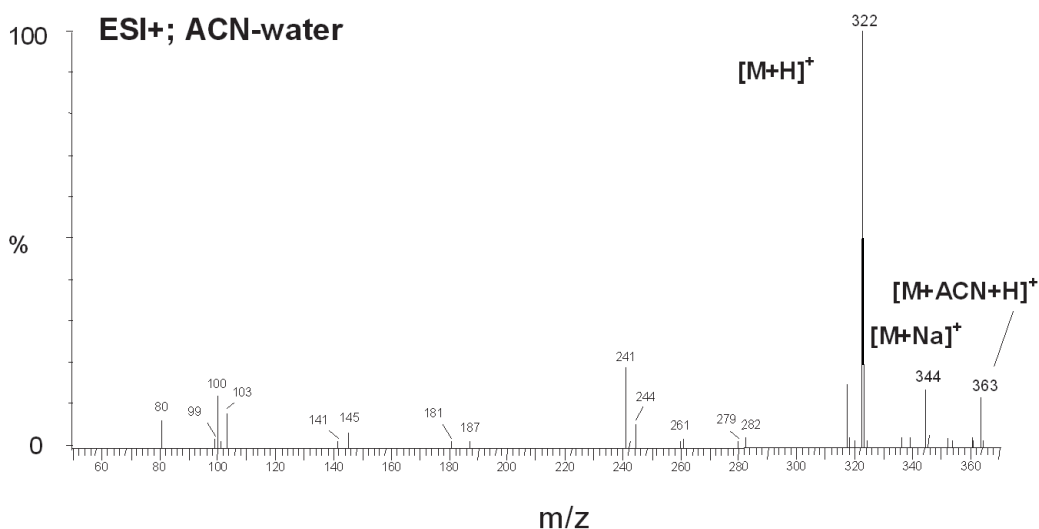


Table 2 lists common adducts for the positive and negative ESI modes.

Table 2. Common adduct ions

Cationized adducts (positive mode)		Anionized adducts (negative mode)	
[M+NH ₄] ⁺	M+18	[M+OAc] ⁻	M+18
[M+Na] ⁺	M+23	[M+Na] ⁻	M+21
[M+CH ₃ OH+H] ⁺	M+33	[M+Cl] ⁻	M+35
[M+K] ⁺	M+39	[M+K] ⁻	M+37
[M+CH ₃ CN+H] ⁺	M+42	[M+HCOO] ⁻	M+59

Take care when determining molecular weights to account for possible adduct ions.

Effect of Isotopes

In some cases, the effect of less abundant isotopes might cause you to use an average molecular weight rather than one based on the most abundant isotopes. When the molecular structure of the target compound contains large numbers of certain elements, the less abundant isotopes become significant. This situation might result in a shift in the mass peaks from their expected *m/z* values.

For example, the most abundant isotope of chlorine is Cl^{35} . However, Cl^{37} occurs with a natural abundance of 24.47 percent. If a compound contains four chlorine atoms, its molecular ion is two mass units greater than that expected from a calculation based solely on Cl^{35} . Using chlorine's average atomic weight (35.453), the molecular ion is correctly identified. Also, you observe a distribution of molecular ions across eight mass units from molecules containing between zero and four Cl^{37} atoms.

Analysis Modes for the Mass Spectrometer

A Thermo Scientific mass spectrometer has these analysis modes:

- [Full Scan](#)
- [Selected Ion Monitoring \(SIM\)](#)
- [MS/MS](#)

Full Scan

In full-scan operation, the MS detector scans repetitively over a wide mass range throughout the analysis and sends the data to the data system computer.

With the Xcalibur data system, you can display the chromatograms (measured intensity versus analysis time) for full-scan MS data in these ways (plot types):

- As a total ion current (TIC) chromatogram. A TIC chromatogram represents the summed intensities of all the ions in the scanned mass range (mass spectrum) plotted against the chromatographic retention time. Each peak in the TIC represents one or more eluting compounds, which can be identified from the mass spectra recorded across the peak.
- As a mass chromatogram for a range of masses within the scan range. Mass chromatograms show the ion intensities of selected mass-to-charge ratios (m/z). The Xcalibur data system extracts these mass spectra from each stored scan and plots them against the analysis time. Use this technique to increase selectivity by displaying an m/z value characteristic of the compound of interest but not present in other sample components.
- As a base peak chromatogram. Base peak chromatograms show the ion intensities of the most intense ions for each time point in the chromatogram.

The full-scan mode is suited to the identification of unknowns and can also be used for trace analysis when sensitivity is not important.

Selected Ion Monitoring (SIM)

In the selected ion monitoring (SIM) mode, the MS detector monitors a limited number of m/z values that are characteristic of a targeted compound or compounds. During an analytical run, the mass analyzer repeatedly switches between the selected m/z values and monitors each m/z value for a programmed dwell time before averaging the measured ion intensities and moving on to the next value.

SIM generates mass chromatograms only of the monitored m/z values, not complete mass spectra as in the full-scan mode. Without a complete mass spectrum, you cannot perform a library search to identify an unknown.

SIM is ideally suited to trace analysis and offers reduced file sizes compared to full-scan operation because SIM records only the information of interest.

MS/MS

Depending on your instrument, you might also be able to do additional stages of mass analysis called MS/MS.

In an MS/MS experiment, an ion from the mass spectrum is selected for fragmentation while all other masses are discarded. The selected ion, called a precursor (parent) ion, is then collided with a neutral background gas. As a result of the collisions, the precursor ion is broken into fragments called product ions. An ion trap mass spectrometer (a mass spectrometer with an ion trap type of mass analyzer) can perform additional stages of MS (called MSⁿ), up to MS¹⁰.

The MS detector can monitor the product ions in either the full-scan mode or the SIM mode. When you set up the MS detector to monitor a specific product ion of a specific precursor (parent) ion, the scan type is called selective reaction monitoring (SRM).

You can create your own libraries of full-scan MS/MS data to use for matching.

You can display the chromatograms for full-scan MS/MS data in these plot types: TIC, mass range, base peak, or neutral fragment. With the neutral fragment plot type, you must specify the neutral fragment.

1 Introduction

Analysis Modes for the Mass Spectrometer

Using the Qual Browser Window

Qual Browser is a powerful and versatile utility for viewing chromatograms and spectra from raw data files (RAW file type) or result files (RST file type).

Note Raw data files contain unprocessed data, and result files contain data that has been processed with a processing method. When you view raw data files in Qual Browser, the data system applies default integration settings to the chromatograms.

For information about the Qual Browser window, toolbars, menus, dialog boxes, and so on, see [Qual Browser Window](#).

These procedures describe how to use some of the basic features of the Qual Browser window.

Contents

- [Opening the Qual Browser Window](#)
- [Using the Qual Browser Toolbars](#)
- [Using the Info Bar](#)
- [Working with Windows](#)
- [Identifying Inactive, Active, and Pinned Cells](#)
- [Changing the Cell State](#)
- [Using the Cursor](#)
- [Viewing Data Files in Qual Browser](#)
- [Working with Cells](#)
- [Managing Layouts](#)
- [Using the Cell Information Page](#)
- [Setting the Global Mass Options for the Qual Browser Window](#)

Opening the Qual Browser Window

You can open the Qual Browser window from the home page, Processing Setup, and Quan Browser windows.

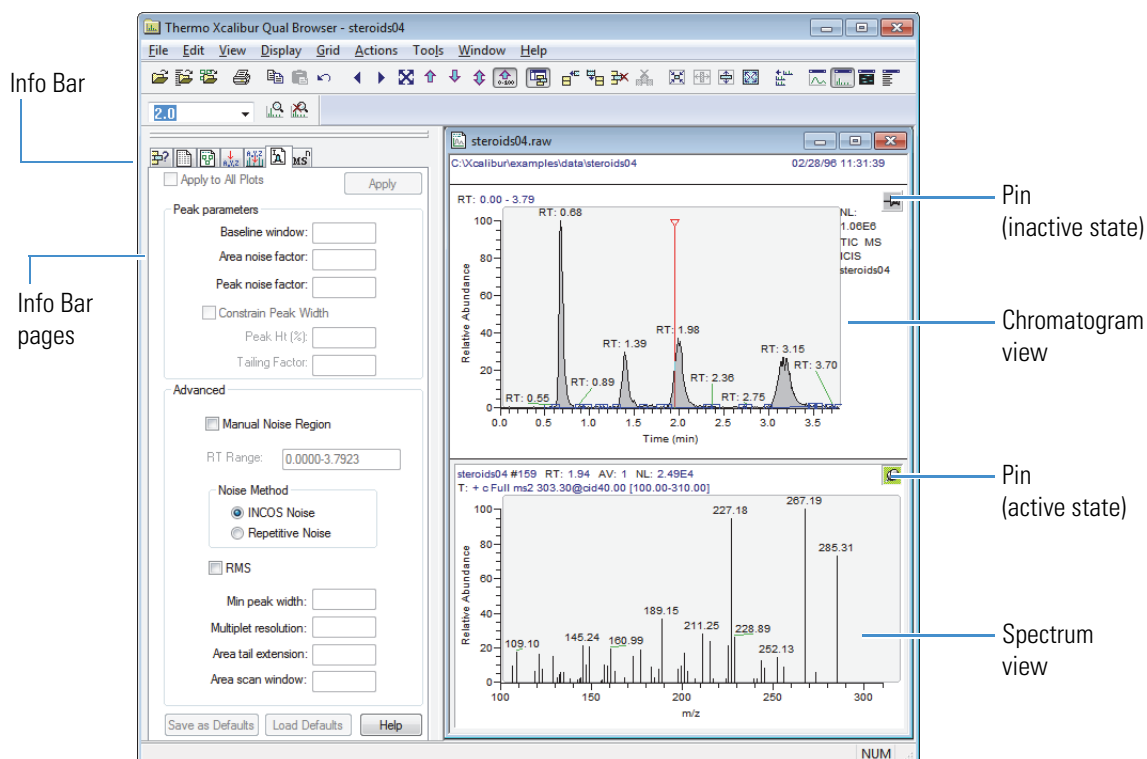
❖ To open the Qual Browser window

Depending where you are in the Xcalibur data system, do one of the following:

- From the home page – Road Map view, click the **Qual Browser** icon, .
- From any view in the home page window, choose **GoTo > Qual Browser** from the menu bar.
- From the home page, Processing Setup, and Quan Browser windows, choose **GoTo > Qual Browser** from the menu bar.
- From the Instrument Setup window, click the **Home Page** icon, , in the toolbar. Then in the home page window, choose **GoTo > Qual Browser**.

Figure 3 shows the Info bar on the left side of the Qual Browser window and a single data window with two cells on the right side of the Qual Browser window. The top cell in the data window contains a chromatogram view with a TIC chromatogram. The bottom cell contains a spectrum view with a mass spectrum extracted from the 1.94 minute time point.

Figure 3. Qual Browser window



The tasks that you can carry out in the Qual Browser window include the following:

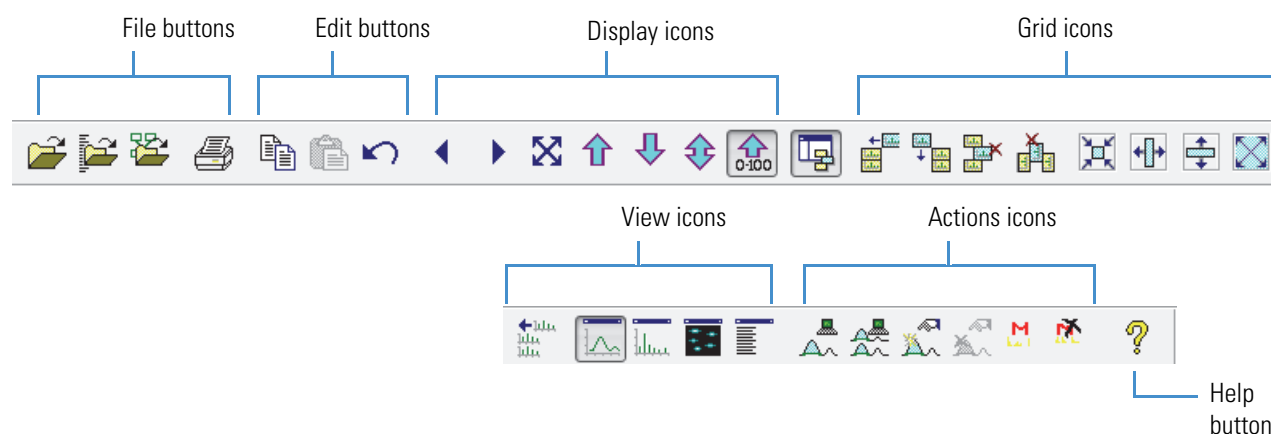
- Generate a variety of chromatogram plots and determine suitable peak detection parameters for subsequent automated analyses that use a processing method.
- Optimize the spectrum for the apex of a chromatographic peak by averaging the scans across the peak apex and subtracting other scans averaged from the baseline on either side of the peak.
- Determine the elemental composition of the peaks in the mass spectrum.
- Simulate the isotopic distribution mass spectrum of a single compound or mixture of compounds.
- Export a spectrum to the Library Browser window to create and maintain user libraries.
- Submit the spectrum of an unknown compound to a library search (if a suitable reference library is present).
- Print a report showing a qualitative data analysis and the library results.

Using the Qual Browser Toolbars

In the Qual Browser window, the buttons (for typical Windows features such as Open File and Print) and icons are divided into two toolbars: Main and Amplify.

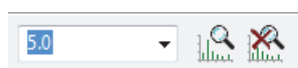
Use the icons and buttons on the Main toolbar to load, save, and print files, and to scale plots, manipulate cells, detect peaks, change views, and arrange windows (Figure 4).

Figure 4. Main toolbar with the default icons and buttons displayed



Use the icons on the Amplify toolbar to adjust the normalization in specific sections of a chromatogram, spectrum, or map plot (Figure 5).

Figure 5. Amplify toolbar



2 Using the Qual Browser Window

Using the Qual Browser Toolbars

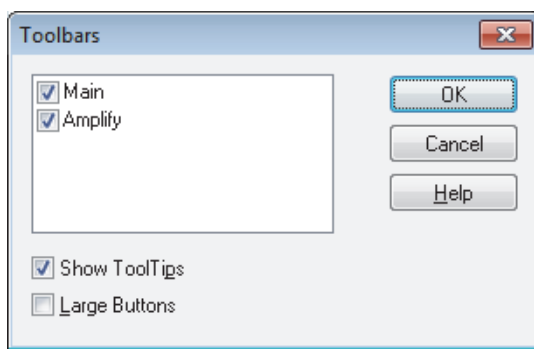
By default these two toolbars are positioned along the top of the Qual Browser window, just beneath the menu bar. Drag them anywhere within the window or dock them along any of the other window edges.

Qual Browser is equipped with a large number of tools. You can view or hide toolbars by using the Toolbars dialog box (see [Figure 6](#)). You can also use the Toolbars dialog box for these tasks:

- Viewing or hiding the display of ToolTips
- Choosing between large or small icons in the toolbar

To open the Toolbar dialog box, choose **View > Toolbars**.

Figure 6. Toolbars dialog box



For more information about displaying and customizing the toolbars in the Qual Browser window, see these topics:

- [Displaying Toolbars](#)
- [Customizing the Toolbar](#)

Displaying Toolbars

Use the Toolbars dialog box to display or hide the Main, Amplify, or both of these Qual Browser toolbars. You can also use the Toolbars dialog box to turn off the tooltips and to enlarge the toolbar icons and buttons.

❖ To display or hide the toolbars

1. Choose **View > Toolbars**.

The [Toolbars Dialog Box](#) opens.

2. To display a toolbar, select its check box. To hide the toolbar, clear its check box.
3. To display ToolTips, select the **Show ToolTips** check box. To hide ToolTips, clear the **ToolTips** check box.

4. Select a button size option.
 - To display large buttons (icons) in the toolbar, select the **Large Buttons** check box.
 - To display small buttons (icons) in the toolbar, clear the **Large Buttons** check box.
5. To save the settings and close the dialog box, click **OK**.

Customizing the Toolbar

You can add application programs to and remove application programs from the Tools menu. You can then launch any added program by double-clicking the added Tool menu command. Application programs have an .exe extension.

- [Adding, Removing, and Repositioning Standard Toolbar Buttons](#)
- [Adding a Program to the Tools Menu](#)
- [Removing a Program from the Tools Menu](#)

Adding, Removing, and Repositioning Standard Toolbar Buttons

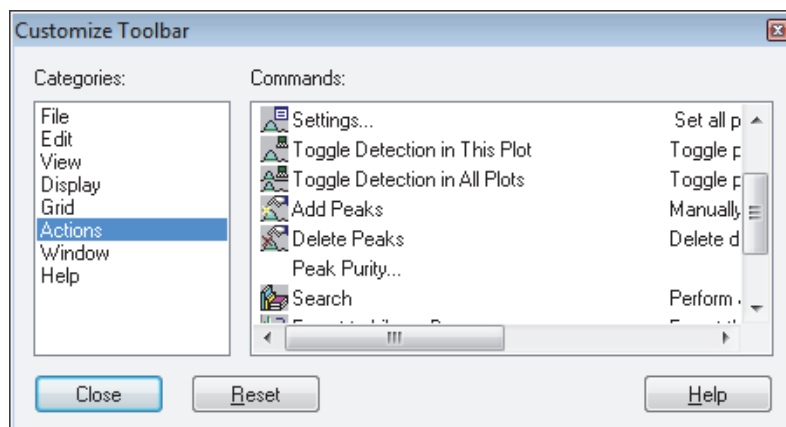
The default toolbar in the Qual Browser window does not display all of the available toolbar buttons (and icons).

❖ To add or remove buttons (and icons) in the toolbar

1. Choose **View > Customize Toolbar**.

The Customize Toolbar dialog box opens (Figure 7). The toolbar commands (buttons or icons) are organized into categories. When you select a category in the Categories list, a different set of commands (buttons or icons) appears in the Commands list.

Figure 7. Customize Toolbar dialog box



2 Using the Qual Browser Window

Using the Qual Browser Toolbars

2. To add a button (or icon), do the following:

- a. In the Categories list, select the appropriate category.

The commands (buttons) for the selected category appear in the Commands list.

- b. In the Commands list, select the command (button) that you want to add to the toolbar and drag it onto the toolbar.

When the cursor reaches the toolbar, a vertical bar and a + sign appear.



- c. Release the mouse button when the vertical bar is in the appropriate location.



3. To remove a button (icon), drag it from the toolbar and into the Commands list.
4. Click **Close** to accept the changes and close the Customize Toolbar dialog box.

❖ To reposition a button in the Main toolbar

1. Open the Customize Toolbar dialog box.
2. Drag the button (or icon) in the Main toolbar to its new position.

Tip Use this technique to group buttons together and to put a space between groups. To close up a space, drag a button to the left. To open up a space, drag to the right.

Adding a Program to the Tools Menu

❖ To add a program to the Tools menu

1. Choose **Tools > Add Tools** from the Qual Browser window or the home page window.

The Add Programs to Tool Menu dialog box opens.

2. Click **Add**.

The Add Tool dialog box opens.

3. To specify the tool to add, click **Browse** to select the path and filename of the tool, or type the path and filename of the tool you want to add in the Locate Programs to be Added dialog box.

4. To store the path and filename of the tool and close the Add Tool dialog box, click **OK**.

The Add Programs to Tool Menu dialog box stays open.

The data system adds the filename without the extension at the bottom of the Menu Contents box and the Menu Text box. The data system also adds the path and filename in the Programs box and the directory path in the Initial Directory box. The Menu Contents box displays the tool commands exactly as the Xcalibur data system displays them in the Tools menu.

5. To edit tool menu entries, select one of these options:
 - To change the command name of a tool listed in the Menu Contents box, select the tool and edit the text in the Menu Text box.
 - To change the tool sequence in the Tools menu, select the tool in the Menu Contents box and click **Move Up** or **Move Down**.
6. When the tools in the Menu Contents box are correct, click **Close** to save settings and close the dialog box. The data system displays the current selection of added tools at the bottom of the Tools menu.

Removing a Program from the Tools Menu

❖ To remove a program from the Tools menu

1. Choose **Tools > Add Tools** from the Qual Browser window or home page window.

The Add Programs to Tool Menu dialog box opens.

2. To select a tool to remove, click the tool in the Menu Contents box.

The data system highlights your selection.

3. Click **Remove**.
4. To store your changes, click **Close**.

The Add Programs to Tool Menu dialog box closes. The data system displays the current selection of added tools at the bottom of the Tools menu.

Using the Info Bar

The Info Bar initially is located on the left side of the Qual Browser window (see [Figure 3](#) on [page 28](#)).

To show or hide the Info Bar, click  on the Main toolbar or choose **View > Info Bar**.

The Info Bar has seven tabs. Each tab displays a separate function on a separate page.

[Table 3](#) describes the tabbed pages on the Info Bar.

Table 3. Info Bar pages listed from left to right

No.	Tab	Page	Description
1		Cell Information	View details of the plots contained in the active cell.
2		Sequence Information	View the raw data files available from an open sequence.
3		Result File Information	View peak data from a result file.
4		Elemental Composition	Calculate the best matching chemical formula for a mass or a list of masses from a spectrum.
5		Spectrum Simulation	Create a simulated isotopic distribution spectrum of a chemical formula.
6	Peak Detection tab		
		ICIC Peak Detection	Set peak parameters and advanced noise methods. The letter in the upper left corner of the tab indicates which algorithm (ICIS, Avalon, or Genesis) is currently selected. This tab appears when you turn on peak detection.
		Avalon Peak Detection	
		Genesis Peak Detection	
7		MS ⁿ Browser Information	View MS ⁿ experimental data for analysis. This tab appears when you open a raw data file.

Working with Windows

The Qual Browser main window displays raw data files, interactive library search results, and qualitative processing. You can view raw data files in the same window or separate windows. Use these Window commands to arrange data windows within Qual Browser:



Cascade Arrange windows diagonally so they overlap.



Tile Arrange windows as non-overlapping tiles.

Each window can be subdivided into a grid of cells, with each cell displaying a view. A view can be a chromatogram, spectrum, mass map, spectrum list, scan header, scan filter list, tune method, experiment method, sample information, status log, or error log view. Chromatogram and spectrum views can contain up to eight plots.

The arrangement of cells within a window is termed a layout. Save layouts to disk for future use. For more information, see [Managing Layouts](#).

You can apply various automatic processing options as follows.

In a chromatogram view

Smoothing to all plots in the cell
Peak detection to the active plot in the current cell or all plots in the current cell

In a spectrum view

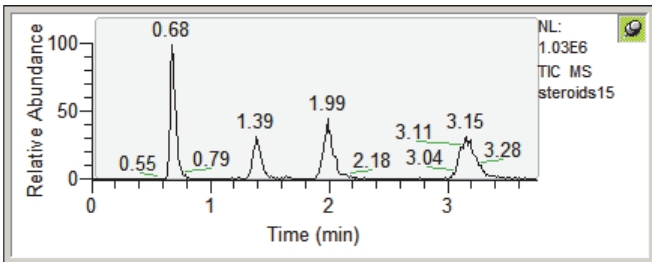
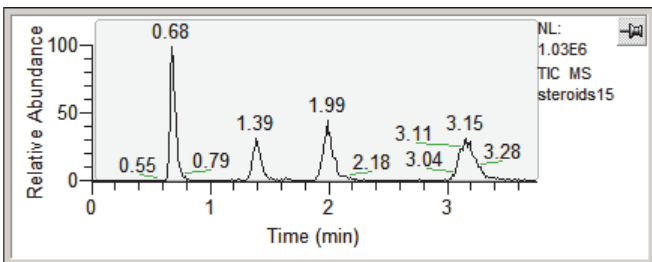
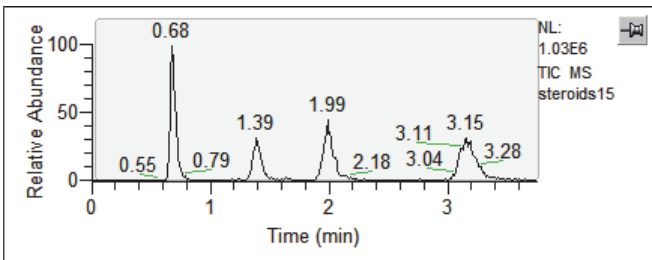
Smoothing
Refine enhancement

Identifying Inactive, Active, and Pinned Cells

There are three hierarchical states for a cell in the grid: active and pinned, active, and inactive. In the cell grid, one cell is active, while all of the other cells are inactive. When you pin the active cell, it remains active when you click another cell in the grid. If no cell is pinned, the active cell is the last cell acted on by a mouse action.

Table 4 describes the three cell states.

Table 4. Cell states

Cell state	Description
Active and pinned	You can identify the active and pinned cell by its light gray border and the green background behind its pinned pin icon. A pinned cell is an active cell that cannot be made inactive by clicking another cell. Instead, actions performed in the inactive cells affect the pinned cell.  Green background and pinned pin Gray border
Active	You can identify the active (but unpinned) cell by its gray border and the light gray background behind its unpinned pin icon. Menu commands, toolbar buttons (icons), and cursor actions affect the active cell.  Light gray background and unpinned pin Gray border
Inactive	You can identify inactive cells by the absence of a gray border and the dark gray background behind its unpinned pin icon. Menu commands, toolbar buttons (icons), and cursor actions do not affect inactive cells.  Dark gray background and unpinned pin

Changing the Cell State

A cell can be inactive, active, or active and pinned (see [Identifying Inactive, Active, and Pinned Cells](#)).

❖ To make a cell active or active and pinned

Tip Clicking a cell's pin icon is the only action required to make a cell active and pinned. Making a cell active (but unpinned) can take up to two actions. If another cell in the grid is active and pinned, you must first unpin it, and then click the target cell to make it active (but unpinned).

Because you can work both directly and interactively with an active and pinned cell, there is no advantage to making a cell active rather than active and pinned. So for practical reasons, make the cell that you want to modify an active and pinned cell by clicking its pin icon.

Do one of the following:

- If the current active view is pinned, click its pin icon to unpin it. Then, click anywhere in the cell that you want to make active.

The selected cell is active (but unpinned). You can modify its contents by using a menu bar command, shortcut menu command, or toolbar button (icon).

—or—

- Click the pin icon of the cell that you want to make active.

The selected cell is active and pinned. You can modify its contents by using a menu bar command, shortcut menu command, or toolbar button (icon). You can also modify its contents by working interactively in other views.

❖ To access the active cell's shortcut menu

Right-click in the active cell.

❖ To select a plot in a multi-plot cell

When a chromatogram or spectrum view contains more than one plot, menu operations target the active plot, which is indicated by a shaded background.

To select an individual plot in a multi-plot cell, click it.

For more information about working interactively with views, see the next topic and [Using Views Interactively](#).

Using the Cursor

Within the chromatogram and spectrum views, use the cursor in three ways:

- To select a point on the view, click the point.
- To select a range, drag a line parallel to any axis.
- To select an area, drag a line in any diagonal direction.

When you place the cursor within the graphic region of a chromatogram, spectrum or map view, the cursor becomes a cross hair. The status bar at the bottom of the Qual Browser window shows the coordinates of the cursor in appropriate units for the view. For example, in a spectrum view the status bar shows the cursor position in terms of the mass-to-charge ratio and intensity.

The effect of clicking or dragging the cursor in a view depends on the cell state and whether another cell in the grid is pinned.

Cursor actions in an active cell (or active and pinned cell) scale the view according to the dimensions of the dragged line or area (see [Table 5](#)).

Table 5. Effect of cursor actions in an active or active and pinned cell

Cursor action in active or active and pinned cell	Effect
Drag parallel to x axis	Rescale graph showing selected x -axis range only, same y -axis range. The y -axis range might rescale depending on the selected Normalization display options.
Drag parallel to y axis	Rescale graph showing selected y -axis range only, same x -axis range.
Drag diagonally over x and y axes	Rescale graph showing both the selected x - and y -axis ranges.

When the grid contains an active and pinned cell, the same actions in an inactive cell have a very different effect. Rather than making the inactive cell active, the action affects the active and pinned cell (see [Table 6](#)). Qual Browser displays a plot or information in the active and pinned cell using data appropriate to the selected point, range, or ranges.

Table 6. Effect of a cursor action in an inactive cell on the active and pinned cell

Active and pinned cell	Inactive cell	Cursor action in inactive cell	Effect on active and pinned cell
Spectrum	Chromatogram	Click retention time (RT) = 1.98 min in the chromatogram view.	Cell displays mass scan that occurs at retention time = 1.98 min.
Status Log	Chromatogram	Click retention time (RT) = 3.16 min in the chromatogram view.	Cell displays status log at retention time = 3.16 min.
Scan Filter	Chromatogram	Click retention time (RT) = 1.36 min in the chromatogram view.	Cell displays the scan filter used for the scan that occurs at retention time = 1.36 min.
Spectrum	Chromatogram	Drag the cursor across a peak of interest.	Cell displays a spectrum that is the average of all the scans recorded across the peak within the selected range of retention times.
Chromatogram	Spectrum	Drag the cursor from m/z 198.4 through 299.7.	Cell displays a mass chromatogram consisting of masses 198.4–299.7.
Chromatogram	Map	Drag the cursor over an area enclosing the ranges 0.5 to 1.0 min and m/z 100 to 200.	Cell displays a mass chromatogram consisting of masses 100–200 with a time range of 0.5 to 1 min.

The preceding table illustrates only a few of the possible effects of the interactive behavior in Qual Browser. To get expected results, remember these actions:

- Pin the target view to keep it active.
- Within an active cell, use the cursor to rescale the view.
- Use the coordinates in the Status bar to select ranges precisely.
- To correct mistakes, choose **Edit > Undo**.

Viewing Data Files in Qual Browser

View data files in Qual Browser by following any of these procedures:

- [Opening Single Raw Files in Qual Browser](#)
- [Opening a Sequence Set of Raw Data Files in Qual Browser](#)
- [Opening and Viewing Result Files in Qual Browser](#)

Raw data files are unprocessed data files from a single injection or a sequence set of injections. Raw data files have a .raw file name extension and sequence files have a .seq file name extension. Result files are the product of processing raw data files with a processing method. Result files have an .rst file name extension. After you run a sequence and acquire data files, the data files are associated with the sequence.

Opening Single Raw Files in Qual Browser

In the Qual Browser window, you can open raw data files (RAW file type), sequence files (SLD file type), or result files (RST file type).

❖ To open a single raw data file

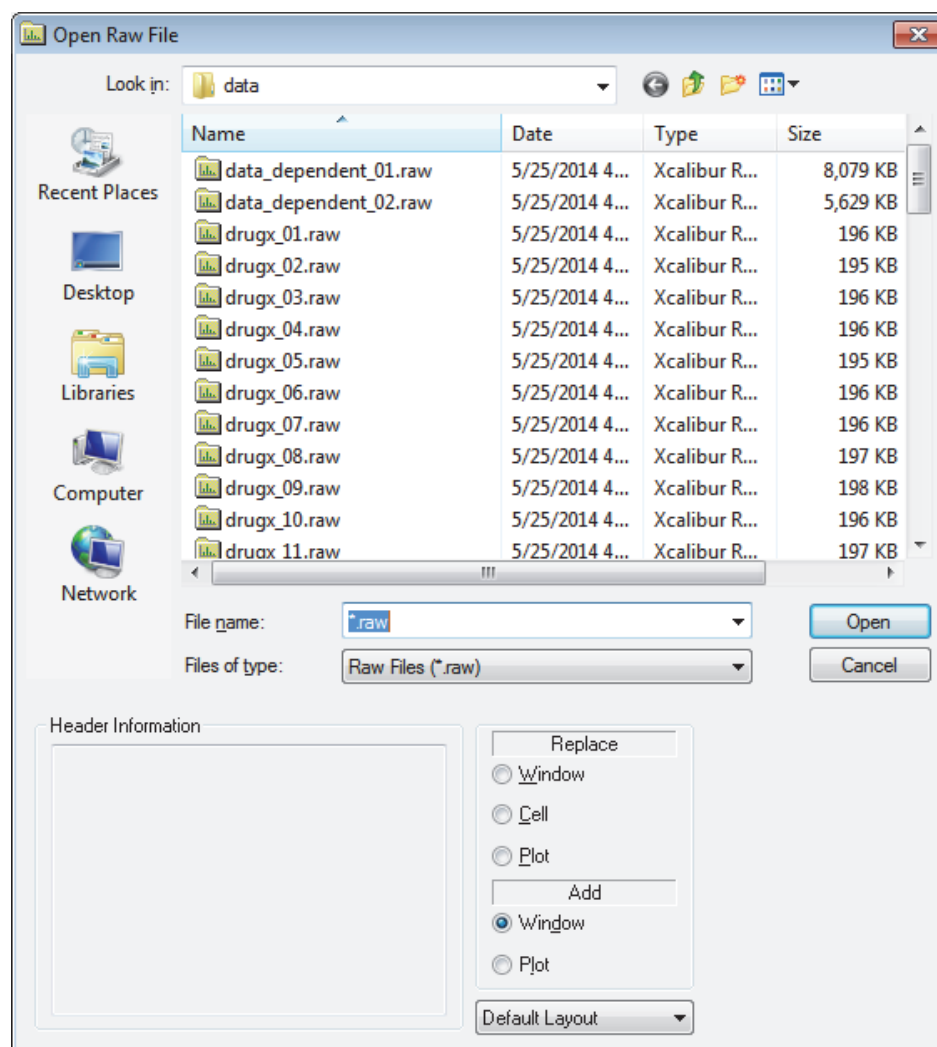
1. Do one of the following:
 - From the menu bar, choose **File > Open**.
 - In the toolbar, click the **Open** icon, .

—or—

- On the keyboard, press CTRL + O.

The Open Raw File dialog box opens (Figure 8).

Figure 8. Open Raw File dialog box



2. Browse to the file that you want to open.
3. Select a Replace option as follows:
 - To replace all the plots in the current window (in all cells) with plots of an equivalent type from the selected raw data file, select **Window**.
 - To replace all plots in the current cell with plots of an equivalent type from the selected file, select **Cell**.
 - To replace the current plot with a plot of an equivalent type from the selected file, select **Plot**.
4. Select an Add option as follows:
 - To open the selected raw data file in a new window using the layout of the currently active window, select **Window**. If no layout is available, Qual Browser applies the most recently saved layout file or, if this is invalid, the default layout.
 - To add the file as a plot in the active cell of the current window, select **Plot**. This option is not available if the cell already contains the maximum number (8) of plots.
5. If you select the **Add Window** option, choose the layout to be applied to the new window.
 - To apply the most recently saved default layout, select **Default Layout**.
 - To apply the layout of the currently active window to the new window, select **Current Layout**. If no layout is available, Qual Browser applies the default layout.

Opening a Sequence Set of Raw Data Files in Qual Browser

After you acquire a set of raw data files with a sequence, the raw data files are associated with the sequence.

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

1. Do one of the following:
 - From the menu bar, choose **File > Open Sequence**.

—or—

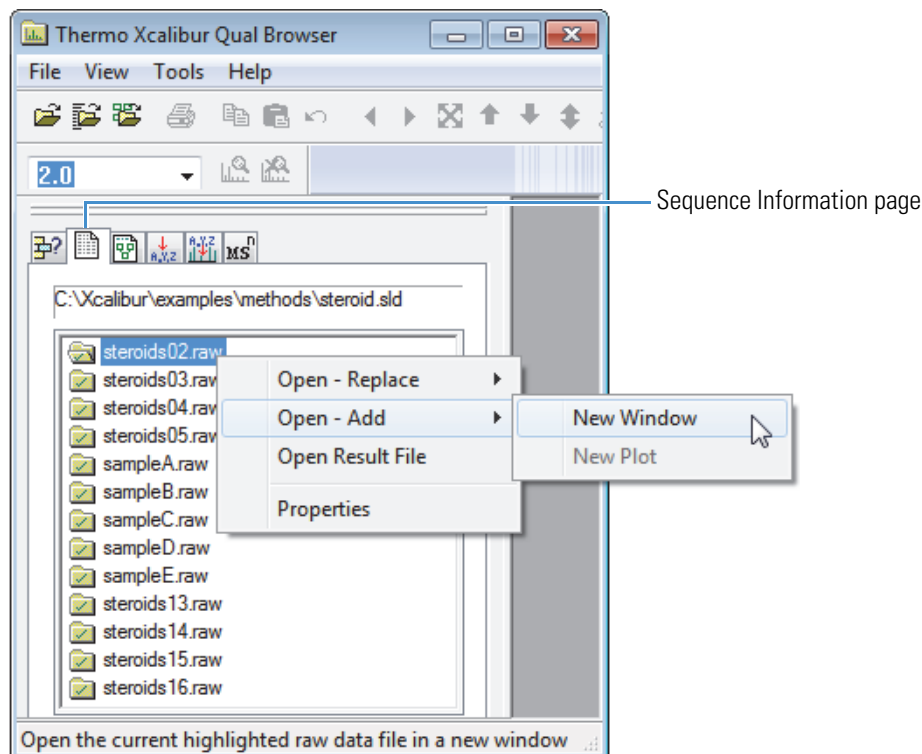
- In the toolbar, click the **Open Sequence** icon, .

The Open Sequence dialog box opens.

2. Browse to the sequence (SLD) that you want to open and click **Open**.

The list of data files associated with the sequence appears on the Sequence Information page of the Info Bar (see Figure 9).

Figure 9. Sequence Information page showing the shortcut menu



❖ To display one or more data files in the Qual Browser window

Do one of the following:

- To replace the data in the current window, double-click the name of the file on the Sequence Information page of the Info Bar or right-click the name of the file and choose **Open - Replace > All In Current Window** from the shortcut menu.
- To replace the data in the active cell, right-click the name of the file and choose **Open - Replace > All In Current Cell** from the shortcut menu.
- To replace data in the active plot, right-click the name of the file and choose **Open - Replace > Current Plot** from the shortcut menu.
- To open the file in a new window using the current layout, right-click the name of the file and choose **Open - Add > New Window** from the shortcut menu.

—or—

- To open the file as a new plot in the active cell, right-click the name of the file and choose **Open - Add > New Plot** from the shortcut menu.

❖ **To open the result file that is associated with the selected raw data file**

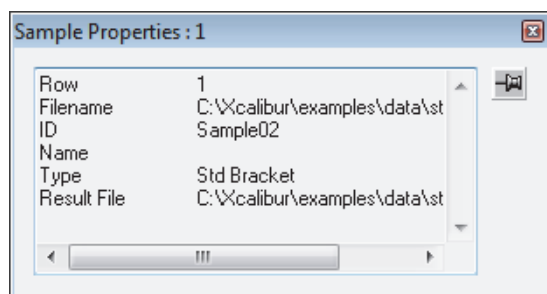
On the Sequence Information page of the Info Bar, right-click the data file name and choose **Open Result File**.

❖ **To view the sample properties for the raw data file**

1. On the Sequence Information page of the Info Bar, right-click the data file name and choose **Properties**.

The Sample Properties dialog box opens (Figure 10), showing basic information about the selected sample. This information includes the row, filename, sample ID, name, sample type, and result filename.

Figure 10. Sample Properties dialog box



When the Sample Properties dialog box is unpinned, it closes when you click outside of it.

2. To keep the Sample Properties dialog box open while you review its contents, click the pin icon.
 3. To close the pinned Sample Properties dialog box, do one of the following:
 - Click the close box icon.
- or—
- Unpin the dialog box by clicking the pin icon again. Then click anywhere outside the dialog box.

Opening and Viewing Result Files in Qual Browser

A result file contains the list of detected peaks from the chromatogram and the qualitative processing results associated with each peak. Qual Browser displays the result file in a fixed, two-cell arrangement (Figure 11). This dialog shows a chromatogram plot in the upper cell, with the detected peaks highlighted and the spectrum associated with the currently selected chromatogram peak in the lower cell. For more information about the result window, see [Qual Browser Result File Window](#).

❖ To open a result file

1. Do one of the following:

- In the toolbar, click the **Open Result File** icon, .

—or—

- From the menu, choose **File > Open Result File**.

The Open Result file dialog box opens.

2. Browse to select the result file (RST) that you want to open.
3. Click **Open**

The result window contains two cells: a chromatogram view and a spectrum view. You cannot add more cells to the window, and you cannot change either view to another view.

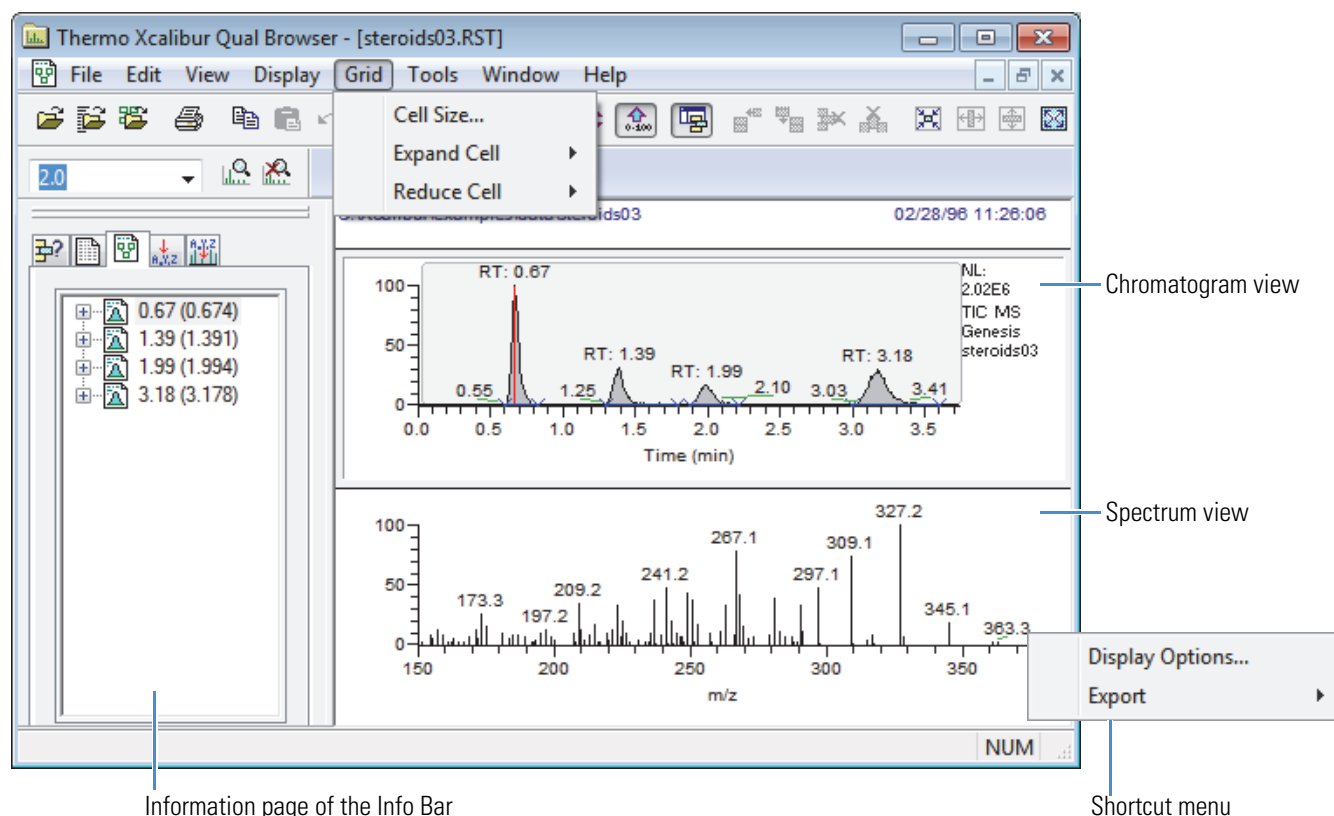
❖ To open a result file for a file in an opened sequence

Right-click the filename on the Sequence Information page of the Info Bar and choose **Open Result File** from the shortcut menu.

Note If no result file exists for the selected file, the menu command is unavailable.

Figure 11 shows the Information page for a result file, as well as the Grid and shortcut menus. Notice that the Insert Cells command is absent from the Grid menu and that the shortcut menu contains only two commands.

Figure 11. Result File view showing the Result File Information page in the Info Bar



Note Many of the features in Qual Browser are not available for use with a result file because the raw data file is not directly available for processing.

It is not possible to submit the spectrum from the results display to a library search. If a library search has been carried out during processing (when the result file was created), search results are stored in the result file and displayed for each detected peak. To submit a spectrum to a library search or to export a spectrum to the Library Browser, open the raw data file. For more information about searching libraries and interpreting library search results, refer to the *Xcalibur Library Browser User Guide*.

❖ **To view result file information**

In the Info Bar, click the **Result File Information** tab  to open the Result File Information page.

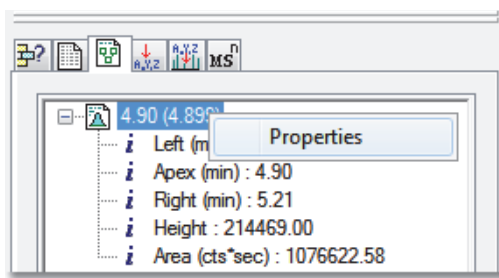
This page shows the following basic information about all detected peaks in the result file:

- Retention times at the peak start (left), peak apex, and peak end (right)
- The peak area and height

For information about the peak, including flags, open the Peak Properties dialog box.

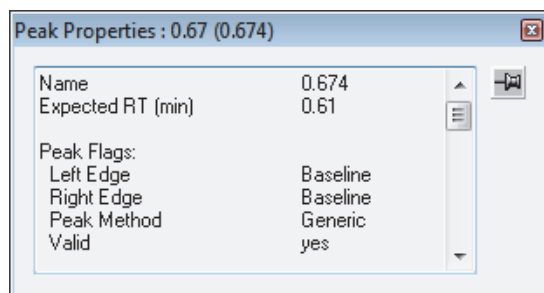
❖ **To view the peak properties**

1. Right-click the peak identifier in the Peak list.
2. Choose **Properties** from the shortcut menu.



The Peak Properties dialog box opens (Figure 12).

Figure 12. Peak Properties dialog box



The unpinned Peak Properties dialog box closes when you click outside of it.

3. To keep the Peak Properties dialog box open while you review its content, click the pin icon.
 4. To close the pinned Peak Properties dialog box, do one of the following:
 - Click the close box icon.
- or—
- Unpin the dialog box by clicking the pin icon again. Then click anywhere outside the dialog box.

Working with Cells

Qual Browser displays chromatograms and spectra in a grid of cells. These topics describe the commands used to manipulate cells:

- [Making a View Active](#)
- [Inserting and Deleting Cells](#)
- [Adjusting the Cell Size](#)
- [Amplifying Regions of a Plot](#)
- [Adding Text to a Plot](#)
- [Adding Graphics to a Plot](#)
- [Removing Text and Graphics from a Plot](#)
- [Opening or Changing Views in Cells](#)
- [Scaling a Plot](#)

Note You can work directly within an active but unpinned cell. However, because there is no advantage to making a cell active rather than active and pinned, the procedures in this topic instruct you to select the active cell by clicking its pin icon.

Making a View Active

The active cell contains the active view. There can only be one active view at a time. The active view can be active (but unpinned) or active and pinned.

Tip There is no advantage to making cells active rather than active and pinned. So to make a cell active, click its pin icon. The cell becomes active and pinned.

❖ To make a view active or active and pinned

Do one of the following:

- If the current active view is pinned, click its pin icon to unpin it. Then, click anywhere in the cell that you want to make active.

The selected cell is active (but unpinned). You can modify its contents by using a menu bar command, shortcut menu command, or toolbar button (icon).

—or—

- Click the pin icon of the cell that you want to make active.

The selected cell is active and pinned. You can modify its contents by using a menu bar command, shortcut menu command, or toolbar button (icon). You can also modify its contents by working interactively in other views.

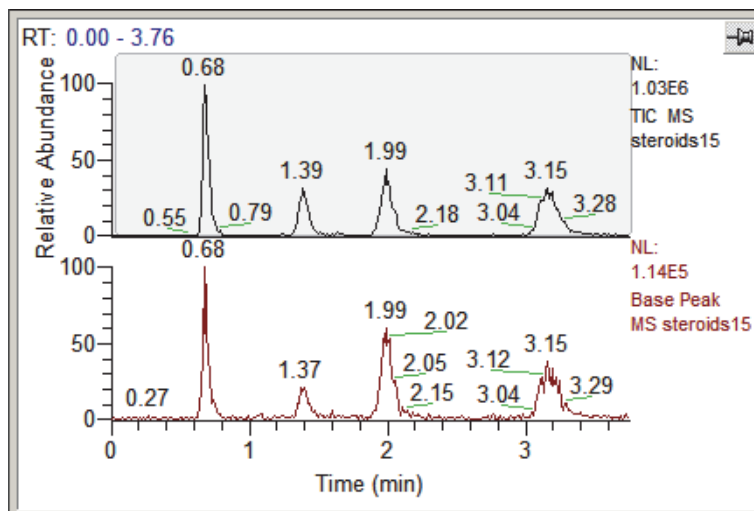
❖ **To make one of the cell plots active**

Click the plot within the view.

To show the plot is active, the data system shades the background of the plot.

Figure 13 shows a cell with a chromatogram view and two plots. The chromatogram and spectrum views can contain up to eight plots.

Figure 13. Cell with two chromatogram plots (TIC and base peak)



❖ **To pin an active but unpinned cell**

Click its pin icon.

Inserting and Deleting Cells

When a raw data file is open, Qual Browser displays one or more cells according to the selected layout.

Note These Grid icons are included in the default Main toolbar: Insert Cells Above, Insert Cells Below, Delete Grid Row, Delete Grid Column, Reduce Size, Full Width, Full Height, and Full Size.



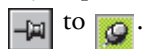
You can use the Customize Toolbars dialog box to add the other icons described in this procedure to the toolbar.

❖ To insert a new cell

1. To select the active cell, click or pin the cell adjacent to the cell or cells that you want to create.

If you click the cell to make it active, but you do not pin it, a gray border appears around the cell.

If you pin the cell, a gray border appears around the cell, and its pin icon changes from



2. To add additional cells, do one of the following:

- To insert a duplicate cell to the left of the active cell, do one of the following:
 - In the toolbar, click the **Insert Cells Left** icon, .
 - From the menu bar, choose **Grid > Insert Cells > Left**.

If the active cell is in a column of cells, the data system inserts a duplicate column of cells to the left of the column containing the active cell.

- To insert a duplicate cell to the right of the active cell, do one of the following:
 - In the toolbar, click the **Insert Cells Right** icon .
 - From the menu, choose **Grid > Insert Cells > Right**.

If the active cell is in a column of cells, the data system inserts a duplicate column of cells to the right of the column containing the active cell.

- To insert a duplicate row of cells above the row containing the active cell, do one of the following:
 - In the toolbar, click the **Insert Cells Above** icon, .
 - From the menu bar, choose **Grid > Insert Cells > Above**.

If the active cell is in a row of cells, the data system inserts a duplicate row of cells above the row containing the active cell.

- To insert a duplicate row of cells below the row containing the active cell, do one of the following:

- In the toolbar, click the **Insert Cells Below** icon, .
- From the menu bar, choose **Grid > Insert Cells > Below**.

If the active cell is in a row of cells, the data system inserts a duplicate row of cells below the row containing the active cell.

Note When you add cells, the data system creates duplicate cells that contain the same view as the active cell. As you add additional cells, the cell size of all cells becomes smaller. the data system might not be able to include all header information in views that are opened in small cells.

❖ **To delete one or more cells**

1. Click the pin icon of the cell in the same row or column of the cell or cells you want to delete to make it active. To delete all of the cells but one, click the pin icon of the cell that you want to keep.
2. Do one of the following:
 - To delete the row of cells that includes the active cell, do one of the following:
 - In the toolbar, click the **Delete Grid Row** icon, .
 - From the menu bar, choose **Grid > Delete > Row**.
 - To delete the column of cells that includes the active cell, do one of the following:
 - In the toolbar, click the **Delete Grid Column** icon, .
 - From the menu bar, choose **Grid > Delete > Column**.
 - To delete all cells except the active cell,
 - In the toolbar, click the **Delete All Grid Cells** icon, .
 - From the menu bar, choose **Grid > Delete > All Cells**.

Note As you delete excess cells, the cell size of the remaining cells becomes larger.

Adjusting the Cell Size

Use the Cell Size dialog box to adjust the size of the active cell in the grid. The Cell Size dialog box is not available if the grid contains a single cell. The Column control has no effect if the view contains a single column. Similarly, the Row Height control has no effect in a grid containing a single row.

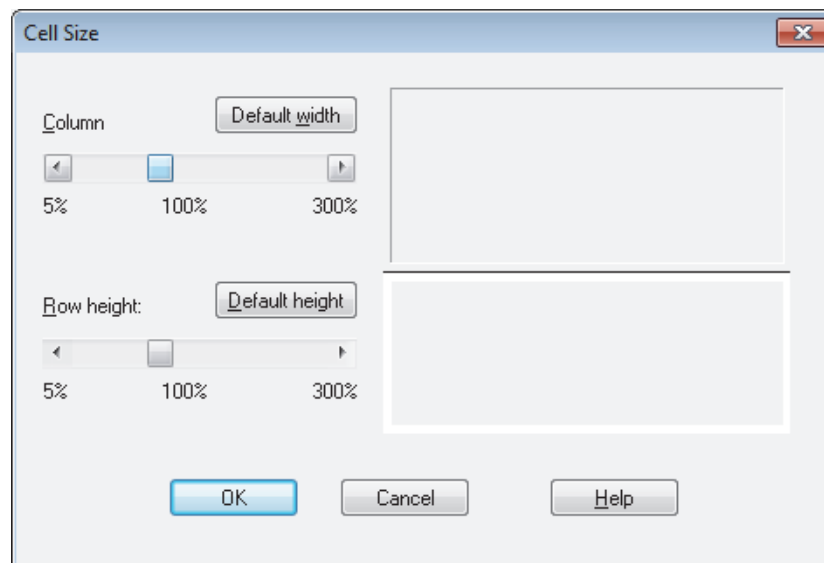
For more information, see [Cell Size Dialog Box](#).

❖ **To adjust the cell size**

1. To make a cell the active and pinned cell or the active cell in the Qual Browser window so that you can adjust its size, click the pin in the upper right corner of the cell or click the cell if no other cell is pinned.
2. Choose **Grid > Cell Size**.

The Cell Size dialog box opens (Figure 14).

Figure 14. Cell Size dialog box



3. To specify the column width, drag the Column width scroll box or click the scroll box left and right arrows until you reach the desired width within the range 5 to 300%.

The current width is displayed below the scroll box.

4. To specify the row height, drag the Row height scroll box or click the scroll box left and right arrows until you reach the desired height within the range of 5 to 300%.

The current height is displayed below the scroll box.

5. To save the settings and close the dialog box, click **OK**.

Amplifying Regions of a Plot

You can use Qual Browser to open a raw data file and display chromatograms, spectra, and maps. Then, you can use the Xcalibur toolbar buttons (icons) or menu commands to amplify selected regions.

❖ To amplify regions of a graph

1. To specify the amplification factor required, select from the following options:
 - Select an amplify factor from the Amplify Factor combo box on the Amplify toolbar. If the value you want is not in the list, type your required factor into the combo box. Click the **Amplify** icon, , in the toolbar.

The data system changes the cursor to .

- Choose **Display > Amplify > Other Factor** to open the Other Factor dialog box. Enter a value in the Amplification Factor text box and click **OK**.

The data system changes the cursor to .

2. To specify the region to amplify, drag the cursor horizontally over the region that you want to amplify.

The data system amplifies the region, places a label above the amplified region such as the following: -----x5-----, and displays the original cursor.

Adding Text to a Plot

You can add text to your chromatogram, spectrum or map plots. Text orientation options are horizontal or vertical. Multiple lines can be aligned to the left, center, or right.

Your annotation text can be placed anywhere on the plot using the  cursor to point to the marked position.

To change the style, color, label, axis, or normalization of a plot, use the [Display Options Dialog Box in Qual Browser](#).

For information about the Add Text dialog box, see [Add Text Dialog Box](#).

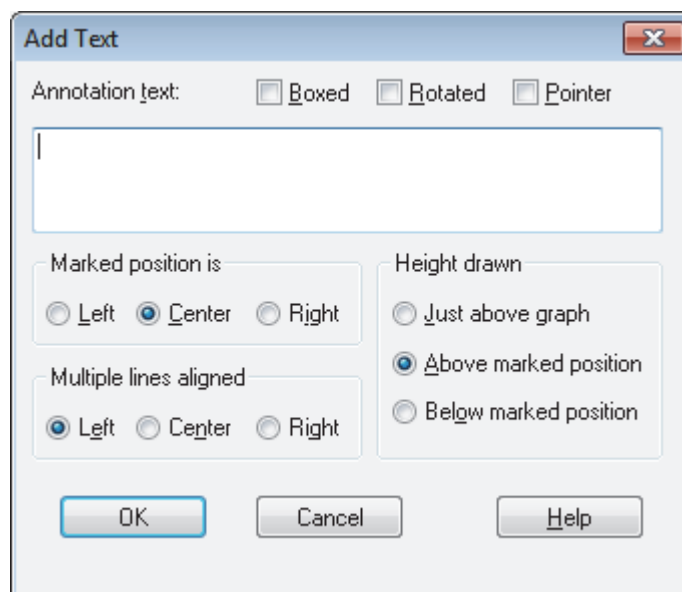
❖ To add text to a spectrum, chromatogram, or map plot

1. Determine what annotation text needs to be added and how you want it to be positioned on the plot.
2. To open the Add Text dialog box ([Figure 15](#)), do one of the following:
 - From the menu bar, choose **Display > Annotate > Add Text**.

—or—

- In the toolbar, click the **Add Text** icon, .

Figure 15. Add Text dialog box



3. Type one or more lines of annotation text in the Annotation Text text box.
Press the ENTER key to enter multiple lines.

4. Use one of the following options in the Multiple Lines Aligned group box to determine the multiple line alignment of text when it appears on the plot:

- To align lines to the left, select the **Left** option (left justification).
- To align lines in the center, select the **Center** option (center justification).
- To align lines to the right, select the **Right** option (right justification).

The data system does not display the text alignment in the Annotation Text text box.

5. Use one of the following options in the Height Drawn group box to determine the vertical alignment of text when it appears on the plot:

- To place the text slightly above a peak, select the **Just Above Graph** option.
- To place the text above where you position the cursor pointer on the plot, select the **Above Marked Position** option.
- To place the text below where you position the cursor pointer on the plot, select the **Below Marked Position** option.

6. Use one of the following options in the Marked Position Is group box to determine the left/center/right alignment where the text is placed relative to the marked position:

- To place the text to the left of the cursor pointer position on the graph, select the **Left** option.
- To place the text in the center of the cursor pointer position on the graph, select the **Center** option.
- To place the text to the right of the cursor pointer position on the graph, select the **Right** option.

7. To save settings and close the Add Text dialog box, click **OK**.

The data system closes the Add Text dialog box and changes the cursor.

8. Place the cursor at the position of the plot where you want your annotation text to appear and click. The data system adds your text and changes the cursor back to your default cursor.

You cannot move the text after it is placed.

If the text is not where you want it, immediately choose **Edit > Undo** or click  to remove the text. Then, repeat this step of the procedure. The data system saves your previous text and settings.

Adding Graphics to a Plot

You can add graphics to a plot. Graphics include horizontal lines, vertical lines, diagonal lines, boxes, and filled boxes. You can also select the color of all added lines and fills. Filled boxes can either appear behind a plot or in front of a plot.

Use the Add Graphics dialog box to specify the appearance of these graphic objects. For more information about the Add Graphics dialog box, see [Add Text Dialog Box](#).

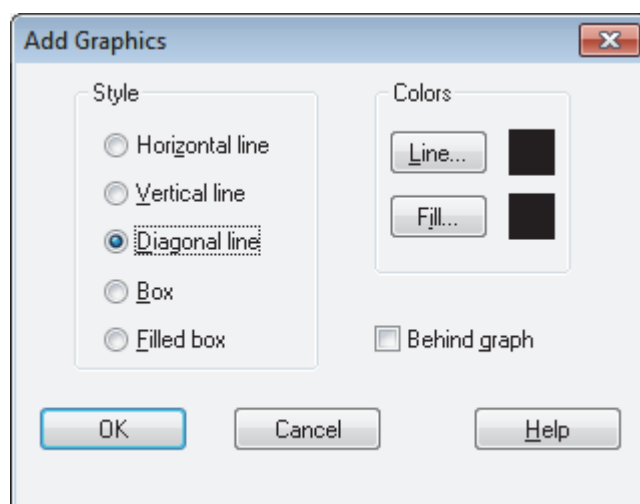
❖ To add graphics to a view

1. Determine what annotation graphic needs to be added and how you want the graphic to be positioned on the plot.
2. To specify the appearance of the graphic object, do the following:
 - a. Open the Add Graphics dialog box ([Figure 16](#)) by doing one of the following:
 - Click the **Add Graphics** icon, , in the toolbar.

—or—

- Choose **Display > Annotate > Add Graphics** from the menu bar.

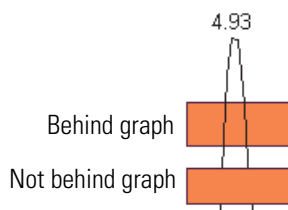
Figure 16. Add Graphics dialog box



- b. To specify the style of the graphic to be added, select one of the following options:
 - To add a horizontal line, select the **Horizontal Line** option. Go to [step 2c](#).
 - To add a vertical line, select the **Vertical Line** option. Go to [step 2c](#).
 - To add a diagonal line, select the **Diagonal Line** option. Go to [step 2c](#).
 - To add a rectangle, select the **Box** option. Go to [step 2c](#).

- To add a filled box, select the **Filled Box** option.
 - If the filled box is to be displayed behind a plot, select the **Behind Graph** check box.
 - If the filled box is to be displayed in front of (on top of) a graph, clear the **Behind Graph** check box.

The following filled boxes use a black line color for the box outline and a brown fill and demonstrate the use of the Behind Graph check box feature. Go to [step 2d](#).



- c. To specify the line color, click **Line** and select a different color. The current line color is displayed to the right of the Line button in the Colors group box.
 - d. To specify the fill color, click **Fill** and select a different color. The current fill color is displayed to the right of the Fill button in the Colors group box.
 - e. To close the Add Graphics dialog box, click **OK** so that you can draw the graphic on the plot.
3. To draw the graphic on the plot, do one of the following:
- To draw a horizontal line, drag the cursor on the plot. You can drag from right-to-left or from left-to-right.
 - To draw a vertical line, drag the cursor on the plot. You can drag from bottom-to-top or from top-to-bottom.
 - To draw a diagonal line, drag the cursor on the plot. You can drag from left-to-right or from right-to-left. You can move the cursor before you release the mouse button to position the angle of the line.
 - To draw a box, start at any corner of the box and then drag the cursor to the opposite corner. The data system draws a box similar to the following.



- To draw a filled box, select a fill color. Start at any corner of the box and then drag any cursor to the opposite corner. The system draws a box similar to the following.



You cannot move the graphic after it is placed. If the graphic is not where you want it, immediately click  or choose **Edit > Undo** to remove the graphic. Then, repeat this step. The system saves your previous text and settings.

Removing Text and Graphics from a Plot

You can easily remove all or selected annotation text and graphics from a plot. You cannot edit or remove the header text.

To change the style, color, label, axis, or normalization of a plot, use the [Display Options Dialog Box in Qual Browser](#).

❖ To remove text and graphics from a plot

1. Specify the text or graphics item to remove by clicking the pin of the cell containing the text or graphics.
2. Do one of the following:
 - To select and remove previously added annotation text or graphics, go to [step 3](#).
 - To remove all previously added annotation text and graphics from a plot, go to [step 4](#).
3. To select and remove text/graphics, do one of the following:
 - In the toolbar, click the **Clear Annotation in Range** icon, .
 - From the menu bar, choose **Display > Annotate > Clear**.

Repeat this step, as required, to remove text and graphics in other locations of the plot.

4. To remove all annotation text and graphics from the active cell, do one of the following:
 - In the toolbar, click the **Clear All Annotation** icon, .
 - From the menu bar, choose **Display > Annotate > Clear All**.
5. If you change your mind, click the **Undo** icon, , in the toolbar or choose **Edit > Undo** from the menu bar.

Opening or Changing Views in Cells

A cell can contain one of eleven views.

❖ To open views in cells

1. To choose a cell to hold the view, click the pin icon of the cell.

The cell pin icon changes from  to . A pinned pin icon with a green background indicates that the cell is the active and pinned cell. Because there can only be one active cell, all other cells are inactive.

2. To choose the view that you want to open in the active cell, select from options in [Table 7](#).

❖ To change the view displayed in a cell

1. Click the cell where you want to change the view.
2. Select the required view from the main toolbar, or choose a view from the View menu or the shortcut menu (right-click the active cell).

The data system replaces the view in the active cell with the view that you selected (see [Table 7](#) for options).

[Table 7](#) lists the eleven possible views and how to open them.

Note These View icons are included in the default Main toolbar: View Chromatogram, View Spectrum, View Map, and View Spectrum List (see [Figure 4](#) on [page 29](#)). You can use the Customize Toolbars dialog box to add the other icons listed in [Table 7](#) to the toolbar.

Table 7. Opening views in cells (Sheet 1 of 2)

View	Select one of these ways to open the view
Chromatogram View	• Choose View > Chromatogram. • Right-click the cell and choose View > Chromatogram from the shortcut menu. • Click the View Chromatogram icon, , in the toolbar.
Spectrum View	• Choose View > Spectrum. • Right-click the cell and choose View > Spectrum from the shortcut menu. • Click the View Spectrum icon, , in the toolbar.
Map View	• Choose View > Map. • Right-click the cell and choose View > Map from the shortcut menu. • Click the View Map icon, , in the toolbar.

Table 7. Opening views in cells (Sheet 2 of 2)

View	Select one of these ways to open the view
Spectrum List View	- Choose View > Spectrum List. - Right-click the cell and choose View > Spectrum List from the shortcut menu. - Click the View Spectrum List icon, , in the toolbar.
Scan Header View	- Choose View > Scan Header. - Right-click the cell and choose View > Scan Header from the shortcut menu. - Click the View Scan Header icon, , in the toolbar.
Scan Filter View	- Choose View > Scan Filters. - Right-click the cell and choose View > Scan Filters from the shortcut menu. - Click the View Scan Filters icon, , in the toolbar.
Tune Method View	- Choose View > Report > Tune Method. - Right-click the cell and choose View > Report > Tune Method from the shortcut menu. - Click the View Tune Method icon, , in the toolbar.
Instrument Method View	- Choose View > Report > Instrument Method. - Right-click the cell and choose View > Report > Instrument Method from the shortcut menu. - Click the View Instrument Method icon, , in the toolbar.
Sample Information View	- Choose View > Report > Sample Information. - Right-click the cell and choose View > Report > Sample Information from the shortcut menu. - Click the View Sample Information icon, , in the toolbar.
Status Log View	- Choose View > Report > Status Log. - Right-click the cell and choose View > Report > Status Log from the shortcut menu. - Click the View Status Log icon, , in the toolbar.
Error Log View	- Choose View > Report > Error Log. - Right-click the cell and choose View > Report > Error Log from the shortcut menu. - Click the View Error Log icon, , in the toolbar.

Scaling a Plot

The chromatogram, spectrum, and map views show plots. Use the Zoom and Pan menu commands to adjust the display of the active plot ([Table 8](#)).

Table 8. Zoom and Pan menu commands

	Zoom In Y	Zoom in on the <i>y</i> axis by a factor of two (2) from the current baseline to show more detail. For example, you can change the <i>y</i> -axis range from 0 to 100 to 0 to 50.
	Zoom Out Y	Zoom out on the <i>y</i> axis by a factor of two (2) to show more data. For example, you can change the <i>y</i> -axis range from 0 to 25 to 0 to 50.
	Auto Range	Display the chromatogram, which is normalized from the minimum to the maximum signal. Auto Range is useful for PDA and UV data.
	Normalize	Normalize the intensity scale of the data display to a fixed range on the <i>y</i> axis, for example, from 0 to 25% to 0 to 100%.
	Zoom In X	Make the <i>x</i> axis larger by a factor of two (2) to show more detail. For example, change the <i>x</i> -axis range from 0 to 20 to 5 to 15.
	Zoom Out X	Make the <i>x</i> axis smaller by a factor of two (2) from the center to show more data. For example, change the <i>x</i> -axis range from 7.5 to 12.5 to 5 to 15.
	Display All	Display all data on the <i>x</i> axis or all text in a report. For example, you can change the <i>x</i> -axis range from 7.5 to 12.5 to 0 to 20.
	Reset	Restore the data display to the full range of the <i>x</i> axis and <i>y</i> axis.
	Pan graph	Use the Pan Graph icon in the toolbar to pan across a zoomed plot by dragging it to the left or right with the mouse.

Managing Layouts

A layout consists of any arrangement of cells, views, and plots within a data window. When you open the Qual Browser window, the data system uses the last layout file to display data from a raw data file in the predefined arrangement and with predetermined option settings. Open a previously created layout or create a new layout at any time.

See these topics for more information:

- [Creating and Saving a Layout](#)
- [Opening and Applying a Layout](#)
- [Displaying Layout Summary Information](#)

Creating and Saving a Layout

You can create and save customized layouts for the Qual Browser window.

❖ To create and save a layout

1. To create the desired arrangement of cells for the data displays, choose **Grid > Insert Cells** to insert cells and **Grid > Delete** to delete cells.
2. To create the desired arrangement of views, do the following for each cell:
 - a. Pin the cell.
 - b. Right-click the pinned cell and choose **View > Desired View** from the shortcut menu. Or, choose the view from the list of views in the View menu
3. To add multiple plots to a cell and change the arrangement of the plots, do the following:
 - a. Pin the cell.
 - b. Right-click the plot of interest and choose one of the following:
 - To insert a plot below the selected plot, choose **Plot > Insert** from the shortcut menu.
 - To delete the selected plot, choose **Plot > Delete** from the shortcut menu.
 - To move the selected plot, choose **Plot > Move Up** or **Plot > Move Down** from the shortcut menu.

You can change the display options for a chromatogram, spectrum, map, ion map, or spectrum list view.

4. To select the display options for a cell, do the following:
 - a. Pin the cell.

- b. Right-click the pinned cell and choose **Display > Display Options** from the shortcut menu.

The Display Options dialog box opens. For information about the display options for the selected view, see [Display Options Dialog Box in Qual Browser](#).

5. To save the layout, do one of the following:

- To save a modified layout with the current name, click the **Save** icon, , in the toolbar or choose **File > Layout > Save** from the menu bar.
- To assign a file name and save a new layout, do the following:
 - a. Click the **Save As** icon, , in the toolbar or choose **File > Layout > Save As** from the menu bar.

The Save Layout dialog box opens.

- b. In the Save In box, browse to the folder where you want to store the layout file.
 - c. In the File Name box, type a name for the file. Then, click **Save**.
- To save the current layout as the new default layout, click the **Save As Default Layout** icon, , in the toolbar or choose **File > Layout > Save As Default**.

For additional information, see [Using Views Interactively](#).

Opening and Applying a Layout

You can open and apply a custom layout file or apply the default layout file to the current Qual Browser window.

❖ To open and apply a custom layout

1. To open a custom layout file, do one of the following:
 - Choose **File > Layout > Apply** from the menu bar.

—or—

- Click the **Apply Layout** icon, , in the toolbar.

The Open Layout File dialog box opens.

2. Browse to the folder where you stored the layout file and select the layout file (LYT) of interest.
3. Click **Open**.

The data system applies the stored layout to the current raw data file.

❖ **To apply the default layout**

Do one of the following:

- Choose **File > Layout > Apply Default** from the menu bar.

—or—

- Click the **Apply Default Layout** icon, , in the toolbar.

❖ **To restore the factory layout**

From the menu bar, choose **File > Layout > Restore Factory Layout**.

Displaying Layout Summary Information

Choose **File > Layout > Summary Info** to display this file's information.

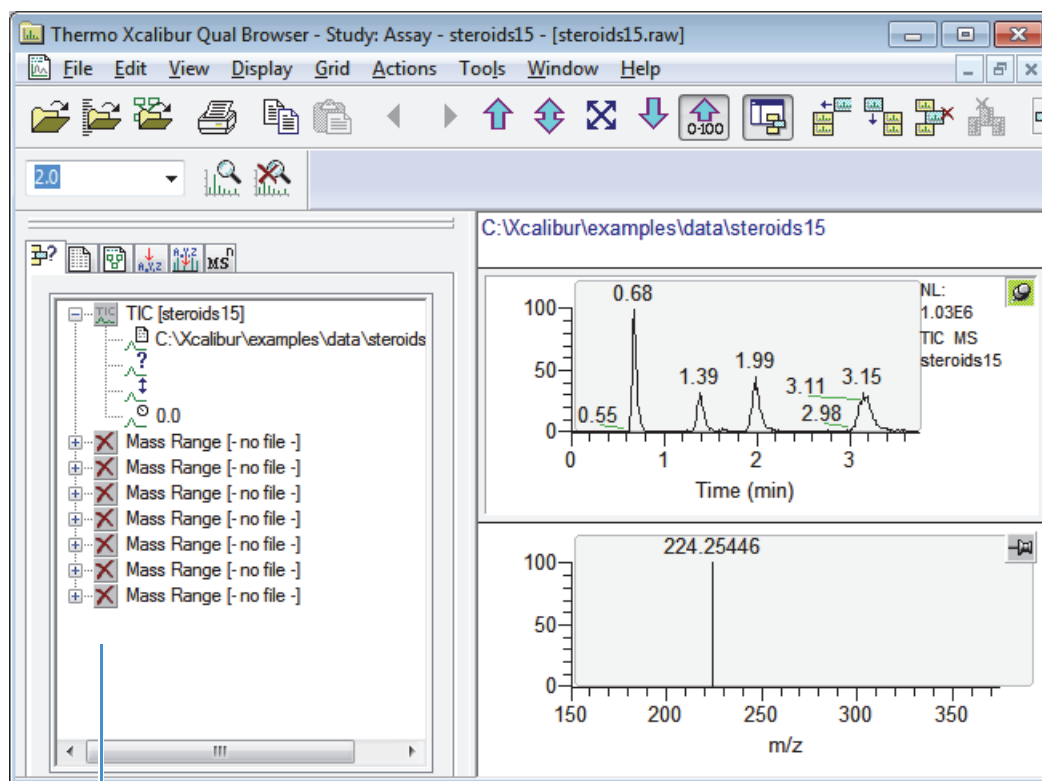
User	The name of the user currently logged in to the Xcalibur data system and Qual Browser.
Header	Basic details about the layout: the File ID, the date the layout was created, and the User ID of the originator of the layout.
Description	Any additional details about the layout such as modifications.

Using the Cell Information Page

The cell information page of the Info Bar displays information about the active cell (Figure 17). Its contents depends on whether the plot is a chromatogram or a spectrum.

For more information, see [Cell Information Page](#).

Figure 17. Cell Information page showing chromatogram cell information



Cell information page for the chromatogram cell

❖ To view cell information

1. Right-click a plot.

The Cell Information page shortcut menu opens.

2. Choose **Ranges**.

The Ranges dialog box opens (see [Setting the Chromatogram Display and Processing Options](#) and [Setting Spectrum Display Options and Processing Options](#)). This dialog box shows the properties of all the plots in the active cell.

3. View or change any of these:
 - Time and mass ranges
 - Background subtraction
 - Smoothing parameters
4. To remove the selected plot from the cell, choose **Delete**.

These topics describe the chromatogram and spectrum information pages:

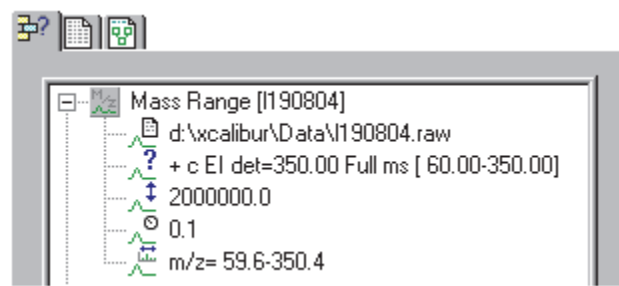
- [Chromatogram Information](#)
- [Spectrum Information](#)

Chromatogram Information

For a chromatogram plot (see [Figure 18](#)), the Cell Information page shows these icons:

	Plot type and filename
	Pathname of the raw data file
	Scan filter (if applied)
	Fixed scale upper limit (if applied)
	Chromatogram delay (if applied)
	Mass range (for mass range plot type only)
	Chromatogram time range or ranges used for background subtraction (if applied)

Figure 18. Cell Information for a chromatogram plot



2 Using the Qual Browser Window

Setting the Global Mass Options for the Qual Browser Window

Spectrum Information

For a spectrum plot, the Cell Information page shows these icons ([Figure 19](#)).



Filename



Pathname of the raw data file



Scan filter (if applied)

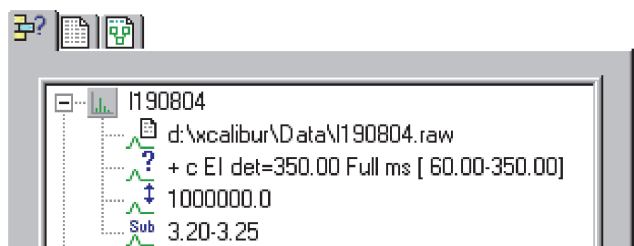


Fixed scale upper limit (if applied)



Chromatogram time range or ranges used for background subtraction (if applied)

Figure 19. Cell Information for a spectrum plot



Setting the Global Mass Options for the Qual Browser Window

Use the Global Mass Options dialog box to specify the mass tolerance and precision for an active cell, the current window, or all the windows in the Qual Browser window.

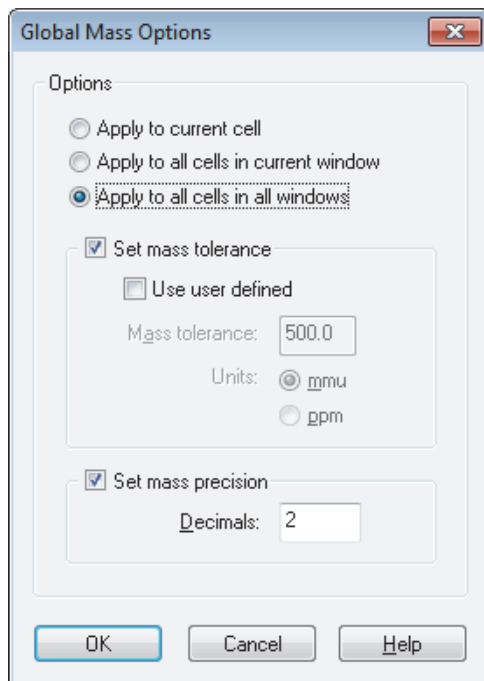
For more information, see [Global Mass Options Dialog Box](#).

❖ To set up the global mass tolerance and precision options

1. Open a raw data file in the Qual Browser window.
2. In the menu bar, choose **Display > Mass Options**.

The Global Mass Options dialog box opens ([Figure 20](#)).

Figure 20. Global Mass Options dialog box



3. Select one of the following options:
 - Apply to Current Cell
 - Apply to All Cells in Current Window
 - Apply to All Cells in All Windows
4. In the Set Mass Tolerance area, do the following to override the mass tolerance setting on the Mass Options page of the Xcalibur Configuration dialog box:
 - a. Select the **Use User Defined** check box.
 - b. In the Mass Tolerance box, type a numeric value for the mass tolerance.
 - c. Select either the mmu or ppm for the mass units to be displayed.
5. In the Set Mass Precision area, type an integer for the number of digits to be displayed after the decimal point.
6. Click **OK**.

❖ **To save these mass options in a layout file**

1. From the menu bar, choose **File > Layout > Save As**.
The Save Layout File dialog box opens.
2. In the File Name box, type a name for the layout file.
3. Click **Save**.

2 Using the Qual Browser Window

Setting the Global Mass Options for the Qual Browser Window

Using Views Interactively

These procedures describe how to work interactively with the Qual Browser views.

Contents

- [Selecting a Point on a Plot](#)
- [Selecting a One-Dimensional Range on a Plot](#)
- [Selecting a Two-Dimensional Range on a Plot](#)
- [Using Scan Filters](#)
- [Scan Filter Format](#)
- [Applying a Scan Filter to a Plot](#)
- [Displaying Multiple Magnifications of a Plot](#)

Use the Qual Browser window to open a raw data file (RAW file type), a sequence file (SLD file type), or a result file (RST file type). With raw data files, opened individually or from a sequence, you can create a grid of interactive cells and display information from the raw data file in any of the cells. From this display, you can use menu commands to select display options or use the cursor to select regions of interest.

A result file contains the list of detected peaks from the chromatogram and the qualitative processing results associated with each peak. Qual Browser displays the result file in a fixed, two-cell arrangement. Many of Qual Browser's features are not available for use with a result file because the raw data file is not available for processing.

You can view a chromatogram, spectrum, map, spectrum list, scan header, scan filter, tune method, processing method sample information, status log, or error log from the current raw data file in any of the cells that appear in the Qual Browser window. With chromatogram, spectrum, and map views, you can display up to eight plots in each cell. You can use the cursor and mouse to select points, ranges, or filters within a view. Cursor actions are always directed toward the active cell.

You can use Qual Browser to do the following:

- Use a chromatogram to generate a mass spectrum (incorporating single or averaged scans, with background subtraction if required) or maps with specific time ranges.
- Use maps to generate a single or averaged spectrum or mass chromatograms with specific mass or time ranges.
- Use a spectrum to generate mass chromatograms.
- Apply scan filters to chromatograms using the drag-and-drop method.

Selecting a Point on a Plot

The following procedure describes how to work interactively with an inactive view and an active and pinned view to display a point of interest in the active and pinned view. For example, you can use this procedure to display the spectrum in the active and pinned view for a particular time point in a chromatogram (inactive view).

Note Working interactively with views requires pinning the view that you want to modify.

❖ To select a point on a plot

1. To activate the cross-hair cursor and status bar, move the cursor to the graphic region of a plot. This is the region above the x axis and to the right of the y axis.

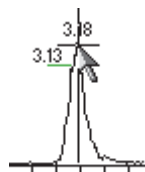
The data system displays a cross-hair cursor (+) and the coordinates in appropriate units for the display in the status bar at the bottom of the Qual Browser window.

For example, this information appears in the status bar:

- Chromatogram view: Time, Intensity
- Spectrum view: Mass (m/z), Intensity
- Map view: Time, Mass (m/z)

The data system only displays the cross-hair and status bar when a view can be used to pick a point, range, or scan filter for application to a plot in the active view.

2. To use the cursor to determine the coordinates of a peak, position the cross-hair cursor on the point on the plot. The application provides the x -axis and y -axis coordinate values.



Time: 3.16, Intensity: 582649, Filter: (none)

3. To select a point in an inactive view to apply to the active and pinned view (or the active plot in an active and pinned view), click a point in one of the inactive views.

A red vertical marker, , indicates the point selected.

When you click any other cell, the red vertical marker disappears.

You can apply these coordinate values from an inactive chromatogram view to the following active views:

- | | |
|---|--|
| • Spectrum: Scan Number and Retention Time | • Tune Method: Segment Number |
| • Map: Retention Time and Mass Range | • Instrument Method: No effect |
| • Spectrum List: Scan Number and Retention Time | • Sample Information: No effect |
| • Scan Header: Scan Number and Retention Time | • Status Log: Scan Number and Status Log Time (RT) |
| • Scan Filter: Scan Number | • Error Log: No effect |

See these examples of selecting a point on a plot:

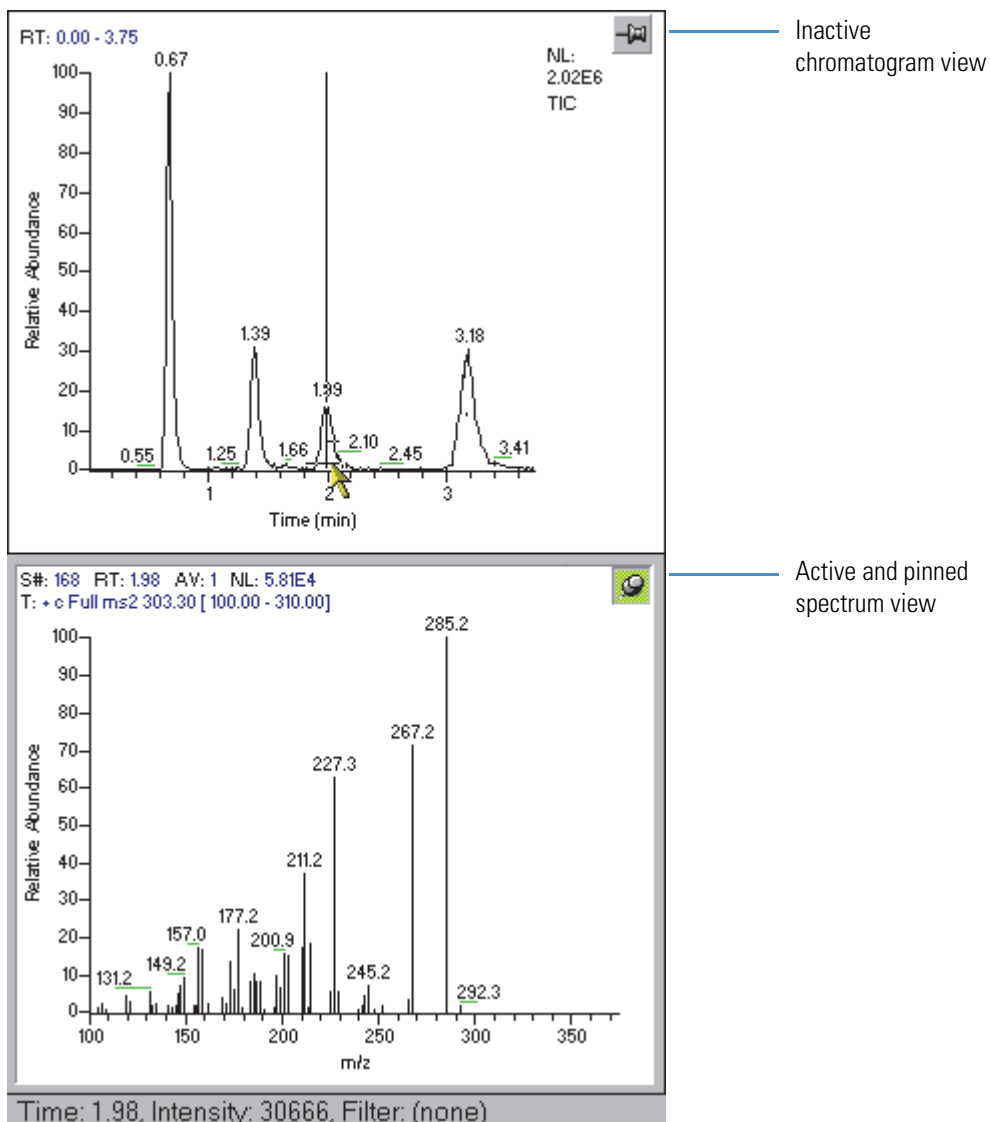
- [Selecting a Point on a Plot: Example 1](#)
- [Selecting a Point on a Plot: Example 2](#)
- [Selecting a Point on a Plot: Example 3](#)

Selecting a Point on a Plot: Example 1

In the following example, the spectrum view is the active and pinned view and the chromatogram view is the inactive view.

- Active and pinned view: spectrum
- Inactive view: chromatogram

When you click the time point at 1.98 minutes in the inactive chromatogram view, the active spectrum view displays the mass spectrum for this time point.

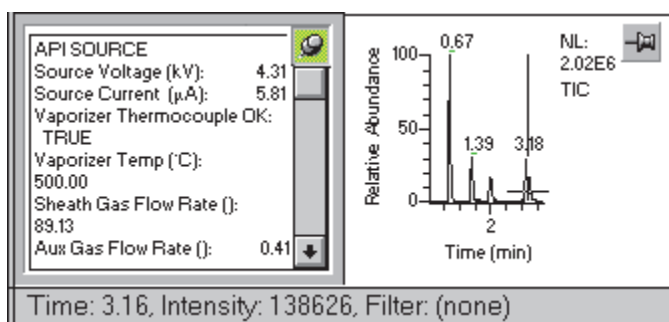


Selecting a Point on a Plot: Example 2

In the following example, the status log view is the pinned view and the chromatogram view is the inactive view.

- Pinned view: status log
- Inactive view: chromatogram

When you click the time point at 3.16 minutes in the inactive chromatogram view, the pinned status log view displays the status log for this time point in the run.

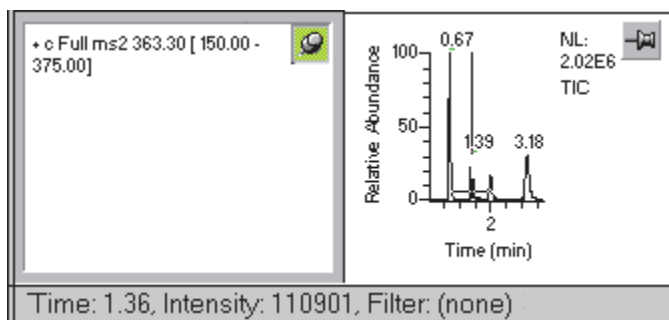


Selecting a Point on a Plot: Example 3

In the following example, the scan filter view is the pinned view and the chromatogram view is the inactive view.

- Pinned view: scan filter
- Inactive view: chromatogram

When you click the time point at 1.36 minutes in the inactive chromatogram view, the active scan filter view displays the scan filter used at this time point.



Selecting a One-Dimensional Range on a Plot

You can select a one-dimensional range in an active plot by dragging the cursor horizontally or vertically across the plot. However, to interactively change the range displayed in one view by selecting a point or range in another view, you must pin the view that you want to modify.

❖ To select a one-dimensional plot range

1. To activate the cross-hair cursor and status bar, move the cursor to the graphic region of a plot. This is the region above the x axis and to the right of the y axis.

The data system displays a cross-hair cursor and the coordinates in the appropriate units for the view in the status bar at the bottom of the Qual Browser window.

This information appears in the status bar of these views:

- Chromatogram view: Time, Intensity, Filter
- Spectrum view: Mass (m/z), Intensity
- Map view: Time, Mass (m/z)

The data system only displays the cross-hair and status bar when a view can be used to pick a point, range, or scan filter for application to the active view.

2. To use the cursor to redraw the active plot using the selected range of axis values, place the cross-hair cursor at the beginning of the desired range in the active plot, and then drag the cursor to the end of the range.

Figure 21 and Figure 22 demonstrate this selection process.

Figure 21. Position the cross-hair

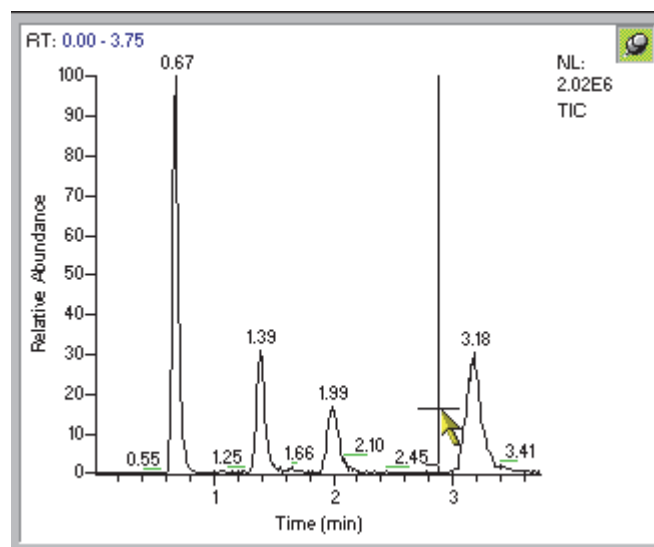
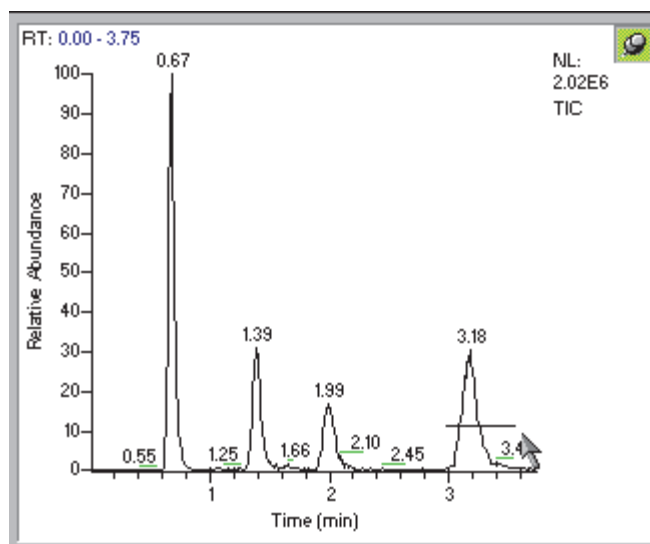


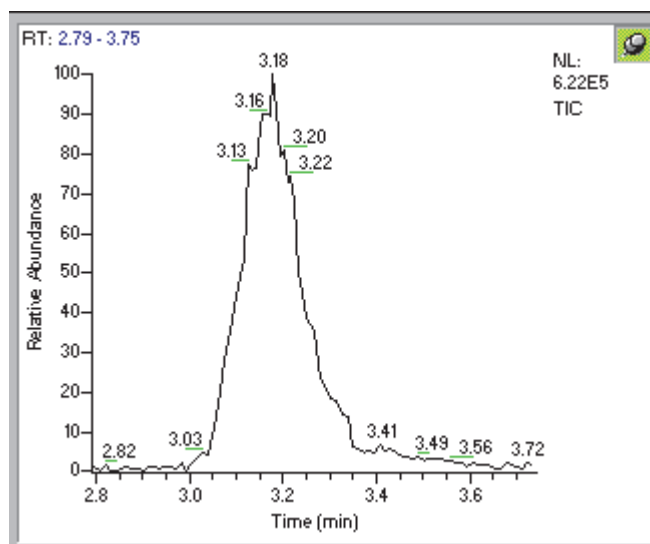
Figure 22. Drag the cursor



A black horizontal line defines the selection range. When you release the mouse button, the line disappears and the data system replots the active plot using the new range (see [Figure 23](#)).

Use this procedure with the *x* axis or *y* axis of the chromatogram, spectrum, and map views.

Figure 23. Xcalibur data system redraws the active plot



3. To use the cursor to apply a different range of values for the active plot, do the following:
 - a. Pin the active plot so that it remains active when you click another cell.
 - b. Drag the cursor across an axis of a plot in an inactive view to apply the selected range to the active and pinned cell.

3 Using Views Interactively

Selecting a One-Dimensional Range on a Plot

See these examples of selecting a one-dimensional range on a plot:

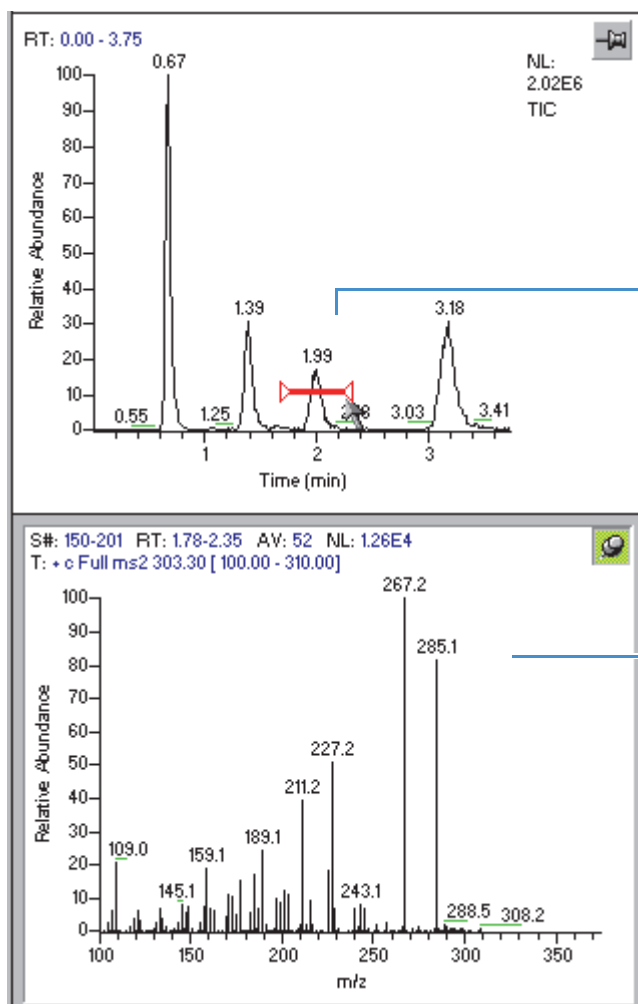
- [Selecting a One-Dimensional Range: Example 1](#)
- [Selecting a One-Dimensional Range: Example 2](#)

Selecting a One-Dimensional Range: Example 1

In the following example, the spectrum view is the pinned view and the chromatogram view is the inactive view.

- Pinned view: spectrum
- Inactive view: chromatogram

When you drag the cursor across a peak of interest in the inactive chromatogram view, a red horizontal marker () defines the selection range, and the pinned spectrum view displays a spectrum that is the average of the scans during the selected time range of 1.78 to 2.35 minutes.



Selecting a One-Dimensional Range: Example 2

In the following example, the chromatogram view is the active and pinned view and the spectrum view is the inactive view.

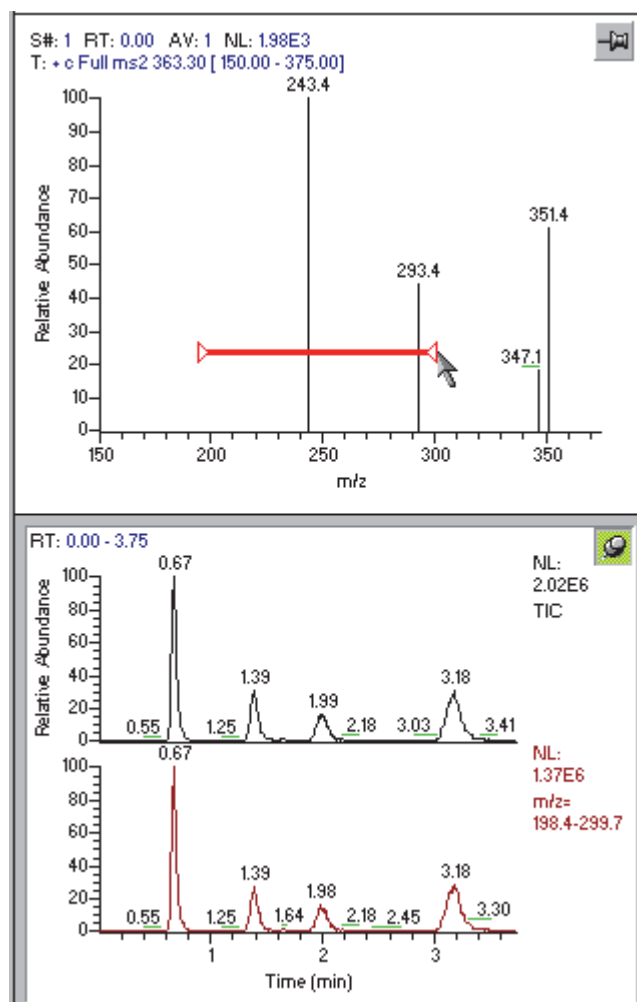
- Active and pinned view: chromatogram
- Inactive view: spectrum

❖ To add a plot to the chromatogram view

1. Click the **Add or Replace Plot** icon, , on the toolbar.
2. In the inactive spectrum view, drag the cursor from m/z 198.4 through 299.7.

In the inactive spectrum view, a red horizontal marker () defines the selection range. In the pinned chromatogram view, a second chromatogram appears below the original chromatogram.

In the following figure, the chromatogram for the selected mass range appears below the original TIC chromatogram.



Selecting a Two-Dimensional Range on a Plot

Use this procedure to isolate a small region of a plot, for example, to select a small peak.

❖ To select a two-dimensional range in the active plot

1. To activate the cross-hair cursor and status bar, move the cursor to the graphic region of a plot. This is the region above the x axis and to the right of the y axis.

The data system displays a cross-hair cursor and the coordinates in the appropriate units for the plot in the status bar at the bottom of the Qual Browser window.

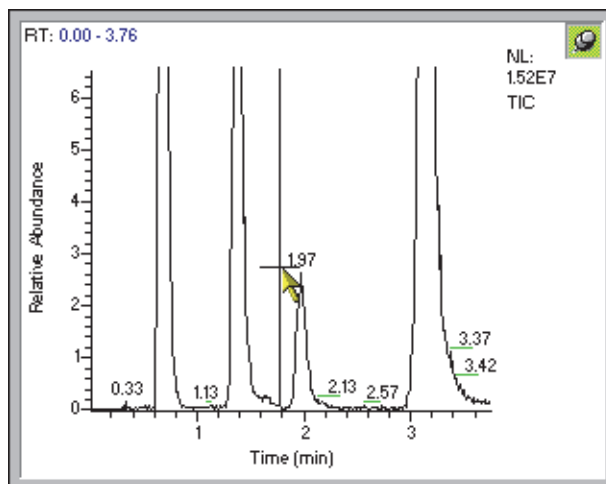
This information appears in the status bar of these views:

- Chromatogram view: Time, Intensity, Filter
- Spectrum view: Mass (m/z), Intensity
- Map view: Time, Mass (m/z)

The data system only displays the cross-hair and status bar when a view can be used to pick a point, range, or scan filter for application to the active plot.

2. To use the cursor to outline a region of interest in the active plot, do the following:
 - a. Position the cross-hair cursor where you want to begin outlining the area of interest (Figure 24).

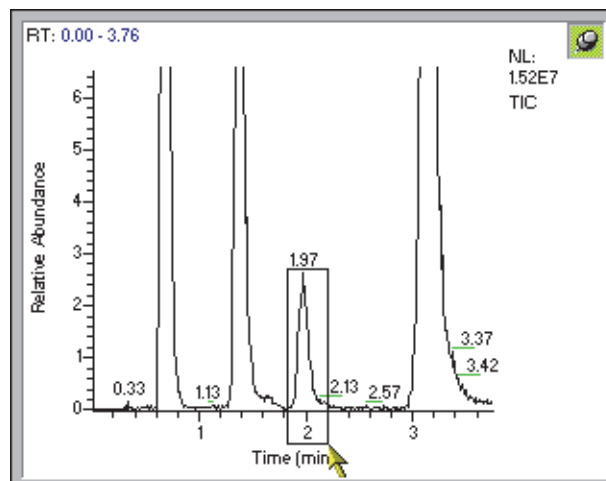
Figure 24. Position the cross-hair



- b. Drag the cursor to the opposite corner of the area. To include the axis, extend the selected area over the axis.

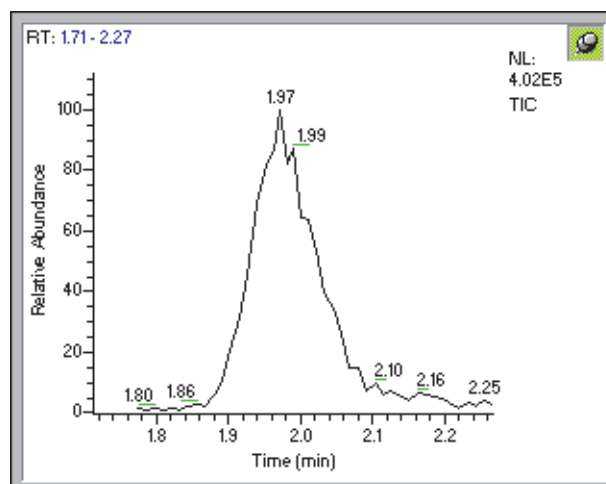
The data system displays a black outline to indicate the area selected (Figure 25).

Figure 25. Drag the cursor to define the area of interest



When you release the mouse button, the data system replots the selected area of the active view (Figure 26).

Figure 26. Plot with area of interest



Use this procedure with the x axis or y axis of the chromatogram, spectrum, and map views.

3. If you do not obtain the desired result, click the **Zoom Reset** icon, , in the toolbar to restore the active plot, and then repeat [step 2](#).

Using Scan Filters

You can use a scan filter to specify that data processing is to be applied to a subset of the scans in a raw data file. The scan filter box is provided in all Xcalibur windows that display raw data files: the home page, Processing Setup, Instrument Setup, Quan Browser, and Qual Browser windows. You can either select a scan filter from the list of filters that the data system creates from the instrument method settings for your mass spectrometer, or you can create a new filter using the scan filter format.

❖ To use scan filters

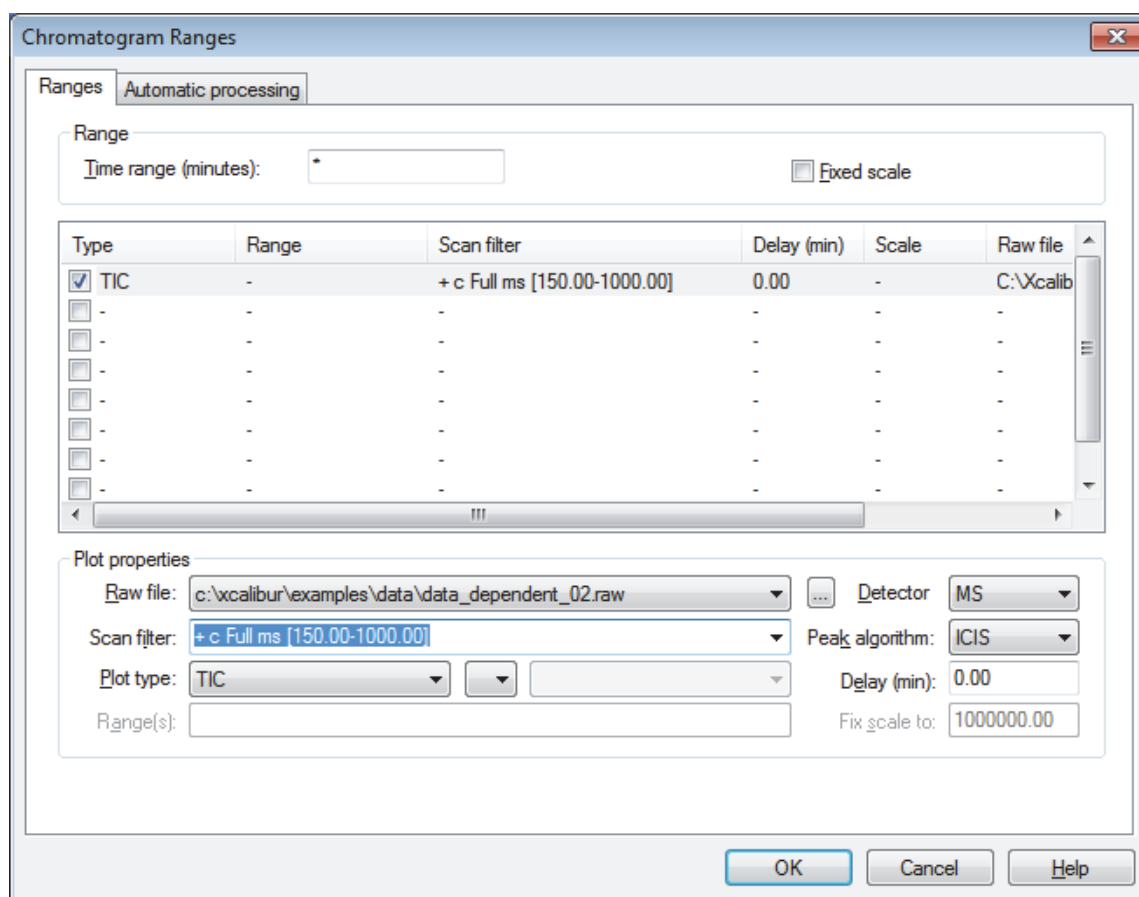
1. Locate the appropriate scan filter list.

Locate the scan filter list (Scan Filter list or Filter list) in one of the following windows: Instrument Setup, Qual Browser, Processing Setup, Quan Browser, or home page.

2. Check the current filter.

The data system displays the current scan filter in the Scan Filter list (see [Figure 27](#)). To view other scan filters available in the raw data file, click the down arrow to display the list.

Figure 27. Example of the scan filter list (Qual Browser window)



3. Do one of the following:
 - To edit the current scan filter, type the change in the Scan Filter box and go to [step 6](#).
 - To modify a different filter in the list, go to [step 4](#).
 - To manually enter a new scan filter, go to [step 5](#).
4. Select a scan filter from the Scan Filter list.

Use the scan filter format to determine the function of each filter in the scan filter list.
Edit the selected scan filter to create a new scan filter, as required. Go to [step 6](#).

5. Type a new scan filter in the Scan Filter list.

Use the scan filter format to create the scan filter that allows you to find only the scans that contain the experiment settings of interest.

- Positive or negative charged ions
 - Centroid or profile data
 - Source CID
 - Scan mode
 - Scan power
 - Parent masses
 - Product mass range
 - TurboScan
 - Constant neutral gain
 - Constant neutral loss
6. Continue to enter other settings.

Scan Filter Format

The data system creates scan filters from scan event settings and stores them with each raw data file. Users can select scan filters to specify that processing is to be applied to a subset of the scans in a raw data file. Make sure to use only fields that apply to your mass spectrometer. You can define additional scan filters by adhering to the following scan filter format.

Note Not all features are applicable for every mass spectrometer.

Table 9. Scan filter format (Sheet 1 of 3)

Feature	Option	Interpretation
Polarity	+, –	Positive, Negative
Data type	p, c	Profile, Centroid
Dependent scans	d, !d	Include dependent scans, Exclude dependent scans
TurboScans	t, !t	Include TurboScan scans, Exclude TurboScan scans
Source CID	sid, !sid	Include Source CID scans, Exclude Source CID scans (Source CID scans are scans for ions produced by source induced dissociation.)
Scan type	FULL, Z, SIM, SRM, CRM, Q1MS, Q3MS	Full scan, ZoomScan, SIM, SRM, CRM, Q1MS, Q3MS
Scan mode	ms, ms2, ms3, ... MS10	MS ⁿ for n = 1 to 10 Each order can be followed by the appropriate number of parents. The parents can also be omitted. Example: “ms3 345.3, 253.2” indicates an MS ³ scan with parents with <i>m/z</i> 345.3 and 253.2.
	pr	Parent (followed by the product mass)
	cng	Constant Neutral Gain (followed by the mass of the neutral)
	cnl	Constant Neutral Loss (followed by the mass of the neutral)
Mass Analyzer	ITMS, TQMS, SQMS, TOFMS, FTMS, Sector	ITMS, TQMS, SQMS, TOFMS, FTMS, Sector
Photo Ionization	pi, !pi	Include photo ionization scans, Exclude photo ionization scans
Compensation Voltage	cv, !cv	Include compensation voltage scans, Exclude compensation voltage scans
Detector Valid	det, !det	Include detector valid scans, Exclude detector valid scans
Enhanced	E, !E	Include enhanced scans, Exclude enhanced scans
Wideband	w, !w	Include wideband scans, Exclude wideband scans

Table 9. Scan filter format (Sheet 2 of 3)

Feature	Option	Interpretation
Supplemental Activation	sa, !sa	Include supplemental activation scans, Exclude supplemental activation scans
Multistate Activation	msa, !msa	Include multistate activation scans, Exclude multistate activation scans
Product masses or mass range of scan	[m1a–m1b, m2a–m2b, m3a–m3b, ...]	Scans with a specific mass range or mass ranges, such as SIM, SRM, and CRM. Example: [50.00 – 1500.00] for a scan from m/z 50.00 to 1500.00 If a scan is exactly 1 u wide, it is displayed as a single value (the center mass). This is typical for SIM, SRM, and CRM. Filters for parents in dependent scans are matched with a tolerance of m/z 1.0 so that minor differences in parent mass measurements from scan to scan do not give different filters.
Segment/scan event number pairs	{segment, scan number}	Example “{3, 4} + c ms” indicates segment 3, scan event 4 for a positive centroid MS scan The curly brackets { } are required.
Ionization mode	APCI, ESI, EI, CI, NSI, FAB, TSP, FD, MALDI, GD	Example: “+ c ESI ms” indicates a positive centroid electrospray MS scan
Corona on/off	corona, !corona	Corona on, Corona off Example: “+ APCI !corona ms” indicates a positive centroid APCI scan with the corona off
Detector value	“det=##.##”	Detector value is “##.##” with no spaces. Example: “+ ESI det= –800.0” indicates a positive electrospray scan at –800.0 detector units (usually volts)
MS/MS and MS ⁿ CID energies	mass@energy	Mass is the parent mass and energy is the CID relative energy (no units) Example: “– c ms2 196.1@25.0” indicates a negative centroid MS/MS scan of m/z 196.1 at 25.0 units of CID energy
Quadrupole identification	Q1MS, Q3MS	Example: “+ c ESI Q3MS” indicates a positive centroid electrospray MS scan using quadrupole 3
Accurate Mass	AM, !AM, AMI, AME	Include accurate mass scans, Exclude accurate mass scans, Include accurate mass internal, Include accurate mass external
Ultra	u, !u	Include ultra scans, Exclude ultra scans

Table 9. Scan filter format (Sheet 3 of 3)

Feature	Option	Interpretation
Sector	BSCAN	Include magnetic sector scans
	ESCAN	Include electric sector scans
LOCK	lock, !lock	Include lock scans, Exclude lock scans
Multiplex	msx, !msx	Include multiplexing scans, Exclude multiplexing scans
Synchronous Precursor Selection	sps	
Rapid scan rate	r	rapid scan rate ion trap scan
Electron Capture Dissociation	ecd, !ecd	Include electron capture dissociation, Exclude electron capture dissociation
Multi Photo Dissociation	mpd, !mpd	Include photo dissociation, Exclude photo dissociation
Electron Transfer Dissociation	etd, !etd	Include electron transfer dissociation scans, Exclude electron transfer dissociation scans
High Energy CID	hcd, !hcd	Include high energy scans, Exclude high energy scans
Source SID	cid, !cid	Include Source SID scans, Exclude Source SID scans (Source SID scans are surface induced scans.)
Free Region	ffr1, ffr2	

Applying a Scan Filter to a Plot

This procedure demonstrates the interactive use of a scan filter view. For the routine application of scan filters to the chromatogram, spectrum, map, or spectrum list views, use the [Ranges Dialog Boxes](#). Choose **Display > Ranges** and select a scan filter from the Scan Filter box.

❖ To familiarize yourself with the scan filter view

1. Open the chromatogram view by clicking the **View Chromatogram** icon, , in the toolbar or by choosing **View > Chromatogram**.

The [Chromatogram View](#) appears in the cell.

2. To display the entire time range for the chromatogram, choose **Display > Zoom > Display All**.
3. To display the entire chromatogram, choose **Display > Zoom > Reset**.
4. If a filter has been applied to the chromatogram view, remove it as follows:

- a. Choose **Display > Ranges**.

The [Chromatogram Display Options Dialog Box](#) opens.

- b. Select the scan filter in the Scan Filter box.
- c. Press the DELETE key and then click **OK** to remove the filter.

5. To open the scan filter view, select another cell and choose **View > Scan Filter**.

The [Scan Filter View](#) opens in that cell.

6. To display all of the scan filters used in the sample, drag the cursor in the chromatogram view parallel to the x axis.
7. To select all of the peaks in the chromatogram, start at the y axis and stop at the end of the x axis. See [Selecting a One-Dimensional Range on a Plot](#) for more information.

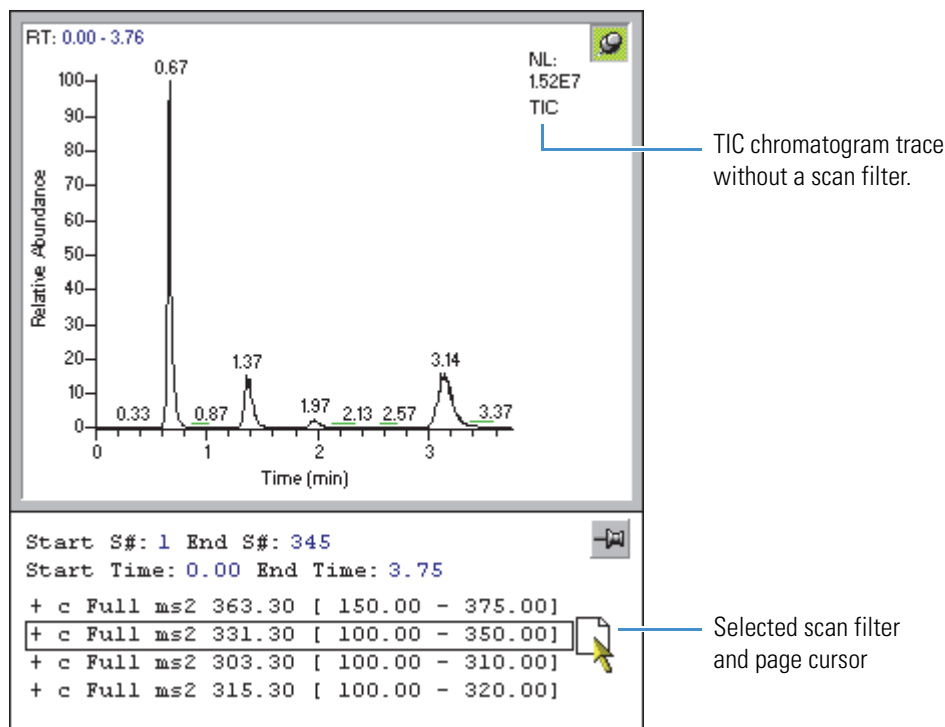
The data system displays all of the scan filters used for the sample run in the scan filter view.

8. To select and apply a scan filter to a plot in the active chromatogram view, drag the scan filter to the active view. Release the mouse button to apply the filter.

Figure 28, Figure 29, and Figure 30 demonstrate this process.

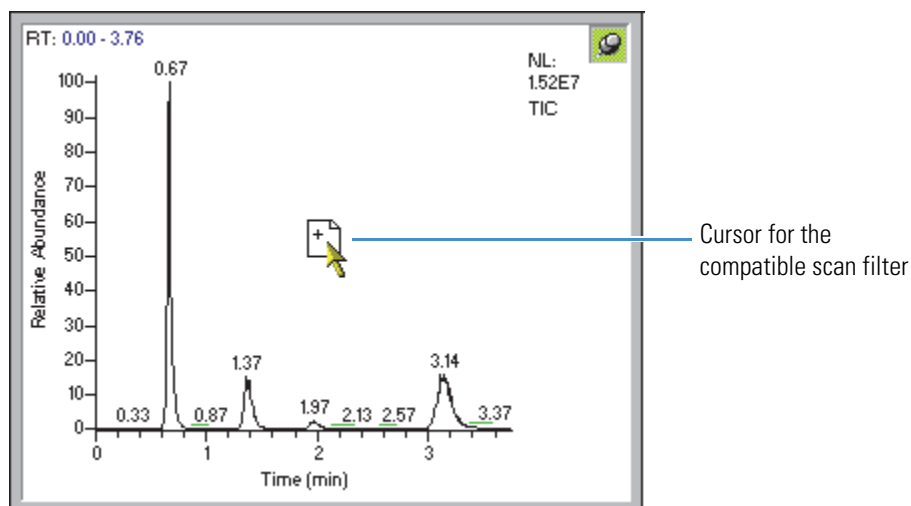
Select a scan filter in the scan filter view. The cursor changes to the page cursor.

Figure 28. Select a scan filter



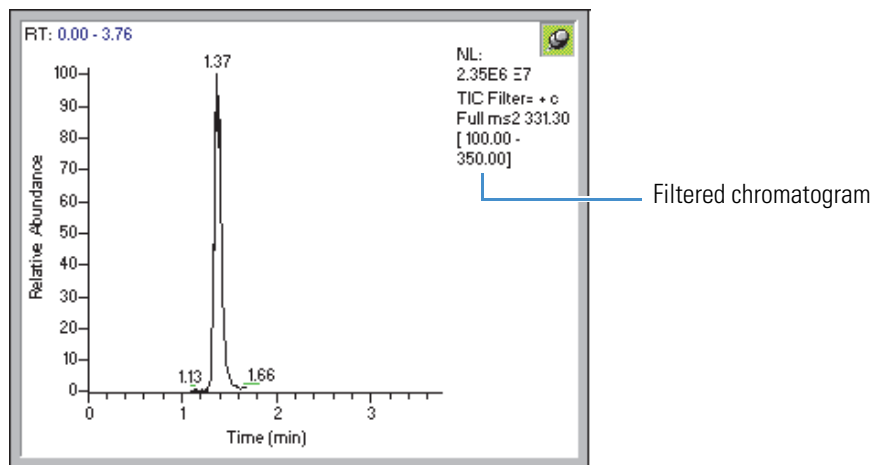
As you drag the scan filter into the active chromatogram view, the cursor changes to the add page cursor, if the scan filter is compatible with the view. Or, the cursor changes to the not allowed cursor, , if the scan filter is incompatible with the view.

Figure 29. Drag the scan filter to a plot in another view



When you release the mouse button, the data system applies the scan filter, redraws the plot, and makes the view that contains the plot with the applied filter the active view.

Figure 30. Xcalibur data system applies the scan filter and redraws the plot



If you do not obtain the desired result, click the **Undo** button, , in the toolbar to restore the previous plot and repeat [step 4](#).

Displaying Multiple Magnifications of a Plot

You can magnify a region of an active plot by dragging the cursor across the region of interest. However, to view the original plot after you magnify a region of interest, or to select a different region of the plot, you must first reset the magnification.

The following procedure describes how to repeatedly magnify different sections of a plot without first resetting the magnification.

❖ To display multiple magnifications of a plot

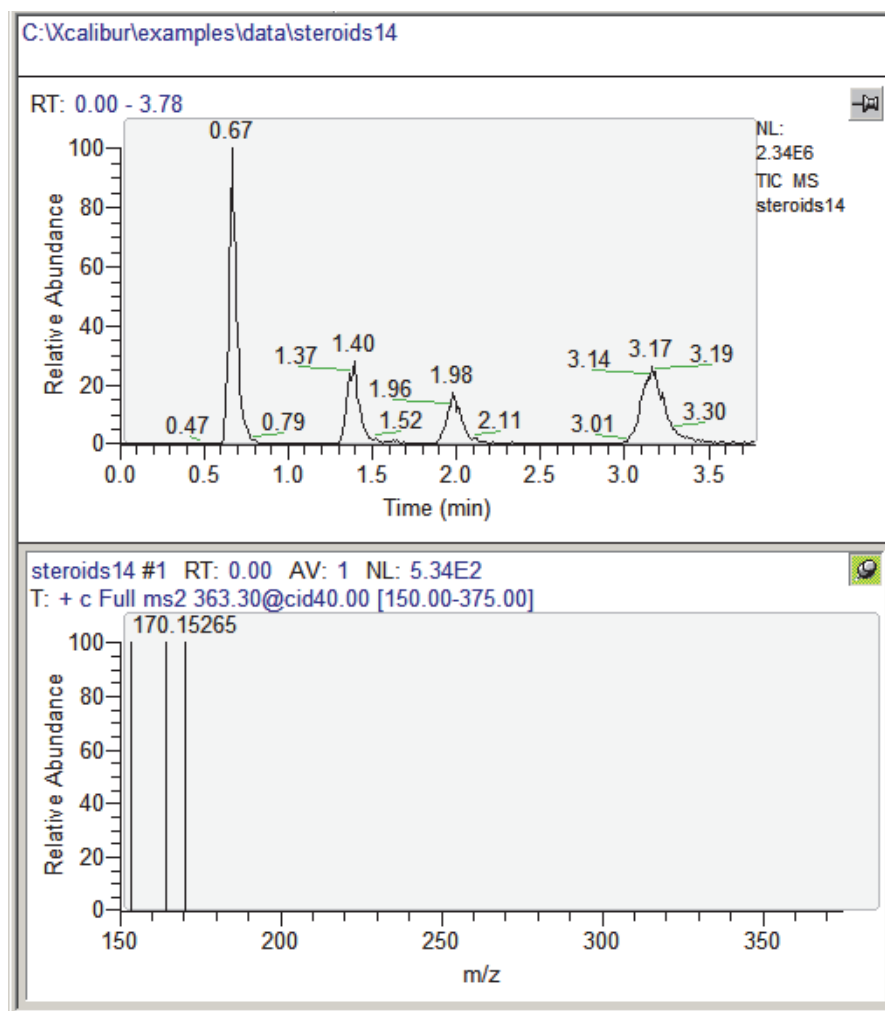
1. Open a raw data file in the Qual Browser window.

[Figure 31](#) shows the default layout for the steroids14.raw example file when you open the raw data file in a new window. The window contains two cells. The upper cell is inactive and displays a chromatogram view with a TIC plot. The lower cell is pinned and displays a spectrum view with the mass spectrum from the beginning of the run (RT = 0).

3 Using Views Interactively

Displaying Multiple Magnifications of a Plot

Figure 31. Default layout for the steroids14 example data file

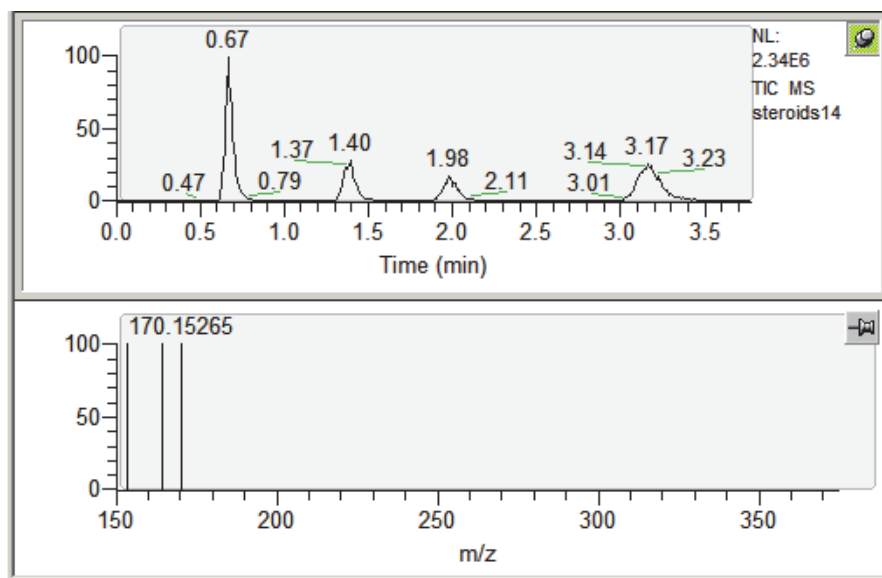


2. Click the pin icon of the target cell.

A gray border appears around the target cell, the background behind the pin turns green, and the pin turns to the pinned position (see [Figure 32](#)).

Note To add a copy of the active cell to the grid, you can make the cell active or active and pinned.

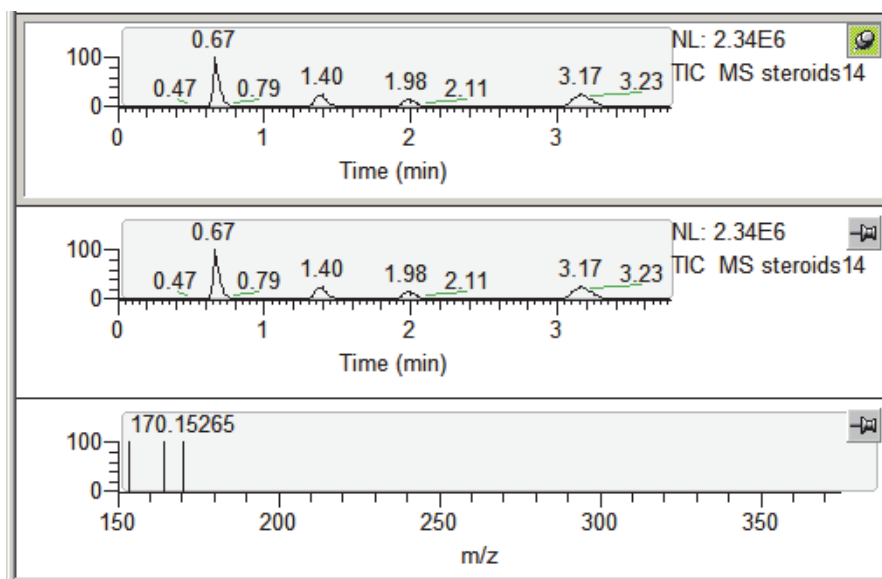
Figure 32. Active and pinned chromatogram view and inactive spectrum view



3. To make a copy of the active cell in a new cell below the current cell, choose **Grid > Insert Cells > Below**.

An inactive copy of the cell appears below the active cell (see [Figure 33](#)).

Figure 33. Cell grid with a copy of the original cell



Note You can magnify a section of an active cell. However, after you modify the display range, you cannot select a range outside this range without first resetting the magnification.

3 Using Views Interactively

Displaying Multiple Magnifications of a Plot

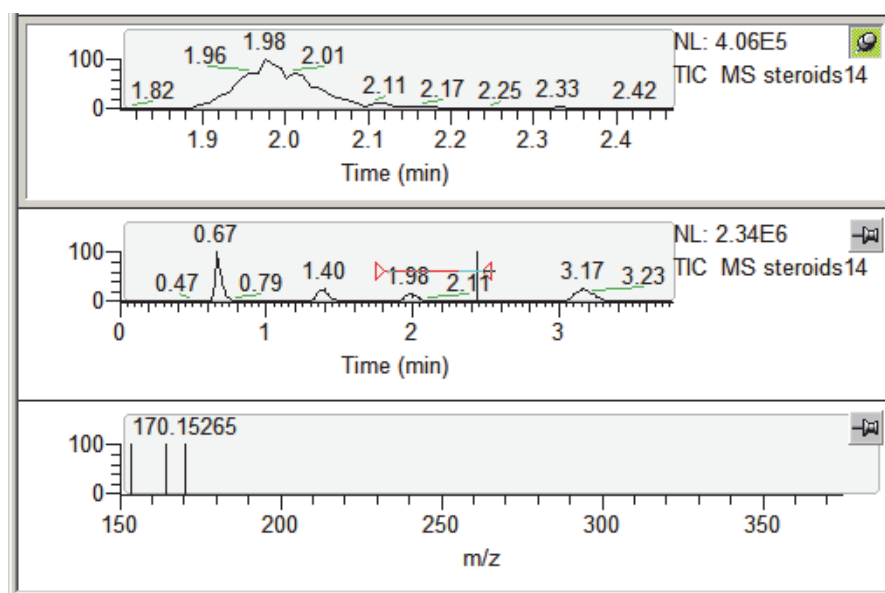
4. In the inactive copy of the cell that you want to modify, select the region of interest as follows:
 - For a chromatogram view or a spectrum view, drag the cursor in the plot parallel to the x axis or y axis (see [Selecting a One-Dimensional Range on a Plot](#)).
 - For a map view, drag the cursor in the plot to select an area from one corner of the region of interest to the opposite corner of the region of interest. For more information about this procedure, see [Selecting a Two-Dimensional Range on a Plot](#).

The selected region appears in the active and pinned cell. The inactive cells are unaffected.

Note To work interactively with cells, the active cell must be pinned.

Figure 34 shows the red horizontal marker that defines the selected region in the inactive cell and the magnified region in the active and pinned cell.

Figure 34. Cell grid with the original chromatogram plot and the magnified section of the plot



5. Repeat [step 4](#) until you are satisfied with the selection.

Working with a Chromatogram View

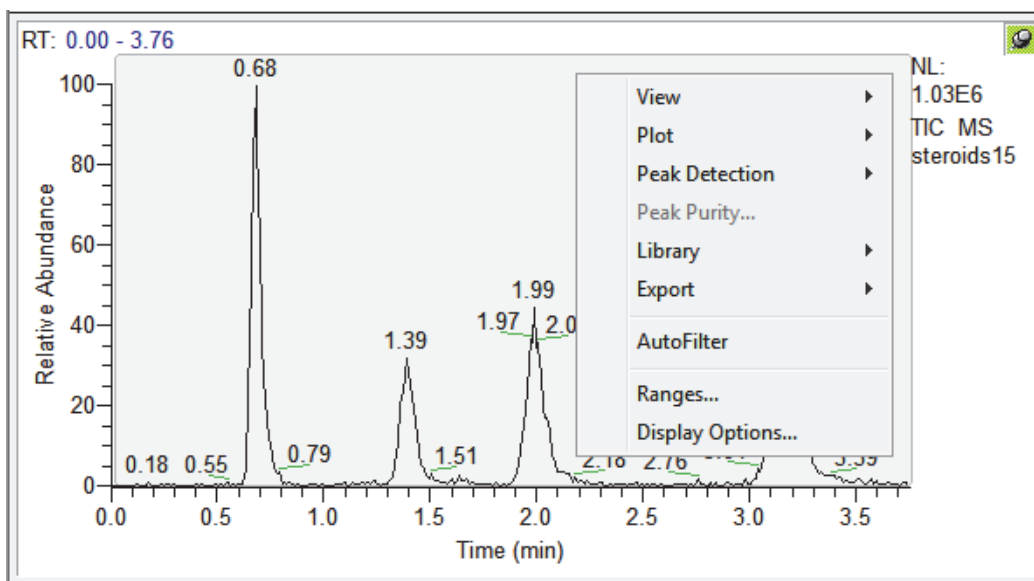
A chromatogram view shows the intensities of one or more masses as a function of time. These procedures describe how to manipulate chromatograms.

Contents

- Inserting and Deleting Chromatogram Plots
- Setting the Chromatogram Display and Processing Options
- Adding Plots to a Chromatogram View with the Autofilter Command
- Setting the Chromatogram Display Options
- Detecting Peaks
- Reviewing the Effect of Different Peak Detection Settings

Figure 35 shows a chromatogram view with the chromatogram shortcut menu displayed. For the y axis, the label is from the detector, the intensity is normalized to the largest peak in the selected time range, and the units are set to relative.

Figure 35. Chromatogram view with the chromatogram shortcut menu displayed



❖ **To view a chromatogram**

To view a chromatogram in the active cell, do one of the following:

- In the toolbar, click the **View Chromatogram** icon, .
- Right-click the cell and choose **View > Chromatogram** from the shortcut menu.

—or—

- From the menu bar, choose **View > Chromatogram**.

Inserting and Deleting Chromatogram Plots

You can display up to eight plots within a chromatogram view.

❖ **To insert a plot in a cell with a chromatogram view**

1. Select the cell containing the view.
2. Right-click the chromatogram above the position for the new plot.
3. Choose **Plot > Insert** from the shortcut menu.

❖ **To delete a plot from a multi-plot chromatogram view**

1. Select the cell containing the view.
2. Right-click the plot that you want to delete.
3. Choose **Plot > Delete** from the shortcut menu.

You can also use the Ranges dialog box to add, delete, or enable plots.

Setting the Chromatogram Display and Processing Options

Use these procedures to select the chromatograms that you want to display and the automatic processing options for the chromatograms:

- [Setting Chromatogram Display Options](#)
- [Setting Automatic Processing for Chromatograms](#)

Setting Chromatogram Display Options

Use the Chromatogram Display Options dialog box to view and edit the mass range and time range for all the plots in a chromatogram view.

For more information about the Ranges page of the Chromatogram Display Options dialog box, see [Chromatogram Display Options Dialog Box](#).

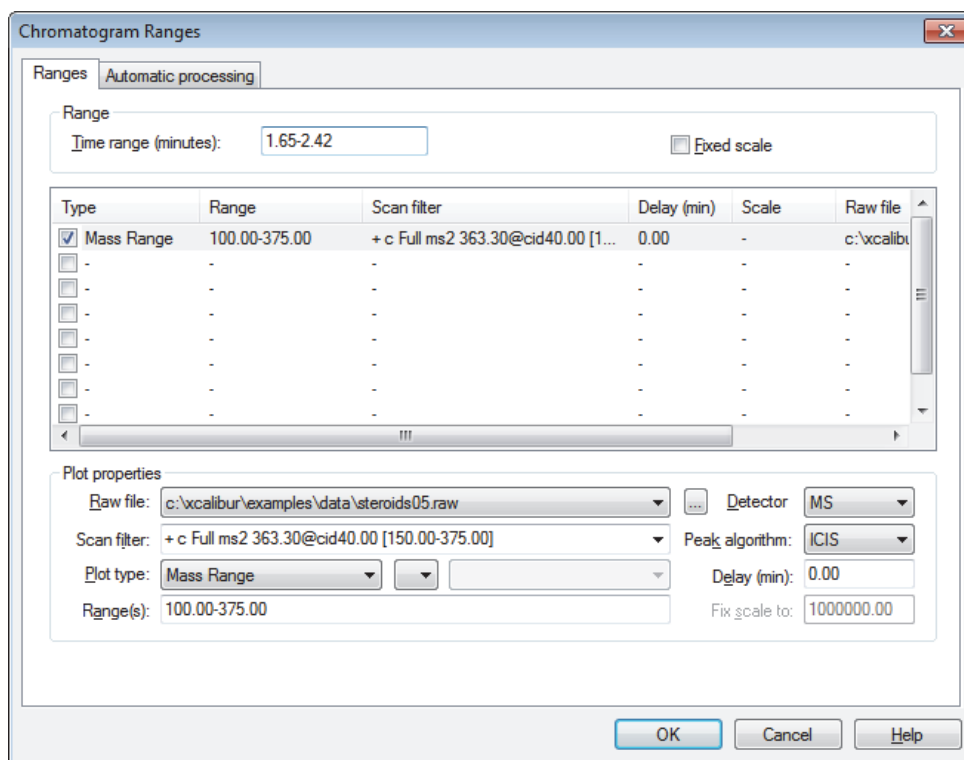
❖ **To set the mass range and time range for a chromatogram**

1. Make the chromatogram view the active view.
2. To open the Chromatogram Ranges dialog box (Figure 36), do one of the following:
 - Click the **Ranges** icon, , in the Qual Browser toolbar.
 - Right-click a chromatogram plot in the cell and choose **Ranges** from the shortcut menu.

—or—

- Choose **Display > Ranges**.

Figure 36. Ranges page of the Chromatogram Ranges dialog box



3. To specify the time range in the Time range box, type the lower and upper time limits in minutes, separated by a dash with no spaces.

Time range (minutes): 1.65-2.42

4. To view or hide the chromatogram, select (or clear) the **Type** check box.

A row of settings in the Chromatogram Ranges dialog box describes the chromatogram.

5. To change the source of the active plot, select a raw data file by doing one of the following:

- Select a file from the Raw File list.

The list contains all of the currently selected raw data files. When you open another raw data file, it appears in the list.

- Click **Browse** adjacent to the list to open the Open dialog box. Then, browse to the required file or type the full path and filename of the required file.

6. To specify the scan filter, select a scan filter from the Scan Filter list.

The Scan Filter list displays the scan filters stored in the raw data file.

7. To specify the chromatogram plot type, use the Plot Type lists. To change the current chromatogram type, click the arrow to display a list of chromatogram type options and select a type option.

8. To specify a range for the specified plot types, type the first mass/wavelength and last mass/wavelength in the Ranges box.

The format for multiple ranges is as follows:

- For an MS detector

First Mass (Range 1) – Last Mass (Range 1), First Mass (Range 2) – Last Mass (Range 2)

- For a PDA detector

First Wavelength (Range 1) – Last Wavelength (Range 1), First Wavelength (Range 2) – Last Wavelength (Range 2)

Use a comma to separate the ranges.

9. In the Plot Properties area, select a detector type and specify a peak algorithm type.
10. Specify the delay time between when a component peak is detected by the MS detector and the same peak is detected by a UV detector or other type of analog detector. To change the value, enter the new delay time in the Delay box. The valid time range is –5.0 to +5.0 minutes.
11. To turn on, change, or turn off the fixed scale setting, do the following:
 - To turn on the maximum range for the y axis of the active chromatogram, select the **Fixed Scale** check box.
 - To change the value, type the new maximum y-axis value in the Fix Scale To box.
 - To turn off the fixed scale setting, clear the **Fixed Scale** check box.
12. To save the settings and close the dialog box, click **OK**.

Setting Automatic Processing for Chromatograms

Use the Automatic Processing page (Figure 37) to apply smoothing or baseline subtraction to all the plots in the active chromatogram view. You can also use this page to set the mass tolerance and precision for the current data file.

You can set default values for mass tolerance and precision for the Qual Browser application by using the Global Mass Options dialog box (see [Global Mass Options Dialog Box](#)).

For more information, see [Automatic Processing Page – Chromatogram Display Options Dialog Box](#).

Follow these procedures to set up the parameters on the Automatic Processing page:

- [Setting Smoothing Area Options](#)
- [Setting Baseline Subtraction Area Options](#)
- [Setting Include Peaks Area Options](#)
- [Setting Mass Tolerance Area Options](#)
- [Setting Mass Precision Area Options](#)

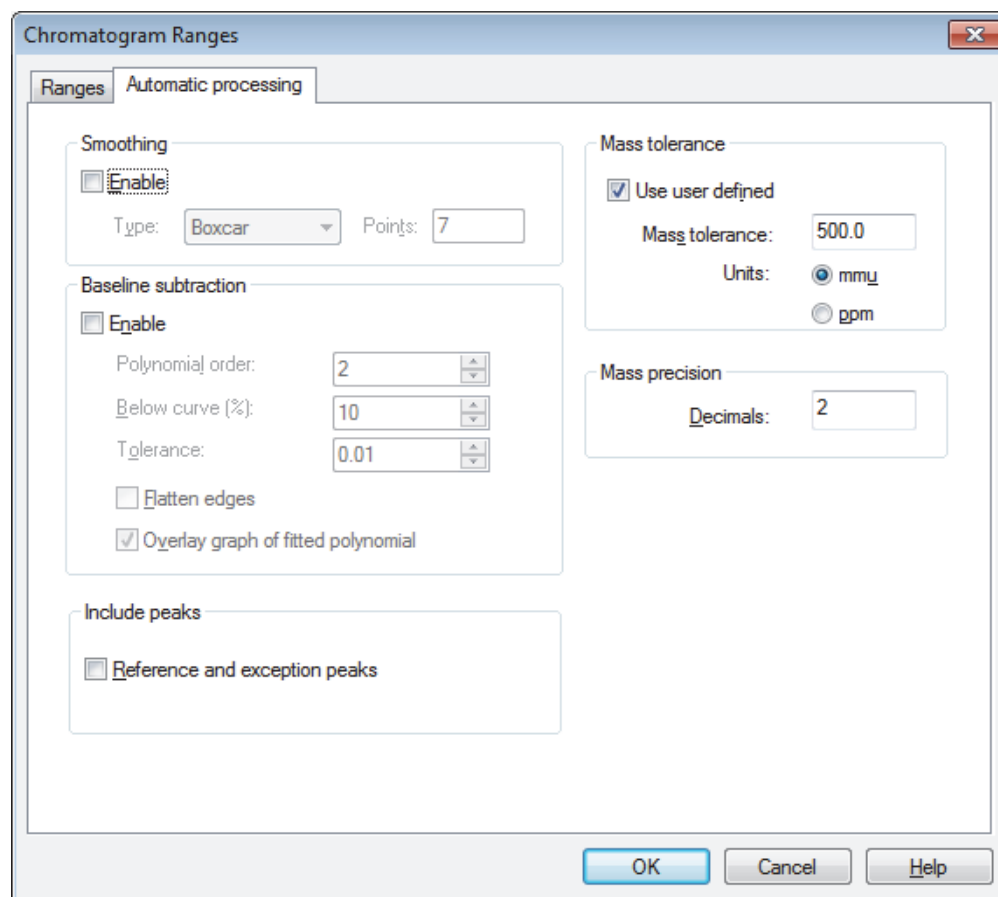
❖ To open the Automatic Processing page for the chromatogram view

1. Open a chromatogram in an active chromatogram view of the Qual Browser window.
 2. To open the Chromatogram Ranges dialog box, do one of the following:
 - In the toolbar, click the **Ranges** icon, .
 - Right-click a chromatogram plot in the cell and choose **Ranges** from the shortcut menu.
- or—
- From the menu bar, choose **Display > Ranges**.
3. Click the **Automatic Processing** tab.

The Automatic Processing page opens (Figure 37). The default values in the Mass tolerance and Mass precision areas are set in the Global Mass Options dialog box. You can override these default values by setting new values on the Automatic Processing page.

Tip To open the Global Mass Options dialog box in Qual Browser, choose **Display > Mass Options** from the menu bar.

Figure 37. Automatic Processing page of the Chromatogram Ranges dialog box



Setting Smoothing Area Options

On the Automatic Processing page of the Chromatogram Ranges dialog box, use the Smoothing area parameters to smooth the chromatograms.

❖ To set the smoothing parameters

1. To turn on chromatogram smoothing, select the **Enable** check box. To turn off chromatogram smoothing, clear the **Enable** check box.
2. To change the type of smoothing, select either **Boxcar** or **Gaussian** from the Type list.
3. To specify the number of points for chromatogram smoothing, type an integer in the Points box.

The valid range for smoothing points includes the odd integers from 3 (minimum smoothing) to 15 (maximum smoothing).

Setting Baseline Subtraction Area Options

On the Automatic Processing page of the Chromatogram Ranges dialog box, use the Baseline Subtraction parameters to apply baseline subtraction to all chromatogram plots in the active view. This algorithm fits a smooth curve through the noise in the chromatogram and subtracts this curve from the chromatogram, leaving the peaks on a flat baseline.

❖ To set baseline subtraction settings

1. To turn on baseline subtraction, select the **Enable** check box. To turn off baseline subtraction, clear the **Enable** check box.
2. To specify the polynomial order, type or select an order for the baseline curve in the Polynomial order box.

The normal range is 3 to 20. For complex chromatograms, use a high polynomial order.

3. To specify the Below curve (%) value, which moves the baseline up or down in the chromatogram noise, type or select a value in the Below Curve (%) box.

The typical range for this parameter is 5 to 30%, depending on the number and width of peaks in the chromatogram. Increase this value as the number of peaks or the peak width increases. The valid range is from 1 to 99.

4. To specify the algorithm's precision, type or select a value in the Tolerance box.

The valid range is from 0.001 to 0.2.

5. To specify how the algorithm fits the beginning and end of the chromatogram, select or clear the **Flatten Edges** check box.

- To make sure the beginning and end of the plot are horizontal, select the check box.
- Clear the check box if this is not required.

6. To display the polynomial function with the chromatogram, select the **Overlay Graph of Fitted Polynomial** check box. Clear the check box to hide the display.

Setting Include Peaks Area Options

On the Automatic Processing page of the Chromatogram Ranges dialog box, the Include peaks area has only one check box. Use this setting to include or exclude the reference peaks (R) and exception peaks (E) for the mass data in all the cells in the Qual Browser window.

❖ To set peaks area settings

To include reference and exception peaks in the chromatogram display, select the **Reference and Exception Peaks** check box. To hide reference and exception peaks, clear this check box.

Setting Mass Tolerance Area Options

Use the Mass Tolerance area of the Automatic Processing page of the Chromatogram Ranges dialog box to specify a mass tolerance for the current data file.

Tip You can set a default value for mass tolerance on the Mass Options page of the Xcalibur Configuration dialog box. Settings on this page affect the display of all the mass data in the Xcalibur data system. You can also set a default value for mass tolerance in the Qual Browser – Global Mass Options dialog box. Settings in this dialog box affect the display of all the mass data in the Qual Browser window.

❖ To set Mass tolerance area settings

1. To use mass tolerance, select the **Use User Defined** check box.
2. Enter a value from **0.1** to **50000.0** in the Mass Tolerance box. Select a unit type.
3. To turn off mass tolerance, clear the **Use User Defined** check box.

Setting Mass Precision Area Options

Use the Mass precision area of the Automatic Processing page of the Chromatogram Ranges dialog box to specify a mass precision for the current data file.

Tip You can set a default value for mass precision on the Mass Options page of the Xcalibur Configuration dialog box. Settings on this page affect the display of all the mass data in the Xcalibur data system. You can also set a default value for mass precision in the Global Mass Options dialog box. Settings in this dialog box affect the display of all the mass data in the Qual Browser window.

❖ To set Mass precision area settings

1. Specify the number of places after the decimal point that display in mass values in the Decimals box.
2. To save the settings and close the dialog box, click **OK**.

Adding Plots to a Chromatogram View with the Autofilter Command

Use the Autofilter command to repopulate a chromatogram view with these possible characteristics:

- A plot showing the chromatogram without any scan filters
- Plots for each scan filter applied to the chromatogram, up to the maximum of eight chromatogram plots

❖ To automatically add plots for all of the scan filters to a chromatogram view

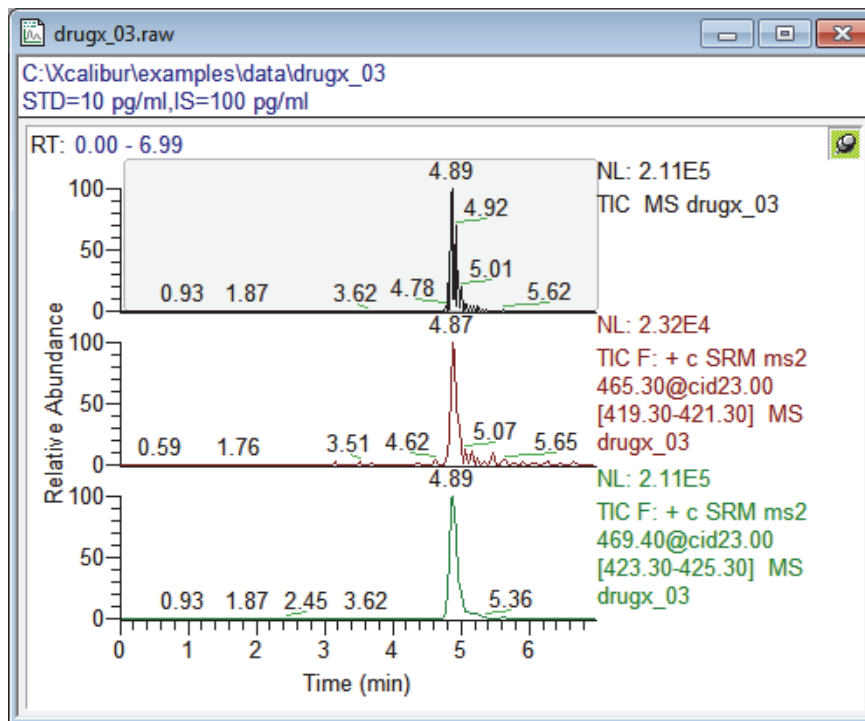
1. Pin the chromatogram view.
2. Do one the following:
 - Choose **Actions > Autofilter** from the menu bar.
 - Right-click the cell and choose **Autofilter** from the shortcut menu.

—or—

- Click the **Autofilter** icon, , in the toolbar.

The data system draws the chromatogram view with a plot for no scan filter applied and one plot for every scan filter applied to the chromatogram up to a maximum of eight chromatogram plots total. Figure 38 shows the result of the Autofilter command on the drugX_03.raw data file (Xcalibur\examples\data).

Figure 38. Chromatogram view for a data file with two scan filters and a TIC



Setting the Chromatogram Display Options

The Display Options dialog box contains a small display area showing the active cell. Use this display to preview the effects of different settings before applying them.

Use one or more of these procedures to set up chromatogram display options:

- [Setting the Chromatogram Axis Options](#)
- [Setting the Chromatogram Color Options](#)
- [Setting the Chromatogram Label Options](#)
- [Setting the Chromatogram Normalization Options](#)
- [Setting the Chromatogram Style Options](#)

Setting the Chromatogram Axis Options

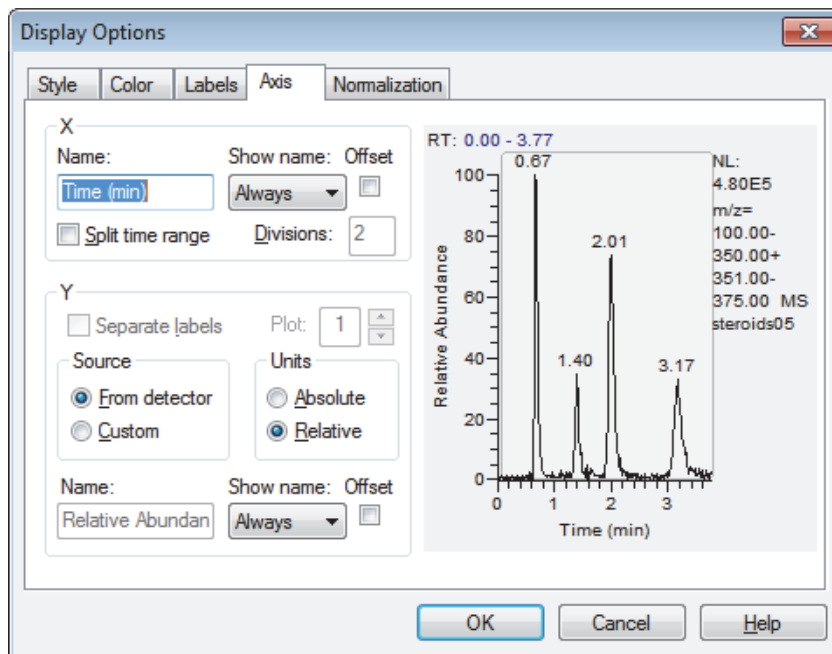
For more information, see [Chromatogram View – Display Options Dialog Box – Axis Page](#).

❖ To set the chromatogram axis options

1. Open a chromatogram in the Qual Browser window and make it active.
2. To open the Display Options dialog box, choose **Display > Display Options** or right-click the cell and choose **Display Options** from the shortcut menu.
3. Click the **Axis** tab.

The Axis page of the Display Options dialog box for the chromatogram view opens ([Figure 39](#)).

Figure 39. Display Options – Axis page for the chromatogram view



4. To change the name of the x or y axis, type the new name in the appropriate axis Name box.
5. To change the time when the data system displays the axis label, select **Never**, **On Print**, or **Always** from the Show name list.
6. To move the displayed plot from the x or y axis, select the appropriate axis **Offset** check box. To turn off axis offset, clear the **Offset** check box.
7. To set time range splitting, do one of the following:
 - To split the time scale, select the **Split Time Range** check box. Then, to change the number of divisions (subsections), type the new number in the Divisions (time) box.
 - To display only one time range, clear the **Split Time Range** check box.
8. To save the settings and close the dialog box, click **OK**.

Setting the Chromatogram Color Options

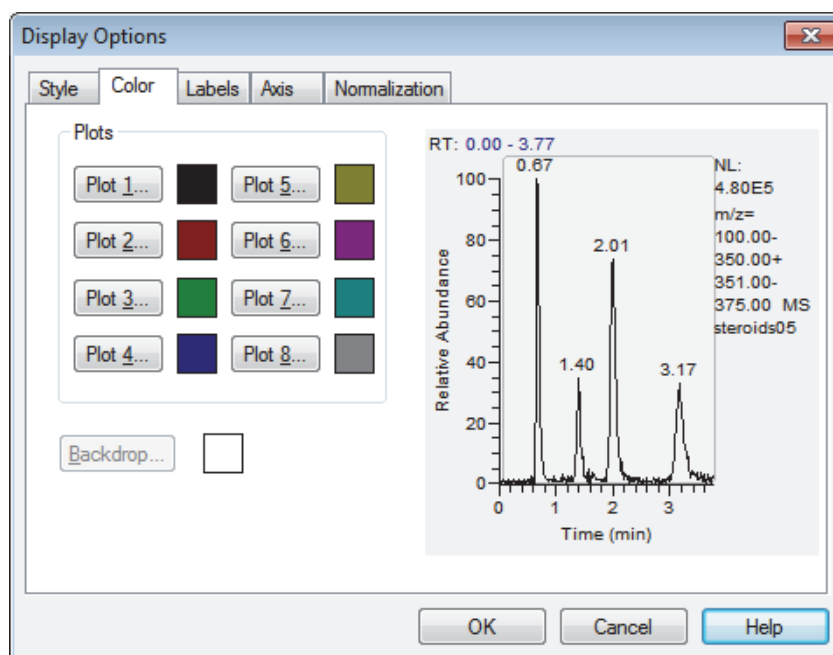
For more information see [Chromatogram View – Display Options Dialog Box – Color Page](#).

❖ To set the chromatogram color options

1. Open a chromatogram in the Qual Browser window and make it active.
2. To open the Display Options dialog box, choose **Display > Display Options** or right-click the cell and choose **Display Options** from the shortcut menu.
3. Click the **Color** tab.

The Color page opens ([Figure 39](#)).

Figure 40. Display Options – Color page for the chromatogram view



4. To select the color of a particular plot, click the Plot *Number* button.

The data system opens the Color dialog box with a color palette so that you can select a preset color or customize a color.

5. To select the color of the backdrop, click **Backdrop**.

The data system opens the Color dialog box with a color palette so that you can select a preset color or customize a color. Backdrop options are available when you have selected the Overlay 3D style.

6. To save the settings and close the dialog box, click **OK**.

Setting the Chromatogram Label Options

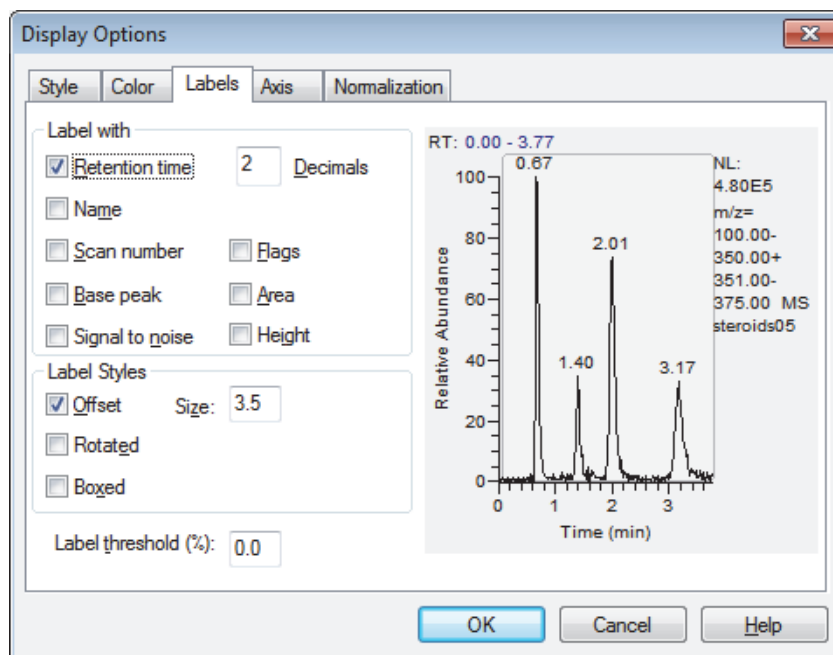
For more information, see [Chromatogram View – Display Options Dialog Box – Labels Page](#).

❖ To set the chromatogram label options

1. Open a chromatogram in the Qual Browser window and make it active.
2. To open the Display Options dialog box, choose **Display > Display Options** or right-click the cell and choose **Display Options** from the shortcut menu.
3. Click the **Labels** tab.

The Labels page opens ([Figure 41](#)).

Figure 41. Display Options – Labels page for the chromatogram view



4. To define the location and contents of chromatogram labels, choose from these options:
 - To display the retention time above chromatogram peaks, select the **Retention Time** check box. To hide the retention time, clear the **Retention Time** check box.
 - To display the active scan number above chromatogram peaks, select the **Scan Number** check box. To hide the scan number, clear the **Scan Number** check box.
 - To display the m/z for the base peak of the active scan above chromatogram peaks, select the **Base Peak** check box. To hide the base peak m/z , clear the **Base Peak** check box.
 - To display letters above chromatogram peaks to provide supplemental information about the peak data, select the **Flags** check box. For example, if a peak is saturated, the data system displays an S above the peak.
5. To specify the style of the labels, choose from these options:
 - To move a label from its normal position to avoid conflict with another label, select the **Offset** check box. Specify the amount of the offset (in number of characters) in the Size box.
 - To write vertical labels, select the **Rotated** check box. To write horizontal labels, clear the **Rotated** check box.
 - To place a box around each peak label, select the **Boxed** check box. If you do not want to have a box around the label, clear the check box.
6. To specify a percent of the base peak so that the data system labels all peaks above that percent, type a value in the Label threshold box.
7. To save the settings and close the dialog box, click **OK**.

Setting the Chromatogram Normalization Options

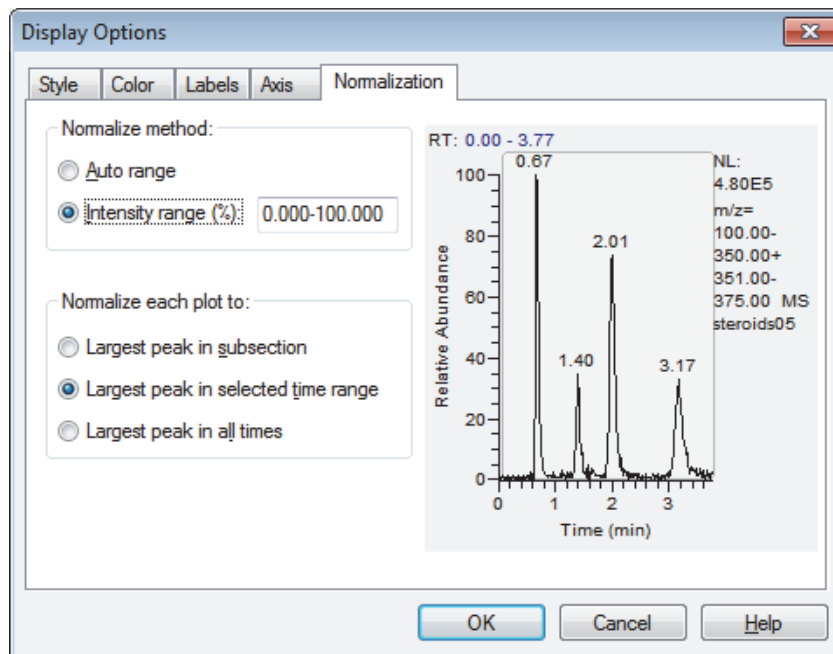
For more information, see [Chromatogram View – Display Options Dialog Box – Normalization Page](#).

❖ To set the chromatogram normalization options

1. Open a chromatogram in the Qual Browser window and make it active.
2. To open the Display Options dialog box, choose **Display > Display Options** or right-click the cell and choose **Display Options** from the shortcut menu.
3. Click the **Normalization** tab.

The Normalization page opens ([Figure 42](#)).

Figure 42. Normalization page for a Chromatogram view in the Display Options dialog box



4. To specify the normalization method, select one of these options:
 - To automatically rescale the y axis to the minimum and maximum signal values, select the **Auto Range** option.
 - To specify the range of values to be plotted on the y axis, select the **Intensity Range** option and type the minimum and maximum intensities you want to display in the Intensity Range box. The valid range is 0.000–100.000 percent.
5. To specify the plot normalization option, select one of these options:
 - To normalize (set the y -axis maximum) to the largest peak in the subsection (division), select the **Largest Peak in Subsection** option.
 - To normalize (set the y -axis maximum) to the largest peak in the time range, select the **Largest Peak in Selected Time Range** option.
 - To normalize (set the y -axis maximum) to the largest peak at all times, select the **Largest Peak in All Times** option.
6. To save the settings and close the dialog box, click **OK**.

Setting the Chromatogram Style Options

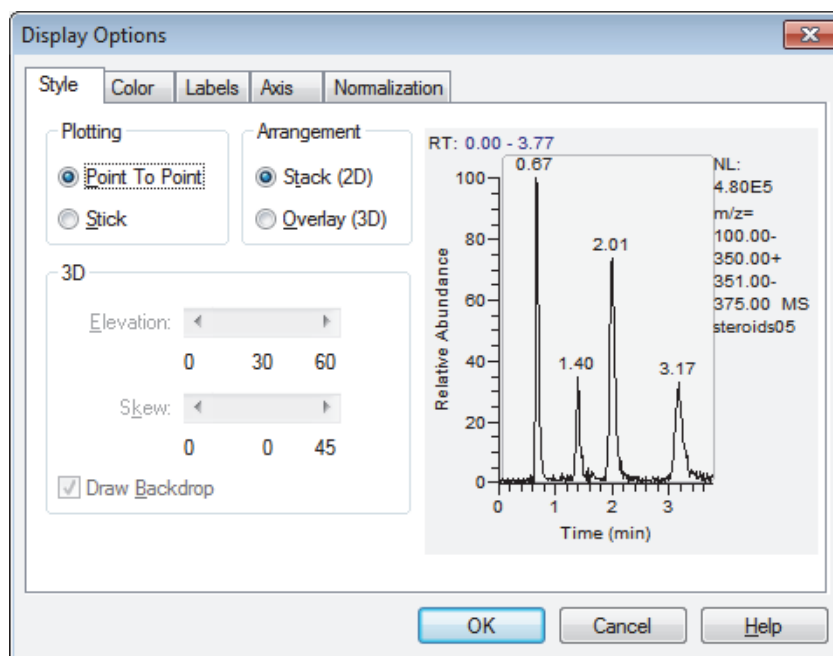
For more information, see [Chromatogram View – Display Options Dialog Box – Style Page](#).

❖ To set the chromatogram style options

1. Open a chromatogram in the Qual Browser window and make it active.
2. To open the Display Options dialog box, choose **Display > Display Options** or right-click the cell and choose **Display Options** from the shortcut menu.

The dialog box opens to the Style page (Figure 43).

Figure 43. Display Options – Style page for the chromatogram view



3. To specify the graphic style, select one of these options:
 - To display point-to-point peak profiles, select the **Point To Point** option.
 - To display the graphic as vertical lines, select the **Stick** option.
4. To specify the arrangement style, select one of these options:
 - To stack plots vertically with no overlap, select the **Stack (2D)** option.
 - To overlay plots vertically with optional horizontal skew (time offset), select the **Overlay (3D)** option.
5. To set the elevation angle for 3D plots from 0 to 60 degrees, either drag the **Elevation** slider or click the Elevation slider left or right arrow until you reach the desired angle.

6. To set the skew angle, either drag the **Skew** slider or click the Skew slider left or right arrow until you reach the desired angle (from 0 to 45 degrees).
7. To add a backdrop to 3D plots, select the **Draw backdrop** check box.
8. To save the settings and close the dialog box, click **OK**.

Detecting Peaks

Qual Browser provides several ways for detecting the chromatographic peaks in a chromatogram view. These topics describe the three most common ways to detect peaks:

- [Automatic Detection of One Plot](#)
- [Automatic Detection of All Plots](#)
- [Manual Detection](#)

The detect peak icons on the Main toolbar and the detect peak menu commands are active only when a raw data file is open in the Qual Browser window and a chromatogram view is the active view.

Icon	Command
	Actions > Peak Detection > Toggle Peak Detection in This Plot
	Actions > Peak Detection > Toggle Peak Detection in All Plots
	Actions > Peak Detection > Add Peaks
	Actions > Peak Detection > Delete Peaks

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

1. Choose **File > Open** from the menu bar or click the **Open** icon, , in the toolbar.
The Open Raw File dialog box appears.
2. Select a raw data file and click **Open**.
The raw data file appears in the Qual Browser window.

❖ To display the Main toolbar

1. From the menu bar, choose **View > Toolbars**.
The Toolbars dialog box opens.
2. Select the **Main** check box and click **OK** to accept the setting and close the dialog box.

Automatic Detection of One Plot

Use the Toggle Peak Detection in This Plot icon or menu command to detect and integrate the chromatographic peaks in the selected plot of a multi-plot chromatogram view. The data system integrates the peaks using the current peak detection and integration settings.

❖ To detect and integrate all peaks in a selected chromatogram plot

1. Click the chromatogram plot in the active cell.

The data system shades the selected plot.

2. To detect and integrate all peaks in the selected chromatogram plot, click  in the toolbar or choose **Actions > Peak Detection > Toggle Detection in This Plot** from the Qual Browser menu bar.

This option uses the current peak detection and integration settings.

3. To undo the peak detection, click the icon in the toolbar a second time or choose **Actions > Peak Detection > Toggle Detection in This Plot** from the menu bar.

Automatic Detection of All Plots

Use the Toggle Peak Detection in All Plots icon or menu command to detect and integrate the chromatographic peaks in all of the plots in a multi-plot chromatogram view. The data system integrates the peaks using the current peak detection and integration settings.

❖ To detect and integrate all peaks in all chromatogram plots in the active cell

1. Click  in the toolbar or choose **Actions > Peak Detection > Toggle Detection in All Plots** from the Qual Browser menu bar.
2. To undo all detected peaks, click the icon in the toolbar a second time or choose **Actions > Peak Detection > Toggle Detection in All Plots** from the menu bar.

Manual Detection

To manually detect and integrate all peaks in all chromatogram plots in the active cell, use either the **Add Peaks** or the **Delete Peaks** icons in the toolbar.

- [Adding Peaks](#)
- [Deleting Peaks](#)

Adding Peaks

Use the Add Peaks icon or menu command to manually detect one or more chromatographic peaks.

❖ To add a peak to a chromatogram plot

1. To detect and integrate any peak in the selected cell, click the **Add Peaks** icon, , in the toolbar or choose **Actions > Peak Detection > Add Peaks** from the Qual Browser menu bar.

The data system changes the cursor to the Add Peaks  cursor.

2. Drag the **Add Peaks** cursor horizontally across the peak to detect and integrate the peak.
The data system marks the added peak with a blue baseline and integrates the peak.
3. To adjust the beginning and ending points of the integrated peak, drag the baseline markers.
4. To restore the default cursor, click the **Add Peaks** icon in the toolbar a second time, or choose **Actions > Peak Detection > Add Peaks** from the menu bar.

Deleting Peaks

The active cell must have one or more chromatographic peaks detected (as indicated by a blue baseline marker, ) for the Delete Peaks icon in the toolbar and the Delete Peaks menu command to be active.

❖ To delete peaks in a raw data file

1. To open the raw data file containing the peaks that you want to delete, click the **Open** file icon, , or choose **File > Open** from the Qual Browser window.

The Open Raw File dialog box opens.

2. Select a raw data file and click **OK**.

The data system displays the raw data file in the Qual Browser window.

3. Turn on peak detection, if it is not already turned on as indicated by a blue baseline marker.

4. To delete specific peaks in an active cell, click the **Delete Peaks** icon, .

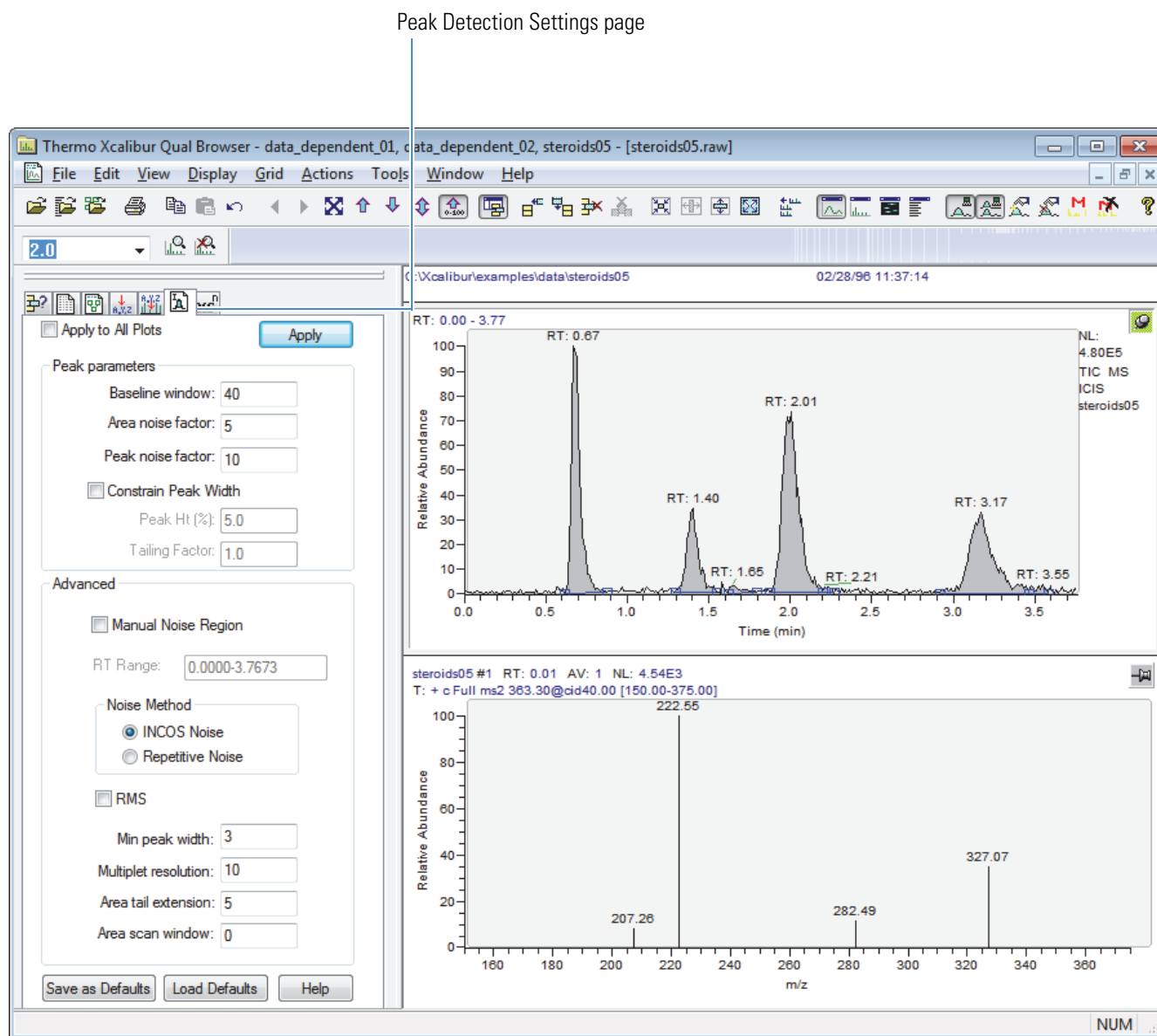
The cursor changes to the delete peaks cursor, .

5. To delete a specific peak, click within the peak's boundary, indicated by the blue baseline, .
6. To return the delete peaks cursor to the default cursor, click  a second time, choose **Actions > Peak Detection > Delete Peaks** from the Qual Browser menu bar, or right-click the plot and select **Peak Detection > Delete Peaks** from the shortcut menu.

Reviewing the Effect of Different Peak Detection Settings

Use the Peak Detection Settings page on the Info Bar of the Qual Browser window to test the effect of changing the peak detection settings (Figure 44).

Figure 44. Peak Detection Settings page in Qual Browser



❖ **To display the Peak Detection Settings page on the Info Bar**

1. Pin the chromatogram view of interest.
2. To add the Peak Detection Settings page to the Info Bar, right-click the pinned chromatogram view and choose **Peak Detection > Set Peak Detection Algorithm and Detect in This Plot** or **Peak Detection > Set Peak Detection in All Plots** from the shortcut menu, and choose the appropriate algorithm (ICIS, Avalon, or Genesis).
3. To display the Peak Detection Settings page, do one of the following:
 - Click the **Peak Detection Settings** tab, , on the Info Bar.
 - Right-click an active chromatogram view and choose **Peak Detection > Settings** from the shortcut menu,—or—
 - Choose **Actions > Peak Detection > Settings** from the menu bar.

❖ **To change the peak detection settings and apply the new settings**

1. Change the settings as appropriate.

For information about the settings on the Peak Detection Settings page, refer to the *Xcalibur Qual Browser User Guide*.

Note The default values on the Peak Detection Settings page are suitable for most analysis requirements. Change these settings only if standard chromatogram detection and integration options do not provide the desired result.

2. Do one of the following:
 - To apply the current chromatogram peak identification and integration settings to all displayed plots in the active view, select the **Apply to All Plots** check box.
 - To apply the settings only to the active plot, clear the **Apply to All Plots** check box.
3. To apply the settings, click **Apply**.

4 Working with a Chromatogram View

Reviewing the Effect of Different Peak Detection Settings

Working with a Spectrum View

A spectrum view shows the intensities of one or more masses as a function of time. These procedures describe how to manipulate spectra.

Contents

- [Setting Spectrum Display Options](#)
- [Setting Spectrum List Display Options](#)
- [Setting Spectrum Display Options and Processing Options](#)
- [Subtracting Background Spectra](#)

For information about exporting mass spectra to a user library, refer to the *Xcalibur Library Browser User Guide*.

Setting Spectrum Display Options

The Display Options dialog box consists of six tabbed pages: Style, Color, Label, Axis, Normalization, and Composition. It contains a small display area showing the active cell. Use these options to preview the effects of different settings before applying them.

Use one or more of these procedures to set up spectrum ranges and options:

- [Setting the Spectrum Axis Options](#)
- [Setting the Spectrum Color Options](#)
- [Setting the Spectrum Label Options](#)
- [Setting the Spectrum Normalization Options](#)
- [Setting the Spectrum Style Options](#)
- [Setting the Spectrum Composition Options](#)

Setting the Spectrum Axis Options

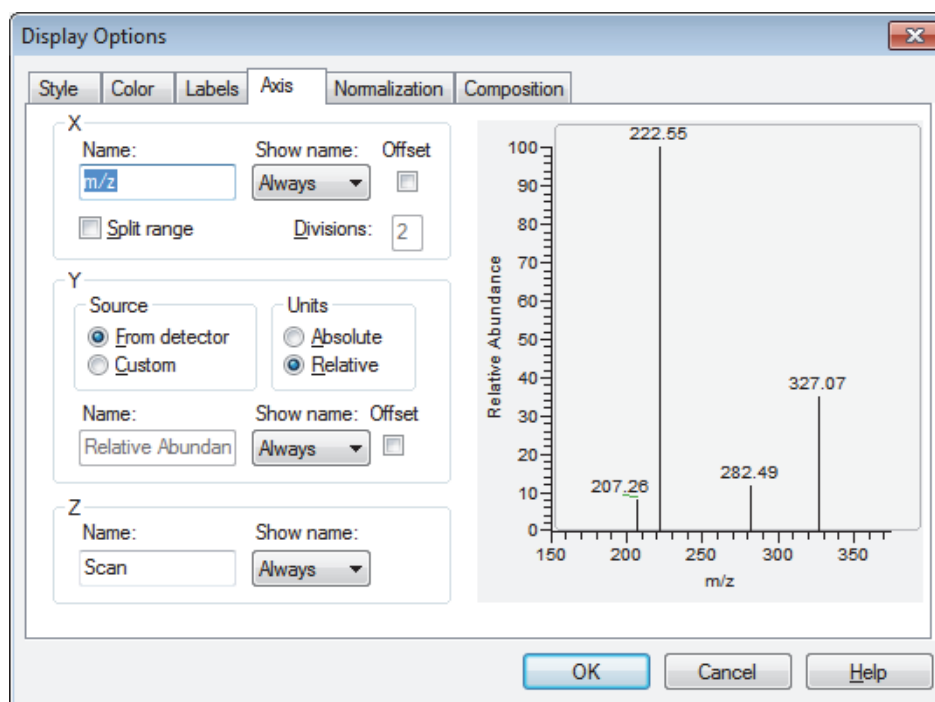
For information about the spectrum axis options, see [Spectrum View – Display Options Dialog Box – Axis Page](#).

❖ To set the spectrum axis options

1. Open a spectrum view in the Qual Browser window and make it active.
2. To open the Display Options dialog box, choose **Display > Display Options** or right-click the cell and choose **Display Options** from the shortcut menu.
3. Click the **Axis** tab.

The Axis page opens (Figure 45).

Figure 45. Display Options – Axis page for the spectrum view



4. To change the name of the *x*, *y*, or *z* axis, type the new name in the X, Y, or Z Name box.
5. To change the time when the data system displays the axis label, select **Never**, **On Print**, or **Always** in the **Show Name** list.
6. To move the displayed plot from the *x* or *y* axes, select the **Offset** check box for X or Y. To turn off axis offset, clear the X or Y **Offset** check box.

7. To set up mass range splitting, choose from these options:
 - To display only one mass range, clear the **Split Range** check box.
 - To split the mass range, select the **Split Range** check box. Then type the new number in the Divisions box to specify the number of divisions (subsections) for the split range.
8. To save the settings and close the dialog box, click **OK**.

Setting the Spectrum Color Options

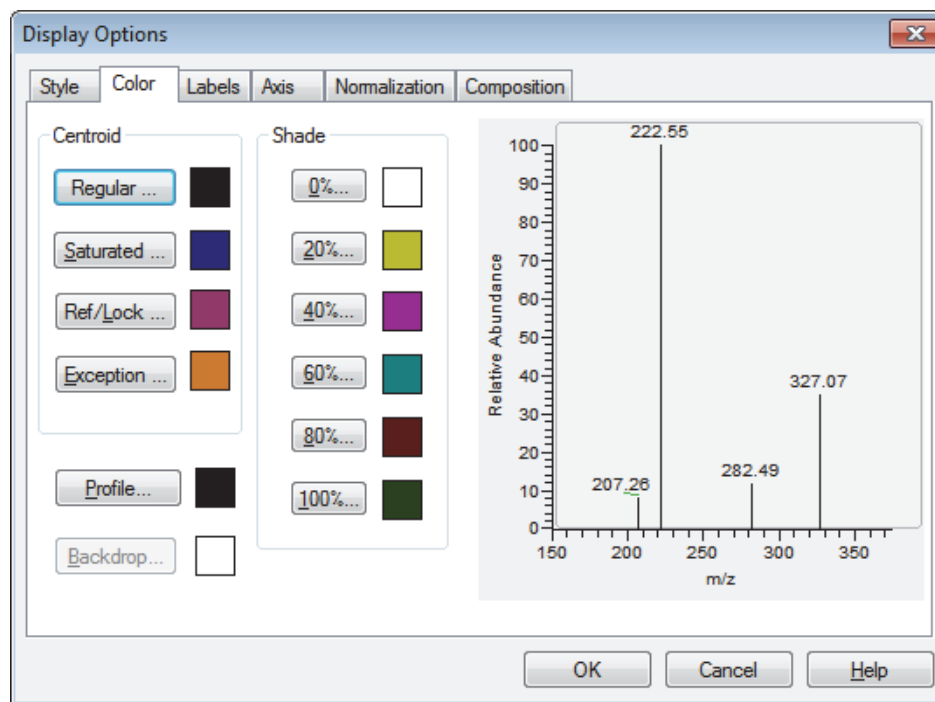
For information about the spectrum color options, see [Spectrum View – Display Options Dialog Box – Color Page](#).

❖ To set the spectrum color options

1. Open a spectrum view in the Qual Browser window and make it active.
2. To open the Display Options dialog box, choose **Display > Display Options** or right-click the cell and choose **Display Options** from the shortcut menu.
3. Click the **Color** tab.

The Color page opens (Figure 46).

Figure 46. Display Options – Color page for the spectrum view



4. To select the color of regular (unflagged) peaks, choose **Regular**. The Color dialog box opens with a color palette so that you can select a preset color or customize a color.

5. To select the color of saturated peaks, choose **Saturated**.

The Color dialog box opens with a color palette so that you can select a preset color or customize a color.

6. To select the color of the profile style, choose **Profile**.

The Color dialog box opens with a color palette where you can select a preset color or customize a color.

7. To select the color of the low intensity areas of the spectrum, click **0%** in the Shade area.

The Color dialog box opens with a color palette where you can select a preset color or customize a color.

8. To select the color of the high intensity areas of the spectrum, click **100%** in the Shade area.

The Color dialog box opens with a color palette where you can select a preset color or customize a color.

9. To save the settings and close the dialog box, click **OK**.

Setting the Spectrum Label Options

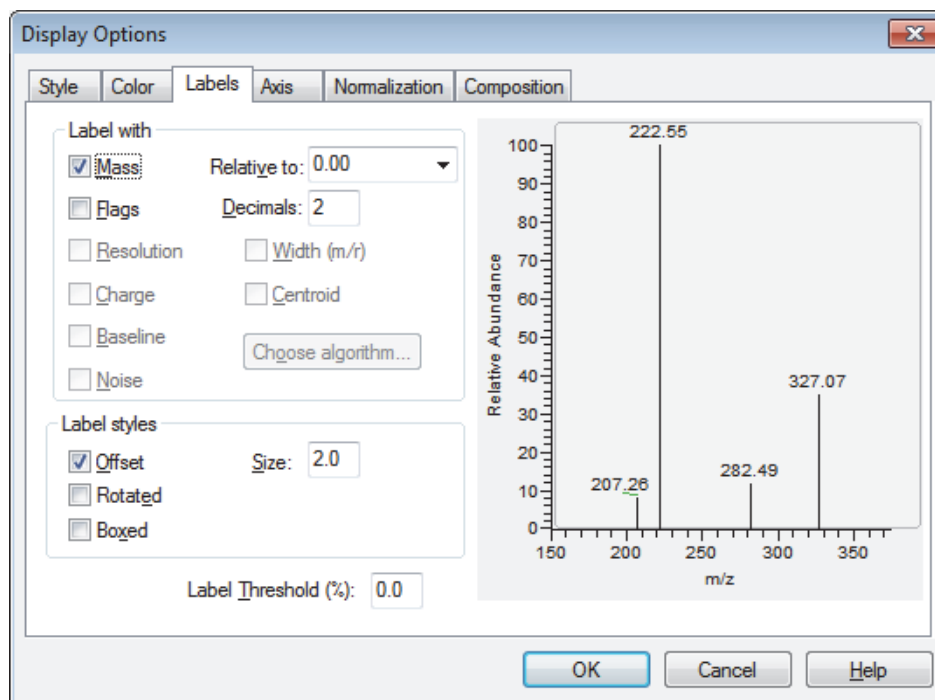
For information about the spectrum label options, see [Spectrum View – Display Options Dialog Box – Labels Page](#).

❖ To set the spectrum label options

1. Open a spectrum view in the Qual Browser window and make it active.
2. To open the Display Options dialog box, choose **Display > Display Options** or right-click the cell and choose **Display Options** from the shortcut menu.
3. Click the **Labels** tab.

The Labels page opens ([Figure 47](#)).

Figure 47. Display Options – Labels page for the spectrum view



4. To define the spectrum labels, do the following:
 - To display an m/z label over spectrum peaks, select the **Mass** check box. In the Decimals box, type a value from 0 to 5 to specify the number of digits to be displayed to the right of the decimal. To hide an m/z label, clear the **Mass** check box.
 - To display letters above spectrum peaks to provide supplemental information about the peak data, select the **Flags** check box. For example, if a peak is saturated, the application displays an S above the peak. To hide supplemental information, clear the **Flags** check box.
5. To specify the style of the spectrum labels, do the following:
 - To move a label from its normal position to avoid conflict with another label, select the **Offset** check box. Type the size of the offset (in number of characters) in the Size box.
 - To write vertical labels, select the **Rotated** check box. To write horizontal labels, clear the **Rotated** check box.
 - To place a box around each peak label, select the **Boxed** check box. If you do not want to have a box around the label, clear the check box.
6. To specify a percent of the base peak so that the data system labels all peaks above that percent, type a value in the Label Threshold box.
7. To save the settings and close the dialog box, click **OK**.

Setting the Spectrum Normalization Options

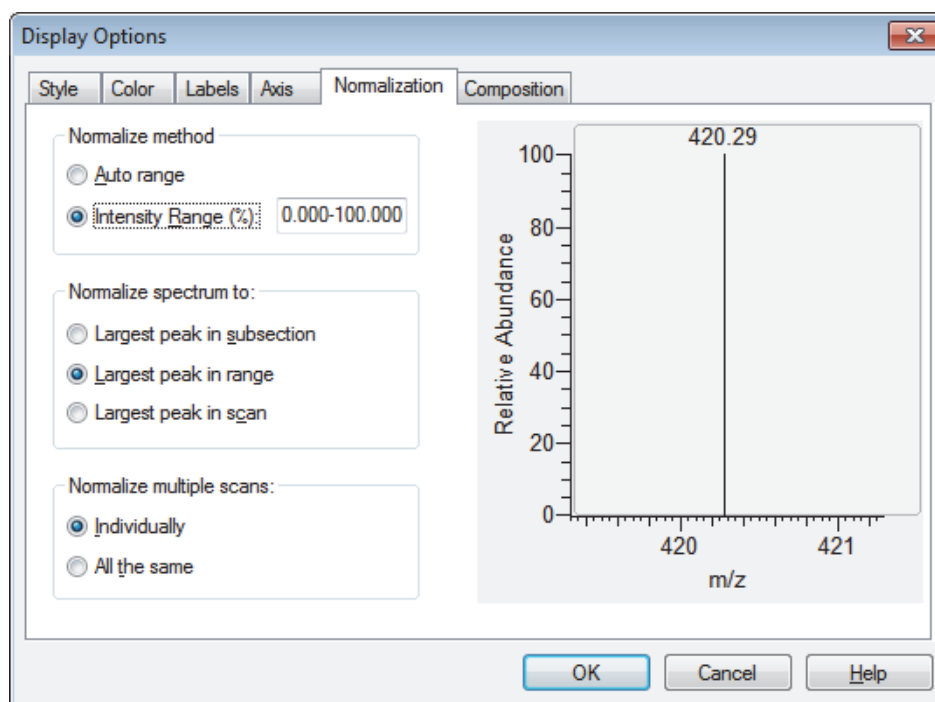
For information about the spectrum normalization options, see [Spectrum View – Display Options Dialog Box – Normalization Page](#).

❖ To set the spectrum normalization options

1. Open a spectrum view in the Qual Browser window and make it active.
2. To open the Display Options dialog box, choose **Display > Display Options** or right-click the cell and choose **Display Options** from the shortcut menu.
3. Click the **Normalization** tab.

The Normalization page opens (Figure 48).

Figure 48. Display Options – Normalization page for the spectrum view



4. To change the intensity range (y -axis range), type the minimum and maximum intensities you want to display in the Intensity Range box. The valid range is 0.000 – 100.000 percent.
5. To specify the spectrum normalization option, select one of these options:
 - To normalize (set the y -axis maximum) to the largest peak in the subsection (division), select the **Largest Peak in Subsection** option.
 - To normalize (set the y -axis maximum) to the largest peak in the mass range, select the **Largest Peak in Range** option.
 - To normalize (set the y -axis maximum) to the largest peak in the scan, select the **Largest Peak in Scan** option.

6. To specify the multiple scan normalization option, select one of these options:
 - To normalize each mass plot individually, select the **Individually** option.
 - To normalize all mass plots equally, select the **All the Same** option.
7. To save the settings and close the dialog box, click **OK**.

Setting the Spectrum Style Options

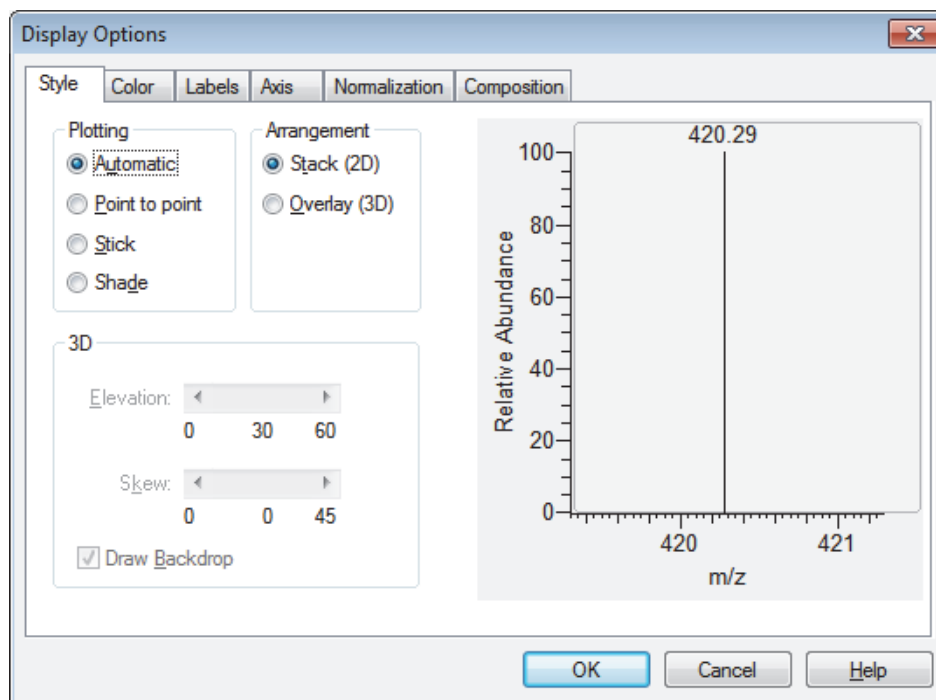
For information about the spectrum style options, see [Spectrum View – Display Options Dialog Box – Style Page](#).

❖ To set the spectrum style options

1. Open a spectrum view in the Qual Browser window and make it active.
2. To open the Display Options dialog box, choose **Display > Display Options** or right-click the cell and choose **Display Options** from the shortcut menu.
3. Click the **Style** tab.

The Style page opens ([Figure 49](#)).

Figure 49. Display Options – Style page for the spectrum view



4. To specify the graphic style, select one of these options in the Plotting area:
 - To choose the graphic style based on the data acquisition method for the active spectrum, select the **Automatic** option.
 - To display point-to-point peak profiles, select the **Point to point** option.
 - To display the graphic as vertical lines, select the **Stick** option.
 - To display the spectrum as a shaded representation of intensity in each amu band for the active spectrum, select the **Shade** option.
5. To specify the arrangement style, select one of these options in the Arrangement area:
 - To stack plots vertically with no overlap, select the **Stack** option.
 - To overlay plots vertically with optional horizontal skew (time offset), select the **Overlay (3D)** option.
6. To set the elevation angle (from 0 to 60 degrees) for 3D plots, drag the **Elevation** slider or click the left or right arrow until you reach the desired angle.
7. To set the skew angle (from 0 to 45 degrees) for 3D plots, drag the **Skew** slider or click the left or right arrow until you reach the desired angle.
8. To add a backdrop to 3D plots, select the **Draw Backdrop** check box. To remove a backdrop, clear the **Draw Backdrop** check box.
9. To save the settings and close the dialog box, click **OK**.

Setting the Spectrum Composition Options

Use the Composition page of the Display Options dialog box for the spectrum view (Figure 50) to add chemical formulas and related labels to the spectrum. The data system determines which chemical formulas have an m/z value most like that of the experimental spectrum peaks.

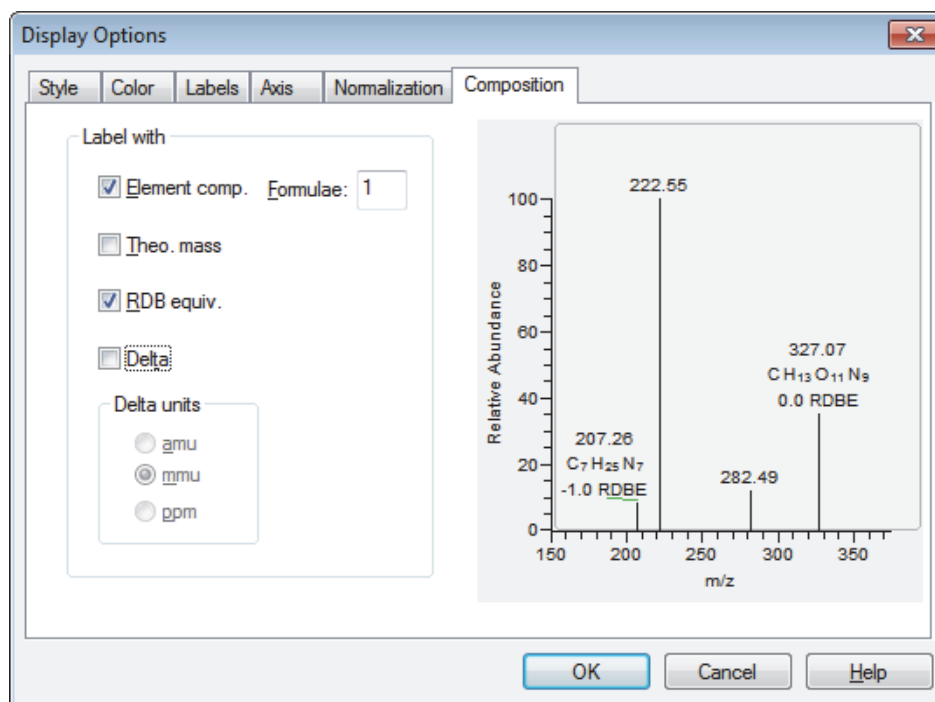
For information about the Composition page, see [Spectrum View – Display Options Dialog Box – Composition Page](#).

❖ To specify the spectrum composition

1. Open a spectrum view in the Qual Browser window and make it active.
2. To open the Display Options dialog box, choose **Display > Display Options** or right-click the cell and choose **Display Options** from the shortcut menu.
3. Click the **Composition** tab.

The Spectrum Composition page of the Display Options dialog box opens (Figure 50).

Figure 50. Display Options – Composition page for the spectrum view



4. To display the chemical formula labels at the top of spectrum peaks, select the **Elemental Comp.** check box.

The data system determines which chemical formulas have a m/z value most like that of the spectrum peaks. The Theo. Mass, RDB Equiv., and Delta check boxes and the Formulae box become available.

5. Do the following:

- To specify how many of the most likely chemical formulas you want the data system to display at the top of spectrum peaks, type a number in the Formulae box.
- To display the theoretical m/z values of the chemical formulas that the data system determines, select the **Theo. Mass** check box.

The data system displays the theoretical m/z values to the right of the formula separated by an equal sign (=).

- To display the value of the ring and double-bond equivalents that the data system calculates for the chemical formulas, select the **RDB Equiv.** check box.

The data system displays the ring and double-bond equivalent value under the chemical formula. Ring and double-bond equivalents provide a measure of the number of unsaturated bonds in a compound. They limit the calculated formulas to only those that make sense chemically.

- To label the peak with the difference between the theoretical and experimental m/z values, select the **Delta** check box. Then, to specify the units to use when calculating the difference between the theoretical and experimental m/z values, select **amu**, **mmu**, or **ppm** in the Delta units area.

6. To save the settings and close the dialog box, click **OK**.

Setting Spectrum List Display Options

Use one or more of these procedures to set up spectrum list display options:

- [Setting the Spectrum List Normalization Options](#)
- [Setting the Spectrum List Style Options](#)
- [Setting the Spectrum List Composition Options](#)

Setting the Spectrum List Normalization Options

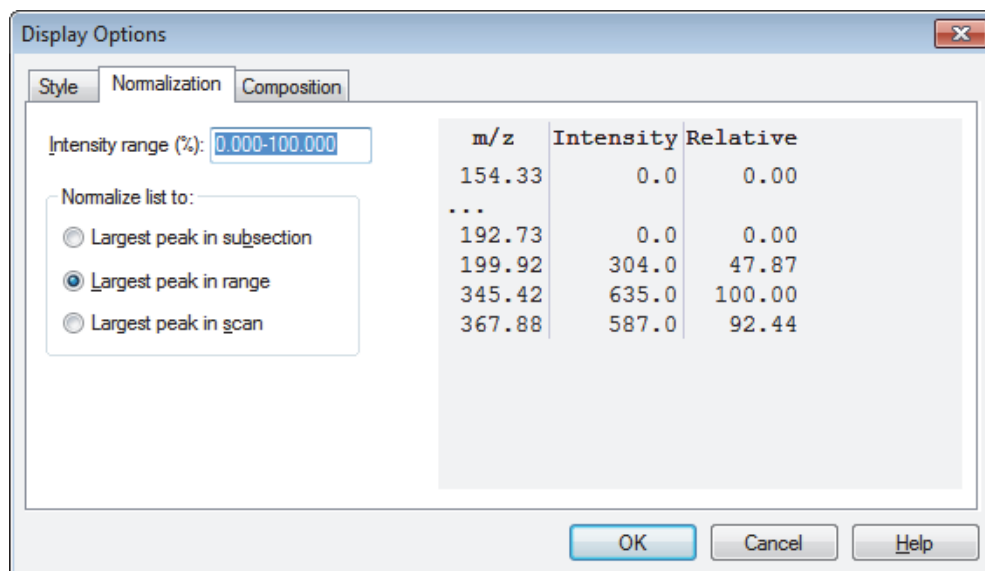
For information about the normalization options for the spectrum list, see [Spectrum List View – Display Options Dialog Box – Normalization Page](#).

❖ To set the spectrum list normalization options

1. Open a spectrum list view in the Qual Browser window and make it active.
2. To open the Display Options dialog box, choose **Display > Display Options** or right-click the cell and choose **Display Options** from the shortcut menu.
3. Click the **Normalization** tab.

The Normalization page opens ([Figure 51](#)).

Figure 51. Display Options – Normalization page for the spectrum list view



4. To change the intensity range, type the minimum and maximum intensities you want to display in the Intensity range box. The valid range is 0.000–100.000 percent.
5. To specify the spectrum list normalization option, do one of the following:
 - To normalize to the largest peak in the subsection, select the **Largest peak in subsection** option.
 - To normalize to the largest peak in the mass range, select the **Largest peak in selected time range** option.

–or–

 - To normalize to the largest peak in the scan, select the **Largest peak in all times** option.
6. To save the settings and close the dialog box, click **OK**.

Setting the Spectrum List Style Options

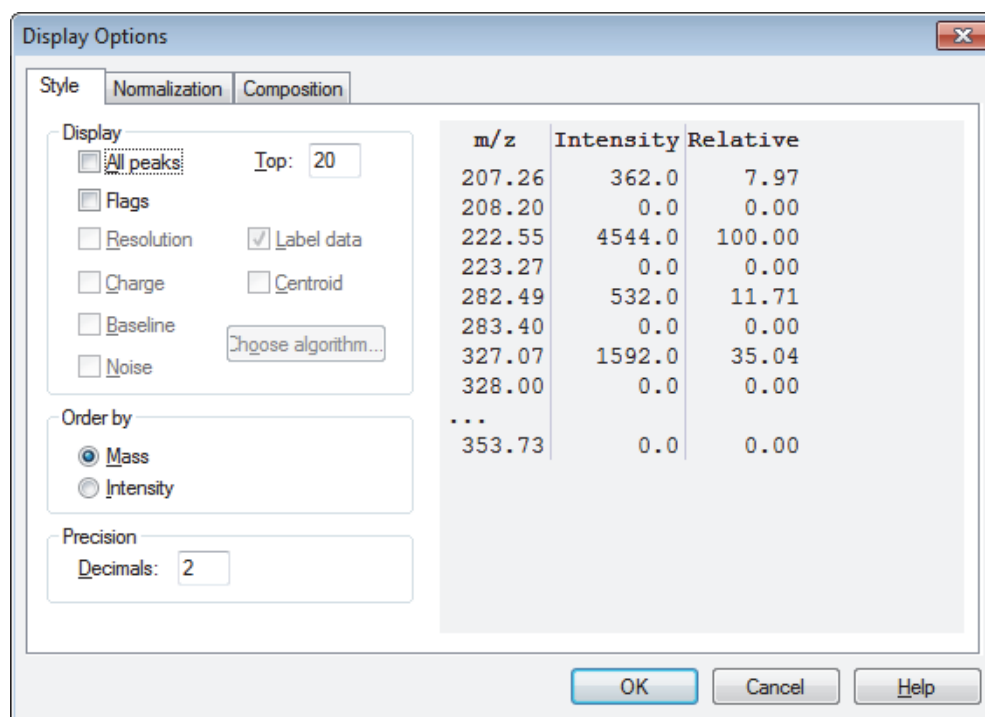
For information about the style options for the spectrum list view, see [Spectrum List View – Display Options Dialog Box – Style Page](#).

❖ To set the spectrum list style options

1. Open a spectrum list view in the Qual Browser window and make it active.
2. To open the Display Options dialog box, choose **Display > Display Options** or right-click the cell and choose **Display Options** from the shortcut menu.
3. Click the **Style** tab.

The Style page opens (Figure 52).

Figure 52. Display Options – Style page for the spectrum list view



4. To specify the number of peaks in the spectrum list, choose one of these options:
 - To display *m/z* values, intensity, and relative intensity of all spectrum peaks in the range specified in the Spectrum List Ranges dialog box or as specified in the active scan filter, select the **All peaks** check box.
 - To specify a maximum number of peaks in the spectrum list, clear the **All peaks** check box and type a maximum number of peaks in the Top box.

5. To specify peak order, choose one of these options in the Order by area:
 - To order the spectrum list by m/z value (in ascending order), select the **Mass** option.
 - To order the spectrum list by intensity (in descending order), select the **Intensity** option.
6. To save the settings and close the dialog box, click **OK**.

Setting the Spectrum List Composition Options

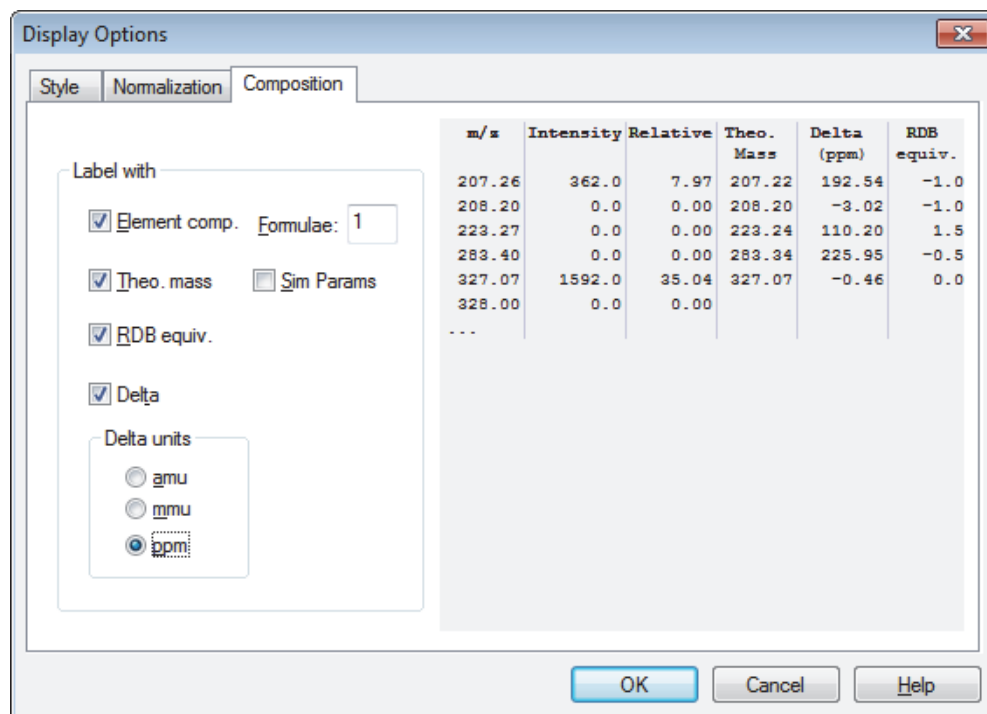
For more information about the composition options for the spectrum list view, see [Spectrum List View – Display Options Dialog Box – Composition Page](#).

❖ To set the spectrum list composition options

1. Open a spectrum list view in the Qual Browser window and make it active.
2. To open the Display Options dialog box, choose **Display > Display Options** or right-click the cell and choose **Display Options** from the shortcut menu.
3. Click the **Composition** tab.

The Composition page opens (Figure 53).

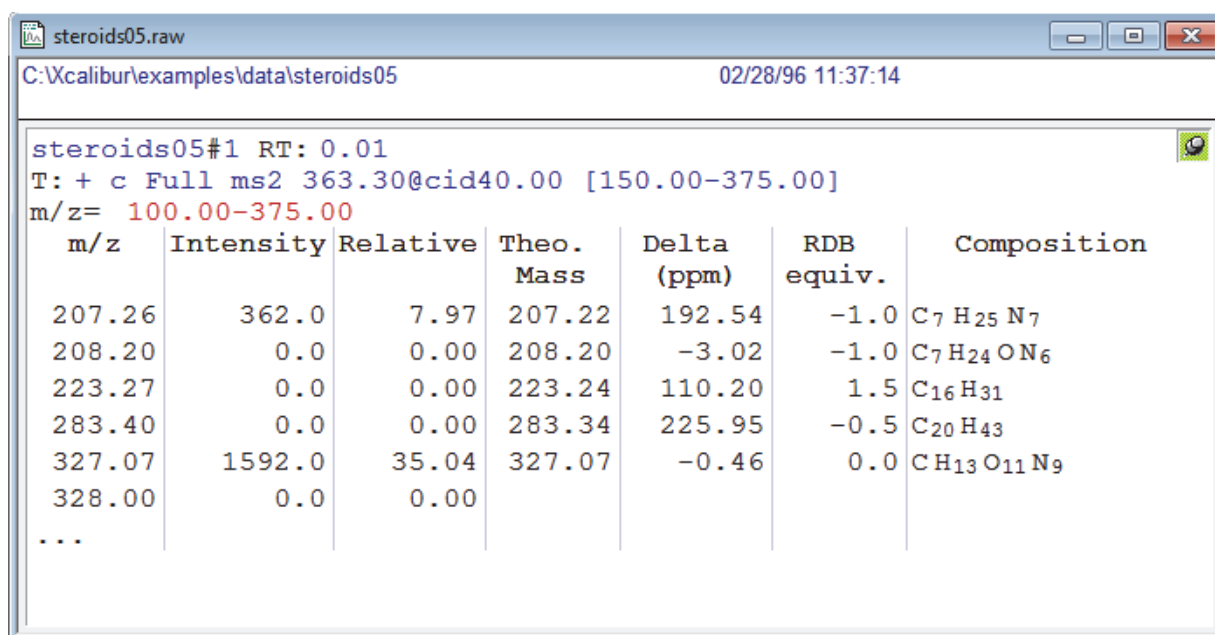
Figure 53. Display Options – Composition page for the spectrum list view



4. Select one or more of the following check boxes:
 - Elemental Comp—select to display the calculated elemental composition for each m/z value.
 - Theo. Mass—select to display the theoretical mass for each m/z value.
 - RDB Equiv.—select to display the calculated RDB equivalents value for each m/z value.
 - Delta—select to display the difference between the measured mass and the theoretical mass.
 - Sim Params
5. In the Formulae box, type the number of theoretical values that you want the data system to calculate for each m/z value.
6. In the Delta Units area, select the units that you want to use to display the calculated mass difference.
7. Click **OK** to close the dialog box.

Figure 54 shows the spectrum list view for the example raw data file, steroids05.raw.

Figure 54. Spectrum list view for an example steroid raw data file



steroids05#1 RT: 0.01
T: + c Full ms2 363.30@cid40.00 [150.00-375.00]
m/z= 100.00-375.00

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
207.26	362.0	7.97	207.22	192.54	-1.0	C ₇ H ₂₅ N ₇
208.20	0.0	0.00	208.20	-3.02	-1.0	C ₇ H ₂₄ O N ₆
223.27	0.0	0.00	223.24	110.20	1.5	C ₁₆ H ₃₁
283.40	0.0	0.00	283.34	225.95	-0.5	C ₂₀ H ₄₃
327.07	1592.0	35.04	327.07	-0.46	0.0	C H ₁₃ O ₁₁ N ₉
328.00	0.0	0.00				
...						

Setting Spectrum Display Options and Processing Options

Use one or more of these procedures to set up spectrum plot ranges:

- [Setting Spectrum Display Options](#)
- [Setting Automatic Processing for Mass Spectra](#)

Setting Spectrum Display Options

Use the Spectrum Display Options dialog box to view and edit the mass range, time range, background subtraction, and smoothing parameters for all the plots in a spectrum cell ([Figure 55](#)).

For more information about the Ranges page, see [Ranges Page – Spectrum Ranges Dialog Box](#).

❖ To set the mass range and time range for a spectrum plot

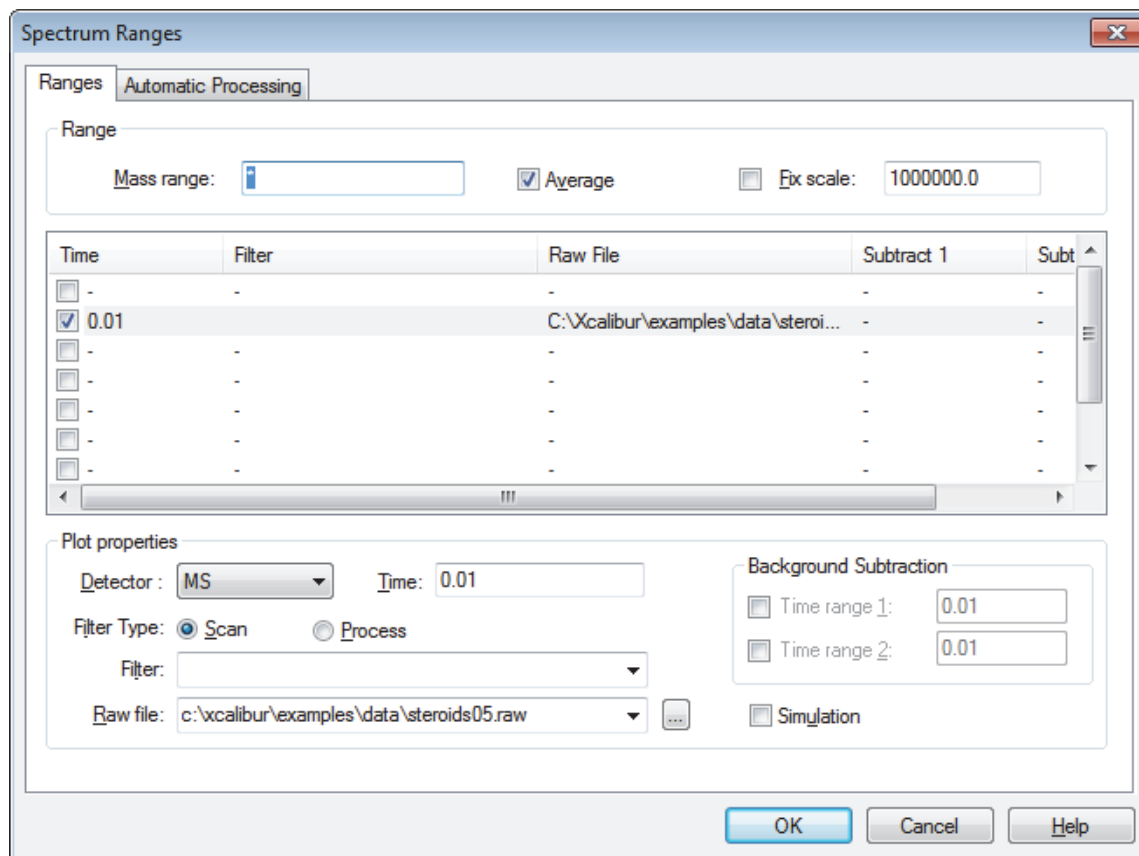
1. Open a spectrum view in the Qual Browser window and make it active.
2. To open the Spectrum Display Options dialog box, do one of the following:
 - Right-click a spectrum plot in the cell and choose **Ranges** from the shortcut menu.
 - From the menu bar, choose **Display > Ranges**.

—or—

 - In the toolbar, click the **Display Ranges** icon, .
3. Click the **Ranges** tab.

The Ranges page of the Spectrum Display Options dialog box opens ([Figure 55](#)).

Figure 55. Spectrum Ranges dialog box – Ranges page



4. To choose a raw data file, select from the table of all active files in the current cell. To change the source of the active plot, choose one of these options:
 - Select a file from the table.
 - Click **Browse** adjacent to the Raw File list and browse to the required file.
 - Type the full path and file name of the required file in the Raw File box.
5. To specify the mass/wavelength range, choose one of these options:
 - To specify the mass range, type the first and last mass of the scan range to be used, separated by a hyphen with no spaces, in the Mass Range box. The format is as follows:
First Mass–Last Mass
 - To specify the wavelength range, type the shortest wavelength and longest wavelength of the scan in the Wavelength Range box. The format is as follows:
shortest wavelength–longest wavelength
6. To specify the time range, type the lower and upper time limits in minutes, separated by a hyphen with no spaces, in the Time Range box.

7. To specify the scan filter, select from options in the Filter list that are stored in the raw data file.

If your MS detector has the MSⁿ Browser feature, first select the Filter Type. Select **Scan** to display the scan filters or select **Process** to display the processing filters.
8. To specify the fix scale setting, choose one of these options in the Range area:
 - To turn on the maximum range for the y axis of the active spectrum, select the **Fix Scale** check box.
 - To change the value, type the new maximum y-axis value in the Fix Scale box.
 - To turn off the fix scale setting, clear the **Fix Scale** check box.
9. To turn spectrum averaging on or off, choose one of these options in the Range area:
 - To average all scans defined by the mass range, time range, and filter settings in the Spectrum Display Options dialog box, select the **Average** check box.
 - To turn off spectrum averaging, clear the **Average** check box.
10. To determine whether background subtraction has been performed, review these settings under Background Subtraction:

The Time range 1 check box and Time range 2 check box indicate whether background subtraction has been performed for the active spectrum. When the check box is selected, the data system displays the time range used for background subtraction in the Time Range 1 or Time Range 2 boxes.

The system enters these settings when you perform a background subtraction by using the Actions > Subtract Spectra commands from the Qual Browser window.
11. To save the settings and close the dialog box, click **OK**.

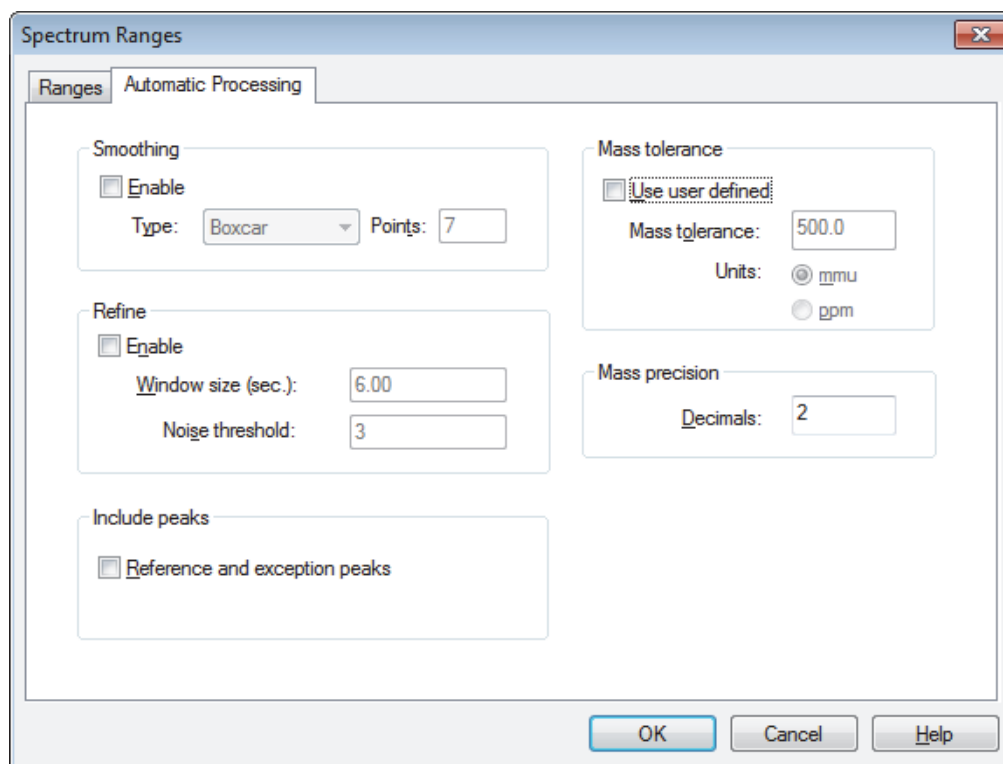
Setting Automatic Processing for Mass Spectra

❖ To set the mass range and time range for a mass spectrum

1. Open a spectrum view in the Qual Browser window and make it active.
2. To open the [Spectrum Ranges Dialog Box](#), right-click a spectrum plot in the cell and choose **Ranges** from the shortcut menu or choose **Display > Ranges**.
3. Click the **Automatic Processing** tab.

The Automatic Processing page of the Spectrum Display Options dialog box opens ([Figure 56](#)).

Figure 56. Spectrum Display Options dialog box – Automatic Processing page



4. To smooth all scans defined by the mass range, time range, and filter settings in the Spectrum Display Options dialog box, do the following:
 - a. Select the **Enable** check box under Smoothing. To turn off spectrum smoothing, clear the **Enable** check box.
 - b. To change the type of smoothing, select either **Boxcar** or **Gaussian** from the Type list.
 - c. To change the number of smoothing points, type the new number of points in the Points box. The valid range for smoothing points includes odd numbers from 3 for minimum smoothing to 15 for maximum smoothing.
5. To refine all scans defined by the mass range, time range, and filter settings in the Spectrum Display Options dialog box, do the following:
 - a. Select the **Enable** check box under Refine. To turn off spectrum smoothing, clear the **Enable** check box.
 - b. Type a time range for Refine in the Window Size box. Set this parameter to the expected peak width.
 - c. Type a limit for low intensity ions in the Noise Threshold box. Start with a value of zero, increasing the setting until the procedure eliminates spurious masses generated by background noise.

6. To include reference and exception peaks in the display of spectra, select the **Reference and Exception Peaks** check box. To exclude reference and exception peaks, clear the **Reference and Exception Peaks** check box.
7. To specify a user-defined mass tolerance, do the following:
 - a. Select the **Use User Defined** check box. To turn off mass tolerance, clear the **Use User Defined** check box.
 - b. Type a value from 0.1 to 50 000.0 in the Mass Tolerance box, and then select units.
8. In the Decimals box under Mass Precision, specify the number of digits the data system displays to the right of the decimal when it displays m/z labels over the peaks in a spectrum.
9. To save the settings and close the dialog box, click **OK**.

Subtracting Background Spectra

Use a chromatogram view to interactively subtract background ions from a spectrum view, subtract background ions from either one range (either side of the chromatogram peak of interest) or two ranges (both sides of the chromatogram peak of interest).

❖ To subtract background spectra

1. Open a chromatogram view in Qual Browser.
2. Open a spectrum view in another cell. You might need to add a new cell to the cell grid.
3. Pin the cell containing the spectrum view.
4. Drag the cursor through the chromatogram peak of interest.

This action updates the pinned spectrum view with an averaged spectrum using the scans in the indicated range.

5. To select one or two ranges for spectrum subtraction, choose one of these options:
 - Choose **Actions > Subtract Spectra > 1 (or 2) Range**.
 - Right-click the spectrum cell and choose **Subtract Spectra > 1 (or 2) Range** from the shortcut menu.
6. Identify a representative baseline region in the chromatogram view close to the peak of interest. Drag the new cursor to select a time range in this region.
7. If you have selected the 2 Range option, choose a region on the other side of the peak of interest.

8. 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. For example, SB: 12 indicates that Qual Browser has applied background subtraction to the spectrum using 12 scans.

9. To see the selected time ranges of the scans that were subtracted, choose **Display > Ranges** to open the Spectrum Display Options dialog box and review the Time Range 1 box.

Working with a Map View

A map is a 2D or 3D representation of an analysis showing all the mass/wavelength scans acquired during an analysis (see [Figure 57](#)). Use the Qual Browser window to open a raw data file, create a grid of interactive cells, and display a map and related header information in any of the cells. Use menu commands to select display options.

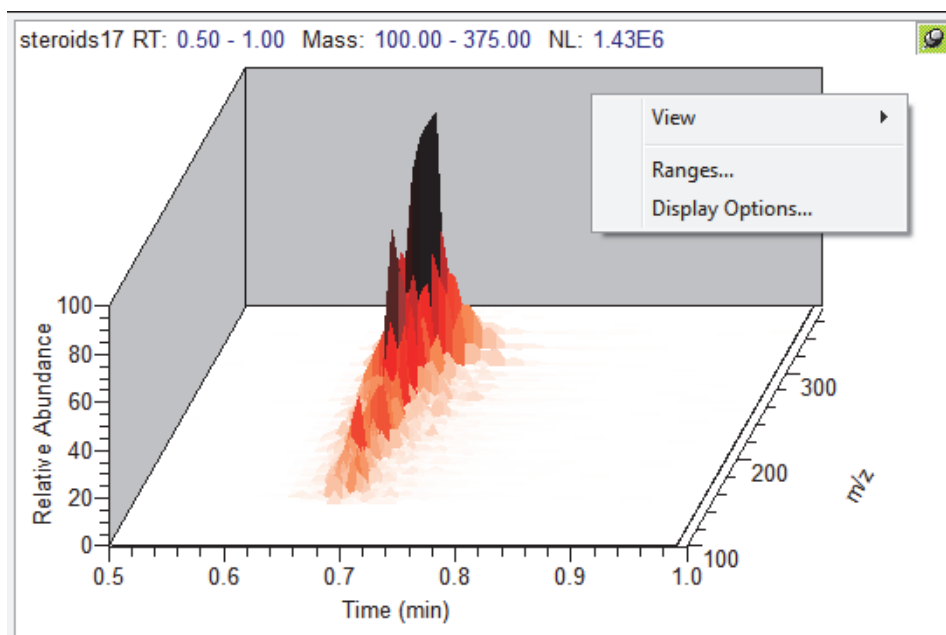
These procedures describe how to set the ranges and display options for a map view.

Contents

- [Setting Map Ranges](#)
- [Setting Map Display Options](#)

The Map view consists of a time point (x axis) versus an m/z value (y axis) versus a relative abundance value (z axis) map plot. An example of a map view is shown below ([Figure 57](#)).

Figure 57. Map view



❖ **To view a map**

Do one of the following:

- Right-click the cell and choose **View > Map** from the shortcut menu (Figure 57 on page 133).
- From the menu bar, choose **View > Map**.
- In the toolbar, click the **View Map** icon, .

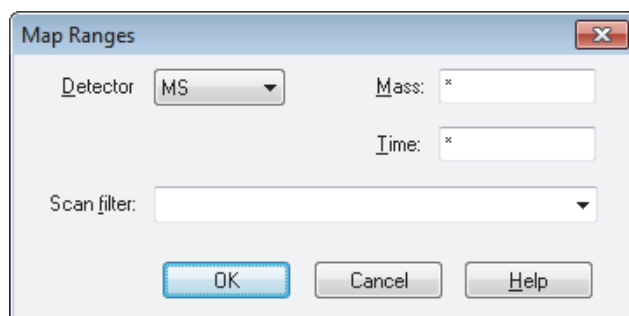
Setting Map Ranges

For more information about the Map Ranges dialog box, see [Map Ranges Dialog Box](#).

❖ **To set the mass range and time range for a map**

1. Make a map view the active view in the Qual Browser window.
2. To open the Map Ranges dialog box (Figure 58), right-click the map view and choose **Ranges** from the shortcut menu.

Figure 58. Map Ranges dialog box



3. To specify the mass range, type the first mass and last mass of the scan in the Mass box.
The format is as follows:
First Mass–Last Mass.
4. Specify the time range in the Time box by typing the lower and upper time limits in minutes, separated by a hyphen with no spaces.
5. Select a desired scan filter from the Scan filter list, which displays filter options stored in the raw data file.
6. To save the settings and close the dialog box, click **OK**.

Setting Map Display Options

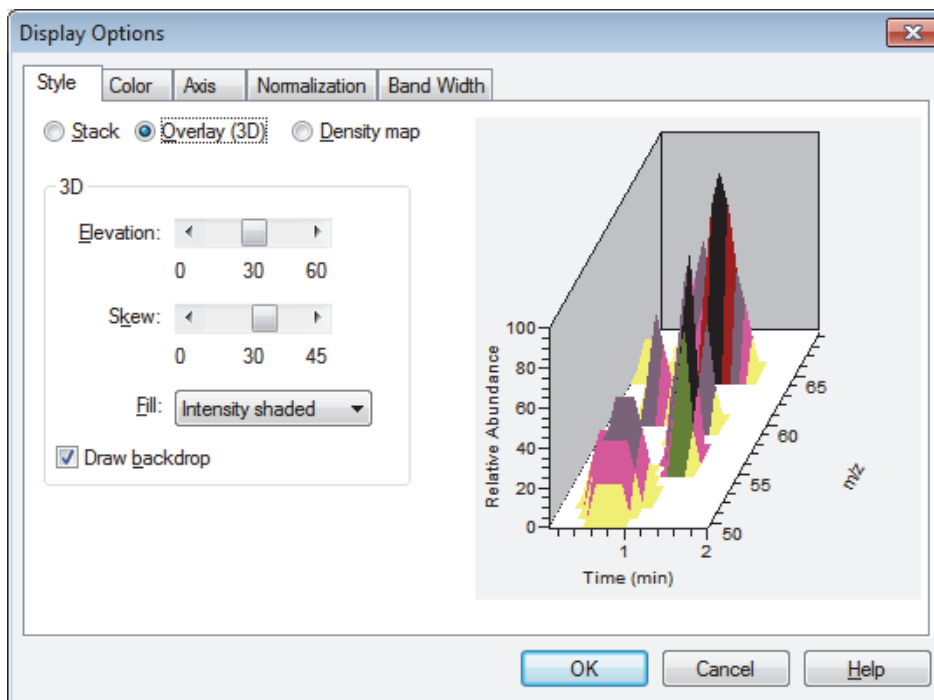
Use the Display Options dialog box to set up the display options for a map view.

❖ **To open the Display Options dialog box for a map view**

1. Make a map view the active view in the Qual Browser window.
2. To open the Display Options dialog box, right-click the cell and choose **Display Options**, or choose **Display > Display Options** from the menu bar.

The Display Options dialog box consists of five tabbed pages: Style, Color, Axis, Normalization, and Band Width (Figure 59). It contains a small display area showing the active cell. Use this set of options to preview the effects of different settings before applying them.

Figure 59. Display Options – Style page for the map view



Follow one or more of these procedures to set up the map display options:

- [Setting the Map Style Options](#)
- [Setting the Map Axis Options](#)
- [Setting the Map Color Options](#)
- [Setting the Map Normalization Options](#)
- [Setting the Band Width](#)

Setting the Map Style Options

For information about the map style options, see [Map or Ion Map View – Display Options Dialog Box – Style Page](#).

❖ To set the map style options

1. Make a map view the active view in the Qual Browser window.
2. To open the Display Options dialog box, choose **Display > Display Options**, or right-click the cell and choose **Display Options** from the shortcut menu.
3. Click the **Style** tab (see [Figure 59](#) on [page 135](#)).

The Style page opens.

4. To specify the arrangement style, select one of these options:
 - To stack plots vertically with no overlap for the active map, select the **Stack** option.
 - To overlay plots vertically with optional horizontal skew (time offset) for the active map, select the **Overlay (3D)** option.

The 3D area becomes available.

 - To display a density map, showing different shades for each intensity, select the **Density map** option.
5. To specify style options for overlaid (3D) plots, do the following in the 3D area:
 - To set the elevation angle (from 0 to 60 degrees), drag the Elevation slider or click the left or right arrow on the Elevation slider until you reach the desired angle.
 - To set the skew angle (from 0 to 45 degrees), drag the **Skew** slider or click the left or right arrow on the Skew slider until you reach the desired angle.
 - To select a different fill option, select a fill option from the Fill list.
 - To add a backdrop to 3D plots, select the **Draw Backdrop** check box. To remove a backdrop, clear the **Draw Backdrop** check box.
6. To save the settings and close the dialog box, click **OK**.

Setting the Map Axis Options

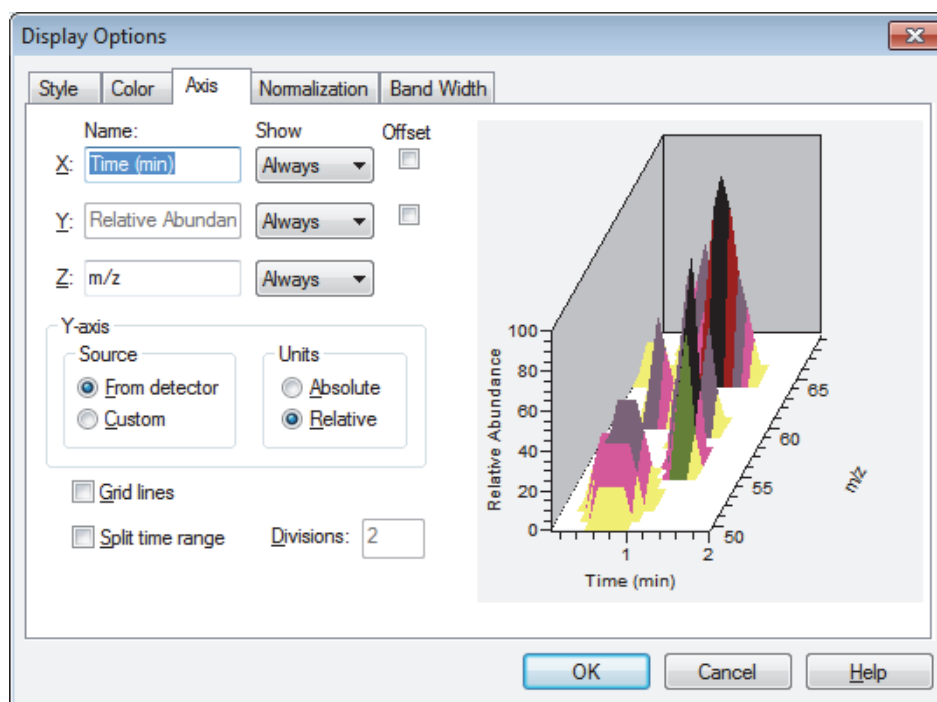
For information about the map axis options, see [Map or Ion Map View – Display Options Dialog Box – Axis Page](#).

❖ To set the map axis options

1. Make a map view the active view in the Qual Browser window.
2. To open the Display Options dialog box, choose **Display > Display Options**, or right-click the cell and choose **Display Options** from the shortcut menu.
3. Click the **Axis** tab.

The Axis page opens (Figure 60).

Figure 60. Axis page for a Map view in the Display Options dialog box



4. To change the name of the x , y , or z axis, type the new name in the X, Y, or Z Name box. For the y axis, first select the **Custom** option in the Source area.
5. To change the time when the data system displays the axis label, select **Never**, **On Print**, or **Always** from the Show list.
6. To move the displayed plot from the x or y axes, select the **Offset** check box for X or Y or both. To turn off axis offset, clear the X or Y **Offset** check box.

7. To set time range splitting, do the following:
 - To split the time scale, select the **Split Time Range** check box. Then, to specify the number of time range subsections, type a number in the Divisions (time) box.
 - To display only one time range, clear the **Split Time Range** check box.
8. To save the settings and close the dialog box, click **OK**.

Setting the Map Color Options

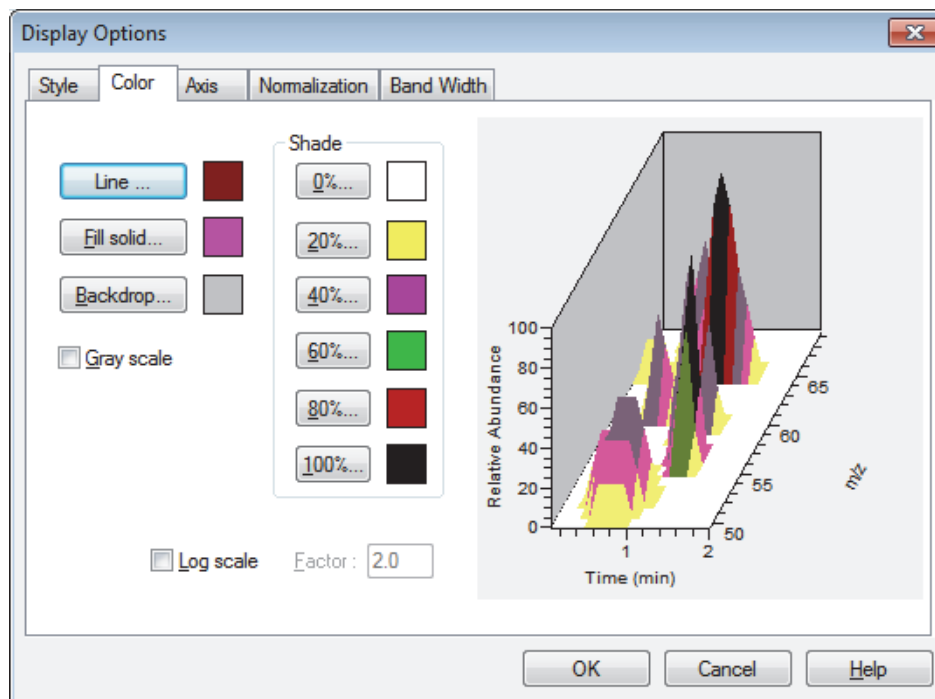
For information about the map color options, see [Map or Ion Map View – Display Options Dialog Box – Color Page](#).

❖ To set the map color options

1. Make a map view the active view in the Qual Browser window.
2. To open the Display Options dialog box, choose **Display > Display Options**, or right-click the cell and choose **Display Options** from the shortcut menu.
3. Click the **Color** tab.

The Color page opens (Figure 61).

Figure 61. Display Options – Color page for the map view



4. To select the color of the framing lines, click **Line**.

The Color dialog box opens with a color palette so that you can select a preset color or customize a color.

5. To select the color of the solid fill for the active map, click **Fill Solid**.

The Color dialog box opens with a color palette so that you can select a preset color or customize a color.

6. To select the color of the backdrop (background), click **Backdrop**.

The Color dialog box opens with a color palette so that you can select a preset color or customize a color. Backdrop is active only when you select the Overlay 3D style.

7. To select grayscale or color, do one of the following:

- To plot the map in grayscale, select the **Grayscale** check box.
- To plot the map in color, clear the **Grayscale** check box.

8. Use the shade buttons (0%, 20%, 40%, 60%, 80%, and 100%) to change the map's color at 0%, 20%, 40%, 60%, 80%, and 100% relative abundance.

9. To select log scale or linear scale, do the following:

- To display the color of the map in a logarithmic scale, select the **Log Scale** check box. The factor width that you set in the Factor box determines the scaling between color bands.
- To display the map in a linear scale, clear the **Log Scale** check box.

10. To save the settings and close the dialog box, click **OK**.

Setting the Map Normalization Options

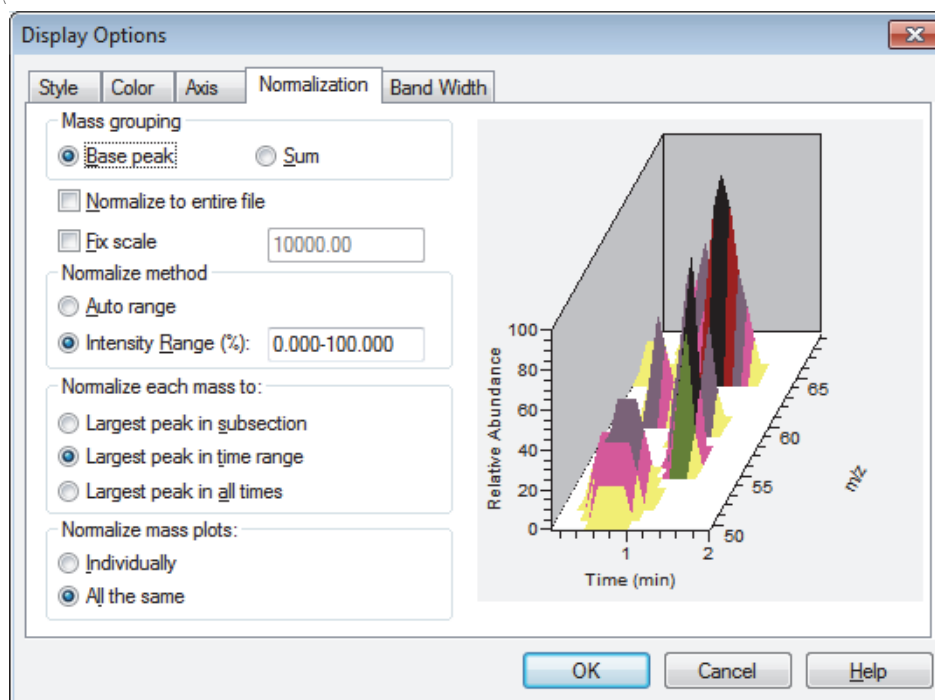
For information about the map normalization options, see [Map or Ion Map View – Display Options Dialog Box – Normalization Page](#).

❖ To set the map normalization options

1. Make a map view the active view in the Qual Browser window.
2. To open the Display Options dialog box, choose **Display > Display Options**, or right-click the cell and choose **Display Options** from the shortcut menu.
3. Click the **Normalization** tab.

The Normalization page opens ([Figure 62](#)).

Figure 62. Display Options – Normalization page for the map view



4. To specify the mass grouping, select one of these options:
 - To use the largest peak within each band (mass range) to determine the intensity of the band, select the **Base peak** option.
 - To use the sum of the intensities within each band (mass range) to determine the intensity of the band, select the **Sum** option.
5. To specify the normalization options, do one of the following:
 - To normalize the map to the largest peak in the raw data file, select the **Normalize to Entire File** check box.
 - To normalize the map to a fixed intensity value, select the **Fix scale** check box. Then type an intensity value between **0.01** and **1e+20** in the Fix Scale box.
 - To determine the intensity range for normalizing the map, select the **Auto Range** option.
 - To change the intensity range (y-axis range), type the minimum and maximum intensities you want to display in the Intensity Range box. The valid range is – 200.000 to 200.000 percent.

6. To specify a peak to normalize the y -axis maximum, select one of these options:
 - To normalize (set the y -axis maximum) to the largest peak in the subsection (division), select the **Largest Peak in Subsection** option.
 - To normalize (set the y -axis maximum) to the largest peak in the time range (all subsections), select the **Largest Peak in Time Range** option.
 - To normalize (set the y -axis maximum) to the largest peak in all times, select the **Largest Peak in All Times** option.
7. To specify the normalization option for multiple mass plots, select one of the following:
 - To normalize each mass plot individually, select the **Individually** option.
 - To normalize all mass plots equally, select the **All the same** option.
8. To save the settings and close the dialog box, click **OK**.

Setting the Band Width

Use the Band Width page to specify the bandwidth in amu units.

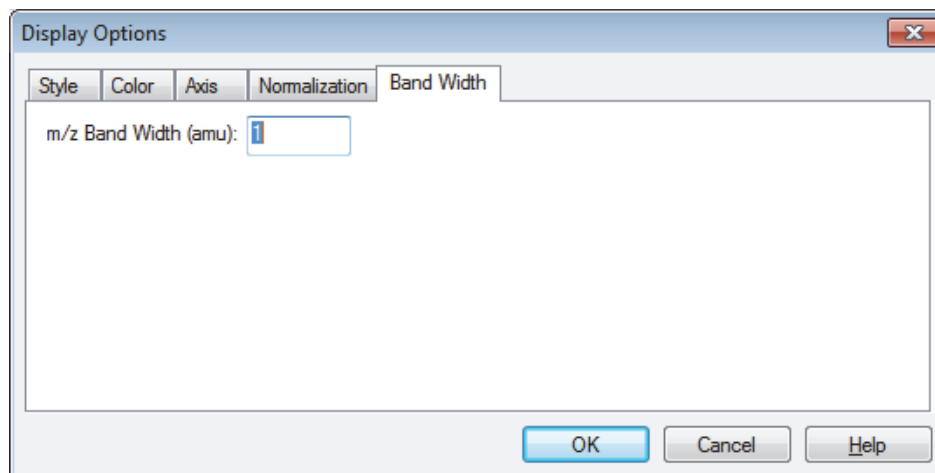
For more information, see [Map or Ion Map View – Display Options Dialog Box – Bandwidth Page](#).

❖ To define the band width in a map view

1. Open a raw data file and make a map view the active view in Qual Browser.
2. To open the Display Options dialog box, choose **Display > Display Options** or right-click the cell and choose **Display Options** from the shortcut menu.
3. Click the **Band Width** tab.

The Band Width page opens ([Figure 63](#)).

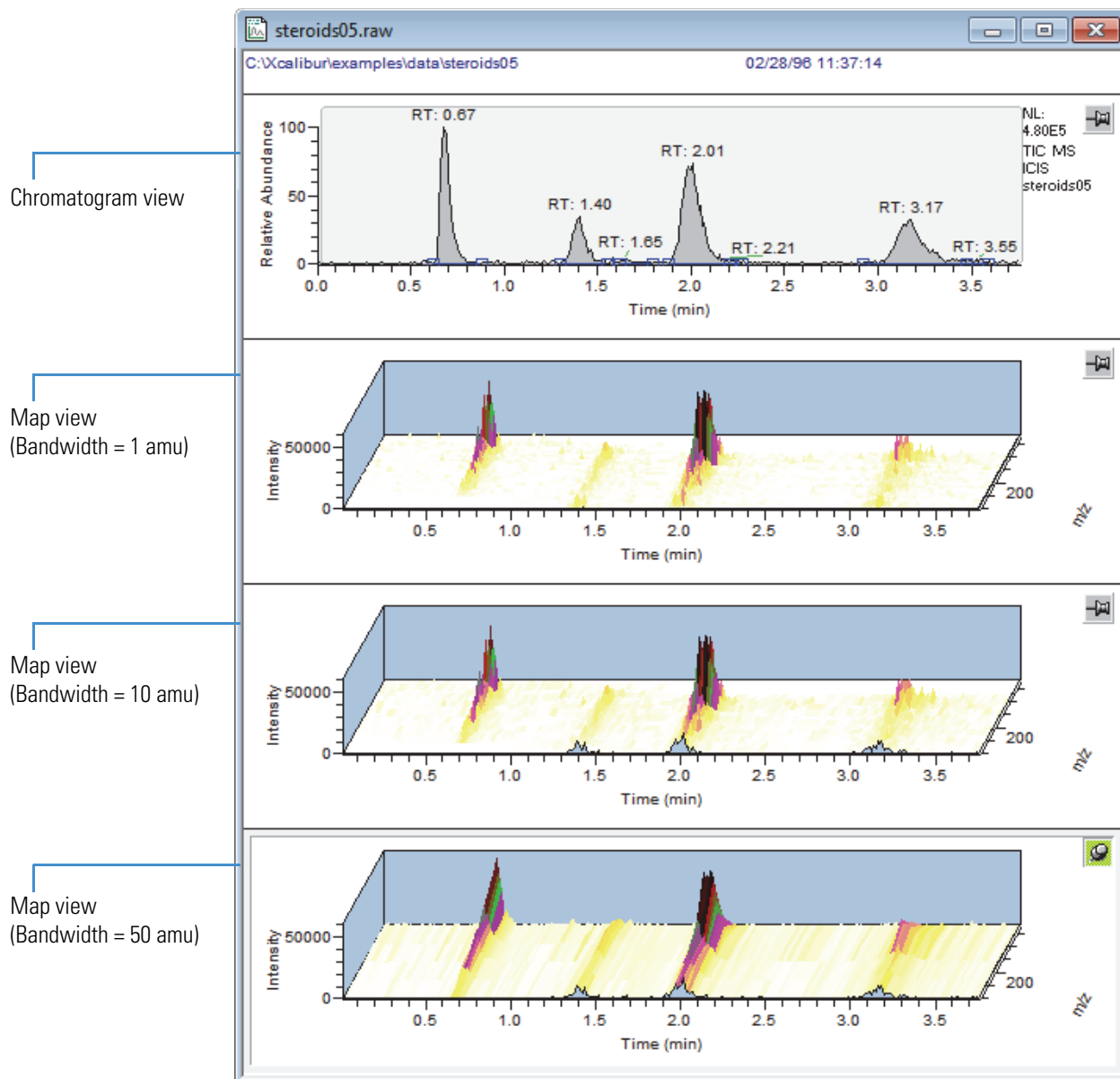
Figure 63. Display Options – Band Width page for the map view



4. In the m/z Band Width (amu) box, type a value from **0.001** to **50**.
5. To save the setting and close the dialog box, click **OK**.

Figure 64 shows the effect of bandwidth on the map view.

Figure 64. Two map views showing how the bandwidth setting affects the visual display



Qual Browser Window

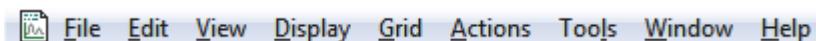
Use Qual Browser to open a raw or result file, display chromatograms, spectra, and maps of the data, choose spectra from chromatograms, average scans, subtract background data, create and save layouts, add text and graphics, apply filters, amplify regions, and print the resulting graphic.

Contents

- [Qual Browser Menus](#)
- [Qual Browser Toolbars](#)
- [Qual Browser Views](#)
- [Qual Browser Info Bar](#)
- [Qual Browser Dialog Boxes](#)
- [Subtract Background Window](#)
- [Qual Browser Result File Window](#)

Qual Browser Menus

This figure shows the Qual Browser menu bar when a raw data file (RAW file type) or a result file (RST file type) is displayed in the window.



For information about the Qual Browser menus, see these topics:

- [Actions Menu – Qual Browser](#)
- [Display Menu – Qual Browser](#)
- [Edit Menu – Qual Browser](#)
- [File Menu– Qual Browser](#)
- [Grid Menu – Qual Browser](#)
- [Help Menu – Qual Browser](#)
- [Tools Menu – Qual Browser](#)
- [View Menu – Qual Browser](#)
- [Window Menu – Qual Browser](#)

Actions Menu – Qual Browser

[Table 10](#) lists the Actions menu commands for the Qual Browser window.

Table 10. Actions menu (Sheet 1 of 4)

Icon	Command	Description
Subtract Spectra		
	1 Range	Perform a peak-by-peak subtraction of selected scans contained in one background region of a chromatogram view from the current spectrum view. Use this command to eliminate background scans that might interfere with the display of spectrum peaks of interest. The subtracted scans must use the same scan filter as the target scans. For more information, see Subtracting Background Spectra .
	2 Ranges	Perform a peak-by-peak subtraction of selected scans contained in two selected background regions of a chromatogram view from the current spectrum view. Use this command to eliminate background peaks that might be interfering with the display of spectrum peaks of interest. The subtracted scans must use the same scan filter as the target scans. For more information, see Subtracting Background Spectra .
	Clear	Remove all subtract spectra modifications to the spectrum view. The data system also removes the SB: xx notation in the spectrum view header to indicate that the spectrum view has been returned to the original display before application of the Subtract Spectra command.

Table 10. Actions menu (Sheet 2 of 4)

Icon	Command	Description
Peak Detection		
	Settings	View a page specific to one of the Xcalibur peak detection algorithms displays and change the parameters used by Qual Browser to identify and integrate chromatogram peaks.
	Toggle Detection in This Plot	Detect and integrate all peaks in the selected chromatogram plot using the current peak detection and integration settings. The data system adds a check mark to the left of the menu command. Choose this command a second time to undo the peak detection and remove the check mark from the left of the menu command. Open a raw data file to make this command active.
	Toggle Detection in All Plots	Detect and integrate all peaks in all selected and unselected chromatogram plots in the active cell using the current peak detection and integration settings. The data system adds a check mark to the left of the menu command. Choose this command a second time to undo all detected peaks and remove the check mark from the left of the menu command. Open a raw data file to make this command active.
	Set Peak Detection Algorithm and Detect in This Plot	View a list of the peak detection algorithms. Click one of the algorithm names in the list to display the page for that algorithm and to use the algorithm to detect chromatogram peaks in the active chromatogram cell. Open a raw data file to make this command active.
	Set Peak Detection Algorithm and Detect in All Plots	View a list of the peak detection algorithms. Click one of the algorithm names in the list to display the page for that algorithm and to use the algorithm to detect chromatogram peaks in all the cells that are currently displayed. Open a raw data file to make this command active.

Table 10. Actions menu (Sheet 3 of 4)

Icon	Command	Description
	Add Peaks	Detect and integrate any peak in the active cell. The data system changes the cursor to the add peaks cursor, . To detect and integrate a peak, drag this cursor horizontally across the peak. The application marks the added peak with a blue baseline, , and integrates the peak. The application also adds a check mark to the left of the menu command. Choose Actions > Peak Detection > Add Peaks a second time to return the add peaks cursor to the default cursor and remove the check mark from the left of the menu command. ❖ To label all detected peaks with their respective area, retention time, or other peak parameters 1. Choose Display > Display Options. The Display Options Dialog Box in Qual Browser opens. 2. Click the Label tab, select peak label parameters. 3. Choose OK. The data system displays the selected labels at the top of all peaks in the plot. Open a raw data file to make this command active.
	Delete Peaks	Delete selected peaks in the active cell. The application changes the cursor to . Click this cursor within each peak boundary, indicated by the blue baseline, , of the peak(s) that you want to delete. One or more peaks must be detected (as indicated by ) for this command to be active.
	Manual Noise Region Selection	Choose this command and drag the cursor horizontally across the region of the chromatogram that you want to select as the noise region. The data system marks the region with a red baseline. The application calculates noise based on the data points you select. It uses all selected data points as noise points and calculates noise based on those points. You can select the noise region from an individual trace or different noise regions from multiple traces. Open a raw data file and select a chromatogram to make this button active.
	Delete Manual Noise Selection	Choose this command and drag the cursor over the region that was previously selected as the noise region. Release the mouse button to delete the noise region.
Peak Purity		
	Peak Purity	View Peak Purity settings. Open a raw data file from a PDA analysis and select PDA from the Detector list in the Ranges dialog box to make this command active.

Table 10. Actions menu (Sheet 4 of 4)

Icon	Command	Description
Library		
	Search	Submit the active spectrum to a library search. The data system displays the results of the search in the Library Search Results window.
	Export to Library Browser	Exports the active spectrum to the Library Browser.
	Export to AMDIS	Exports the active spectrum to AMDIS.
	Options	Choose the libraries used during a library search. You can also change various parameters that determine how the search is carried out.
AutoFilter		
	AutoFilter	Apply all of the scan filters in the current raw data file and open an AutoFilter display in the active cell. The AutoFilter display consists of a vertical sequence of chromatogram plots. The first chromatogram displays the TIC with no scan filter. Below the first chromatogram are up to seven TIC scan filter chromatograms, one chromatogram plot for each scan filter. For additional information, see the Scan Filter View. You can also apply scan filters to one or more plots from the Chromatogram Display Options Dialog Box.

Display Menu – Qual Browser

Table 11 lists the Display menu commands for the Qual Browser window.

Table 11. Display menu (Sheet 1 of 3)

Icon	Command	Description
	Ranges	Open a Ranges dialog box for the active view. There is a Ranges dialog box for each of these view types: Chromatogram view: Chromatogram Display Options Dialog Box Spectrum view: Spectrum Ranges Dialog Box Map or Ion Map views: Map Ranges Dialog Box Spectrum List view: Spectrum List Ranges Dialog Box Scan Header view: Scan Header Range Dialog Box Scan Filter view: Scan Filter View The Ranges command is not available for Report views.
	Mass Options	Specify parameters for mass tolerance and mass precision for the displayed chromatogram, spectrum, and spectrum list plots.
	Display Options	Select the style, color, label [chromatogram and spectrum only], axis, normalization, and smooth [chromatogram only] options for your chromatogram, spectrum, or map.
Annotate		
	Add Text	Add text to the active plot.
	Add Graphics	Add simple graphic objects such as lines or boxes to the active plot.
	Clear	Activate the  cursor so that you can selectively remove text or graphics annotation entries. To remove graphics or text, drag the cursor horizontally above or below the text or graphic. The data system removes the text or graphic(s) and changes the cursor back to your default cursor. Repeat this procedure to remove other annotations. Click  on the toolbar or choose Display > Annotate > Clear from the menu bar. The  cursor appears. To remove all of the annotations from the active cell, choose Display > Annotate > Clear All.
	Clear All	Remove all text and graphics annotation entries in the active cell. To remove annotations one at a time, use the Clear command.

Table 11. Display menu (Sheet 2 of 3)

Icon	Command	Description
Zoom		
	Zoom In Y	Zoom in on the <i>y</i> axis by a factor of two (2) from the current baseline to show more detail. For example, you can change the <i>y</i> -axis range from 0–100 to 0–50.
	Zoom Out Y	Zoom out on the <i>y</i> axis by a factor of two (2) to show more data. For example, you can change the <i>y</i> -axis range from 0–25 to 0–50.
	Auto Range	View the chromatogram, which is normalized from the minimum to the maximum signal. Auto Range is useful for PDA and UV data.
	Normalize	Normalize the intensity scale of the data display to a fixed range on the <i>y</i> axis. For example, from 0–25 percent to 0–100 percent.
	Zoom In X	Make the <i>x</i> axis larger by a factor of two (2) to show more detail. For example, you can change the <i>x</i> -axis range from 0–20 to 5–15.
	Zoom Out X	Make the <i>x</i> axis smaller by a factor of two (2) from the center to show more data. For example, you can change the <i>x</i> -axis range from 7.5–12.5 to 5–15.
	Display All	View all data on the <i>x</i> axis or all text in a report. For example, you can change the <i>x</i> -axis range from 7.5–12.5 to 0–20.
	Reset	Restores the data display to the full range of the <i>x</i> axis and <i>y</i> axis.
Pan		
	Drag With Cursor	Change the cursor to  so that you can drag the cursor to the left or right to pan the plot left or right.
	Forward	Display data to the left of the active displayed range. This command is incremental so you might need to use it multiple times to display the region of interest. To move the display to the right, choose Display > Pan > Back .
	Back	Display data to the right of the active displayed range. This command is incremental so you might need to use it multiple times to display the region of interest. To move the display to the left, choose Display > Pan Forward .
	Next Scan	Display the next mass scan with its scan number.
	Previous Scan	Display the previous mass scan with its scan number.

Table 11. Display menu (Sheet 3 of 3)

Icon	Command	Description
Amplify		
	Other Factor	Enter an amplification factor in the range 1.1 to 1000.0. You can apply this factor to a region of a chromatogram view, spectrum view, or map view. The value is placed and displayed in the Amplify Factors box. When you click OK, the data system displays this cursor: . To amplify a region, drag the cursor horizontally over the region. The application amplifies the region, places this label above the amplified region: -----x3.2-----, and displays the original cursor. To turn off  before using it, click . To cancel one or more amplified regions of a graph, click the Cancel Amplified Region icon, , or choose Amplify > Clear. To cancel all amplified regions of a graph, choose Amplify > Clear All.
	Clear	Cancel one or more amplified regions of a plot. The data system change the cursor to . To clear an amplified region, drag the cursor horizontally extending slightly beyond the start and end of the region. The application removes the amplification, removes the amplification labels (such as -----x5-----), and displays the original cursor. To turn off  before using it, click .
	Clear All	Cancel all amplified regions of an active plot. The data system removes the amplification, removes the amplification labels (such as -----x5-----), and displays the original cursor. To cancel one or more amplified regions of a graph, click the Cancel Amplified Region icon, , or choose Amplify > Clear All.

Edit Menu – Qual Browser

Table 12 describes the Edit menu commands for the Qual Browser window.

Table 12. Edit menu

Button	Command	Description
	Undo	Cancel your previous action. For example, if you have just deleted an entry or annotation, choose the Undo command to replace the deleted entry or annotation. Also, if you have just completed an entry or annotation, choose the Undo command to delete the entry or annotation. If you complete two actions, the Undo command only undoes the previous action and not the first action.
	Copy Cell	Copy the active cell to the Clipboard.
	Paste Cell	Paste a cell that is stored on the Clipboard to the active cell. This command is often used after a Copy Cell command or after choosing the Copy Cell button.
	Copy View	Copy the active window to the Clipboard. You can then use the Paste command of another application, such as Microsoft Word or Microsoft Excel™, to copy the window object to a document or spreadsheet. To edit the window object after it is pasted, return to the Xcalibur data system to edit the window object and repeat the copy/paste procedure.
	Copy Special	Enter the height and width to be used to format the output to the Clipboard. You can also specify the units for the height and width as either millimeters or inches.

File Menu– Qual Browser

Table 13 lists the File menu commands in the Qual Browser window.

Table 13. File menu (Sheet 1 of 2)

Button	Command	Description
Open		
	Open	Find and open a raw data file or a layout file that already exists.
	Open Sequence	Select a sequence file.
	Open Result File	Select a result file. The data system displays a warning message if your selected result file does not contain any qualitative data. To view the result file for a raw data file in an opened sequence, right-click the file name on the Sequence Information page of the Info Bar. Then, choose Open Result File from the popup context menu. The result file is displayed in the Qual Browser workspace and the Result File Information page of the Info Bar.
Layout		
	Apply	Select a layout file.
	Apply Default	Apply the default layout to the active window.
	Save	Save the current layout. If the file has not been named, The Save Layout File dialog box opens. Provide a name. The data system applies the layout file name extension .lyt.
	Save As	Save the current layout with a new name. The data system applies the layout file name extension .lyt.
	Save As Default	Save the current layout as the default layout for new windows.
	Summary Information	Read, modify, or delete file summary information about the active file.
Other Commands		
	Close All	Close all the windows in Qual Browser.
	Save Composite Spectrum Data	Save a document as a different name or location. Display composite spectrum data with MSⁿ Browser to make this command active.

Table 13. File menu (Sheet 2 of 2)

Button	Command	Description
	Change Dataset Name	Select a dataset from a predefined list of names. The text of this menu item might be different if the administrator chose to use another name for a dataset. For example, this menu item might be Change Job Name.
	Audit Trail	View all auditable events and changes made to data files in the current application.
	Print	Specify what you want to print and how to print it.
	Print Preview	Preview the pages before printing.
	Page Setup	Opens the Page Setup dialog box, where you can select from these options: printer, form, orientation, and margins.
	Recent Files	View the paths and names of the most recently used four files. These are located above the Exit command. The data system displays both open and closed files. Click a displayed file to load it. If the selected file was closed, the data system opens it.
	Exit	Close the active window. If you exit before clicking OK from an active dialog box, the data system prompts you to save your changes.

Grid Menu – Qual Browser

Table 14 lists the Grid menu commands in the Qual Browser window.

Table 14. Grid menu (Sheet 1 of 3)

Icon	Command	Description
Insert Cells		
	Left	Insert a cell or cells to the left of the active cell.
	Right	Insert a cell or cells to the right of the active cell.
	Above	Insert a cell or cells above the active cell.
	Below	Insert a cell or cells below the active cell.
Delete		
	Row	Delete the grid row containing the active cell.
	Column	Delete the grid column containing the active cell.
	All Cells	Delete all cells in the view except the active cell.
Cell Size		
	Cell Size	Adjust the column width and row height. You can make adjustments relative to other columns and rows. This menu item is not available if you have only one cell.
Expand Cell		
	Full Width	Expand a cell to the full width of the grid.
	Full Height	Expand a cell to the full height of the grid.
	Full View	Expand a cell to the full size of the grid.

Table 14. Grid menu (Sheet 2 of 3)

Icon	Command	Description
Reduce Cell		
	10%	Temporarily reduce the grid column size of the active cell to 10% of the original size. The data system responds by expanding the right or left neighboring grid columns so that the cells in these grid columns can be viewed at increased resolution. If there is only one column in the grid, this command temporarily reduces the grid row size of the active cell to 10% of the original size. The data system responds by expanding the top or bottom neighboring grid rows so that the cells in these grid rows can be viewed at increased resolution. To restore the grid column size to the original width, click the Reduce Size icon, , in the toolbar again.
	20%	Temporarily reduce the grid column size of the active cell to 20% of the original size. The data system responds by expanding the right or left neighboring grid columns so that the cells in these grid columns can be viewed at increased resolution. If there is only one column in the grid, this command temporarily reduces the grid row size of the active cell to 20% of the original size. The data system responds by expanding the top or bottom neighboring grid rows so that the cells in these grid rows can be viewed at increased resolution. To restore the grid column size to the original width, click the Reduce Size icon, , in the toolbar again.
	50%	Temporarily reduce the grid column size of the active cell to 50% of the original size. The data system responds by expanding the right or left neighboring grid columns so that the cells in these grid columns can be viewed at increased resolution. If there is only one column in the grid, this command temporarily reduces the grid row size of the active cell to 50% of the original size. The data system responds by expanding the top or bottom neighboring grid rows so that the cells in these grid rows can be viewed at increased resolution. To restore the grid column size to the original width, click the Reduce Size icon, , in the toolbar again.

Table 14. Grid menu (Sheet 3 of 3)

Icon	Command	Description				
Group Row						
	Group Row	Group a row containing two or more cells in a view containing two or more rows. After you have grouped cells, the data system updates any changes you make to ungrouped cells in the same view to all of the grouped cells. To group a row, you must have at least two rows of cells in your view and the grouped row need to have at least two cells. The data system makes the grouped row cells active, indicated by a gray border around the grouped row cells and deactivates most menu commands and buttons in the toolbar. For example, consider the following view. <table><tr><td colspan="2">Chromatogram</td></tr><tr><td>Spectrum</td><td>Mass List</td></tr></table> If your group spectrum and mass list cells using the Group Row command, the application simultaneously updates mass list and spectrum cells as you make changes in the Chromatogram cell.	Chromatogram		Spectrum	Mass List
Chromatogram						
Spectrum	Mass List					
Group Column						
	Group Column	Group a column containing two or more cells in a view containing two or more columns. After you have grouped cells, the data system updates any changes you make to ungrouped cells in the same view to all of the grouped cells. To group a column, you must have at least two columns of cells in your view and the grouped column needs to have at least two cells. The application makes the grouped column cells active, indicated by a gray border around the grouped cells, and deactivates most menu commands and buttons in the toolbar. For example, consider the following view. <table><tr><td rowspan="2">Chromatogram</td><td>Spectrum</td></tr><tr><td>Mass List</td></tr></table> If you group spectrum and mass list cells using the Group Column command, the application simultaneously updates mass list and spectrum cells as you make changes in the Chromatogram cell.	Chromatogram	Spectrum	Mass List	
Chromatogram	Spectrum					
	Mass List					
Grid Lines						
	Grid Lines	View or hide grid lines between cells.				

Help Menu – Qual Browser

Table 15 lists the Help menu commands in the Qual Browser window.

Table 15. Help menu

Command	Description
Qual Browser Help	Open Xcalibur Help and display Help for the Qual Browser window.
Xcalibur Help	Open Xcalibur Help.
Glossary	Open the glossary.
How To Use Online Help	Open Help that describes how to use the Help viewer.
About Qual Browser	View the version information for the Xcalibur data system, the installed Thermo Scientific applications, and the instrument drivers. Also view the Thermo Fisher Scientific copyright notice.

Tools Menu – Qual Browser

Table 16 lists the Tools menu commands in the Qual Browser window.

Table 16. Tools menu

Command	Description
Background Subtract	Create a new raw data file by subtracting one raw data file from another.
Add Tools	Add and remove tools [programs] on the Qual Browser window menu bar. The data system displays the added programs as menu commands when you choose the Tools menu from the Qual Browser window.

View Menu – Qual Browser

Table 17 lists the View menu commands in the Qual Browser window.

Table 17. View menu (Sheet 1 of 2)

Icon	Command	Description
Views		
	Chromatogram	View one or more chromatograms in the active cell. The data system displays any chromatograms defined by the settings in the Chromatogram Display Options Dialog Box .
	Spectrum	View a spectrum in the active cell. The application displays the spectrum defined by the settings in the Spectrum List Ranges Dialog Box .
	Map	View a three-dimensional x, y, z map of the parameters time, relative peak height, and m/z in the active cell. The application displays the map defined by the settings in the Map Ranges Dialog Box .
	Ion Map	View a three-dimensional x, y, z map of the parameters time, relative peak height, and m/z in the active cell. The application displays the map defined by the settings in the Map Ranges Dialog Box .
	Spectrum List	View the instrument method in the active cell. The instrument method contains the scan number and retention time for the scan and tabular data for m/z , intensity, and relative intensity. The application displays the instrument method defined by the settings in the Spectrum List Ranges Dialog Box .
	Scan Header	View the scan header of the current scan in the active cell. The application displays the scan header for the scan that is closest to the time set in the Scan Header Range Dialog Box .
	Scan Filters	View all of the scan filters used in all scans of the active raw data file in the active cell. The application displays the Scan Filter for the scan that is closest to the time set in the Scan Filter Range Dialog Box .
Reports		
	Tune Method	View the tune method stored in the active raw data file in the active cell.
	Instrument Method	View the instrument method stored in the active raw data file in the active cell. If there is more than one instrument method, click the right and left arrows   located in the toolbar to browse to the pages of the instrument methods for the other instruments. These right and left arrow buttons are not active for raw data files that contain only one instrument method.
	Sample Information	View the sample list information stored in the active raw data file.

Table 17. View menu (Sheet 2 of 2)

Icon	Command	Description
	Status Log	View the status log stored with the active raw data file.
	Error Log	View the error log stored with the active raw data file.
Other Commands		
	Add Plot	Activate automatic plot addition mode for grids containing multiple cells. Use this option to build a layout quickly. ❖ To add a plot 1. Activate a mode (indicated by a check mark ✓ alongside the menu item). 2. Pin the cell where you want to add a plot. 3. Click in another cell. A plot is added to the pinned cell. 4. Repeat this procedure to add further plots to pinned cells.
	Toolbars	Show or hide the Main and Amplify toolbars. You can also turn ToolTips on or off and choose to display large or small buttons in the toolbar.
	Customize Toolbar	Customize the Main toolbar. You can add buttons for most Qual Browser menu commands. You can also change the order of the buttons in the toolbar or remove them from the toolbar.
	Status Bar	Shows or hides the Status bar.
	Info Bar	Shows or hides the Info bar.
	Refresh	Update a view that is showing a chromatogram or a map from a raw data file that is currently being acquired. The data system expands the display range to show the full range of the data acquired so far. The range is reset only in the currently active cell. The application refreshes other cells, but does not adjust their ranges.

Window Menu – Qual Browser

Table 18 lists the Window menu commands in the Qual Browser window.

Table 18. Window menu

Icon	Command	Description
	New Window	Open a new data window in Qual Browser. The new window uses the default layout and displays the most recently opened raw data file.
	Cascade	Arrange the current open windows in an overlapped arrangement with all the title bars visible.
	Tile	Arrange the current open windows in a tiled arrangement so that each window has the same area of Qual Browser's workspace.
	Arrange Icons	Arrange iconized (minimized) windows along the bottom of the Qual Browser workspace.

Qual Browser Toolbars

The Qual Browser window provides these toolbars:

- [Amplify Toolbar – Qual Browser](#)
- [Main Toolbar – Qual Browser](#)

Amplify Toolbar – Qual Browser

Use the Qual Browser window Amplify toolbar to amplify a region of a plot. [Table 19](#) describes the icons on the Amplify toolbar.

Table 19. Qual Browser Amplify toolbar

Icon	Description
	Amplify Factor Set the Amplify Factor to apply to a region of a plot using the Amplify button. Select an amplify factor from the preset values or type your own. For example, to amplify a region by a factor of 10.0, type or select 10 in the Amplify Factor box.
	Amplify Enlarge a region of the active plot by the factor selected in the Amplify Factor box. The data system changes the cursor to . To amplify a region, drag the cursor horizontally over the region. The application amplifies the region, places the following label above the amplified region: -----x5-----, and displays the original cursor. To turn off  before using it, click . To cancel one or more amplified regions of a graph, click the Cancel Amplified Region icon, , or the choose Display > Amplify > Clear. The  cursor appears. Drag the cursor across the amplified region. To cancel all amplified regions of a graph, choose Display > Amplify > Clear All.
	Cancel Amplified Region Cancel one or more amplified regions of a plot. The data system change the cursor to . To clear an amplified region, drag the cursor horizontally extending slightly beyond the start and end of the region. The application removes the amplification, removes the amplification labels (such as -----x5-----), and displays the original cursor. To turn off  before using it, click . To remove all amplified regions from a graphic, choose Display > Amplify > Clear All.

Main Toolbar – Qual Browser

You can customize the Qual Browser window Main toolbar to display buttons for most menu commands. The [Amplify Toolbar – Qual Browser](#) is fixed. When you start Qual Browser for the first time the Main toolbar contains buttons for some of the most frequently used commands. You can fully customize the main toolbar.

For information about customizing the Main toolbar, see [Customizing the Toolbar](#).

All of the buttons available for the Qual Browser Main toolbar are displayed below under the menu bar name that contains the corresponding command. Buttons in the toolbar are also arranged in this manner in the Customize Toolbar dialog box.

[Table 20](#) describes the buttons and icons on the Main toolbar.

Table 20. Qual Browser Main toolbar (Sheet 1 of 9)

Button/ Icon	Command	Description
File		
	Open	Find and open a file that already exists.
	Open Sequence	Select a sequence file (SLD).
	Open Result File	Select a result file (RST).
	Apply	Select a layout file (LYT).
	Apply Default	Apply the default layout to the active data window.
	Save	Enter audit information about the active file and select the location (disk and directory) for the saved file. After you have entered audit information, click Continue . The Save As dialog box opens.
	Save As	Save the layout of the active data window. If it has not been saved before, the Save Layout File dialog box opens. Provide a name for the layout.
	Save As Default	Save the layout of the active data window as the default layout for new windows.
	Summary Information	View summary information.
	Close All	Close all data windows.
	Print Preview	Specify what you want to print and how to print it before previewing the pages. You can print your selection or return to Qual Browser.

Table 20. Qual Browser Main toolbar (Sheet 2 of 9)

Button/ Icon	Command	Description
	Print	Select print range and print quality.
Edit		
	Undo	Cancel your previous action. For example, if you have just deleted an entry or annotation, choose the Undo command to replace the deleted entry or annotation. Also, if you have just completed an entry or annotation, choose the Undo command to delete the entry or annotation. If you complete two actions, the Undo command only undoes the previous action and not the first action.
	Copy Cell	Copy the active cell to the Clipboard.
	Paste Cell	Paste a cell that is stored on the Clipboard to the active cell.
	Copy View	Copy the active grid to the Clipboard.
	Copy Special	Scale the output size of the Clipboard image from the current cell or window.
View		
	Chromatogram	Change the view in the active cell to a chromatogram view.
	Spectrum	Change the view in the active cell to a spectrum view.
	Map	Change the view in the active cell to a map view.
	Spectrum List	Change the view in the active cell to a spectrum list view.
	Scan Header	Change the view in the active cell to a scan header view.
	Scan Filters	Change the view in the active cell to a scan filters view.
	Tune Method	Change the view in the active cell to a tune method view.
	Instrument Method	Change the view in the active cell to an instrument method view.
	Sample Information	Change the view in the active cell to a sample information view.
	Status Log	Change the view in the active cell to a status log view.

Table 20. Qual Browser Main toolbar (Sheet 3 of 9)

Button/ Icon	Command	Description
	Error Log	Change the view in the active cell to an error log view.
	Add Plot	Activate automatic plot addition mode for grids containing multiple cells. Use this option to build a layout quickly. ❖ To add a plot 1. Activate a mode (indicated by a check mark ✓ alongside the menu item). 2. Pin the cell where you want to add a plot. 3. Click in another cell. A plot is added to the pinned cell. 4. Repeat this procedure to add further plots to pinned cells. When you have finished adding plots, click the button in the toolbar again.
	Info Bar	View or hide the Info Bar. The Help button on the Genesis Peak Detection Settings Page appears at the extreme bottom of the page.
	Refresh	Update a view that is showing a chromatogram or a map from a raw data file that is currently being acquired. The data system expands the display range to show the full range of the data acquired so far. The range is reset only in the currently active cell. The application refreshes other cells, but does not adjust their ranges.
Display		
	Ranges	View ranges for the active view. The Ranges command is not available for Report views. There is a Ranges dialog box for each of these view types: Chromatogram view: Chromatogram Display Options Dialog Box Spectrum view: Spectrum Ranges Dialog Box Map or Ion Map views: Map Ranges Dialog Box Spectrum List view: Spectrum List Ranges Dialog Box Scan Header view: Scan Header Range Dialog Box Scan Filter view: Scan Filter Range Dialog Box

Table 20. Qual Browser Main toolbar (Sheet 4 of 9)

Button/ Icon	Command	Description
	Display Options	Select the style, color, label [chromatogram and spectrum only], axis, normalization, and smoothing [chromatogram only] options for your chromatogram, spectrum, or map.
	Add Text	Add text to the active plot.
	Add Graphics	Add simple graphic objects such as lines or boxes to the active plot.
	Clear	Activates the  cursor so that you can selectively remove text or graphics annotation entries. To remove graphics or text, drag the cursor horizontally above or below the text or graphic. The data system removes the text or graphic(s) and changes the cursor back to your default cursor. Repeat this procedure to remove other annotations. To remove annotations one at a time, click the Clear, , icon in the toolbar.
	Clear All	Remove all text and graphics annotation entries in the active cell.
	Zoom In Y	Zoom in on the <i>y</i> axis by a factor of two (2) from the current baseline to show more detail. For example, you can change the <i>y</i> -axis range from 0–100 to 0–50.
	Zoom Out Y	Zoom out on the <i>y</i> axis by a factor of two (2) to show more data. For example, you can change the <i>y</i> -axis range from 0–25 to 0–50.
	Auto Range	View the chromatogram, which is normalized from the minimum to the maximum signal. Auto Range is useful for PDA and UV data.
	Normalize (0 to 100%)	Normalizes the intensity scale of the data display to a fixed range on the <i>y</i> axis. For example, from 0–25 percent to 0–100 percent.
	Zoom In X	Zoom in on the <i>x</i> axis by a factor of two (2) to show more detail. For example, you can change the <i>x</i> -axis range can from 0–20 to 5–15.
	Zoom Out X	Zoom out on the <i>x</i> axis by a factor of two (2) from the center to show more data. For example, you can change the <i>x</i> -axis range from 7.5–12.5 min to 5–15 min.
	Display All	View all data on the <i>x</i> axis or all text in a report. For example, you can change the <i>x</i> -axis range from 7.5–12.5 min to 0–20 min.
	Reset	Restores the data display to the full range of the <i>x</i> axis and <i>y</i> axis.
	Drag With Cursor	Move (pan) the active plot horizontally left and right along the <i>x</i> axis by dragging the cursor. The data system changes the cursor to . Click  again to turn off .

Table 20. Qual Browser Main toolbar (Sheet 5 of 9)

Button/ Icon	Command	Description
	Forward	Display data to the left of the active displayed range. This command is incremental so you might need to use it multiple times to display the region of interest.
	Back	Display data to the right of the active displayed range. This command is incremental so you might need to use it multiple times to display the region of interest.
	Next Scan	View the next mass scan with its scan number.
	Previous Scan	View the previous mass scan with its scan number.
Grid		
	Left	Insert a cell or cells to the left of the active cell.
	Right	Insert a cell or cells to the right of the active cell.
	Above	Insert a cell or cells above the active cell.
	Below	Insert a cell or cells below the active cell.
	Row	Delete the grid row containing the active cell.
	Column	Delete the grid column containing the active cell.
	All Cells	Delete all the cells in the active window.
	Cell Size	Adjust the column width and row height. You can make adjustments relative to other columns and rows.
	Full Width	Zoom the active cell to the full width of the grid.
	Full Height	Zoom the active cell to the full height of the grid.
	Full View	Zoom the active cell to the full size of the grid.

Table 20. Qual Browser Main toolbar (Sheet 6 of 9)

Button/ Icon	Command	Description				
	Reduce Cell	Temporarily reduces the grid column size of the active cell to 20% of the original size. The data system expands the right or left neighboring grid columns so that you can view the cells in these grid columns at increased resolution. This command is only active if the grid has two or more rows or columns. If there is only one column in the grid, this command temporarily reduces the grid row size of the active cell to 20%. The system responds by expanding the top or bottom neighboring grid rows so that the cells in these grid rows can be viewed at increased resolution.				
	Group Row	Group a row containing two or more cells in a view containing two or more rows. After you have grouped cells, the data system updates any changes you make to ungrouped cells in the same view to all of the grouped cells. To group a row, you must have at least two rows of cells in your view and the grouped row needs to have at least two cells. The data system makes the grouped row cells active, draws a blue border around the grouped row cells, and deactivates most menu commands and buttons in the toolbar. The data system also makes all ungrouped row cells in the view inactive. For example, consider the following view: <table border="1"><tr><td colspan="2">Chromatogram</td></tr><tr><td>Spectrum</td><td>Mass List</td></tr></table> If you group spectrum and mass list cells using the Group Row command, the system simultaneously updates mass list and spectrum cells as you make changes in the Chromatogram cell.	Chromatogram		Spectrum	Mass List
Chromatogram						
Spectrum	Mass List					

Table 20. Qual Browser Main toolbar (Sheet 7 of 9)

Button/ Icon	Command	Description			
	Group Column	Group a column containing two or more cells in a view containing two or more columns. After you have grouped cells, the data system updates any changes you make to ungrouped cells in the same view to all of the grouped cells. To group a column, you must have at least two columns of cells in your view and the grouped column needs to have at least two cells. The data system makes the grouped column cells active, draws a blue border around the grouped cells, and deactivates most menu commands and buttons in the toolbar. The application also makes all ungrouped column cells in the view inactive. For example, consider the following view: <table data-bbox="563 728 943 890"><tr><td rowspan="2">Chromatogram</td><td>Spectrum</td></tr><tr><td>Mass List</td></tr></table> If you group spectrum and mass list cells using the Group Column command, the application simultaneously updates mass list and spectrum cells as you make changes in the Chromatogram cell.	Chromatogram	Spectrum	Mass List
Chromatogram	Spectrum				
	Mass List				
	Grid Lines	View or hide grid lines.			
Actions					
	1 Range	Perform a peak-by-peak subtraction of selected scans contained in one background region of a chromatogram view from the current spectrum view. Use this command to eliminate background scans that might interfere with the display of spectrum peaks of interest. The subtracted scans need to use the same scan filter as the target scans. For more information, see Subtracting Background Spectra .			
	2 Ranges	Perform a peak-by-peak subtraction of selected scans contained in two selected background regions of a chromatogram view from the current spectrum view. Use this command to eliminate background peaks that might be interfering with the display of spectrum peaks of interest. The subtracted scans need to use the same scan filter as the target scans. For more information, see Subtracting Background Spectra .			
	Clear	Remove all subtract spectra modifications to the spectrum view. The data system also removes the SB: xx notation in the spectrum view header to indicate that the spectrum view has been returned to the original display before applying the Subtract Spectra command.			
	Settings	View a page specific to one of the Xcalibur peak detection algorithms and change the parameters used by Qual Browser to identify and integrate chromatogram peaks.			

Table 20. Qual Browser Main toolbar (Sheet 8 of 9)

Button/ Icon	Command	Description
	Toggle Detection in This Plot	Detect and integrate all peaks in the selected chromatogram plot using the current peak detection and integration settings. Click the icon a second time to undo the peak detection. A raw data file must be open for this button to be active.
	Toggle Detection in All Plots	Detect and integrate all peaks in all selected and unselected chromatogram plots in the active cell using the current peak detection and integration settings. Click the icon a second time to undo all detected peaks. A raw data file must be open for this button to be active.
	Add Peaks	Detect and integrate any peak in the active cell. The data system changes the cursor to the add peaks cursor, . To detect and integrate a peak, drag this cursor horizontally across the peak. The data system marks the added peak with a blue baseline, , and integrates the peak. Click the icon a second time to return the add peaks cursor to the default cursor. ❖ To label all detected peaks with peak parameters 1. Choose Display > Display Options. The Display Options Dialog Box in Qual Browser opens. 2. Click the Label tab, and select peak label parameters. 3. Choose OK. The application displays the selected labels at the top of all peaks in the plot. A raw data file must be open for this button to be active.
	Delete Peaks	Delete selected peak(s) in the active cell. The data system changes the cursor to the delete peaks cursor, . Click this cursor within each peak boundary, indicated by the blue baseline  of the peak(s) that you want to delete. Click  a second time to return the delete peaks cursor to the default cursor. One or more peaks must be detected (as indicated by ) for this button to be active.

Table 20. Qual Browser Main toolbar (Sheet 9 of 9)

Button/ Icon	Command	Description
	Add Manual Noise Region	Select an area as the noise region. Click  and drag the cursor horizontally across the chromatogram region you want to select. The data system marks the region with a red baseline. The application calculates noise based on the data points you select. It uses all selected data points as noise points and calculates noise based on those points. You can select the noise region from an individual trace or different noise regions from multiple traces. Open a raw data file and select a chromatogram to make this button active.
	Delete Manual Noise Region	Delete a selected noise region. Click  and drag the cursor over the region that was previously selected as the noise region. Release the mouse button to delete the noise region.
	Search	Submit the active spectrum to a library search. The data system displays the results of the search in the Library Search Results window.
	Export to Library Browser	Exports the active spectrum to the Library Browser.
	Options	Choose the libraries used during a library search. You can also change various parameters that determine how the search is carried out.
	Autofilter	Apply all of the scan filters in the current raw data file and open an AutoFilter display in the active cell. The AutoFilter display consists of a vertical sequence of chromatogram plots. The first chromatogram displays the TIC with no scan filter. Below the first chromatogram are up to seven TIC scan filter chromatograms, one chromatogram plot for each scan filter. You can also apply scan filters to one or more plots from the Chromatogram Display Options Dialog Box.
Window		
	New Window	Open a new data window in Qual Browser. The new window uses the default layout and displays the most recently opened raw data file.
	Cascade	Arrange the current open windows in an overlapped arrangement with all the title bars visible.
	Tile	Arrange the current open windows in a tiled arrangement so that each window has the same area of Qual Browser's workspace.
Help		
	Qual Browser Help Command	Open Xcalibur Help for Qual Browser. This window displays procedures and reference topics for the Qual Browser window.

Qual Browser Views

The Qual Browser window contains a grid of cells. A cell displays only one view; however, you can change the view displayed by a cell to any of the following views.

- [Chromatogram View](#)
- [Error Log View](#)
- [Instrument Method View](#)
- [Ion Map View](#)
- [Map View](#)
- [Sample Information View](#)
- [Scan Filter View](#)
- [Scan Header View](#)
- [Spectrum List View](#)
- [Spectrum View](#)
- [Status Log View](#)
- [Tune Method View](#)

Each of these views has a shortcut menu. Use the View command in the short cut menu to change the view. [Figure 65](#) shows the shortcut menu for the chromatogram view and the expanded View menu.

Figure 65. Chromatogram view shortcut menu and View menu commands

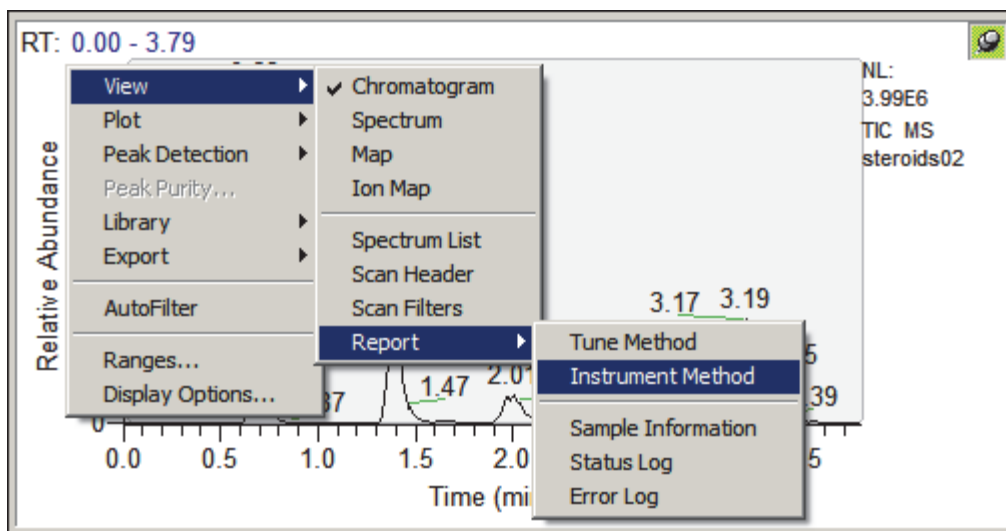


Table 21 describes the views that you can open with the View menu commands.

Table 21. View menu (Sheet 1 of 2)

Command	Description
View	
View > Chromatogram	Changes the view in the active cell to the chromatogram view. The data system displays any chromatograms defined by the settings in the Chromatogram Display Options Dialog Box .
View > Spectrum	Changes the view in the active cell to the spectrum view. The data system displays the spectrum defined by the settings in the Spectrum Ranges Dialog Box .
View > Map	Changes the view in the active cell to a three-dimensional x, y, z map of the parameters time, relative peak height, and m/z value. The data system displays the map defined by the settings in the Map Ranges Dialog Box .
View > Ion Map	Changes the view in the active cell to a three-dimensional x, y, z map of the parameters time, relative peak height, and m/z value. The data system displays the map defined by the settings in the Map Ranges Dialog Box .
View > Spectrum List	Changes the view in the active cell to the instrument method view. The instrument method contains the scan number and retention time for the scan and tabular data for m/z , intensity, and relative intensity. The application displays the spectrum list defined by the settings in the Spectrum List Ranges Dialog Box .
View > Scan Header	Changes the view in the active cell to the scan header view. The data system displays the scan header for the scan that is closest to the time set in the Scan Header Range Dialog Box .
View > Scan Filters	Changes the view in the active cell to the scan filter view where you can view all of the scan filters used in all scans of the active raw data file. The data system displays the scan filter for the scan that is closest to the time set in the Scan Filter Range Dialog Box .
View > Reports >	
View > Reports > Tune Method	Changes the view in the active cell to the tune method view where you can view the tune parameters stored in the active raw data file.
View > Reports > Instrument Method	Changes the view in the active cell to the instrument method view where you can view the instrument method parameters stored in the active raw data file. If the instrument method controls more than one device, click the right and left arrows  located in the toolbar to browse to the through the pages of the instrument method for each device. These right and left arrow buttons are not active for raw data files that contain only one device; for example, only a mass spectrometer.
View > Reports > Sample Information	Changes the view in the active cell to the sample information view where you can view the sample list information stored in the active raw data file.

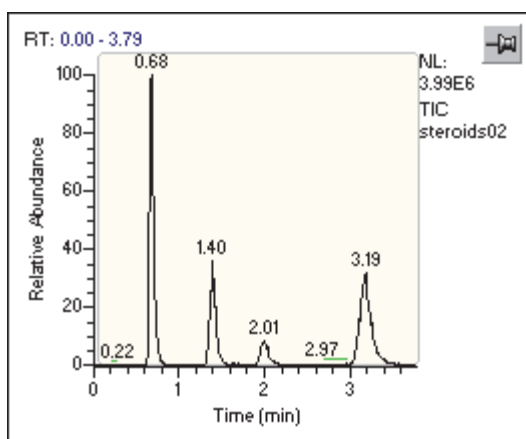
Table 21. View menu (Sheet 2 of 2)

Command	Description
View > Reports > Status Log	Changes the view in the active cell to the status log view where you can view the status log stored with the active raw data file.
View > Reports > Error Log	Changes the view in the active cell to the error log view where you can view the error log stored with the active raw data file.

Chromatogram View

Use the Qual Browser window to open a raw data file, create a grid of interactive cells, and display a chromatogram and related header information in any of the cells. Use menu commands to select view options.

The chromatogram view consists of up to eight chromatogram plots. This figure shows an example of a chromatogram view plot with a retention time label.



For information about the view header and the shortcut menu, see these topics:

- [View Header Information](#)
- [Chromatogram View Shortcut Menu](#)

View Header Information

- RT
- NL
- m/z [Mass Range]
- TIC
- Base Peak
- Analog UV 1
- Analog UV 2
- Analog UV 3
- Analog UV 4
- Scan Filter

Chromatogram View Shortcut Menu

Right-click the chromatogram view to display the shortcut menu commands.

Table 22 describes the shortcut menu commands for the chromatogram view.

Table 22. Chromatogram view shortcut menu commands (Sheet 1 of 3)

Command	Description
View	
Use the commands on the View menu to change the view in the active cell. For a brief description of each view, see Table 17 on page 158.	
Plot	
Plot > Insert	Insert a copy of the selected (grayed) plot above the selected plot. Select a plot.
Plot > Delete	Delete the selected (grayed) plot. Select a plot.
Plot > Move Up	Switch positions of the selected (grayed) plot with the one above it. Select a plot.
Plot > Move Down	Switch positions of the selected (grayed) plot with the one below it. Select a plot.
Peak Detection	
Peak Detection > Settings	View or change the parameters used by Qual Browser to identify and integrate chromatogram peaks.
Peak Detection > Toggle Detection in This Plot	Detect and integrate all peaks in the selected chromatogram plot using the current peak detection and integration settings. The data system adds a check mark to the left of the menu command. Choose Peak Detection > Toggle Detection In This Plot a second time to undo the peak detection and remove the check mark from the left of the menu command. Open a raw data file to make this command active.
Peak Detection > Toggle Detection in All Plots	Detect and integrate all peaks in all selected and unselected chromatogram plots in the active cell using the current peak detection and integration settings. The data system adds a check mark to the left of the menu command. Choose Peak Detection > Toggle Detection In All Plots a second time to undo all detected peaks and remove the check mark from the left of the menu command. Open a raw data file to make this command active.

Table 22. Chromatogram view shortcut menu commands (Sheet 2 of 3)

Command	Description
Peak Detection > Set Peak Detection Algorithm and Detect in This Plot	View a list of the Xcalibur peak detection algorithms. Select one of the algorithm names in the list to display the page for that algorithm and to use the algorithm to detect chromatogram peaks in the active chromatogram cell. Open a raw data file to make this command active.
Peak Detection > Set Peak Detection Algorithm and Detect in All Plots	View a list of the Xcalibur peak detection algorithms. Select one of the algorithm names in the list to display the page for that algorithm and to use the algorithm to detect chromatogram peaks in all the cells that are currently displayed. Open a raw data file to make this command active.
Peak Detection > Add Peaks	Detect and integrate any peak in the active cell. The data system changes the cursor to the add peaks cursor, . To detect and integrate a peak, drag this cursor horizontally across the peak. The application marks the added peak with a blue baseline, , and integrates the peak. The application also adds a check mark to the left of the menu command. Choose Peak Detection > Add Peaks a second time to return the add peaks cursor to the default cursor and remove the check mark from the left of the menu command. For information about labeling the detected chromatographic peaks, see Setting the Chromatogram Label Options.
Peak Detection > Delete Peaks	Delete selected peaks in the active cell. The data system changes the cursor to . Click this cursor within each peak boundary, indicated by the blue baseline, , of the peak(s) that you want to delete. One or more peaks must be detected (as indicated by ) for this command to be active.
Peak Purity	
Peak Purity	View or change Peak Purity settings. Open a raw data file from a PDA analysis and select PDA from the Detector list in the Ranges dialog box to make this command active.
Library	
Library > Search	Submit the active spectrum to a library search. The data system displays the results of the search in the Library Search Results window.
Library > Export to Library Browser	Export the active spectrum to the Library Browser.
Library > Options	Choose the libraries used during a library search. You can also change various parameters that determine how the search is carried out.

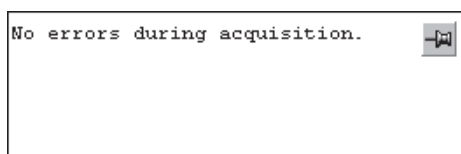
Table 22. Chromatogram view shortcut menu commands (Sheet 3 of 3)

Command	Description
Export	
Export	Export the time versus intensity values of the chromatogram to the Clipboard.
AutoFilter	
AutoFilter	Apply all of the scan filters in the current raw data file and open an AutoFilter display in the active cell. For more information, see Adding Plots to a Chromatogram View with the Autofilter Command. The AutoFilter display consists of a vertical sequence of chromatogram plots. The first chromatogram displays the TIC with no scan filter. Below the first chromatogram are up to seven TIC scan filter chromatograms, one chromatogram plot for each scan filter. For more information, see the Scan Filter View. You can also apply scan filters to one or more plots from the Chromatogram Display Options Dialog Box.
Ranges	
Ranges	View and edit the mass range, time range, and other properties of a chromatogram plot.
Display Options	
Display Options	Select the Style, Color, Labels, Axis, and Normalization settings.

Error Log View

Use the Qual Browser window to open a raw data file, create a grid of interactive cells, and view an error log in any of the cells. Use menu commands to select view options.

The error log view lists errors that occurred during a sample run. This figure shows an error log with no errors.



Right-click the error log view to open the Error view shortcut menu, which lists the Qual Browser views.

Use the commands on the View menu to change the view in the active cell. For a brief description of each view, see [Table 17](#) on [page 158](#).

Instrument Method View

Use the Qual Browser window to open a raw data file, create a grid of interactive cells, and view the instrument method for the current raw data file in any of the cells.

If there is more than one instrument, click the show previous and show next buttons  located in the toolbar to browse to the pages of the instrument method for the other instruments.

Note These right and left arrow buttons are not active for raw data files that contain only one instrument method.

[Figure 66](#) shows the method parameters in a raw data file that a Thermo Fisher Scientific application chemist acquired with an LC/MS system made up of an Accela™ Open AS, an Accela 1250 Pump, and a Q Exactive™ mass spectrometer.

Figure 66. Instrument method view for an LC/MS instrument

Nor_0_A
Accela Open AS

Description:

Standard Accela Open AS Injection

Sample pickup

Needle dip in Wash 1

Sample Injection

Valve Clean with Solvent 2

Post Clean with Solvent 2

Valve Clean with Solvent 1

Post Clean with Solvent 1

(Stator Wash)

Syringe: 100ulDLW

Macro Sequence

Standard Injection Accela Open_Rev03 (Step 1 of 1)

Airgap Volume (ul): 3

Front Volume (ul): 5

Autosampler
section

Click the Show Next icon, .

Nor_0_A
Accela 1250 Pump

Method creator: Thermo

Last modified: 5/1/2011 6:00:30 PM by Thermo

Instrument: Accela 1250 Pump

Common settings:

Pressure units: bar

Pressure stability: 10.00

Pump 1 settings:

Name: Pump 1

Comment:

Solvent A:

Solvent B:

Solvent C:

Solvent D:

Start settings: Accela AS injection

LC pump
section

Click the Show Next icon, .

Nor_0_A
Q Exactive - Orbitrap MS

Method of Q Exactive

OVERALL METHOD SETTINGS

Global Settings

use lock masses off

Time

Method duration 3.00 min

Experiment

FS-AIF

Time

runtime 0 to 3 min

General

Mass
spectrometer
section

View Header Information

- Instrument Method: *Drive:\Path*
- Created

Instrument Method Information

- Creator
- Last Modified
- Summary
- MS Run Time

Instrument Method Settings

For an LC/MS instrument, the instrument method settings for the autosampler, LC pump, and mass spectrometer are listed on separate pages.

Example parameters for the mass spectrometer:

Syringe Settings	MS Detector Settings	Dependent Data Settings
• Syringe Type • Flow Rate • Volume • Stop Syringe Pump at End of Run [Yes/No]	• Segments • Duration • Tune Method • Scan Events • Scan Type	• Reject Spectrum List • Parent Spectrum List • Default Charge State • Collision Energy • Min Signal Required

Instrument Method View Shortcut Menu

Right-click in the instrument method view to open the Instrument Method view shortcut menu, which lists the Qual Browser views.

Use the commands on the View menu to change the view in the active cell. For a brief description of each view, see [Table 17](#) on [page 158](#).

Ion Map View

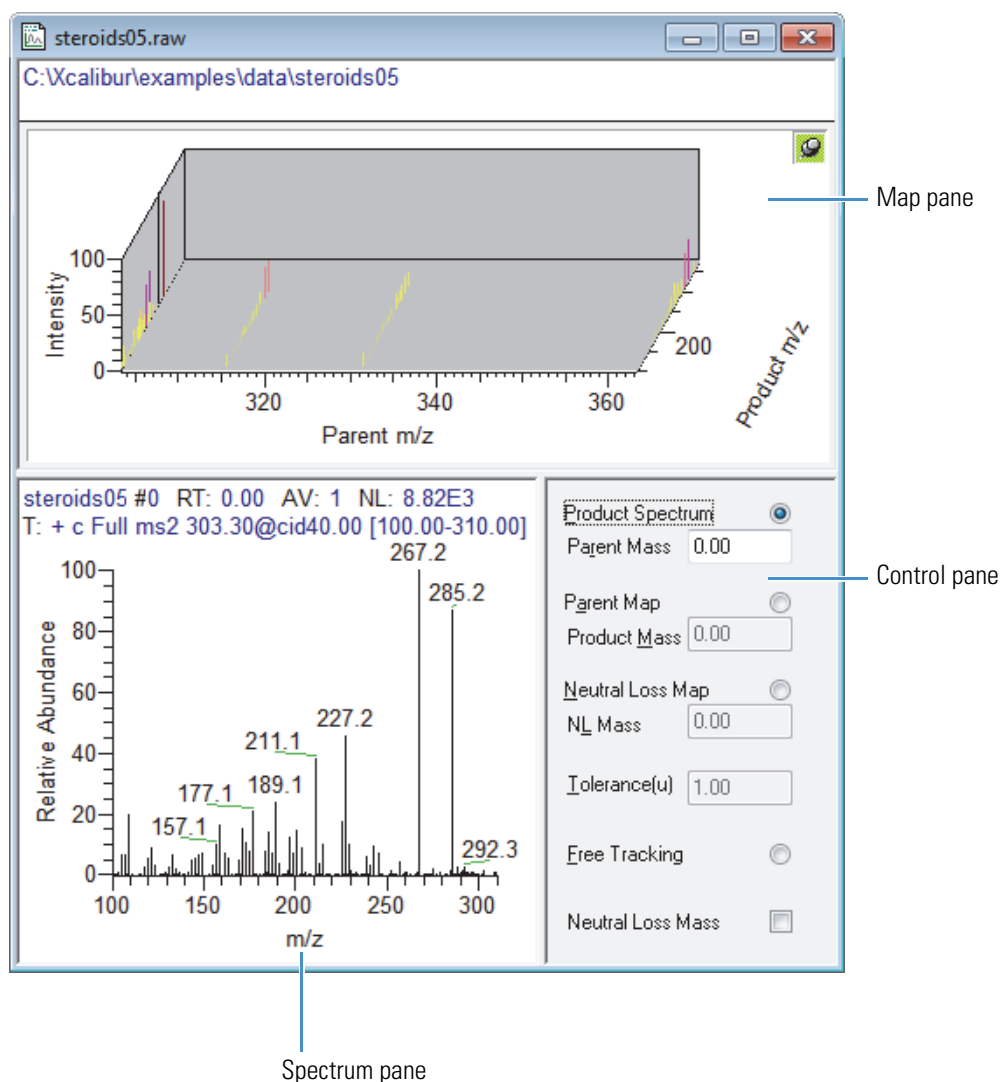
Use the ion map view to analyze the precursor (parent), product, and neutral loss of MSⁿ data. The ion map view consists of three panes. The map pane on the top, the control pane on the right side, and the spectrum pane on the bottom. For information about the ion map view see these topics:

- [Map Pane](#)
- [Control Pane](#)
- [Spectrum Pane](#)

Note The ion map view in the Qual Browser window is not available for all MS detectors.

Figure 67 shows the ion map view with a 3D ion map.

Figure 67. Ion map view



Map Pane

The Map pane of the ion map view can display the MSⁿ data as a Stack (2D), Overlay (3D), or Density Map (2D).

❖ To select the map type that you want to display

1. Choose **Display > Display Options**.

The Display Options dialog box opens.

2. Click the Style tab to display the Style page and select one of the three options.
 - The Density Map (2D) style displays the precursor (parent) mass (*x* axis) and product mass (*y* axis) as a density map with different colors for each intensity. This is the default display style.
 - The 2D Stack style displays the precursor (parent) mass on the *x* axis and stacks the individual product mass spectra on the *y* axis.
 - The 3D Map style displays the precursor (parent) mass on the *x* axis, product mass on the *y* axis, and relative abundance on the *z* axis. Neutral loss masses are calculated using the following formula:

$$parent - product$$

❖ To change the spectrum in the spectrum pane

In the map pane, drag the cursor to the mass region of interest.

The spectrum pane displays the corresponding spectrum, and the control pane displays the coordinates.

[Table 23](#) describes the shortcut menu commands for the map pane in the ion map view. To display these commands, right-click the map pane.

Table 23. Map pane shortcut menu

Command	Description
View	Use the commands on the View menu to change the view in the active cell. For a brief description of each view, see Table 17 on page 158 .
Ranges	Opens the Map Ranges dialog box where you can set the precursor (parent) mass range, product mass range, and scan filter for an ion map.
Display Options	Opens the Display Options dialog box. Select the style, color, axis, and normalization settings.
Toggle Neutral Loss	--

Control Pane

Use the Control pane to specify that the precursor (parent), product, or neutral loss is to remain constant while other parameters are varied.

Table 24 describes the parameters in the Control pane of the ion map view.

Table 24. Control pane parameters (Sheet 1 of 3)

Parameter	Description
Product Spectrum	Create a product spectrum consisting of products from the specified parent mass. The Activate the Parent Mass box opens.
Parent Mass	View the product spectrum for the selected parent in the Spectrum pane. This spectrum consists of all of the products from the parent in the data that is the closest to the selected parent mass coordinate. Drag the cursor in the Map pane along the Parent axis. The data system displays the parent mass coordinate in the Parent Mass box. Also, you can enter the parent mass coordinate in the Parent Mass box. The valid range is m/z 0.00 to 100 000.00. To make this box available, select the Product Spectrum option.
Parent Map	Produce a parent map consisting of parents that decompose to form the specified product mass. When you select this option, the Product Mass box becomes available.
Product Mass	View the parent map for the selected product in the Spectrum pane. This reconstructed spectrum consists of all of the parents that produced the products defined in the product mass window. The parents and products were extracted from the array of MS/MS data. The product mass window is defined by the m/z value in the Product Mass box and the m/z value in the Tolerance box, as follows: <i>product mass +/- Tolerance</i>. To make this box available, select the Parent Map option. Drag the cursor in the Map pane along the Product axis. The data system displays the product mass coordinate in the Product Mass box. Also, you can enter the product mass coordinate in the Product Mass box. The valid range is m/z 0.00 to 100 000.00.

Table 24. Control pane parameters (Sheet 2 of 3)

Parameter	Description
Neutral Loss Map	When you select this option, the Neutral Loss box becomes available so that you can create a neutral loss map consisting of parents that lose the specified neutral loss mass.
NL Mass	View the neutral loss map for the selected neutral loss mass in the Spectrum pane. This reconstructed spectrum consists of all of the parents that produced product(s) within the neutral loss mass window selected. The neutral loss window is defined by the m/z value in the Neutral Loss box and the m/z value in the Tolerance box, as follows: $\text{Neutral Loss Mass} \pm \text{Tolerance}$ The neutral loss mass is <i>parent mass</i> – <i>product mass</i>. To make this box available, select the Neutral Loss option. Drag the cursor in the Map pane along the diagonal neutral loss axis. The data system displays the neutral loss mass coordinate in the Neutral Loss box. Also, you can enter the neutral loss coordinate in the Neutral Loss box. The valid range is m/z – 100 000.00 to 100 000.00.
Tolerance	Select the window where the data system selects either product masses or neutral loss masses, depending upon which option you select. - When you select the Product Mass option, the product window is defined by the m/z value in the Product Mass box and the m/z value in the Tolerance box, as follows: $\text{Product Mass} \pm \text{Tolerance}$ - When you select the Neutral Loss option, the neutral loss window is defined by the m/z value in the Neutral Loss box and the m/z value in the Tolerance box, as follows: $\text{Neutral Loss Mass} \pm \text{Tolerance}$ The neutral loss mass is <i>parent mass</i> – <i>product mass</i>.

Table 24. Control pane parameters (Sheet 3 of 3)

Parameter	Description
Free Tracking	Disconnect the map pane from all controls provided by the spectrum pane and the control pane. If you select the Free Tracking option, you can drag the cursor in the map pane to select specific regions of the map.
Neutral Loss Mass/Product Mass	Provide a double label at the top of each ion peak displayed in the Spectrum pane. The title of this check box changes depending upon whether you have selected the Product Spectrum option, Parent Map option, or Neutral Loss Map option in the Control pane. - Product Spectrum option: The check box is labeled Neutral Loss Mass. The spectrum displays all products from the specified parent mass. Peaks are labeled as follows: Product Mass (Neutral Loss Mass) - Parent Map option: The check box is labeled Neutral Loss Mass. The spectrum displays all parents that produce the specified product mass. Peaks are labeled as follows: Parent Mass (Neutral Loss Mass) - Neutral Loss Map option: The check box is labeled Product Mass. The spectrum displays all parents that produce a product by losing the specified neutral loss (NL) mass. Peaks are labeled as follows: Parent Mass (Product Mass)

Spectrum Pane

View the spectrum that you select using the cursor controls in the map pane and the settings in the control pane. Depending on the settings, you can display the following:

- Product Spectrum
- Parent Map
- Neutral Loss Map

Right-click in the spectrum pane to open the shortcut menu.

[Table 25](#) describes the shortcut menu commands for the spectrum pane.

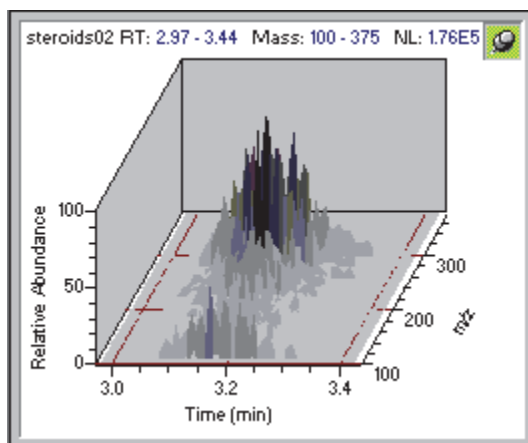
Table 25. Spectrum pane shortcut menu

Command	Description
View	
Use the commands on the View menu to change the view in the active cell. For a brief description of each view, see Table 17 on page 158 .	
Ranges	
Ranges	Opens the Spectrum Ranges dialog box.
Display Options	
Display Options	Opens the Display Options dialog box. Select the style, color, labels, axis, and normalization settings.

Map View

Use the Qual Browser window to open a raw data file, create a grid of interactive cells, and display a map and related header information in any of the cells. Use menu commands to select display options.

The map view consists of a time (x axis) versus m/z (y axis) versus relative abundance (z axis) map plot. This figure shows an example of a map view.



View Header Information

- RT: retention time range
- Mass: mass-to-charge range
- NL: normalization value
- T: Scan type
- F: Scan filter

Map View Shortcut Menu

Right-click the map view to open the shortcut menu for the map view.

Table 26 describes the commands in the shortcut menu for the map view.

Table 26. Map view shortcut menu commands

Command	Description
View	Use the commands on the View menu to change the view in the active cell. For a brief description of each view, see Table 17 on page 158.
Ranges	Opens the Map Ranges dialog box, where you can set the mass and time range and scan filter for a map.
Display Options	Opens the Display Options dialog box, where you can select the style, color, axis, normalization, and bandwidth settings.

Sample Information View

Use the Qual Browser window to open a raw data file, create a grid of interactive cells, and view sequence information for the current sample in any of the cells.

This figure shows an example of the sample information view.

steroids02
Type: Std Bracket Start Level: 3 ID: Sample02 Row: 1

Sample Name:
Study:
Client:
Laboratory:
Company:
Phone:
Experiment Method: C:\pitcontrial2\steroidMSMSis
Processing Method: C:\pitcontrial2\steroidmsmslS
Vial: 1
Injection Volume (µl): 20.00
Sample Weight: 0.00
Sample Volume (µl): 0.00
ISTD Amount: 0.00

Right-click the sample information view to open the Sample Information view shortcut menu. Use the commands on the View menu to change the view in the active cell. For a brief description of each view, see [Table 17](#) on [page 158](#).

[Table 27](#) describes the parameters in the sample information view. The settings are read-only.

Table 27. Sample information view parameters (Sheet 1 of 2)

Parameter	Description
Raw File name	Displays the file name of the raw data file.
Type	Displays the sequence bracket type.
ID	Displays the sample ID.
Row	
Sequence Information	
Sample Name	--
Heading	Displays information about a user-defined column heading that is pertinent to the active sample row in the sequence. Set the headings in the Sequence Setup view.
Instrument Method:	Displays the <i>Drive:\Path</i> for the instrument method used to acquire the raw data file.
Processing Method	Displays the <i>Drive:\Path</i> for the processing method listed in the sequence if applicable.
Vial	Displays the position of a sample in the autosampler.
Injection Volume	Displays the sample injection volume in microliters.
Sample Weight	Displays the amount of a component that has been placed in the sample. The data system reports only include this information. It does not convert units.
Sample Volume	Displays the volume of a component that has been placed in the sample. The data system reports only include this information. It does not convert units.

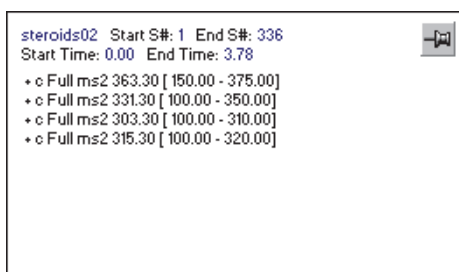
Table 27. Sample information view parameters (Sheet 2 of 2)

Parameter	Description
ISTD Amount	Displays the value entered in the ISTD Corr Amt column of a sequence table. If the value in this box is not 0.000, the value is used in an algorithm to correct for a case when any internal standard amounts specified in the active instrument method are correct, but when the amount of internal standard actually in one or more samples is different than the amount specified in the instrument method. This correction eliminates the necessity of remaking any samples to the internal standard concentrations or amounts specified in the instrument method and re-running the samples.
Dil Factor	Displays the dilution factor that was used to prepare the sample.

Scan Filter View

Use the Qual Browser window to open a raw data file, create a grid of interactive cells, and display a list of scan filters in the scan filter format. Use menu commands to select view options.

This figure shows an example of the scan filter view.



View Header Information

- Start S#
- End S#
- Start Time
- End Time

Scan Filter View Shortcut Menu

Right-click the scan filter view to open the scan filter view shortcut menu. [Table 28](#) describes the commands in the shortcut menu for the scan filter view.

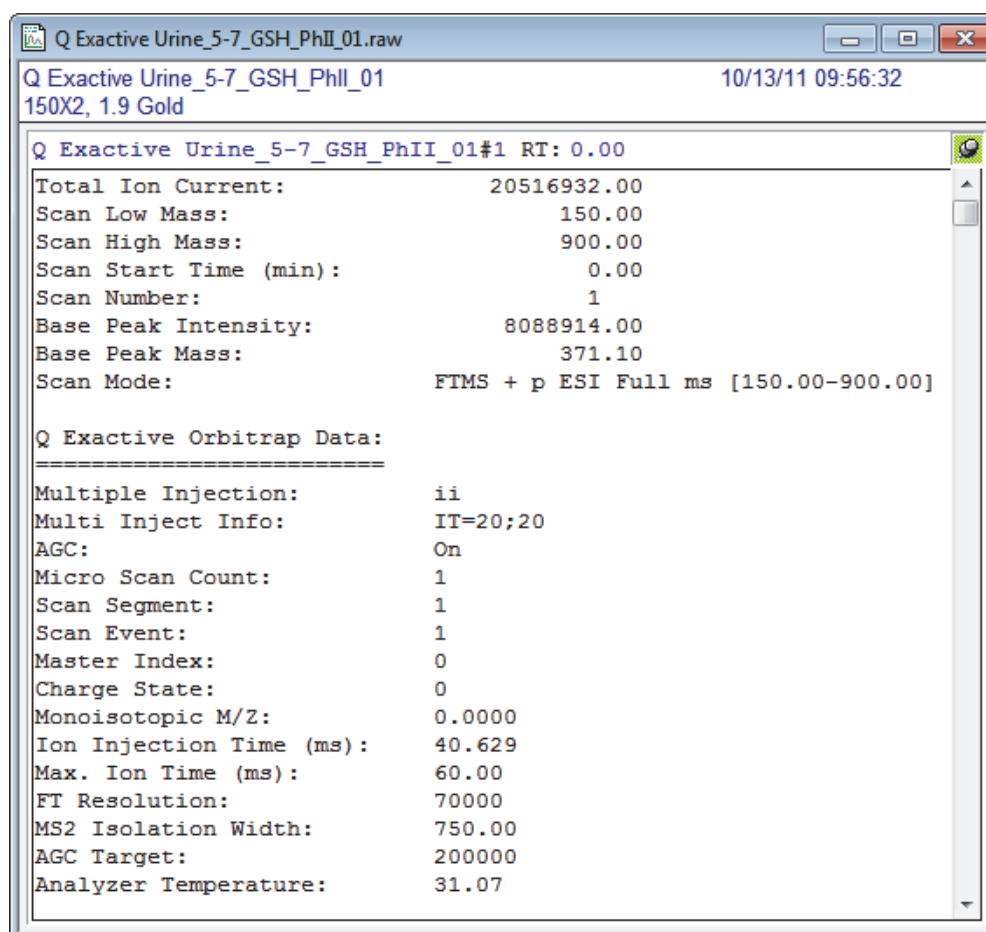
Table 28. Scan Filter view shortcut menu commands

Command	Description
View	Use the commands on the View menu to change the view in the active cell. For a brief description of each view, see Table 17 on page 158 .
Ranges	Opens the Scan Filter Range dialog box where you can set the scan filter time.

Scan Header View

Use the Qual Browser window to open a raw data file, create a grid of interactive cells, and display scan header information for a selected scan in any of the cells. Use menu commands to select view options.

This figure shows an example of the scan header view.



Display Header Information

- S#:
- RT:

Scan Header Information

The master scan number is an integer value assigned to the precursor scan for the current data-dependent scan. This value is listed in the scan header of the data-dependent scan.

- Total Ion Current
- Scan Low Mass
- Scan Start Time
- Scan End Time
- Scan Number
- Master Scan Number (for some mass spectrometers)
- Micro Scan Count
- Base Peak Intensity
- Base Peak Mass
- Ion Injection Time
- Scan Mode
- Scan Segment
- Scan Event
- Elapsed Scan Time
- API Source CID Energy
- Resolution
- Data Type
- Polarity
- Average Scan by Inst.
- Backgd Subtracted by Instrument
- Charge State
- Number of Data Packets
- MS Order
- Parent Mass(es)
- Isolation Width(s)
- Collision Energy(s)

Scan Header View Shortcut Menu

Right-click the scan header view to open the scan header view shortcut menu. [Table 29](#) describes the commands in the shortcut menu for the scan header view.

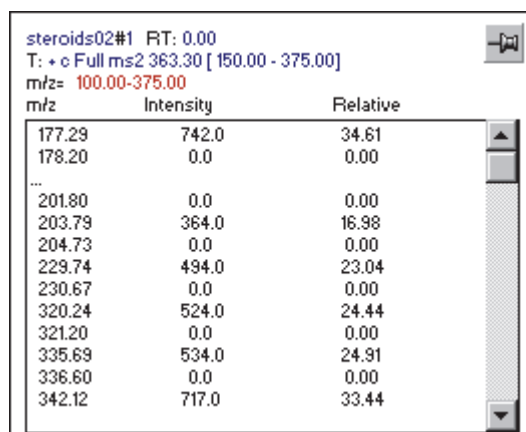
Table 29. Scan Header view shortcut menu commands

Command	Description
View	Use the commands on the View menu to change the view in the active cell. For a brief description of each view, see Table 17 on page 158 .
Ranges	Opens the Scan Header Range dialog box, where you can set the scan header time.

Spectrum List View

The spectrum list view can display either of these lists:

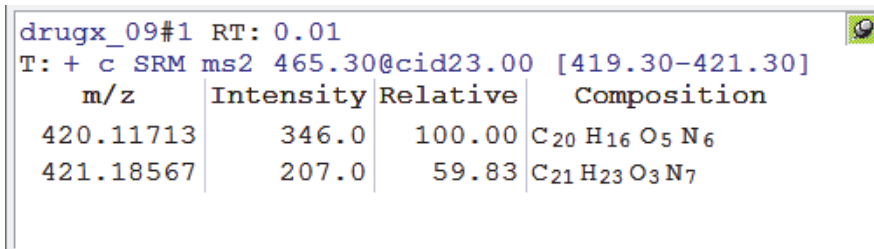
- A list containing m/z , absolute intensity, and relative intensity for each of the selected ions. If you have label stream data, you can also include Resolution, Charge, Baseline, and Noise. If you have a profile scan, you can also display centroided data. This figure shows an example of the spectrum list view.



steroids02#1 RT: 0.00
T: + c Full ms2 363.30 [150.00 - 375.00]
m/z= 100.00-375.00

m/z	Intensity	Relative
177.29	742.0	34.61
178.20	0.0	0.00
...		
201.80	0.0	0.00
203.79	364.0	16.98
204.73	0.0	0.00
229.74	494.0	23.04
230.67	0.0	0.00
320.24	524.0	24.44
321.20	0.0	0.00
335.69	534.0	24.91
336.60	0.0	0.00
342.12	717.0	33.44

- A list containing m/z , theoretical mass, delta (mms), RDB equivalents, and composition from your simulation data.



drugx_09#1 RT: 0.01
T: + c SRM ms2 465.30@cid23.00 [419.30-421.30]

m/z	Intensity	Relative	Composition
420.11713	346.0	100.00	C ₂₀ H ₁₆ O ₅ N ₆
421.18567	207.0	59.83	C ₂₁ H ₂₃ O ₃ N ₇

For information about the display options for the spectrum list view, see these topics:

- [Spectrum List View – Display Options Dialog Box – Normalization Page](#)
- [Spectrum List View – Display Options Dialog Box – Style Page](#)
- [Spectrum List View – Display Options Dialog Box – Composition Page](#)

View Header Information

- S# Scan number
- RT Retention time
- AV Averaged (followed by the number of averaged scans)
- SB Subtracted (followed by subtraction information)
- NL Neutral loss
- T Scan type
- F Scan filter

Spectrum List View Shortcut Menu

To open the spectrum list view shortcut menu, right-click the spectrum list view. [Table 30](#) describes the commands in the shortcut menu for the spectrum list view.

Table 30. Spectrum list view shortcut menu commands (Sheet 1 of 2)

Command	Description
View	Use the commands on the View menu to change the view in the active cell. For a brief description of each view, see Table 17 on page 158 .
Subtract Spectra > 1 Range	Perform a peak-by-peak subtraction of selected scans contained in one background region of a chromatogram view from the current spectrum view. Use this command to eliminate background scans that might interfere with the display of spectrum peaks of interest. The subtracted scans need to use the same scan filter as the target scans. For more information, see Subtracting Background Spectra .
Subtract Spectra > 2 Ranges	Perform a peak-by-peak subtraction of selected scans contained in two selected background regions of a chromatogram view from the current spectrum view. Use this command to eliminate background peaks that might be interfering with the display of spectrum peaks of interest. The subtracted scans need to use the same scan filter as the target scans. For more information, see Subtracting Background Spectra .

Table 30. Spectrum list view shortcut menu commands (Sheet 2 of 2)

Command	Description
Export > Clipboard (Exact Mass)	Export the exact m/z versus intensity values of the spectrum to the Clipboard. The data system also copies the raw data file name, scan filter, scan number, and retention time information to the Clipboard.
Export > Clipboard (Nominal Mass)	Export the rounded m/z versus intensity values of the spectrum to the Clipboard. The application also copies the raw data file name, scan filter, scan number, and retention time information to the Clipboard.
Elemental Composition	Determine which chemical formulas have m/z values most like that of the spectrum peaks. The application then displays the chemical formula labels at the top of the spectrum peaks. If the application displays the elemental composition values in light gray, close Qual Browser and choose Xcalibur Roadmap > Tools > Configuration. The Configuration page opens. Click the Fonts tab and set all font sizes to a minimum of 10 points.
Ranges	View and edit the mass range, time range, and other properties of a spectrum list.
Display Options	Change the appearance of your spectrum list.

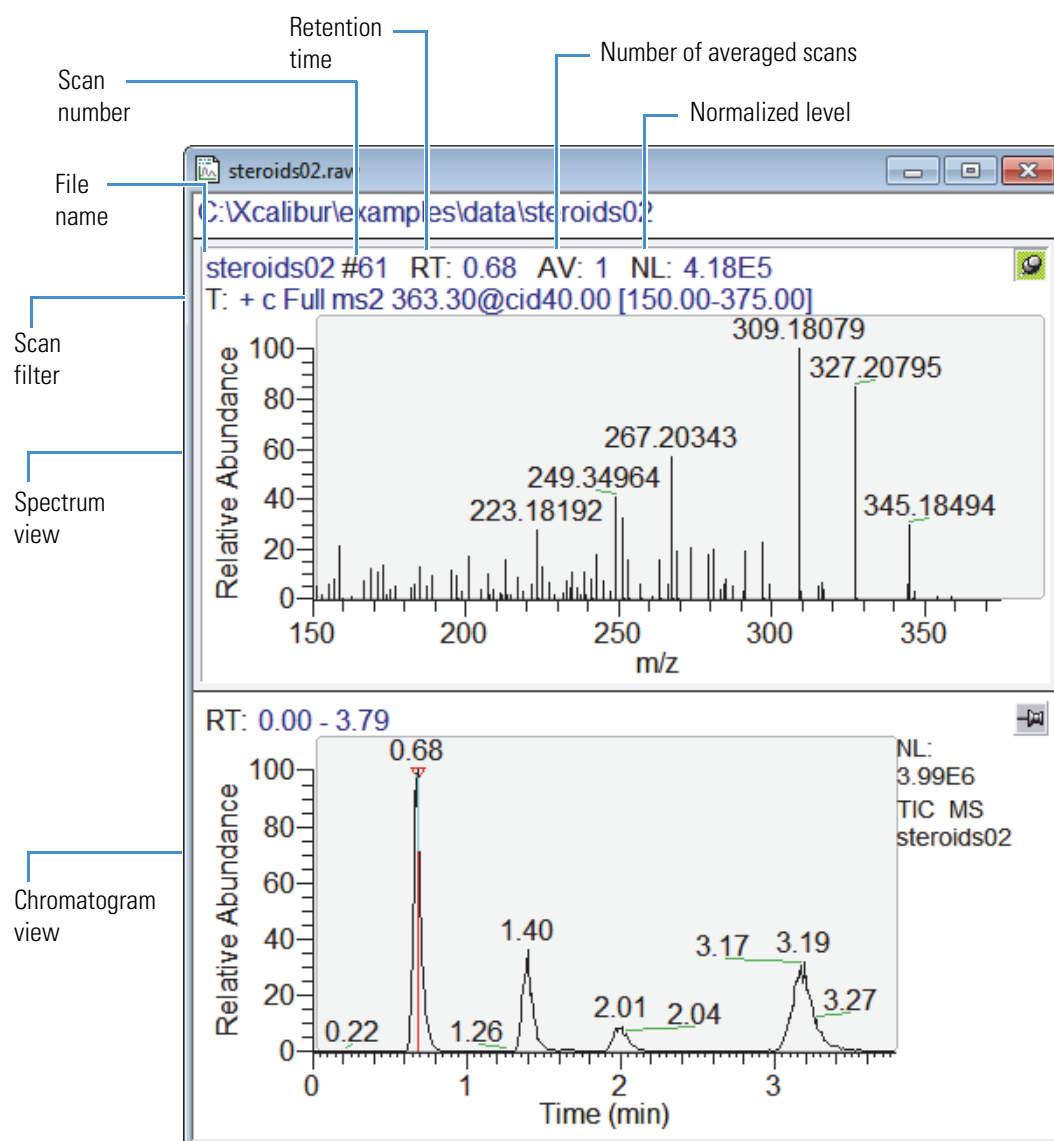
Spectrum View

Use the Qual Browser window to open a raw data file, create a grid of interactive cells, and display a spectrum and related header information in any of the cells. Use menu commands to select display options.

The spectrum view contains a scan header and a plot of the relative abundance versus mass-to-charge (m/z) ratio of an ion. From left to right, the first line of the scan header lists the file name, scan number, retention time, number of averaged scans, and the normalized level of the scan. The second line lists the scan filter.

Figure 68 shows a spectrum view with a data-dependent MS/MS product ion scan (#61) that has been selected from the TIC MS chromatogram at a retention time of 0.68 minutes.

Figure 68. Spectrum view (top cell) and chromatogram view (bottom cell)



View Header Information

- S# Scan number
- RT Retention time
- AV Averaged (followed by the number of averaged scans)
- SB Subtracted (followed by subtraction information)
- NL Normalized level
- T Scan type
- F Scan filter

Spectrum View Shortcut Menu

To open the spectrum view shortcut menu, right-click the spectrum view.

[Table 31](#) describes the commands in the shortcut menu for the spectrum view.

Table 31. Spectrum view shortcut menu commands (Sheet 1 of 2)

Command	Description
View	Use the commands on the View menu to change the view in the active cell. For a brief description of each view, see Table 17 on page 158 .
Plot	
Plot > Insert	Insert a copy of the selected (grayed) plot above the selected plot. Select a plot.
Plot > Delete	Delete the selected (grayed) plot. Select a plot.
Plot > Move Up	Switch positions of the selected (grayed) plot with the one above it. Select a plot.
Plot > Move Down	Switch positions of the selected (grayed) plot with the one below it. Select a plot.
Subtract Spectra	
Subtract Spectra > 1 Range	Perform a peak-by-peak subtraction of selected scans contained in one background region of a chromatogram view from the current spectrum view. Use this command to eliminate background scans that might interfere with the display of spectrum peaks of interest. The subtracted scans need to use the same scan filter as the target scans. For more information, see Subtracting Background Spectra .
Subtract Spectra > 2 Ranges	Perform a peak-by-peak subtraction of selected scans contained in two selected background regions of a chromatogram view from the current spectrum view. Use this command to eliminate background peaks that might interfere with the display of spectrum peaks of interest. The subtracted scans need to use the same scan filter as the target scans. For more information, see Subtracting Background Spectra .
Subtract Spectra > Clear	Remove all subtract spectra modifications to the spectrum view. The data system also removes the SB: xx notation in the spectrum view header to indicate that the spectrum view has been returned to the original display before application of the Subtract Spectra command.

Table 31. Spectrum view shortcut menu commands (Sheet 2 of 2)

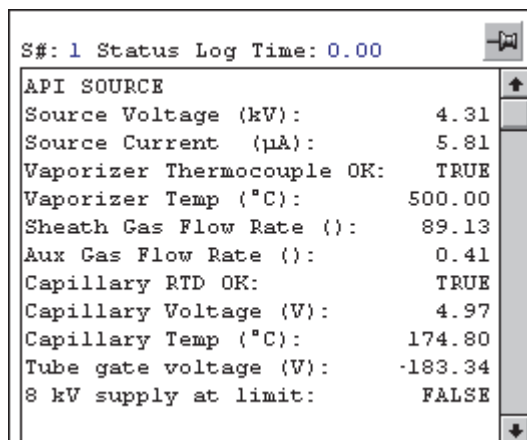
Command	Description
Library	
Library > Search	Submit the active spectrum to a library search. The application displays the results of the search in the Library Search Results window.
Library > Export to Library Browser	Export the active spectrum to the Library Browser application.
Library > Options	Opens the Search Properties dialog box, where you can select the libraries used during a library search. You can also change various parameters that determine how the search is carried out.
Export	
Export > Clipboard (Exact Mass)	Export the exact m/z versus intensity values of the spectrum to the Clipboard. The data system also copies the raw data file name, scan filter, scan number, and retention time information to the Clipboard.
Export > Clipboard (Nominal Mass)	Export the rounded m/z versus intensity values of the spectrum to the Clipboard. The application also copies the raw data file name, scan filter, scan number, and retention time information to the Clipboard.
Export > Write to Raw File	Save the mass spectrum that is displayed in the spectrum view as a raw data file. The data system appends –qb to the end of the original raw data file name, adds information about the origin of the mass spectrum to the status log, and saves the file as a raw data file. When you open a raw data file that contains only a single mass spectrum, see the Extended Information section of the status log for formation about the origin of the mass spectrum.
Elemental Composition	
Elemental Composition	Determine which chemical formulas have m/z values most like that of the spectrum peaks. The data system then displays the chemical formula labels at the top of the spectrum peaks. If the data system displays the elemental composition values in light gray, close Qual Browser and choose Xcalibur Roadmap > Tools > Configuration. The Configuration page opens. Click the Fonts tab and set all font sizes to a minimum of 10 points.
Ranges	
Ranges	View and change the mass range, time range, and other properties of a spectrum plot.
Display Options	
Display Options	Select the style, color, labels, axis, and normalization settings.

Status Log View

Use the Qual Browser window to open a raw data file, create a grid of interactive cells, and view status log information for a selected scan in any of the cells.

For a list of the available views, see [Qual Browser Views](#).

This figure shows an example of the status log view.



S#: 1 Status Log Time: 0.00	
API SOURCE	
Source Voltage (kV):	4.31
Source Current (µA):	5.81
Vaporizer Thermocouple OK:	TRUE
Vaporizer Temp (°C):	500.00
Sheath Gas Flow Rate (l/min):	89.13
Aux Gas Flow Rate (l/min):	0.41
Capillary RTD OK:	TRUE
Capillary Voltage (V):	4.97
Capillary Temp (°C):	174.80
Tube gate voltage (V):	-183.34
8 kV supply at limit:	FALSE

View Header Information

- S#:
- Status Log Time

Status Log Information

API Source

- Source Voltage
- Source Current
- Vaporizer Thermocouple OK: [True/False]
- Vaporizer Temp
- Sheath Gas Flow Rate
- Aux Gas Flow Rate
- Capillary RTD OK: [True/False]
- Capillary Voltage
- Capillary Temp
- Tube Gate Voltage
- 8 kV Supply at Limit: [True/False]

Vacuum

- Vacuum OK: [True/False]
- Ion Gauge Pressure OK: [True/False]
- Ion Gauge On: [True/False]
- Ion Gauge (Torr $\times 10^{-5}$)
- Convectron Pressure OK: [True/False]
- Convectron Gauge

Turbo Pump

- Status
- Life
- Speed
- Power
- Temperature

Ion Optics

- Octapole Frequency On: [True/False]
- Octapole 1 Offset
- Octapole 2 Offset
- Lens Voltage
- Trap DC Offset
- Analyzer Temperature

Main RF

- Reference Sine Wave OK: [True/False]
- Standing Wave Ratio Failed: [True/False]
- Main RF DAC (steps)
- Main RF Detected
- RF Detector Temperature
- Main RF Modulation
- Main RF Amplifier
- RF Generator Temp

Ion Detection System

- Multiplier Actual

Power Supplies

- +5V Supply Voltage
- –15V Supply Voltage
- +15V Supply Voltage
- +24V Supply Voltage
- –28V Supply Voltage
- +28V Supply Voltage
- +28V Supply Current
- +35V Supply Voltage
- +36V Supply Voltage
- –150V Supply Voltage
- +150V Supply Voltage
- –205V Supply Voltage
- +205V Supply Voltage
- Ambient Temp

Instrument Status

- Instrument: On/Off
- Analysis
- Retention Time

Autosampler

- Status
- Current Vial Position
- Number of Injections

LC Pump

- Status
- Run Time
- Flow Rate
- Pump Pressure [Minimum]
- Solvent Composition

Analog Inputs

- Number Activated

Syringe Pump

- Status
- Flow Rate
- Infused Volume
- Syringe Diameter

Digital Inputs

- Ready In is active:
[True/False]
- Start In is active:
[True/False]
- Divert/Inject Valve

UV Detector

- Status

Tune Method View

Use the Qual Browser window to open a raw data file, create a grid of interactive cells, and view a tune method for a specified run segment in any of the cells. Use menu commands to select view options.

For a list of the available cell views, see [Qual Browser Views](#).

This figure shows an example of the Tune method view.

Segment: 1		
Capillary Temp (°C):	175.00	↑
APCI Vaporizer Temp (°C):	500.00	
Source Voltage (kV):	8.00	
Source Current (µA):	6.00	
Sheath Gas Flow (l):	90.00	
Aux Gas Flow (l):	10.00	
Capillary Voltage (V):	5.00	
Tube Lens Offset (V):	55.00	
Octapole RF Amplifier (Vp-p):	400.00	
Octapole 1 Offset (V):	-2.25	
Octapole 2 Offset (V):	-5.50	
InterOctapole Lens Voltage (V):	-16.00	
Trap DC Offset Voltage (V):	-10.00	
Multiplier Voltage (V):	0.00	
Maximum Ion Time (ms):	400.00	
Ion Time (ms):	5.00	
Data Type:	Centroid	
Source Type:	APCI	
Polarity:	Positive	↓

View Header Information

- Segment

Tune Method Information

- Capillary Temp
- APCI Vaporizer Temp
- Source Voltage (APCI)
- Source Voltage (API)
- Source Current (APCI)
- Source Current (API)
- Sheath Gas Flow
- Aux Gas Flow
- Capillary Voltage (API)
- Tube Lens Offset (API)
- Octapole RF Amplifier
- Octapole 1 Offset
- Octapole 2 Offset
- InterOctapole Lens Voltage
- Trap DC Offset Voltage
- Multiplier Voltage
- Maximum Ion Time
- Ion Time
- Data Type
- Source Type
- Polarity
- Zoom Micro Scans
- Zoom AGC Target
- Full Micro Scans
- Full AGC Target
- MSⁿ Micro Scans
- MSⁿ AGC Target

Qual Browser Info Bar

The Qual Browser Info Bar displays information about the active grid cell for chromatogram or spectrum views. It consists of these pages.



Cell Information Page



Elemental Composition Page



MSⁿ Browser Information Page



Avalon Peak Detection Settings Page



ICIS Peak Detection Settings Page



Genesis Peak Detection Settings Page



Result File Information Page



Sequence Information Page



Spectrum Simulation Page

Cell Information Page

Use the cell information page of the Info Bar view to view information about the active grid cell for spectrum or chromatogram views.

For more information, see [Using the Cell Information Page](#).

[Table 32](#) describes the parameters on the cell information page of the Info Bar view.

Table 32. Cell Information page parameters (Sheet 1 of 2)

Parameter	Description
Spectrum Views	
 Plot type and Raw File Name	View information about a raw data file created by the mass spectrometer when a sample is run, containing raw analysis data. The icon changes to reflect the type of plot present.
 Raw File Path	View a listing of the directories that lead from the current drive and directory to the raw data file.
 Scan Filter (if applied)	View scan filters used in a raw data file. The data system uses scan filters to specify that processing is to be applied to a subset of the scans in a raw data file. The application creates scan filters from instrument method settings and can be selected using the Scan Filter boxes in the data system windows.
 Fix Scale (if applied)	View the current maximum range for the y axis of the active spectrum. This box is only active when you select the Spectrum Fix Scale check box. The maximum y -axis value can range from 10 to 10^{10} . To change the value, input the new maximum y -axis value in the Spectrum Fix Scale box.
 Background Subtraction: Time Range 1, Time Range 2 (if applied)	The chromatogram time range or ranges used for background subtraction.
Chromatogram Views	
 Raw File Name	View information about a raw data file (.raw) created by the mass spectrometer when a sample is run, containing raw analysis data.
 Raw File Path	View a listing of the directories that lead from the current drive and directory to the raw data file.
 Scan Filter (if applied)	View applied scan filters. The data system uses scan filters to specify that processing is to be applied to a subset of the scans in a raw data file. Scan filters are created by the application from instrument method settings and can be selected using Scan Filter boxes in the data system windows.

Table 32. Cell Information page parameters (Sheet 2 of 2)

Parameter	Description
 Fix Scale (if applied)	View or change the current maximum range for the <i>y</i> axis of the active chromatogram. This box is only active when you select the Spectrum Fix Scale check box. The maximum <i>y</i> -axis value can range from 10 to 10^{10} . To change the value, input the new maximum <i>y</i> -axis value in the Spectrum Fix Scale box.
 Detector Delay	View the time difference in minutes between data acquisition for the UV or analog detector and the mass spectrometer. To align the chromatographic information from two detectors, the data system corrects for the delay time between the detectors. The delay time is a user-specified value.
 Mass Range (for mass range plot type only)	View the mass spectrometer mass ranges for a type of chromatogram where the application sums all ions from one or more specified mass spectrometer mass ranges plots them as a function of time.
 Background Subtraction Time Range 1, Time Range 2 (if applied)	View the chromatogram time range or ranges used for background subtraction.

Right-click the cell information page to open a shortcut menu.

[Table 33](#) describes the commands in the shortcut menu for the cell information page.

Table 33. Cell Information page shortcut menu commands

Command	Description
Ranges	View or change the properties of all the plots in the active cell. You can view or modify the time and mass ranges and change background subtraction and smoothing parameters.
Delete	Delete the selected plot from the cell.

Elemental Composition Page

Use the Elemental Composition page, , of the Info Bar to calculate the best matching chemical formula for a mass or a list of masses from a spectrum.

Table 34 describes the parameters on the Elemental Composition page of the Info Bar view.

Table 34. Elemental Composition page parameters (Sheet 1 of 4)

Parameter	Description
Elemental Composition	
Elemental Composition	Specify the mass and the charge state and whether to include the Nitrogen Rule in the calculation of possible formulas. See Nitrogen Rule for more information. If the data system displays the elemental composition values in light gray, close Qual Browser and choose Xcalibur Roadmap > Tools > Configuration . The Configuration page opens. Click the Fonts tab and set all font sizes to a minimum of 10 points.
Mass	View or change the mass you want the data system to use to calculate probable chemical formulas. To change the mass value, type or select a mass from 0.5 to 100000 . To calculate formulas and display them in the results list, click Calculate .
Max Results	View or change the maximum number of formulas you want the data system to display. To increase or decrease the number of results, type or select a number from 1 to 400 . To calculate formulas and display them in the results list, click Calculate .
Calculate button	Calculate formulas and display them in the results list after you type a mass from 0.5 to 100 000 in the Mass box.
Results table	
View a table displaying the results of the formula calculation using the values specified in the Calculate Composition box. The list is presented in order of best fit and contains rows that you can select to compute a spectrum or to print the results to a file.	
Idx	The Index (Idx) column displays the number of the row in the results list. The Index column displays an incremental list of numbers in order of Best Fit after specifying that the data system calculate probable chemical formulas. To display the simulated mass spectrum for a formula in the results table, click anywhere in the row of interest and click Simulate . A view opens to the right of the Info Bar with a simulated mass spectrum. To view the information as a spectrum list, right-click the view and choose Spectrum List from the shortcut men.
Formula	This column displays the formulas calculated using the values specified in the Calculate Composition box and the limits specified in the Limits area.
RDB	View the ring and double-bond equivalents calculated for each of the formulas in the Results List. See also Double Bond/Ring Equivalent box.

Table 34. Elemental Composition page parameters (Sheet 2 of 4)

Parameter	Description
Delta [units]	View the difference between the specified mass and the calculated mass, in amu, mmu, or ppm units, for each of the formulas in the results table.
File button	Write a formula or a group of formulas to a CSV file. ❖ To save one or more formulas to a CSV file 1. Do one of the following: - While pressing the SHIFT key, select a contiguous set of rows in the result list to be copied. —or— - While pressing the CTRL key, select the rows in the results list to be copied. 2. Click File . The Save As dialog box opens. 3. Select the directory where you want to store the file, type a name in the File Name box, and then click Save . The application automatically saves the file as a CSV file.
List button	View the information from the results list in the spectrum list view. The spectrum list view lists the m/z value, theoretical mass, delta (mmu), RDB equivalents, and composition (formula) for each selected ion.
Simulate button	Simulate the spectrum of a selected formula in the results table. The spectrum is based on the full isotope distribution for that formula.
Limits area	
Limits	Limit the number of possible elemental compositions. You can specify limits on peak width and on sites of unsaturation (or double bond and ring equivalents.)
Charge	View or change the charge state you want Isotope Viewer to use to calculate probable formulas. To change the charge state, type or select a number from –99 to +99 . To calculate formulas and display them in the results table, click Calculate .

Table 34. Elemental Composition page parameters (Sheet 3 of 4)

Parameter	Description
Nitrogen Rule	Select whether to use the Nitrogen Rule in the formula calculation. The choices in the list are as follows: Do Not Use, Even, and Odd. For molecular ions of even or odd molecular weight, specify that formulas contain either an even or an odd number of nitrogen atoms, respectively, in the Nitrogen-Rule list. Conversely, for fragment ions of even or odd molecular weight, specify the reverse; that is, specify odd or even, respectively, in the Nitrogen-Rule list. McLafferty states the Nitrogen Rule as follows: “If an odd-electron ion contains no (or an even number of) nitrogen atoms, its molecular ion will be at an even mass number. [Similarly,] an odd-electron ion will be at an odd mass number if it contains an odd number of nitrogen atoms.”
Mass Tolerance	Specify a mass tolerance to restrict the number possible elemental compositions. The data system returns results of the elemental composition search only if the computed formula matches the entered mass within the specified tolerance. The value must be between 0.00 and 1000.00.
Units	View the units that you can associate with mass tolerance: amu (atomic mass units), mmu (millimass units), and ppm (parts-per-million). If you specify error limits in ppm, the errors are mass-dependent and get larger at low masses and smaller at high masses.
Double Bond/Ring Equivalents	View or change a range of values for double bonds and ring equivalents—a measure of the number of unsaturated bonds in a compound—and limits the calculated formulas to only those that make sense chemically. You can specify limits in a range from –1000.0 to +1000.0. The value is calculated by the following formula: $D = 1 + \frac{\sum_i^{i_{\max}} N_i (V_i - 2)}{2}$ where D is the value for the RDB $i_{\max}$ is the total number of different elements in the composition N_i is the number of atoms of element i V_i is the valence of atom i The calculation results in an exact integer such as 3.0, indicating an odd-electron ion, or an integer with a remainder of 0.5, indicating an even-electron ion. A value of –0.5 is the minimum value and corresponds to a protonated, saturated compound (for example, H_3O^+).

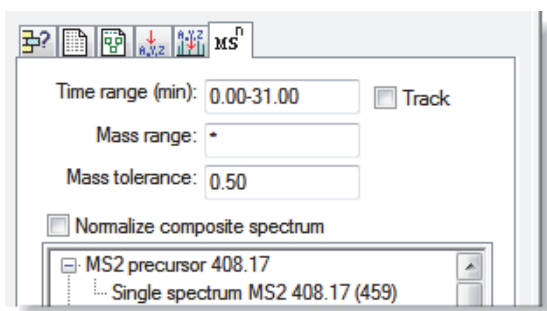
Table 34. Elemental Composition page parameters (Sheet 4 of 4)

Parameter	Description
Elements in Use	
Elements in Use	Defines which isotopes, and the number of occurrences for each isotope, to consider when the data system calculates possible elemental compositions for a specified mass value.
Isotope	View the isotopes that you want the data system to consider when it calculates elemental compositions for a given mass. To add an isotope, click in an empty area in the Isotope column. The Select Isotopes Dialog Box opens. Also, you can right-click in the grid and choose Add Isotopes from the shortcut menu. To remove an isotope, right-click an isotope and choose Delete Isotope from the shortcut menu.
Min	View the minimum number of occurrences of a specified isotope for a determination of formula composition.
Max	View the maximum number of occurrences of a specified isotope for a determination of formula composition.
DB Eq.	View the values of the lower and upper limits for double bond and ring equivalents that IsotopeViewer calculates for each isotope in the Elements In Use List. See also Double Bond/Ring Equivalent box.
Mass	View the exact isotopic mass for each isotope specify in the Elements In Use List.
Buttons	
Load	Select an isotope limits file (.lim) that contains a set of isotope limits.
Save As	Save a list of isotopes as an isotope limits file with a .lim file name extension.
	❖ To select multiple isotopes in the Elements In Use list 1. Click an isotope symbol. 2. Press CTRL + click or SHIFT + click to select other isotope symbols you want in the isotope limits file.
Apply	Apply the Elemental Composition box settings to the spectrum.

MSn Browser Information Page

Use the MSⁿ browser information page of the Info Bar to display and analyze MSⁿ experimental data.

Figure 69. Information page – MSⁿ Browser



Note The MSⁿ browser information page is not available for all mass spectrometers.

Table 35 describes the parameters on the MSⁿ browser information page of the Info Bar view.

Table 35. MSⁿ Browser Information page parameters (Sheet 1 of 4)

Parameter	Description
 MS2 Precursor	Select MSⁿ spectra. The  icon is the top of the tree view displayed in the Info bar of the MSⁿ Browser feature available in the Qual Browser window. A typical starting view is shown below.   MS2 precursor 1108.16   MS2 precursor 1122.17   MS2 precursor 1208.12   MS2 precursor 1222.17   MS2 precursor 1308.23 The MS2 precursor ion <i>m/z</i> is displayed to the right of the icon. The MS2 precursor ion is the parent ion mass from the MS1 experiment that is used for the MS2 (MS/MS) experiment. If you click the plus (+) sign, all of the MS3 precursor icons appear and the icon for the MS2 average spectrum appears. See the example below. -  MS2 precursor 1108.16 -  MS3 precursor 775.98  Composite spectrum MS3 1108.16,775.98  Average spectrum MS3 1108.16,775.98 (38-185)  Average spectrum MS2 1108.16 (37-184) +  MS2 precursor 1122.17 +  MS2 precursor 1208.12 +  MS2 precursor 1222.17 +  MS2 precursor 1308.23 To view a spectrum, click the  icon of interest.

Table 35. MSⁿ Browser Information page parameters (Sheet 2 of 4)

Parameter	Description
 Composite Spectrum	View a spectrum that is the sum of all MS², MS³, MS⁴, MS⁵,...MS¹⁰ spectra, as defined by your instrument method. • A spectrum that has not been normalized When the Normalize Composite Spectrum check box is unavailable on the MSⁿ page of the Info bar, the data system normalizes the composite spectrum (NL) to the highest intensity of the MS² experiment. When you choose this option, the data system displays the intensities of consecutive MS experiments at lower and lower intensities. An example follows for a processing filter for a composite spectrum (not normalized) of an MS³ experiment where four microscans were averaged. The precursor (parent) mass of the MS² experiment is m/z 1108.16 and the precursor (parent) mass of the MS³ experiment is m/z 775.98. The relative collision energy used for both experiments was 30 percent: <pre>Msnbrows#38-185 RT:0.98-4.91 AV:4 NL: 2.73E3 T: + c CMP ms3 1108.16@30.00 776.03@30.00 [200.00-1560.00]</pre> These peaks are labeled: (Parent Mass) PM MS² and PM MS³. • Normalized spectrum When the Normalize Composite Spectrum check box is active on the MSⁿ page of the Info bar, each MSⁿ spectrum is individually normalized (NL) so that its highest peak is displayed at Relative Abundance 100. The relative peak heights of this display are therefore not meaningful. For example, a composite spectrum (CMP) for an MS³ experiment displays both the MS² base peak and the MS³ base peak at Relative Abundance 100 and maintains all other relative abundances of the other ions in each spectrum. Use this display normalization option to view multiple spectra simultaneously, even if the absolute value of the intensities are significantly different. An example follows for a process filter for a normalized composite spectrum of an MS³ experiment in which four microscans were averaged. The precursor (parent) mass of the MS¹ experiment is m/z 1108.16 and the precursor (parent) mass of the MS² experiment is m/z 775.98. The relative collision used was 30 percent: <pre>Msnbrows#38-185 RT:0.98-4.91 AV:4 NL: 2.73E3 T: + c CMP ms3 1108.16 775.98 [200.00-2000.00]</pre>

Table 35. MSⁿ Browser Information page parameters (Sheet 3 of 4)

Parameter	Description
 Average Spectrum	View a spectrum that is the sum of all of the microscans taken for a particular MSⁿ experiment. An average spectrum can be independently displayed for MS², MS³, MS⁴, MS⁵, ...MS¹⁰ experiments. The average spectrum is displayed normalized (NL) to the average base peak. In the event that there is only one spectrum with one scan to average, the data system displays the term single spectrum instead of average spectrum. In other words, single spectrum is a special case of average spectrum. An example of a processing filter for the average spectrum of an MS³ experiment in which two microscans were averaged follows. The precursor (parent) mass of the MS¹ experiment is <i>m/z</i> 1108.07 and the precursor (parent) mass of the MS² experiment is <i>m/z</i> 776.03: Msnbrows#38–185 RT:1.01–4.91 AV:2 NL: 2.73E3 T: + MS3 1108.07@30.00 776.03@30.00 [200.00–1560.00]
 Scan Number At RT	Select single scans (individual scans) on the MS ⁿ Browser Information page if you right-click the MS ⁿ Information page and choose Include Single Scans .
Time Range	Enter a chromatogram time range. The MSⁿ browser changes the Time axis on the chromatogram (View > Chromatogram) and limits the spectra available for display to those taken during the specified time range. There are two ways to change the Time Range: • Enter the time range in minutes in the Time Range box. The valid range is 0.00 to 999.0 minutes. The format is <i>From–To</i>. For example, to view the chromatogram time range from 0.01 to 5.10 minutes, type 0.01–5.10. • Select the Track check box to track the time range using the chromatogram view. Then, drag the cursor horizontally across the chromatogram view from the minimum time to the maximum time of interest. The data system changes the range in the Time Range box and displays the chromatogram with its revised range. To return to the original range, click the Zoom Reset icon, .
Track	Track the time range using the chromatogram view. Then, drag the cursor horizontally across the chromatogram view (View > Chromatogram) from the minimum time to the maximum time of interest. The data system changes the range in the Time Range box and displays the chromatogram with its revised range. To return to the original range, click the Zoom Reset icon, .

Table 35. MSⁿ Browser Information page parameters (Sheet 4 of 4)

Parameter	Description
Mass Range	Enter the mass range that you are interested in viewing. The MSⁿ browser limits the viewable spectra to the specified mass range. To change the mass range, type the range in the Mass Range box. The valid range is <i>m/z</i> 65.00 to 2000.00. The format is <i>From–To</i>. For example, to view spectra having mass range <i>m/z</i> 100 to 500, type 100.00–500.00.
Mass Tolerance	View or change the current mass range over which spectra are not distinguished (grouped). The valid range is <i>m/z</i> 0.00 to 10.00. The default value is <i>m/z</i> 0.50. • If the mass tolerance is large (<i>m/z</i> >0.50), the data system groups scans that meet the range tolerance so that the number of individual scans can be reduced. • If the mass tolerance is small (<i>m/z</i> <0.50), the data system displays each scan from the specified precursor.
Normalize Composite Spectrum	Normalize the composite spectrum displayed in the spectrum view (View > Spectrum). This option results in a composite of individual spectra (MS², MS³, MS⁴, and so on), normalizing each spectrum to the highest intensity in the MS² experiment, not using the relative number of counts. This option provides easy comparison of MSⁿ experimental data. However, the data system does not retain the peak ratio of the MSⁿ data. Clear this check box if you do not want to normalize the composite spectrum displayed in the spectrum view (View > Spectrum). This option results in a composite of individual spectra (MS², MS³, MS⁴, and so on), normalizing the MS² spectrum to Relative Abundance 100 and displaying all other spectra relative to their actual number of counts. This option increases the difficulty of comparison of MSⁿ experimental data, however it retains the peak ratio information.

Table 36 describes the commands in the shortcut menu for the MSⁿ browser information page of the Info Bar view.

Table 36. MSⁿ browser Information page shortcut menu commands

Ranges	View or change the properties of all the plots in the active cell. You can view or modify the time and mass ranges and change background subtraction and smoothing parameters.
Include Individual Scans	If you clear this command, the MSⁿ Browser displays the MS² Average Spectrum and all MSⁿ Average Spectra and Composite Spectra that are included in the raw data file. If you select this command, the MSⁿ Browser displays the MS² Average Spectrum and all of the individual scans that make up the average spectrum. The number of individual scans is controlled by the selection of the Mass Tolerance value. If the Mass Tolerance is small (<0.50), individual scans are available for display. Individual scans might be grouped if the Mass Tolerance is large ($m/z > 0.50$). In addition, the MSⁿ Browser displays MSⁿ Average Spectra, MSⁿ Composite Spectra, and all of the MSⁿ individual scans. The functionality of the Mass Tolerance value is the same for all MSⁿ scans as that for MSⁿ scans as described above. Individual scans appear in the following format:  <i>Scan Number at Retention Time</i> For example, the icons for scan numbers 76, 115, and 154 appear below: <pre> + MS MS2 precursor 1222.138 - MS MS2 precursor 1307.958 + MS MS3 precursor 975.968  Average spectrum MS2 1307.958 (76-154)  76 at 2.012 mins  115 at 3.047 mins  154 at 4.088 mins </pre>
Normalize Composite Spectrum	View the selected spectrum as either normalized or not normalized.
Expand/Collapse List	View or hide the subentries in the list.
Export	Export the information to your computer Clipboard.
Print	Open the Print dialog box.

Avalon Peak Detection Settings Page

Use the Avalon Peak Detection Settings page of the Info Bar to specify peak identification and peak integration criteria to be applied to the active chromatogram displayed in the Qual Browser window.

❖ To calculate values for initial value events

1. Open a raw data file and make the chromatogram view active.
2. Click **Auto Calculate Initial Events**.

❖ To modify the settings for events in the event list

1. Select the row that you want to modify.
2. Enter the revised settings in the boxes below the list. Type values in the Time and Value boxes.

There are seven initial entry integration events, identified by the initial value setting in the Time column. These are the default integration events required by the Avalon integration algorithm. You can change the value of an initial entry integration event, but you cannot delete it or change its time value.

3. Click **Change** to automatically update both the event list and the chromatogram display.

❖ To add an event to the event list

1. Type values in the Time (Min) box and the Value box and select an event in the Event list.
2. Click **Add**.

❖ To delete an event

1. Select the row that you want to delete.
2. Click **Delete**.

Table 37 describes the parameters on the Avalon peak detection settings page, , of the Info Bar view.

Table 37. Avalon peak detection settings page parameters (Sheet 1 of 3)

Parameter	Description
Application of Settings	
Apply to All Plots	Apply the current chromatogram peak identification and integration settings to all displayed plots. To apply criteria to all plots, select the Apply to All Plots check box. To apply the criteria to only the active plot, clear this check box.
Event Table	
There are seven initial value integration events, identified by the initial value setting in the Time column. These are the default integration events required by the Avalon integration algorithm. You can change the value of an initial entry integration event, but you cannot delete it or change its time value. Use the Time and Value boxes and the Event list below the table to modify the list of events.	
Event column	Displays the integration events.
Time column	Displays the time for each event. You cannot change the time value for an Initial Value event; however, you can add the same event with a non-zero time value to the table.
Value column	Displays the values associated with each event. The range of factors allowed for each value is specific to each event.
Time box	Use this box to change the time for existing timed events or to specify the time for new events. You cannot change the time value for an initial value event, but you can add these events as events with non-zero time values to the table.
Event list	Use this list to add new events to the table.
Value box	Use this box to change the event values.
Events	
There are seven initial value events: Start/End Threshold, Bunch Factor, Area Threshold, P-P Threshold, Negative Peaks, Tension, and Tangent Skim. Of the seven initial value events, the Threshold and Bunch Factor parameters are the most important ones in controlling peak detection. The data system provides the following events.	
Start/End Threshold	Directly related to the RMS noise in the chromatogram, this value is Threshold, the fundamental control used for peak detection.
Bunch Factor	The Bunch Factor is the number of points grouped together during peak detection. It controls the bunching of chromatographic points during integration and does not affect the final area calculation of the peak. The Bunch Factor must be an integer between 1 and 6; a high bunch factor groups peaks into clusters.

Table 37. Avalon peak detection settings page parameters (Sheet 2 of 3)

Parameter	Description
Area Threshold	Controls the area cutoff. The application does not detect any peaks with a final area less than the area threshold. This control is in units of area for the data.
P-P Threshold	The peak to peak resolution threshold controls how much peak overlap must be present before two or more adjacent peaks create a peak cluster. Peak clusters have a baseline drop instead of valley to valley baselines. This integration event is specified as a percent of peak height overlap.
Negative Peaks	Automatically resets after a negative peak has been found.
Tension	Controls how closely the baseline should follow the overall shape of the chromatogram. A lower tension traces the baseline to follow changes in the chromatogram more closely. A high baseline tension follows the baseline less closely over longer time intervals. Set a value in minutes.
Tangent Skim	For fused peaks that are significantly different in size, the tangent skim method provides a method of allocating area to the various peaks. By default, the application chooses the tallest peak in a cluster as the parent (solvent). You can also identify which peak in the cluster is the parent. The application detects tangent skim peaks on either side (or both sides) of the parent peak. Tangent skim automatically resets at the end of the peak cluster.
These events are not required.	
Shoulders On	Turns on the detection of shoulders.
Shoulders Off	Shoulders Off Turns off the detection of shoulders.
Force Cluster On	Turns on the grouping of peaks into a single peak.
Force Cluster Off	Turns off the grouping of peaks into a single peak.
Disable Cluster On	Enables the grouping effect in the specified time range.
Disable Cluster Off	Disables the grouping effect in the specified time range.

Table 37. Avalon peak detection settings page parameters (Sheet 3 of 3)

Parameter	Description
Buttons	
Auto Calc Initial Events	Search for the best values of initial events that detect peaks in the data. This button is active with the event list of the Avalon peak detection algorithm only if you have a raw data file open. When you click the button, Avalon automatically estimates the initial values for peak detection based on the data in the current raw data file, and then displays those initial values in the event list. Any timed event in the event list is unchanged when you click this button. Auto Calculate Initial Events determines initial values for the following events only: Start Threshold, End Threshold, Area Threshold, P-P [Resolution] Threshold, Bunch Factor, Negative Peaks, and Tension. Additionally, you can specify timed events for these events in the same event list.
Add	Add a time/event/value entry for a timed event in the event list. When you click the Add button, both the event list and the chromatogram display update automatically with the added specification in the currently selected chromatogram.
Delete	Remove a highlighted event from the event list. You cannot delete initial values.
Change	Update a highlighted time/event/value entry in the event list. When you click the Change button, peak detection with the updated specification occurs automatically in the currently selected chromatogram. For initial events, the application changes only the values, and not the events.

ICIS Peak Detection Settings Page

Use the ICIS peak detection settings page, , of the Info Bar view to specify peak detection and integration criteria that the data system applies to the active raw data file displayed in the Qual Browser window.

Table 38 describes the parameters on the ICIS peak detection settings page of the Info Bar view.

Table 38. ICIS peak detection settings page parameters (Sheet 1 of 3)

Parameter	Description
Application of Settings	
Apply to All Plots	Apply the current chromatogram peak identification and integration settings to all displayed plots. To apply criteria to all plots, select the Apply to All Plots check box. To apply the criteria to only the active plot, clear this check box.
Peak Parameters	
Baseline Window	Specify the number of scans to review, looking for a local minima. The valid range is 1 through 500. The default value is 40 scans. This value is used by the ICIS peak detection algorithm.
Area Noise Factor	Specify the noise level multiplier used to determine the peak edge after the location of the possible peak. The valid multiplier range is 1 through 500. The default multiplier is 5. This value is used by the ICIS peak detection algorithm.
Peak Noise Factor	Specify the noise level multiplier used to determine the potential peak signal threshold. The valid multiplier range is 1 through 1000. The default multiplier is 10. This value is used by the ICIS peak detection algorithm.
Constrain Peak Width	Limit the peak width of a component during peak integration of a chromatogram. You can then set values that control when peak integration is turned on and off by specifying a peak height threshold and a tailing factor. To constrain a peak width, select the Constrain Peak Width check box and type values in the Peak Height (%) box and the Tailing Factor box.

Table 38. ICIS peak detection settings page parameters (Sheet 2 of 3)

Parameter	Description
Peak Ht (%)	View or change the percent of the total peak height (100%) that a signal needs to be above the baseline before integration is turned on or off. This box is active only when you select the Constrain Peak Width check box. The valid range is 0.0 to 100.0%. To enter a height, type the appropriate value in the Peak Ht(%) box.
Tailing Factor	View or change a factor that controls how the data system integrates the tail of a peak. This factor is the maximum ratio of the trailing edge to the leading side of a constrained peak. This box is active only when you select the Constrain Peak Width check box. The valid range is 0.5 through 9.0.
Advanced	
Advanced	Specify advanced criteria to detect your chromatographic peak. The data system provides these advanced settings: Manual Noise Region, INCOS Noise, Repetitive Noise, RMS, Minimum Peak Width, Multiplet Resolution, Area Tail Extension, and Area Scan Window.
Manual Noise Region	Specify a region of the chromatogram that the data system uses to determine noise. You can enter the retention time (RT) in the RT Range box. Also, you can click  and drag the cursor horizontally across the region of the chromatogram that you want to select as the noise region. The application marks the region with a red baseline.
RT Range	Enter the retention time (RT) range in the RT Range box that you want the data system to use to determine noise. The RT range should be within the chromatogram range. Also, you can click  and drag the cursor horizontally across the region of the chromatogram that you want to select as the noise region. The application marks the region with a red baseline.
INCOS Noise	Use a single pass algorithm to determine the noise level. This value is used by the ICIS peak detection algorithm.
Repetitive Noise	Use a multiple pass algorithm to determine the noise level. This value is used by the ICIS peak detection algorithm. In general, this algorithm is more accurate in analyzing the noise than the INCOS Noise algorithm, but it takes longer.
RMS	Calculate noise as RMS. By default, the data system uses Peak To Peak for the noise calculation. If you determine the noise region manually, the application automatically selects RMS.

Table 38. ICIS peak detection settings page parameters (Sheet 3 of 3)

Parameter	Description
Min Peak Width	Enter the minimum number of scans required in a peak. The valid range is 0 to 100 scans. The default value is 3 scans. This value is used by the ICIS peak detection algorithm.
Multiplet Resolution	Enter the minimum separation in scans between the apexes of two potential peaks. This criteria determines if two peaks are resolved. The valid range is 1 to 500 scans. The default value is 10 scans. This value is used by the ICIS peak detection algorithm.
Area Tail Extension	Enter the number of scans past the peak endpoint to use in averaging the intensity. The valid range is 0 to 100 scans. The default value is 5 scans. This value is used by the ICIS peak detection algorithm.
Area Scan Window	Enter the number of scans on each side of the peak apex to include in the area integer. The valid range is 0 to 100 scans. The default value of 0 scans specifies that all scans from peak start to peak end are to be included in the area integration. This value is used by the ICIS peak detection algorithm.
Buttons	
Apply	Apply the settings displayed in the dialog box.
Save As Default	Use the current settings as default settings. If you save the settings as defaults, you can restore these values at any time by using the Load Default button.
Load Default	Restore the current default settings. To set default settings, click Save As Default .

Genesis Peak Detection Settings Page

Use the Genesis peak detection settings page, , of the Info Bar view to specify peak identification and peak integration criteria to be applied to active raw data file displayed in the Qual Browser window.

Table 39 describes the parameters on the Genesis peak detection settings page of the Info Bar view.

Table 39. Genesis peak detection settings page parameters (Sheet 1 of 4)

Parameter	Description
Application of Settings	
Apply to All Plots	Apply the current chromatogram peak identification and integration settings to all displayed plots. To apply criteria to all plots, select the Apply to All Plots check box. To apply the criteria to only the active plot, clear this check box.
Peak Parameters	
Percent of Highest Peak	Enter a percentage threshold to limit the number of peaks submitted for further processing. The data system discards any detected peaks with an intensity less than the threshold percentage of the most intense peak.
Minimum Peak Ht (S/N)	View or change the peak signal-to-noise criteria to equal or exceed as a criteria for peak detection. The application ignores all chromatogram peaks that have signal-to-noise values that are less than the Minimum Peak Height (S/N) value. To enter a peak signal-to-noise criteria, type the value in the Minimum Peak Height (S/N) box. The valid range is 1.0 (all peaks) to 999.0.
S/N Threshold	View or change the threshold for detecting peak edges. The default value is 0.5 and the valid range is 0.0 to 999.0. The data system calculates the signal-to-noise ratio using only baseline signal. Any extraneous, minor, detected peaks are excluded from the calculation.
Valley Detection Enabled	Use the valley detection approximation method to detect unresolved peaks. This method drops a vertical line from the apex of the valley between unresolved peaks to the baseline. The intersection of the vertical line and the baseline defines the end of the first peak and the beginning of the second peak. To turn this method on, select the Valley Detection check box. To turn this method off, clear the check box.

Table 39. Genesis peak detection settings page parameters (Sheet 2 of 4)

Parameter	Description
Expected Width	View or change the expected peak width parameter (in seconds). This value controls the minimum width that a peak is expected to have if valley detection is selected. With valley detection selected, any valley points nearer than the <i>expected width</i>/2 to the top of the peak are ignored. If a valley point is found outside the expected peak width, the data system terminates the peak at that point. The application always terminates a peak when the signal reaches the baseline, independent of the value set for the expected peak width. The valid range is 0.0 to 999.0 seconds. To change the current value, type a new width in the Expected Width box.
Constrain Peak Width	Limit the peak width of a component during peak integration of a chromatogram. You can then set values that control when peak integration is turned on and off by specifying a peak height threshold and a tailing factor. To limit a peak width, select the Constrain Peak Width check box.
Peak Ht	View or change the Peak Height where the data system tests the width of target peaks. You can enter any value from 0 to 100%. The default value is 5.0%.
Tailing Factor	View or change a factor that controls how the data system integrates the tail of a peak. This factor is the maximum ratio of the trailing edge to the leading side of a constrained peak. This box is active only when you select the Constrain Peak Width check box. The valid range is 0.5 through 9.0.
Advanced	
RMS	Calculate noise as RMS.
Peak to Peak	Calculate noise as peak-to-peak.
Manual Noise Region	Specify a region of the chromatogram that the data system uses to determine noise. You can enter the retention time (RT) in the RT Range box. Also, you can click the Manual Noise Region icon, , and drag the cursor horizontally across a region of the chromatogram to select the region as the noise region. The application marks the region with a red baseline.

Table 39. Genesis peak detection settings page parameters (Sheet 3 of 4)

Parameter	Description
RT Range	Enter the retention time (RT) range in the RT Range box that you want the data system to use to determine noise. The RT range should be within the chromatogram range. Also, you can click the Manual Noise Region icon, , and drag the cursor horizontally across a region of the chromatogram to select the region as the noise region. The application marks the region with a red baseline.
Baseline Noise Tolerance (%)	View or change a value that controls how the baseline is drawn in the noise data. The higher the baseline noise tolerance value, the higher the baseline is drawn through the noise data. The valid range is 0.0 to 100.0. To change the baseline noise tolerance, type the new value in the Baseline Noise Tolerance box. When you click Apply, the data system applies the new peak integration parameter.
Min Number of Scans in Baseline	View or change the minimum number of scans that the data system uses to calculate a baseline. A larger number includes more data in determining an averaged baseline. The valid range is 2 to 100.0. To change the minimum number of scans, type the new value in the Minimum Number of Scans in Baseline box. When you click Apply, the data system applies the new baseline parameter.
Baseline Noise Rejection Factor	View or change the current baseline noise rejection factor. This factor controls the width of the rms noise band above and below the peak detection baseline. This factor is applied to the raw rms noise values to raise the effective rms noise used by the data system during peak detection. The system responds by assigning the left and right peak boundaries above the noise and therefore closer to the peak apex value in minutes. This action effectively raises the peak integration baseline above the rms noise level. The valid range of this factor is 0.1 to 10.0. The default value is 2.0.
Peak S/N Cutoff	View or change the signal-to-noise level that the data system defines as the top of the peak edge. For example, if the signal-to-noise at the apex is 500 and the Peak S/N Cutoff value is 200, the application will define the right and left edges of the peak when the S/N reaches a value less than 200. The valid range is 50.0 to 10 000.0. To change the cutoff value, type the new value in the Peak S/N Cutoff box. When you click Apply, the application applies the new peak detection parameter.

Table 39. Genesis peak detection settings page parameters (Sheet 4 of 4)

Parameter	Description
Rise Percentage	View or change the percentage that the peak trace can rise above the baseline after passing through a minimum (before or after the peak). If the trace exceeds this value, the data system applies valley detection peak integration criteria. This test is applied to both the left and right edge of the peak. This criteria is useful for integrating peaks with long tails. The valid range is 0.1 to 500.0. To change the rise percentage, type the new value in the Rise Percentage box. When you click Apply, the data system applies the new peak detection criteria.
Valley S/N	View or change the signal-to-noise criteria that the data system uses for valley detection. The valid range is 1.0 to 100.0. To change the valley detection signal-to-noise criteria, type the new value in the Valley S/N box. When you click Apply, the data system applies the new peak detection criteria.
Background Recomputation Interval	The data system periodically recalculates the representative background scan it uses for background subtraction. This is to compensate for the possibility that the composition of the background might change over the course of a run. The Background Recomputation Interval is the time interval in minutes between these recalculations. To change the interval, type the new value in the Background Recomputation Interval box. The valid range is 0.5 to 10.0 minutes.
Number of Scans in Background	View or change the number of background scans used to determine the background. The valid range is 2 to 100. To change the number of background scans, type the new value in the Number of Scans in Background box. When you click Apply, the data system applies the new baseline parameter.
Buttons	
Apply	Apply the settings displayed in the dialog box.
Save As Default	Specify to use the current settings as default settings. Once the settings are saved as defaults, you can restore these values at any time by using the Load Default button.
Load Default	Restore the current default settings. To set default settings, click Save As Default.

Result File Information Page

The result file information page contains a peak list for the selected result file.

To open the result file information page, click the tab, , on the Info Bar view.

Table 40 describes the parameters on the result file information page of the Info Bar view.

Table 40. Result File Information page parameters

Command	Description
Retention Time 	Specify the time after injection when an analyte elutes. This is the total time that the analyte is retained on the chromatographic column. If the maximum signal from an analyte is detected 5 min and 14 s after injection, then the analyte has a retention time of 5:14.
Left	View the retention time corresponding to the start of the chromatographic peak, where the detection signal increases beyond the threshold criteria.
Apex	The retention time corresponding to the uppermost point of a chromatogram peak.
Right	The retention time corresponding to the end of the chromatographic peak, where the detection signal decreases below the threshold criteria.
Height	The number of counts at the peak apex.
Area	The area of the peak in units of counts * seconds.

Sequence Information Page

The sequence information page of the Info Bar view lists the file name and path of the sequence. It also lists the raw data files in the sequence.

To open the sequence information page, click the tab, , on the Info Bar view.

Double-click any file in the sequence to open it in the active window, replacing the plots in all cells with equivalent spectra, chromatograms, or maps.

Right-click any file within the sequence information page to display a shortcut menu.

[Table 41](#) describes the commands on the sequence information page of the Info Bar view.

Table 41. Sequence information page parameters

Command	Description
Open-Replace	
All in Current Window	Open the selected file in the active window, replacing the plots in all cells with equivalent spectra or chromatograms (you can also double-click a file).
All in Current Cell	Replace all plots in the active cell with equivalent plots from the selected file.
Current Plot	Replace the current plot in the active window with an equivalent from the selected file.
Open-Add	
New Window	Open the selected raw data file in a new window.
New Plot	Open the selected file as a plot in the active cell.
Other	
Open Result File	Open a result file associated with the selected raw data file.
Properties	View basic information about the selected sample including the row, filename, sample ID, name, sample type and result file name. The dialog box closes if you click anywhere outside it. Click the pin icon to keep the Sample Properties dialog box open. You must then click the close icon to close the dialog box or unpin the dialog box (by clicking the pin icon again) and click anywhere outside the dialog box.

Spectrum Simulation Page

Use the spectrum simulation page to create a simulated isotopic distribution spectrum of a chemical formula.

To open the spectrum simulation (Isotope Simulation) page, click the tab, , on the Info Bar view.

These tables describe the following:

- [Spectrum simulation page parameters](#)
- [One- and three-letter abbreviations for the standard amino acids](#)
- [Three-letter abbreviations for less common amino acids](#)

Table 42 describes the parameters in the Isotope Simulation area on the spectrum simulation page of the Info Bar view.

Table 42. Spectrum simulation page parameters (Sheet 1 of 5)

Parameter	Description
New	Place the simulated spectrum in a new view.
Insert	Place the simulated spectrum above the selected (highlighted) spectrum. Select a spectrum to make the Insert button active.
Replace	Replace the selected (highlighted) spectrum with the simulated spectrum. Select a spectrum to make the Replace button active.
Chemical Formula	Enter or select the chemical formula for the simulated spectrum. Then, click the Insert or Replace button to display the spectrum. The maximum molecular weight for the formula is less than 600 000 amu. You can enter both upper and lower case letters, however the data system interprets all lower case input as two-letter symbols. For example, the string <i>inau</i> will be parsed as <i>In Au</i>. You can force other interpretations by being more specific in capitalization, namely <i>INaU</i> or <i>INaU</i>. The application interprets all upper case input as single-letter element names. For example, <i>COSI</i> is interpreted as <i>C O S I</i>. Specify a specific isotope by naming it in the following fashion: $[13]\text{C}$ using square brackets about the isotope mass number. You can specify mixtures of substances by using additional symbols + (addition) and * (multiplication). Both symbols are required to specify a mixture. A valid mixture has the format substance*quantity + substance*quantity, for example, C4H8*2+H2O*5.

Table 42. Spectrum simulation page parameters (Sheet 2 of 5)

Parameter	Description
Peptide/Protein	Enter or select the peptide/protein formula for the simulated spectrum. Then, click the Insert or Replace button to display the spectrum. The maximum molecular weight for the formula is less than 600 000 amu. You can use both single capital letter abbreviations for amino acids (for example, CAT), and the standard three letter abbreviations with the first letter capitalized. To enter multiple copies of an amino acid, type a number directly after the one- or three-letter abbreviation. For example: Tyr3 represents three Tyrosine residues. You can specify mixtures of substances by using additional symbols '+' (addition) and '*' (multiplication). Both symbols are required to specify a mixture. A valid mixture has the format substance*quantity + substance* quantity, for example, A*2+C*5. See List of One- and Three-Letter Abbreviations for the Standard Amino Acids. See List of Three-Letter Abbreviations for Less Common Amino Acids.
Plus H2O	Specify that the simulated spectrum for a peptide formula includes a water molecule. This check box becomes active when you select the Peptide/Protein option.
Mass readback	View the sum of the masses of the lightest naturally occurring isotopes of the elemental formula in amu. When mixtures are simulated, the value of Mass readback will be blank.
Change Mixture button	Opens the Change Mixture for Simulation dialog box, where you can specify the compounds and amounts you want to include in the mixture.
Adduct	
Adduct	Specify that the simulated spectrum is an adduct. The Spectral Simulation feature in the data system supports two general modes of ionization: addition or subtraction of protons and addition/subtraction of electrons. If you clear the Adduct check box, the data system calculates the mass to charge ratio based on the loss or addition of electrons according to this general formula: $\text{formula mass} - (\text{sign of charge} * \text{the number of charges} * \text{electron mass}) / \text{number of charges}$ If you select the Adduct check box, the data system calculates the mass to charge ratio based on protonation/deprotonation according to this general formula: $\text{formula mass} + (\text{sign of charge} * \text{the number of charges} * \text{proton mass}) / \text{number of charges}$ When a formula does not contain any hydrogen atoms, the system does not subtract the mass of a proton even though the you select the Adduct check box. See Concentration below for more information on how the data system calculated the mass to charge ratio for multiply charged ions when an adduct without any hydrogen atoms is selected.

Table 42. Spectrum simulation page parameters (Sheet 3 of 5)

Parameter	Description
Identity	Select the adduct for the simulated spectrum. Selections: H, K, or Na
Concentration	There are four possibilities for how the adduct is added to the ion: One, Low, High, and 100%. - One adduct For positive charge states and positively charged adducts, the data system creates the specified charge state by adding the positive adduct for the first charge and H⁺ ions for subsequent charges. For example, a charge distribution of Most abundant=2 and Half width = 2 (2,2) and a K⁺ adduct shows these ions: +1 C10K⁺ +2 C10HK⁺2 +3 C10H2K⁺3 +4 C10H3K⁺4 For negative charge states, each charge state shows loss of H⁺ to attain the specified charge. If the molecule does not contain hydrogen, nothing is removed. For example, for 2 ions C6H6 and C4 and a K adduct, the (–2,2) charge state gives: –1 C6H5K–C4K– –2 C6H4K–2 C4K–2 –3 C6H3K–3 C4K–3 –4 C6H2K–4 C4K–4 The second and third cases produce a distribution of adducts for charges where the absolute values are greater than 1. It is possible to specify both a distribution of charge states and a distribution of adducts. This case can result in an extremely complicated spectrum when the adduct distribution overlaps the charge state distribution. - Low The ion with no adduct will be included at 100% intensity, 1 adduct at 25% intensity, 2 adducts at 11% intensity, and so on. (To the limit of the charge distribution.) - High The ion with N adducts are included at 100% intensity, N-1 adduct at 25% intensity, N-2 adducts at 11% intensity, and so on, where N is the absolute value of the maximum charge simulated. (To the limit of the charge distribution.) 100% The ion of charge N contains M adducts (where M is the absolute value of N.)

Table 42. Spectrum simulation page parameters (Sheet 4 of 5)

Parameter	Description
Charge Distribution	
Charge Distribution	Specify limits on charge distribution. Change the values of the settings to simulate the effect on ions. See Adduct for more information.
Most Abundant	Select the most abundant charge of the ion, and the data system calculates the masses accordingly. The range is -99 to +99, and the default value is +1.
Half Width	Simulate the number of additional charges on each side of the most abundant. Select a value from 0 to 99. For example: If you simulate charge 10 and a half width of 3, then the data system draws charges 10 ± 3, giving 7, 8, 9, 10, 11, 12, 13 (with the largest peak at charge 10). If you simulate charge 2 and a half width of 3, then the application draws positive charges from the range 2 ± 3, giving 1, 2, 3, 4, 5. (with the largest peak at charge 2). If you simulate charge 1 and a half width of 3, then the application draws charges 1, 2, 3, 4. To simulate an intensity distribution, the peaks at the edge of the distribution are shown at 5% of the height of the most abundant peak.
Output Style	
Output Style	Select how you want the data system to display the simulated spectrum. The options are Pattern, Profile, and Centroid.
Pattern	Plot the exact pattern of isotopic peaks generated by the simulation.
Profile	Plot the pattern spectrum convolved with a gaussian, cosine, triangular, or Lorentzian broadening function (see below). Use the Samples Per Peak box to specify the number of data points across the peak.

The figure displays four stacked plots illustrating different broadening functions for a mass spectrum. The x-axis for all plots is labeled 'm/z' and ranges from 106 to 112. The y-axis represents intensity. The top plot, labeled 'Gaussian', shows a single smooth peak centered at 109.1. The second plot, labeled 'Cosine', shows a peak centered at 109.1 with smaller peaks at 110.1, 111.1, and 112.1. The third plot, labeled 'Triangular', shows a triangular peak centered at 109.1. The bottom plot, labeled 'Lorentzian', shows a Lorentzian peak centered at 109.1.

Table 42. Spectrum simulation page parameters (Sheet 5 of 5)

Parameter	Description
Samples/Peak	Set the Samples Per Peak to the number of data points across the width of the peak. The peak definition depends on which valley option you selected: - FWHM: the width of the peak is measured at 50% height 10% Valley: the width of the peak is measured at 5% height 5% Valley: the width of the peak is measured at 2.5% height After resolving 2 peaks, the data system creates a valley by the sum of the signals from the newly resolved peaks, so the peak height of each contributing peak at the valley bottom is half of the valley height.
Centroid	Select this option to apply the same algorithm used in the firmware to convert from profile data to centroid. When you select centroid, both the Samples/Peak box and the Choose Algorithm button become active.
Choose Algorithm	Select a centroiding algorithm.
Resolution	
Specify the type of unit for peak width to associate with the value in the adjacent boxes. You can select resolution in Daltons, parts per million (ppm), or resolving power. Simulate MS results from a quadrupole detector with a fixed mass peak width (Daltons), or simulate results from a magnetic sector detector with a relative mass peak width (ppm or resolving power).	
Daltons	Specify a value for simulated peak width in Daltons. When you select the option, the box becomes active.
PPM	Specify a value for simulated peak width in parts per million. When you select the option, the box becomes active.
Resolving Power	Specify the resolving power for simulated peak width. When you select the option, the box becomes active. Resolving power is a measurement of the ability of a mass spectrometer to resolve close peaks. For example: A resolving power of 1000 at 10% valley implies that if there are 2 equal height peaks at mass 1000 and 1001, then there will be a valley between those peaks at 10% of the peak height, at mass 1000.5 (and that at 999.5 and 1001.5 the profile will be at 5% of the peak height).
Valley	
FWHM	Select this option to make the peak width at half maximum equal to the resolution. For example, if you select a resolution of 1 Dalton, then the peak is 1 Dalton wide at half maximum.
10%	Select this option to simulate a valley at 10% height between just resolved peaks.
5%	Select this option to simulate a valley at 5% height between just resolved peaks.

List of One- and Three-Letter Abbreviations for the Standard Amino Acids

Table 43 lists the one- and three-letter abbreviations for the standard amino acids as well as the formulas of the amino acid residues. Use these abbreviations or formulas to enter the peptide/protein formula for the simulated spectrum (see [Peptide/Protein](#)).

Note Table 43 also includes the one- and three-letter abbreviation for ornithine, a non-standard amino acid.

Table 43. One- and three-letter abbreviations for the standard amino acids

One letter	Amino acid name	Residue formula	Three letter
A	Alanine	C ₃ H ₅ NO	Ala
C	Cysteine	C ₃ H ₅ NOS	Cys
D	Aspartate	C ₄ H ₅ NO ₃	Asp
E	Glutamate	C ₅ H ₇ NO ₃	Glu
F	Phenylalanine	C ₉ H ₉ NO	Phe
G	Glycine	C ₂ H ₃ NO	Gly
H	Histidine	C ₆ H ₇ N ₃ O	His
I	Isoleucine	C ₆ H ₁₁ NO	Ile
K	Lysine	C ₆ H ₁₂ N ₂ O	Lys
L	Leucine	C ₆ H ₁₁ NO	Leu
M	Methionine	C ₅ H ₉ NOS	Met
N	Asparagine	C ₄ H ₆ N ₂ O ₂	Asn
O	Ornithine	C ₅ H ₁₁ N ₂ O	Orn
P	Proline	C ₅ H ₇ NO	Pro
Q	Glutamine	C ₅ H ₈ N ₂ O ₂	Gln
R	Arginine	C ₆ H ₁₂ N ₄ O	Arg
S	Serine	C ₃ H ₅ NO ₂	Ser
T	Threonine	C ₄ H ₇ NO ₂	Thr
V	Valine	C ₅ H ₉ NO	Val
W	Tryptophan	C ₁₁ H ₁₀ N ₂ O	Trp
Y	Tyrosine	C ₉ H ₉ NO ₂	Tyr

List of Three-Letter Abbreviations for Less Common Amino Acids

Table 44 lists three-letter abbreviation for less common amino acids.

Use these abbreviations to enter the peptide/protein formula for the simulated spectrum (see [Peptide/Protein](#)).

Table 44. Three-letter abbreviations for less common amino acids (Sheet 1 of 3)

Three letter	Name	Formula
Abu	2-Aminobutyric acid (2-aminobutanoic acid)	C ₄ H ₇ NO
Aec	Aminoethylcysteine	C ₅ H ₁₀ N ₂ OS
Aib	Aminoisobutyric acid	C ₄ H ₇ NO
Aln	--	C ₁₃ H ₁₁ NO
Aly	Alveolysin	C ₁₂ H ₂₂ N ₂ O ₆
Amc	--	C ₆ H ₁₀ N ₂ O ₂ S
Bcy	--	C ₁₀ H ₁₁ NOS
Bgl	--	C ₁₂ H ₁₃ NO ₃
Bly	--	C ₁₆ H ₂₆ N ₄ O ₃ S
Bse	--	C ₁₀ H ₁₁ NO ₂
Bth	--	C ₁₁ H ₁₃ NO ₂
Cmc	Carboxymethylcysteine	C ₅ H ₇ NO ₃ S
Cml	--	C ₈ H ₁₄ N ₂ OS
Cph	Chlorophenylalanine	C ₉ H ₈ NOCl
Cya	Cysteic acid	C ₃ H ₅ NO ₄ S
Dha	Dehydroalanine	C ₃ H ₃ NO
Dhb	Dehydro-2-aminobutyric acid	C ₄ H ₅ NO
Dpr	D-proline	C ₅ H ₅ NO
Dty	Diiodotyrosine	C ₉ H ₇ NO ₂ I ₂
Fcy	--	C ₁₈ N ₂₉ NOS
Fph	--	C ₉ H ₈ NOF
Ftr	--	C ₁₂ H ₁₀ N ₂ O ₂
Gaa	--	C ₄ H ₇ NO
Gcg	--	C ₅ H ₅ NO ₄
Gla	Carboxyglutamic acid	C ₆ H ₇ NO ₅
Glp	--	C ₅ H ₅ NO ₂

Table 44. Three-letter abbreviations for less common amino acids (Sheet 2 of 3)

Three letter	Name	Formula
Hse	Homoserine	C ₄ H ₇ NO ₂
Hsl	Homoserine lactone	C ₄ H ₅ NO
Hya	Beta-hydroxyaspartate	C ₄ H ₅ NO ₄
Hyg	Hydroxyglycine	C ₅ H ₇ NO ₄
Hyl	Hydroxylysine	C ₆ H ₁₂ N ₂ O ₂
Hyp	Hydroxyproline	C ₅ H ₇ NO ₂
Ils	Isolysine	C ₉ H ₁₈ N ₂ O
Ity	Iodotyrosine	C ₉ H ₈ NO ₂ I
Iva	Isovaline	C ₅ H ₉ NO
Mar	--	C ₇ H ₁₄ N ₄ O
Mas	--	C ₅ H ₇ NO ₃
Mbt	--	C ₁₇ H ₁₇ NO ₂
Mes	--	C ₅ H ₉ NO ₃ S
Mga	--	C ₆ H ₁₀ N ₂ O ₂
Mgl	--	C ₆ H ₉ NO ₃
Mhi	--	C ₇ H ₉ N ₃ O
Mls	--	C ₇ H ₁₄ NO
Mme	--	C ₆ H ₁₁ NOS
Mph	--	C ₁₀ H ₁₁ NO
Mso	Methioninesulfoxide	C ₅ H ₉ NO ₂ S
Mty	--	C ₁₀ H ₁₁ NO ₂
Nle	Norleucine	C ₆ H ₁₁ NO
Nls	Norlysine	C ₁₂ H ₁₅ N ₃ O ₂
Pal	--	C ₈ H ₈ N ₂ O
Pcy	--	C ₁₉ H ₃₅ NO ₂ S
Pec	--	C ₁₀ H ₁₂ N ₂ OS
Pip	2-Piperidinecarboxylic acid	C ₆ H ₉ NO
Psr	Phosphoserine	C ₃ H ₆ NO ₅ P
Pth	Phosphothreonine	C ₄ H ₈ NO ₅ P
Pty	Phosphotyrosine	C ₉ H ₁₀ NO ₅ P
Pyr	Pyroglutamic acid	C ₅ H ₅ NO ₂

Table 44. Three-letter abbreviations for less common amino acids (Sheet 3 of 3)

Three letter	Name	Formula
Sar	Sarcosine	C ₃ H ₅ NO
Sas	--	C ₈ H ₈ NO ₅
Tml	E-amino trimethyl-lysine	C ₉ H ₁₉ N
Tys	Tyrosinesulfonic acid Tyr(SO ₃ H)	C ₉ H ₉ NO ₅ S

Qual Browser Dialog Boxes

The Qual Browser window has these dialog boxes:

- [Add Graphics Dialog Box](#)
- [Add Text Dialog Box](#)
- [Amplify by Other Factor Dialog Box](#)
- [Average Filter Selection Dialog Box](#)
- [Cell Size Dialog Box](#)
- [Choose Centroiding Algorithm Dialog Box](#)
- [Color Dialog Box](#)
- [Copy to Clipboard Dialog Box](#)
- [Display Options Dialog Box in Qual Browser](#)
- [Global Mass Options Dialog Box](#)
- [Heading Editor Dialog Box](#)
- [Peak Purity Dialog Box](#)
- [Print Dialog Box](#)
- [Ranges Dialog Boxes](#)
- [Search Properties Dialog Box](#)
- [Select Isotopes Dialog Box](#)
- [Specify Mixture for Simulation Dialog Box](#)
- [Toolbars Dialog Box](#)

For information about the Add Programs To Tool Menu and Add Tool dialog boxes, refer to the reference section of the *Xcalibur Data Acquisition and Processing User Guide*.

Add Graphics Dialog Box

Use the Add Graphics dialog box to add graphic elements to a spectrum, chromatogram, or map. For more information, see [Adding Graphics to a Plot](#).

Table 45 describes the parameters in the Add Graphics dialog box.

Table 45. Add Graphics dialog box parameters (Sheet 1 of 3)

Parameter	Description
Style	
Horizontal Line	Draw a horizontal line on a plot. ❖ To draw a horizontal line 1. Select the Horizontal Line option and select a line color. 2. Click OK to close the Add Graphics dialog box. 3. Drag the cursor on the plot to draw the horizontal line. You can drag from right-to-left or from left-to-right.
Vertical Line	Draw a vertical line on a plot. ❖ To draw a vertical line 1. Select the Vertical Line option and select a line color. 2. Click OK to close the Add Graphics dialog box. 3. Drag the cursor on the plot to draw the vertical line. You can drag from bottom-to-top or from top-to-bottom.
Diagonal Line	Draw a diagonal line on a plot. ❖ To draw a diagonal line 1. Select the Diagonal Line option and select a line color. 2. Click OK to close the Add Graphics dialog box. 3. Drag the cursor on the plot to draw the diagonal line. You can drag from left-to-right or from right-to-left. Move the cursor before you release the mouse button to position the angle of the line.

Table 45. Add Graphics dialog box parameters (Sheet 2 of 3)

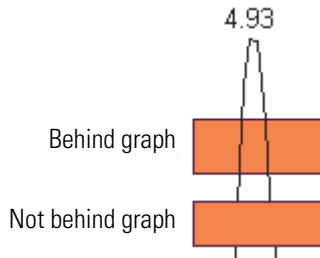
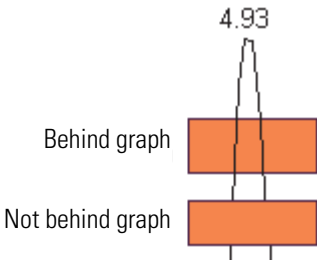
Parameter	Description
Box	Draw a rectangle on a plot. ❖ To draw a box 1. Select the Box option and select a line color. 2. Click OK to close the Add Graphics dialog box. 3. Drag the cursor diagonally to draw the box. You can click to start at any corner of the box and then drag the cursor to the opposite corner. The data system draws a box similar to the following: 
Filled Box	Draw a rectangle on a plot. ❖ To draw a filled box 1. Select the Filled Box option and select a line color and a fill color. 2. Determine whether the filled box is behind or not behind a graph. 3. Click OK to close the Add Graphics dialog box. 4. Drag the cursor diagonally to draw the box. You can click to start at any corner of the box and then drag any cursor to the opposite corner. These filled boxes have a black box and a brown fill and demonstrate the use of the Behind Graph check box feature. 

Table 45. Add Graphics dialog box parameters (Sheet 3 of 3)

Parameter	Description
Colors	
Line	Select the color of the added line or box outline. The current color for an added line or box outline is displayed to the right of the Line button. The Color dialog box opens with a color palette so you can select a preset color or customize a color. Use the adjacent graphic to view the result of the current color selection.
Fill	Select the color of the added filled box. The current color for the added filled box is displayed to the right of the Fill button. The Color dialog box opens with a color palette so you can select a preset color or customize a color. Use the adjacent graphic to view the result of the current color selection.
Behind Graph	Draw a filled box either in front of a plot or behind a plot. To draw a filled box behind a graph, select the Behind Graph check box. To draw an opaque filled box in front of (on top of) a graph, clear the Behind Graph check box. This figure shows the difference between the two options: 

Add Text Dialog Box

Use the Add Text dialog box to type, format, and position text on a spectrum, chromatogram, or map plot. For information, see [Adding Text to a Plot](#).

[Table 46](#) describes the parameters in the Add Text dialog box.

Table 46. Add Text dialog box parameters (Sheet 1 of 8)

Parameter	Description
Annotation Text	View the annotation text that the data system adds to your plot if you click OK and click your plot with the Add Text cursor . Text alignment and position options in the Add Text dialog box are not displayed until you select the position on the plot. To change the text, select the current text and type the new caption. Use the ENTER key for multiple lines.
Boxed	Include a visible box around the annotation text you add to a plot. To add a box around the text, select the Boxed check box. If you do not want to include a box with the text, clear the Boxed check box.
Rotated	Rotate the annotation text you add to a plot so that it reads vertically from bottom to top. To rotate the text, select the Rotated check box. If you want your text to read horizontally from left to right, clear the Rotated check box. A sample of rotated text follows. Annotation Text

Table 46. Add Text dialog box parameters (Sheet 2 of 8)

Parameter	Description
Pointer	Draw a pointer line from the annotation text to a point on the plot. To include a pointer with your annotation text, select the Pointer check box. If you do not want your annotation text to include a pointer, clear the Pointer check box. To point above the annotation text, select the Below Marked Position option. To point below the annotation text, select the Above Marked Position option. These precautions make sure the pointer line does not cross over the annotation text. An example of the proper use of pointers is shown below.

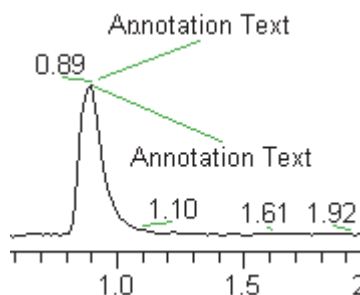


Table 46. Add Text dialog box parameters (Sheet 3 of 8)

Parameter	Description
Marked Position Is	
Left	Orient annotation text so that the position marked with the I_{Abc} text cursor is to the left of the placed text. In other words, the text is to the right of the point that you position the arrow of the text cursor. The data system activates the text cursor when you click OK from the Add Text dialog box. If you select the Left option in the Marked Position Is area, the exact placement of annotation text also depends upon the option you select in the Height Drawn area, as follows: If you also select the Just Above Graph option, the text is placed as follows.  If you also select the Above Marked Position option, the text is placed as follows.  If you also select the Below Marked Position option, the text is placed as follows. 

Table 46. Add Text dialog box parameters (Sheet 4 of 8)

Parameter	Description
Center	Orient annotation text so that the position marked with the text cursor I_{Abc} is in the center of the placed text. The data system activates the text cursor when you click OK from the Add Text dialog box. If you select the Center option in the Marked Position Is area, the exact placement of annotation text also depends upon the option you select in the Height Drawn area, as follows: If you also select the Just Above Graph option, the text is placed as follows.  If you also select the Above Marked Position option, the text is placed as follows.  If you also select the Below Marked Position option, the text is placed as follows. 

Table 46. Add Text dialog box parameters (Sheet 5 of 8)

Parameter	Description
Right	Orient annotation text so that the position marked with the I_{Abc} text cursor is to the right of the placed text. In other words, the text is to the left of the point that you position the arrow of the text cursor. The data system activates the text cursor when you click OK from the Add Text dialog box. If you select the Right option in the Marked Position Is area, the exact placement of annotation text also depends upon the option you select in the Height Drawn area, as follows: If you also select the Just Above Graph option, the text is placed as follows.  If you also select the Above Marked Position option, the text is placed as follows.  If you also select the Below Marked Position option, the text is placed as follows. 

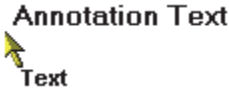
Table 46. Add Text dialog box parameters (Sheet 6 of 8)

Parameter	Description
Multiple Lines Aligned	
Left	Align multiple rows of annotation text so that each row is aligned on the left side. The data system does not display the left alignment of the text until it is placed onto the plot with the text cursor, as follows: Line One This is Line Two Line Three
Center	Align multiple rows of annotation text so that each row is aligned on a center axis. The application does not display the center alignment of the text until it is placed onto the plot with the text cursor, as follows: Line One This is Line Two Line Three
Right	Align multiple rows of annotation text so that each row is aligned on the right side. The application does not display the right alignment of the text until it is placed onto the plot with the text cursor I_{Abc}, as follows. Line One This is Line Two Line Three

Table 46. Add Text dialog box parameters (Sheet 7 of 8)

Parameter	Description
Height Drawn	
Just Above Graph	Orient the height of annotation text so that it is positioned directly above the plot position marked with the I_{Abc} text cursor. If you select the Just Above Graph option in the Height Drawn area, the exact placement of annotation text also depends upon the option you select in the Marked Position Is area, as follows: If you also select the Left option, the text is placed as follows. Annotation Text  If you also select the Center option, the text is placed as follows. Annotation Text  If you also select the Right option, the text is placed as follows. Annotation Text 

Table 46. Add Text dialog box parameters (Sheet 8 of 8)

Parameter	Description
Above Marked Position	Orient the height of annotation text so that it is positioned above the position marked with the  text cursor. If you select the Above Marked Position option, the exact placement of annotation text also depends upon the option you select in the Marked Position Is area, as follows: If you also select the Left option, the text is placed as follows.  If you also select the Center option, the text is placed as follows.  If you also select the Right option, the text is placed as follows. 
Below Marked Position	Orient the height of annotation text so that it is positioned below the position marked with the  text cursor. If you select the Below Marked Position option, the exact placement of annotation text also depends upon the option you select in the Marked Position Is box, as follows: If you also select the Left option, the text is placed as follows.  If you also select the Center option, the text is placed as follows.  If you also select the Right option, the text is placed as follows. 

Amplify by Other Factor Dialog Box

Use the Amplify by Other Factor dialog box to specify an amplification factor to apply to a region of an active plot. For more information, see [Amplifying Regions of a Plot](#).

The valid range is 1.1 to 1000.0. When you click OK, the data system changes the cursor to  so that you can drag the cursor horizontally to amplify a region of the active graph or type a value into the Amplify Factor box.

[Table 47](#) describes the parameter in the Amplify by Other Factor dialog box.

Table 47. Amplify by Other Factor dialog box parameter

Parameter	Description
Amplification Factor	Type an amplification factor to be applied to a region of an active plot. The valid range is 1.1 to 1000.0.

Average Filter Selection Dialog Box

The Average Filter Selection dialog box opens whenever you try to average scans in a chromatogram time range in which two or more types of scan types are defined. Use this dialog box to select one of the scan filters defined for the selected time range.

Table 48 describes the parameter in the Average Filter Selection dialog box.

Table 48. Average Filter Selection dialog box parameter

Parameter	Description
Filter	View the current scan filter for the active raw data file. You can use a scan filter to specify that processing is to be applied to a subset of the scans in a raw data file. To apply a different scan filter, select a new filter from the scan filter list (most common method), select a new filter from a list and edit the scan filter or type a new scan filter command string into the box using the scan filter format. ❖ To select from the list of scan filters used to create the raw data file 1. Open the Filter list. 2. Select one of the scan filters. The data system displays the scan filter in the Filter box. For example, this scan filter: <pre>c full ms [26.81–251]</pre> finds all scans in a raw data file that have these properties: <pre>centroid data Scan Mode: Full Scan Power: MS Product Ion Mass Range: m/z 26.81 to 251.00</pre>

Cell Size Dialog Box

Use the Cell Size dialog box to define the size of a cell. For more information, see [Adjusting the Cell Size](#).

Table 49 describes the parameters in the Cell Size dialog box.

Table 49. Cell Size dialog box parameters

Parameter	Description
Column Width	To set the column width of a cell, drag the Column Width scroll box or click the scroll box left and right arrows until you reach the desired width within the range 5 to 300%. The current width is displayed below the scroll box. To quickly set the column width to 100%, choose the Default Width button. Use the adjacent graphic to view the result of the column width setting. Changing the Column Width has no effect if you have only one column of cells.
Row Height	To set the row height of a cell, drag the Row Height scroll box or click the scroll box left and right arrows until you reach the desired height within the range of 5 to 300%. The current height is displayed below the scroll box. To quickly set the column height to 100%, choose the Default Height button. Use the adjacent graphic to view the result of the column height setting. Changing the Row Height has no effect if you have only one row of cells.

Choose Centroiding Algorithm Dialog Box

Use the Choose Centroiding Algorithm dialog box (Figure 70) to choose which algorithm the data system uses to calculate the centroid of profile data and to specify values of parameters used by the centroiding algorithm.

Figure 70. Choose Centroiding Algorithm dialog box

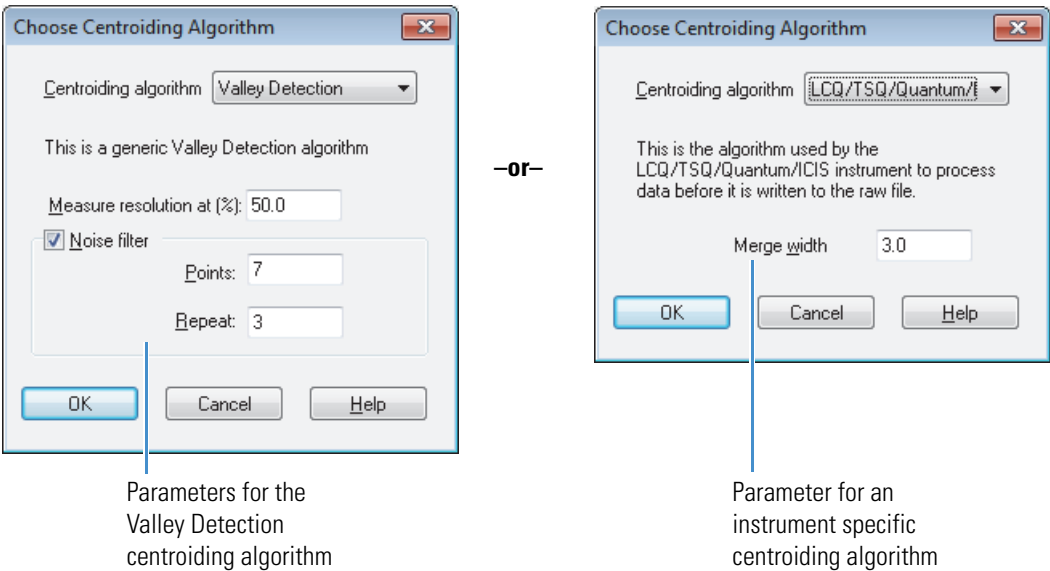


Table 50 describes the parameters in the Choose Centroiding Algorithm dialog box.

Table 50. Choose Centroiding Algorithm dialog box parameters (Sheet 1 of 2)

Parameter	Description
Centroiding Algorithm	Select the algorithm that you want the data system to use to convert the simulated spectrum from profile data to centroid data. Select the algorithm that is appropriate for the mass spectrometer whose spectrum you want to simulate, or select the generic Valley Detection algorithm. Selections: • LCQ/TSQ/Quantum/ICIS • DSQ/PolarisQ/GCQ • Valley Detection (default)

Table 50. Choose Centroiding Algorithm dialog box parameters (Sheet 2 of 2)

Parameter	Description
Measure Resolution At	Specify where to measure the resolution of a peak. The valley detection algorithm can measure the resolution of each peak (resolving power) by determining when the signal crosses a threshold on both sides of the peak. The data system measures the threshold relative to the apex height of the peak. This option is available only when you are using the Valley Detection algorithm.
Noise Filter	
Noise Filter	Check this box to turn on a filter to reject noise on peaks and prevent splitting peaks with a dip in the peak apex. A moving mean filter is applied to the signal, averaging the indicated number of points. The filter is repeatedly applied, as set by the Repeat parameter. This filtered data is only used to determine the start and end points of peaks. After this has been determined, peaks are centroided from the original (unfiltered) signal. For example: If peaks are being split at the apex, turn on filtering, and increase the points value until peaks are no longer split.
Points	The number of points to consider in filtering. The value must be between 3 and 99.
Repeat	The repeat count to use in filtering. The value must be between 1 and 9.
Other	
Merge Width	Merge data points that are within this range. The value can be between 0.0 and 100.0. Merge Width is used only for the LCQ/TSQ/Quantum/ICIS and DSQ/PolarisQ/GCQ algorithms.

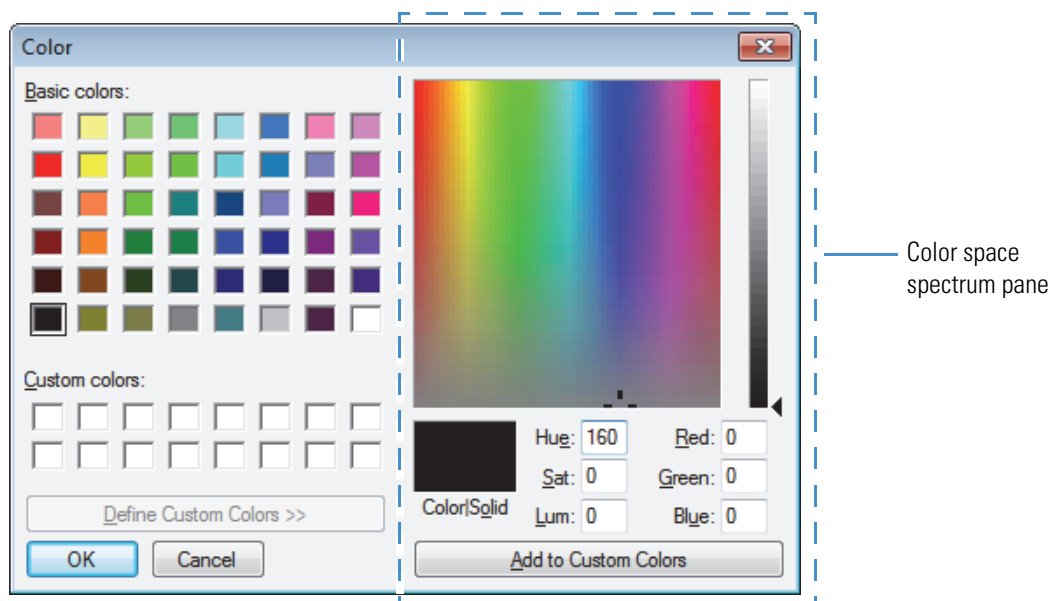
Color Dialog Box

Use the Color dialog box to select one of 48 basic colors or 16 (maximum) preselected custom colors.

Click **Define Custom Colors** to display the color space spectrum pane where you can choose colors from a continuous palette containing millions of colors. A selected color can then be added to your palette of 16 preselected colors that are displayed in the Color dialog box.

Figure 71 shows the color space spectrum pane on the right side of the Color dialog box.

Figure 71. Color dialog box with the color space spectrum pane displayed



When you choose a point in the Color Space Spectrum box, the selected color appears in the Color/Solid box and the data system displays the corresponding Hue, Saturation, Luminosity, as well as Red, Green, and Blue color coordinates. You can change the Luminosity (amount of white) of the selected color by dragging the triangular cursor located to the right of the Luminosity Scale up or down while monitoring the corresponding color in the Color/Solid box.

You can also define a particular color by typing its Hue, Saturation, and Luminosity or Red, Green, and Blue color coordinates into the corresponding boxes.

Copy to Clipboard Dialog Box

Use the Copy to Clipboard dialog box to copy either the current cell or the entire grid in the active window to the Clipboard. You can also specify the height and width of the copied object in either millimeters or inches.

Table 51. Copy to Clipboard dialog box parameters

Parameter	Description
Copy	
Current Cell	Copy the active cell to the Clipboard or copy all the cells in the active window grid by using the Grid option.
Grid	Copy the entire grid within a window to the Clipboard or you can copy just the active cell by using the Cell option.
Output Size	
Width	View the current width of an object copied to the Clipboard. The units of the value are either millimeters or inches, depending upon the selected units option.
Height	View the current height of an object copied to the Clipboard. The units of the value are either millimeters or inches, depending upon the selected units option.
Millimeters	View the units used for the size of a cell or grid copied to the Clipboard as millimeters.
Inches	View the units used for the size of a cell or grid copied to the Clipboard as inches.

Display Options Dialog Box in Qual Browser

Use the pages of the Display Options dialog box to select Style, Color, Labels, Axis, Band Width, Normalization, and Composition settings. The available parameters on these pages depend on whether the view in the active cell is a chromatogram, spectrum, map, ion map, or spectrum list.

View	Pages
Chromatogram	Chromatogram View – Display Options Dialog Box – Axis Page
	Chromatogram View – Display Options Dialog Box – Color Page
	Chromatogram View – Display Options Dialog Box – Labels Page
	Chromatogram View – Display Options Dialog Box – Normalization Page
	Chromatogram View – Display Options Dialog Box – Style Page
Spectrum	Spectrum View – Display Options Dialog Box – Axis Page
	Spectrum View – Display Options Dialog Box – Color Page
	Spectrum View – Display Options Dialog Box – Labels Page
	Spectrum View – Display Options Dialog Box – Normalization Page
	Spectrum View – Display Options Dialog Box – Style Page
	Spectrum View – Display Options Dialog Box – Composition Page
Map and Ion Map	Map or Ion Map View – Display Options Dialog Box – Axis Page
	Map or Ion Map View – Display Options Dialog Box – Bandwidth Page
	Map or Ion Map View – Display Options Dialog Box – Color Page
	Map or Ion Map View – Display Options Dialog Box – Normalization Page
	Map or Ion Map View – Display Options Dialog Box – Style Page
Spectrum List	Spectrum List View – Display Options Dialog Box – Normalization Page
	Spectrum List View – Display Options Dialog Box – Style Page
	Spectrum List View – Display Options Dialog Box – Composition Page

Chromatogram View – Display Options Dialog Box – Axis Page

Use the Axis page of the Display Options dialog box to modify the appearance of your chromatogram. The data system displays the results of the current settings in the graphic on the right side of the page.

For more information, see [Setting the Chromatogram Axis Options](#).

[Table 52](#) describes the parameters on the Display Options – Axis page for the chromatogram view.

Table 52. Chromatogram Axis page parameters (Sheet 1 of 3)

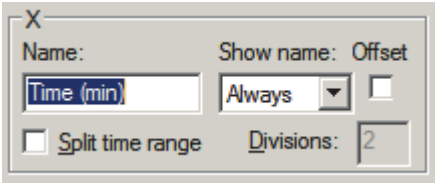
Parameter	Description
X	
	
Name (X)	View or change the current <i>x</i>-axis name, as appropriate for the active chromatogram, spectrum, or map. To change the <i>x</i>-axis name, type the new name in the Name box. The data system displays the results of the current settings in the adjacent graphic. The default <i>x</i>-axis name is Time (min).
Show Name (X or Y)	View or change when the data system displays the axis name next to the corresponding axis. The data system can display the axis label displayed in the axis Name box at the following times: • Never: The data system does not display the axis label when the graphic is displayed or printed. • On Print: The application displays the axis label whenever the graphic is printed as a report. • Always: The application displays the axis label whenever the graphic is displayed or printed. The current option is displayed in the list. To change the time when the application displays the axis label, select from the Show name list of options. Click Never, On Print, or Always. Since standard reports are not displayed on the screen, the On Print and Always Show name list options for standard reports are identical.

Table 52. Chromatogram Axis page parameters (Sheet 2 of 3)

Parameter	Description
Offset (X)	Set the location for the displayed plot a specified distance from the x axis. The x -axis offset moves the y axis slightly above the x axis so that you can see baseline details.
Split Time Range (X)	Split the time scale of the active chromatogram into two or more divisions. To split the time scale, select the Split Time Range check box. The data system activates the divisions box so that you can select the number of divisions.
Divisions	View or change the current number of divisions for a chromatogram with a split time range. This box is only active if you select the Split time range check box. The number of divisions can be two, three, or four. To change the number of divisions, type the new number in the Divisions (time) box. The data system displays the multiple chromatograms in the adjacent graphic.

Y

The screenshot shows a dialog box for configuring the Y-axis. It has a 'Separate labels' checkbox. Below it is a 'Plot' dropdown menu currently set to '1'. There are two main sections: 'Source' with radio buttons for 'From detector' (selected) and 'Custom'; and 'Units' with radio buttons for 'Absolute' and 'Relative' (selected). At the bottom, there is a 'Name' text field with 'Relative Abundant' and a 'Show name' section with a dropdown set to 'Always' and an unchecked checkbox.

Separate Labels	This box is available when the chromatogram view contains two or more plots. Apply a distinct label to the y axis of each plot in the active chromatogram view. To label the chromatogram plots separately, select the Separate Labels check box. The data system activates the Plot box so you can specify the plot to get a specific label. Select multiple plots on the Ranges Page – Chromatogram Display Options Dialog Box .
Plot	Specify a plot to apply a particular label to.

Table 52. Chromatogram Axis page parameters (Sheet 3 of 3)

Parameter	Description
Source	Specify that the data system apply either a custom (user-defined) label or a label from the detector to the y axis of a chromatogram plot. When you specify a custom label in Qual Browser, the application retrieves the parameters from a layout (.lyt) file or the Name box. If you are using the default layout file, the application retrieves the parameters from the default values you specified on the Labeling And Scaling Page Labeling and Scaling Page of the Xcalibur Configuration dialog box.
Units	Apply absolute or relative scaling to the y axis of a chromatogram plot.
Name	The default y-axis name is Relative Abundance. View or change the current y-axis name, as appropriate for the active chromatogram. To change the y-axis name, select the Custom option in the Source area, and then type the new name in the Name box. The data system displays the results of the current settings in the adjacent graphic.
Show Name	See the x -axis description.
Offset (Y)	Set the location for the displayed plot a specified distance from the y axis. The y-axis offset moves the x axis slightly to the right of the y axis so that you can see plot details at low x-axis values.

Chromatogram View – Display Options Dialog Box – Color Page

Use the Color page of the Display Options dialog box to modify the appearance of a chromatogram view. The data system displays the results of the current settings in the graphic on the right side of the page.

For information about the Color dialog box, see [Color Dialog Box](#). For information about working with the Color page, see [Setting the Chromatogram Color Options](#).

[Table 53](#) describes the parameters on the Display Options – Color page for the chromatogram view.

Table 53. Chromatogram Color page parameters

Parameter	Description
Plots	Change the colors of any of the plots within a chromatogram view. In Processing Setup, the chromatogram preview on the Color page corresponds to Plot 1. Plot buttons 2 through 8 are not used.
Plots 1 to 8	Change the color of a plot. The current plot color is displayed to the right of its plot number button. To select the color of a plot, click the Plot number button, for example, Plot 3. The data system opens the Color Dialog Box with a color palette so that you can select a preset color or customize a color.
Backdrop	Change the color of the backdrop (background) of a map view, overlaid (3D) spectrum view, or overlaid (3D) chromatogram view. Click Backdrop to display a background. The data system displays the current plot color to the right of the Backdrop button. To select the color of the backdrop, click Backdrop. The application opens the Color Dialog Box with a color palette so that you can select a preset color or customize a color. The application displays the results of the current settings in the adjacent graphic.

Chromatogram View – Display Options Dialog Box – Labels Page

Use the Labels page of the Display Options dialog box to modify the appearance of your chromatogram. The data system displays the results of the current settings in the graphic on the right side of the page.

For more information, see [Setting the Chromatogram Label Options](#).

[Table 54](#) describes the Display Options – Labels page for the chromatogram view.

Table 54. Chromatogram Labels page parameters (Sheet 1 of 3)

Parameter	Description
Label with	
Retention Time	Add a retention time label above chromatogram peaks. The order of chromatogram labels for an undetected peak, from top to bottom, is scan number, retention time, and base peak. The application displays the retention time on all peaks that meet the selection criteria set in the Label threshold box. The retention time of a detected peak is indicated by the letters <i>RT</i> to the left of the value.
Decimals	View or change the number of decimal places in the retention time label. The range is 0 to 5.
Name	Add the component name in a Quan view.
Scan Number	Add the active scan number in the label above chromatogram peaks. The scan number of a detected peak is indicated by the letters <i>S#</i> to the left of the value.
Base Peak	Add <i>m/z</i> for the base peak of the active scan above chromatogram peaks. The base peak of a detected peak is indicated by the letters <i>BP</i> to the left of the value.

Table 54. Chromatogram Labels page parameters (Sheet 2 of 3)

Parameter	Description
Signal-To-Noise	Add the signal-to-noise ratio above chromatogram peaks. When you select this check box and use the Genesis peak detection algorithm, The data system displays the calculated signal-to-noise ratio above the peaks. When you select this check box and use either the ICIS or the Avalon peak detection algorithm, the application displays SN: NA (not applicable) above the peaks, because these algorithms do not calculate a value for signal-to-noise ratio. The signal to noise of a detected peak is indicated by the letters SN to the left of the value.
Flags	Add letters above chromatogram peaks to provide supplemental information about the peak data. For chromatograms, the only possible flag is S, which indicates that a peak is saturated— the signal is too large to measure (over range from A to D converter).
Area	Add m/z labels for the area of each integrated peak in the chromatogram peaks. The integrated area of a detected peak is indicated by the letters MA or AA to the left of the value. MA indicates manual integration, and AA indicates automatic integration.
Height	Show the peak height above chromatogram peaks. The height of a detected peak is indicated by the letters MH or AH to the left of the value. MH indicates manual integration. AH indicates automatic integration.
Label Styles	
Offset	Set the location for the displayed plot at a specified distance from the x or y axes. The x-axis offset moves the y axis slightly above the x axis so that you can see baseline details. The y-axis offset moves the x axis slightly to the right of the y axis so that you can see plot details at low x axis values. The amount of the offset is specified in the Size box.
Rotated	Select whether the data system writes peak labels vertically upwards or horizontally. For vertical labels, select the Rotated check box. For horizontal labels, clear the Rotated check box. Use the adjacent graphic to view the result of the current label settings.

Table 54. Chromatogram Labels page parameters (Sheet 3 of 3)

Parameter	Description
Boxed	Select whether the data system places a box around each peak label. To box your label, select the Boxed check box. If you do not want to have a box around the label, clear the check box. Use the adjacent graphic to view the result of the current label settings.
Size	View or change the amount that the data system moves a label from its normal position to avoid conflict with another label. This box is only activated when you select the Offset check box. The valid range is 0.1 to 15.0. The default value is 2.0.
Label threshold (%)	View or change the percent of the base peak so that the data system labels peaks above that percent. The valid range is 0.0 to 100.0%. For example, if the base peak is 100% and the label threshold setting is 50.0%, the data system labels all peaks at or above 50%.

Chromatogram View – Display Options Dialog Box – Normalization Page

Use the Normalization page of the Display Options dialog box to modify the appearance of your chromatogram. The data system displays the results of the current settings in the graphic on the right side of the page.

Table 55 describes the Display Options – Normalization page for the chromatogram view.

Table 55. Chromatogram Normalization page parameters (Sheet 1 of 2)

Parameter	Description
Normalize Method	
Auto Range	Select the auto range normalization method for chromatograms. The data system reviews the chromatogram data, detects the minimum and maximum signal data points, and assigns these values to the extremes on the <i>y</i> axis. The entire dynamic range of the chromatogram is then displayed in the active view, normalized over the full range of the <i>y</i> axis.
Intensity Range	Specify the minimum and maximum ranges of the chromatogram plot to display in the <i>y</i> axis. The valid range of values is –200.000 to 200.000%. The default range is 0.000–100.000%.
Normalize Each Plot To	
Largest Peak in Subsection	Set the <i>y</i> -axis maximum for each subsection (division) equal to the largest peak in the subsection (division). Set the number of subsections on the Axis page.

Table 55. Chromatogram Normalization page parameters (Sheet 2 of 2)

Parameter	Description
Largest Peak in Selected Time Range	Set the <i>y</i> -axis maximum equal to the largest peak in the time range. The time range is the sum of all subsections [divisions]. Each subsection (division) has the same <i>y</i> -axis maximum. Set the number of subsections on the Axis page.
Largest Peak in All Times	Set the <i>y</i> -axis maximum equal to the largest peak in all times. Each subsection (division) has the same <i>y</i> -axis maximum. Set the number of divisions on the Axis page.

Chromatogram View – Display Options Dialog Box – Style Page

Use the Style page of the Display Options dialog box to modify the appearance of a chromatogram view. The data system displays the results of the current settings in the graphic on the right side of the page.

For more information, see [Setting the Chromatogram Style Options](#).

[Table 56](#) describes the parameters on the Display Options – Style page for the chromatogram view.

Table 56. Chromatogram Style page parameters (Sheet 1 of 2)

Parameter	Description
Plotting	
Point To Point	Select a graphic style that displays the active chromatogram or spectrum using a point-to-point peak profile.
Stick	Select a graphic style that displays the active chromatogram or spectrum using vertical lines.
Arrangement	
Stack (2D)	Stack plots vertically, with no overlap, for plots in the active cell.
Overlay (3D)	Overlay plots vertically with optional horizontal skew (time offset) for chromatogram or spectrum plots in the active cell.

Table 56. Chromatogram Style page parameters (Sheet 2 of 2)

Parameter	Description
3D	
This area becomes available when you select the Overlay (3D) option in the Arrangement area.	
Elevation	Set the elevation angle (amount of overlay) to a value from 0 to 60 degrees for an overlay arrangement of plots in the active cell. To set the elevation angle, either drag the Elevation slider or click the Elevation slider left or right arrow until you reach the desired angle. The data system displays the current angle setting below the scroll box.
Skew	Set the skew angle (time offset) to a value from 0 to 45 degrees for an overlay arrangement of plots in the active cell. To set the skew, either drag the Skew slider or click the Skew slider left or right arrow until you reach the desired angle. The application displays the current angle setting below the scroll box.
Draw Backdrop	Select a graphic style that includes a drawn perspective backdrop for an overlay arrangement of plots in the active cell.

Spectrum View – Display Options Dialog Box – Axis Page

Use the Axis page of the Display Options dialog box to modify the appearance of your spectrum. The data system displays results of the current settings in the graphic on the right side of the page.

For more information, see [Setting the Spectrum Axis Options](#).

[Table 57](#) describes the parameters on the Display Options – Axis page for the spectrum view.

Table 57. Spectrum Axis page parameters (Sheet 1 of 2)

Parameter	Description
X, Y, Z	
Name	View or change the current axis names for the x, y, and z axes, as appropriate for the active spectrum view. To change an x- or z-axis name, type the new name in the Name box. The data system displays results of the current settings in the adjacent graphic. The default axis names are as follows: • X: m/z • Y: Relative Abundance • Z: Scan
Show Name (X, Y, Z)	View or change when the data system displays the axis name next to the corresponding axis. The data system can display the axis label displayed in the axis Name box at the following times: • Never: The data system does not display the axis label when the graphic is displayed or printed. • On Print: The application displays the axis label whenever the graphic is printed as a report. • Always: The application displays the axis label whenever the graphic is displayed or printed. The current option is displayed in the list. To change the time when the system displays the axis label, select Never, On Print, or Always in the Show Name list. Since standard reports are not displayed on the screen, the On Print and Always selections for standard reports are identical.

Table 57. Spectrum Axis page parameters (Sheet 2 of 2)

Parameter	Description
Offset (X and/or Y)	Set the location for the displayed plot at a specified distance from the x and/or y axes. The x-axis offset moves the y axis slightly above the x-axis so that you can see baseline details. The y-axis offset moves the x axis slightly to the right of the y axis so that you can see plot details at low x-axis values. The amount of the offset is specified in the Size box.
Split Time Range (X)	Split the m/z scale of the active spectrum into two or more divisions. To split the mass scale, select the Split Time Range check box. The data system activates the Divisions box so that you can enter the number of divisions.
Divisions	View or change the current number of divisions for a spectra with a split mass range. This box is only active if you select the Split time range check box. The number of divisions can be two, three, or four. To change the number of divisions, type the new number in the Divisions (m/z) box. The data system displays the multiple spectra in the adjacent graphic.
Y	
Source	Specify that the data system apply either a custom (user-defined) label or a label from the detector to the y axis of a spectrum plot. When you specify a custom label in Qual Browser, the application retrieves the parameters from a layout (.lyt) file. If you are using the data system's default layout file, the application retrieves the parameters from the default values you specified on the Labeling and Scaling page of the Xcalibur Configuration dialog box.
Name	View or change the y-axis name. To change the y-axis name, select the Custom option in the Source area, and then type the new name in the Name box. The data system displays results of the current settings in the adjacent graphic.

Spectrum View – Display Options Dialog Box – Color Page

Use the Color page of the Display Options dialog box to modify the appearance of a Spectrum view. The Xcalibur system displays the results of the current settings in the graphic on the right side of the page.

For more information, see [Setting the Spectrum Color Options](#).

[Table 58](#) describes the parameters on the Display Options – Color page for the spectrum view.

Table 58. Spectrum Color page parameters (Sheet 1 of 2)

Parameter	Description
Centroid	
Regular (peaks)	Change the color of regular, unflagged, peaks. The current color for regular peaks is displayed to the right of the Regular (peaks) button. To select the color of regular peaks, click Regular. The data system opens the Color Dialog Box with a color palette so that you can select a preset color or customize a color. It displays the results of the current settings in the adjacent graphic.
Saturated (peaks)	Change the color of saturated peaks (amplitude is greater than range). The current color is displayed to the right of the Saturated (peaks) button. To change the color of saturated peaks, click Saturated. The data system opens the Color Dialog Box with a color palette so that you can select a preset color or customize a color. It displays the results of the current settings in the adjacent graphic.
Reference/Lock	Change the color of reference peaks. The current color is displayed to the right of the Ref/Lock button. To change the color of reference peaks, click Ref/Lock. The data system opens the Color Dialog Box with a color palette so that you can select a preset color or customize a color. The data system displays the results of the current settings in the adjacent graphic.
Exception	Change the color of the exception peak. The current color is displayed to the right of the Exception (peaks) button. To change the color of exception peaks, click Exception. The data system opens the Color Dialog Box with a color palette so that you can select a preset color or customize a color. The system displays the results of the current settings in the adjacent graphic.

Table 58. Spectrum Color page parameters (Sheet 2 of 2)

Parameter	Description
Other	
Profile	Change the color of the profile style. The data system displays the current color to the right of the Profile button. To change the color of the profile, click Profile. The Color Dialog Box opens with a color palette. You can select a preset color or customize a color. The application displays the results of the current settings in the adjacent graphic.
Backdrop	Change the color of the backdrop (background) of a map view, overlaid (3D) spectrum view, or overlaid (3D) chromatogram view. The data system displays the current plot color to the right of the Backdrop button. To select the color of the backdrop, click Backdrop. The application opens the Color Dialog Box with a color palette so that you can select a preset color or customize a color. It displays the results of the current settings in the adjacent graphic.
Shade	
Shade (%)	Change the color of the map at 0%, 20%, 40%, 60%, 80%, and 100% relative abundance. To change the color, click a (%) button. The data system opens the Color Dialog Box with a color palette so that you can select a preset color or customize a color. These changes are only visible if you have selected the Shade option on the Spectrum View – Display Options Dialog Box – Style Page.

Spectrum View – Display Options Dialog Box – Labels Page

Use the Labels page of the Display Options dialog box to modify the appearance of your spectrum. The data system displays the results of the current settings in the graphic on the right side of the page.

For more information, see [Setting the Spectrum Label Options](#).

[Table 59](#) describes the parameters on the Display Options – Labels page for the spectrum view.

Table 59. Spectrum Labels page parameters (Sheet 1 of 4)

Parameter	Description
Label with	
Mass (MS data only)	Display a m/z label at the top of spectrum peaks. To turn on peak mass labeling, select the Mass check box. The Decimals box becomes active. The data system displays the Mass check box only if you are using MS data.
Relative To	Move the m/z label at the top of spectrum peaks by the amount typed in the Relative to box.
Wavelength (non-MS data only)	Display a wavelength label at the top of spectrum peaks. The Decimals box becomes active. The data system displays the Wavelength check box only if you are not using MS data.
Flags	Display letters above the colored spectrum peaks. The letters indicate why the peaks are colored. The possible flags are as follows: • S Saturated peaks are peaks with a signal too large to measure (over range from A to D converter). • R Reference peaks are peaks from a reference compound used for an internal recalibration of a scan (for example, in MAT95 series). • L Lock peaks are local references used to calculate accurate mass of nearby peaks (for example, in Quantum™ AM). • E Exception peaks are also peaks from a reference compound, but not used for recalibration. These are typically small isotopes or fragments of the main references.

Table 59. Spectrum Labels page parameters (Sheet 2 of 4)

Parameter	Description
Decimals	View or change the number of digits the data system displays to the right of the decimal when it positions m/z labels over the peaks in a spectrum. This box is only active if you select the Mass check box. The valid range is 0 to 5.
Resolution	Display the resolution information only when your instrument is set to acquire additional peak labeling information. This check box is available only if resolution information is stored in the raw data file. If you acquire profile data and the instrument has not acquired the resolution information, you can select to have the data system centroid the data after acquisition by selecting the centroid check box. This action turns on the Resolution check box.
Charge	Display the charge state information that is stored in the raw data file. The charge is stored in the raw data file only when your instrument is set to acquire additional peak labeling information. This check box is available only if charge state information is stored in the raw data file.
Baseline	Display the baseline information that is stored in the raw data file. The baseline is stored in the raw data file only when your instrument is set to acquire additional peak labeling information. This check box is available only if baseline information is stored in the raw data file.
Noise	Display the noise information that is stored in the raw data file. The noise is stored in the raw data file only when your instrument is set to acquire additional peak labeling information. This check box is available only if noise information is stored in the raw data file.
Width (m/r)	Specify the peak width (mass $\div$ resolution) at the peak height used for the resolution measurement. For example: With profile data, select the Centroid check box, select the Valley Detection algorithm, and type 50.0 for Measure resolution at (%). With this method, the peak width shown on labels is at 50% (also called FWHM). This check box is available only if resolution information is stored in the raw data file or if you have applied a centroiding algorithm.

Table 59. Spectrum Labels page parameters (Sheet 3 of 4)

Parameter	Description
Centroid	Use centroid data for mass labels. This check box is active only if you display profile data (this is not true for LTQ-FT™, Orbitrap™, and Exactive™ instruments, because they already have centroid data used for mass labels). If you acquire profile data, select the Centroid check box to have the data system centroid the data after acquisition for use in the labels feature. This action turns on the Resolution check box. In this case, the Resolution and Width settings are available.
Choose algorithm	Opens the Choose Centroiding Algorithm dialog box, where you can select the centroiding algorithm. This button becomes available when you select the Centroid check box. To turn on the Centroid check box, you must display profile data.
Label styles	
Offset	Make the location for the displayed plot a specified distance from the <i>x</i> and/or <i>y</i> axes. The <i>x</i>-axis offset moves the <i>y</i> axis slightly above the <i>x</i> axis so that you can see baseline details. The <i>y</i>-axis offset moves the <i>x</i> axis slightly to the right of the <i>y</i>-axis so that you can see plot details at low <i>x</i>-axis values. The amount of the offset is specified in the Size box.
Size	View or change the amount that the data system moves a label from its normal position to avoid conflict with another label. This box is activated when you select the Offset check box. The valid range is 0.1 to 15.0. The default value is 2.0.
Rotated	Select whether the data system writes peak labels vertically upwards or horizontally. For vertical labels, select the Rotated check box. For horizontal labels, clear the Rotated check box. Use the adjacent graphic to view the result of the current label settings. Only the peak labels are rotated. The flags are not rotated.
Boxed	Select whether the data system places a box around each peak label. To box your label, select the Boxed check box. If you do not want to have a box around the label, clear the check box. Use the adjacent graphic to view the result of the current label settings. Only the peak labels are boxed. The flags are not boxed.

Table 59. Spectrum Labels page parameters (Sheet 4 of 4)

Parameter	Description
Threshold	
	Label peaks that are at or above a minimum percent of the base peak. This option sets the minimum percent. The valid range is 0.0 to 100.0%. For example, if the base peak is 100% and the label threshold setting is 50.0%, the data system labels all peaks at or above 50%.
	To change the label threshold, type a different percent value in the Label Threshold box. Use the adjacent graphic to view the result of the current label settings.

Spectrum View – Display Options Dialog Box – Normalization Page

Use the Spectrum Normalization page of the Display Options dialog box to modify the appearance of your spectrum by specifying the following normalization parameters. The data system displays the results of the current settings in the graphic on the right side of the page.

For more information, see [Setting the Spectrum Normalization Options](#).

[Table 60](#) describes the parameters on the Display Options – Normalization page for the spectrum view.

Table 60. Spectrum Normalization page parameters (Sheet 1 of 2)

Parameter	Description
Normalize method	
Auto range	Select the auto range normalization method for chromatograms. The data system reviews the chromatogram data, detects the minimum and maximum signal data points, and assigns these values to the extremes on the y axis. The entire dynamic range of the chromatogram is then displayed in the active view, normalized over the full range of the y axis.
Intensity Range	View or change the relative abundance range of mass spectrum peaks that the data system includes in the current spectrum view. The valid range must fall between 0.000 and 200.000 percent. To change the range of relative abundances, type the minimum and maximum relative abundance you want to display in the Intensity Range box, separated by a dash. For example, to display all peaks in a mass spectrum with relative abundances ranging from 50 to 100 percent, enter 50.000–100.000 . The data system then excludes spectrum peaks with relative abundances that range from 0.000 to 49.999 from the displayed spectrum.

Table 60. Spectrum Normalization page parameters (Sheet 2 of 2)

Parameter	Description
Normalize Spectrum To	
Largest Peak in Subsection	Set the <i>y</i> -axis maximum for each subsection (division) equal to the largest peak in the subsection (division). Set the number of subsections on the Axis page.
Largest Peak in Mass Range	Set the <i>y</i> -axis maximum equal to the largest peak in the mass range. (The mass range is the sum of all subsections [divisions]). Each subsection (division) has the same <i>y</i> -axis maximum. Set the number of divisions on the Axis page.
Largest Peak in Scan Range	Set the <i>y</i> -axis maximum equal to the largest peak in the scan range. (The scan range is all <i>m/z</i> in the scan.) Each subsection (division) has the same <i>y</i> -axis maximum. Set the number of divisions on the Axis page.
Normalize Multiple Scans	
Individually	Normalize mass plots individually.
All the Same	Normalize all mass plots equally.

Spectrum View – Display Options Dialog Box – Style Page

Use the Spectrum Style page of the Display Options dialog box to modify the appearance of a Spectrum view. The data system displays the results of the current settings in the graphic on the right side of the page.

For more information, see [Setting the Spectrum Style Options](#).

[Table 61](#) describes the parameters on the Display Options – Style page for the spectrum view.

Table 61. Spectrum Style page parameters (Sheet 1 of 2)

Parameter	Description
Plotting	
Automatic	Have the data system choose the graphic style based upon the data acquisition method used for the active spectrum.
Point to Point	Select a graphic style that displays the active chromatogram or spectrum using a point-to-point peak profile.
Stick	Select a graphic style that displays the active chromatogram or spectrum using vertical lines.
Shade	Select a graphic style that uses a shaded representation of intensity in each amu band for the active spectrum.

Table 61. Spectrum Style page parameters (Sheet 2 of 2)

Parameter	Description
Arrangement	
Stack (2D)	Stack plots vertically, with no overlap, for plots in the active cell.
Overlay (3D)	Overlay plots vertically with optional horizontal skew (time offset) for chromatogram or spectrum plots in the active cell.
3D	
This area becomes available when you select the Overlay (3D) option in the Arrangement area.	
Elevation	Set the elevation angle (the amount of overlay) to a value between 0 and 60 degrees for an overlay arrangement of plots in the active cell. To set the elevation angle, either drag the Elevation slider or click the Elevation slider left or right arrow until you reach the desired angle. The data system displays the current angle setting below the scroll box.
Skew	Set the skew angle (time offset) to a value between 0 and 45 degrees for an overlay arrangement of plots in the active cell. To set the skew, either drag the Skew slider or click the Skew slider left or right arrow until you reach the desired angle. The data system displays the current angle setting below the scroll box.
Draw Backdrop	Select a graphic style that includes a drawn perspective backdrop for an overlay arrangement of plots in the active cell.

Spectrum View – Display Options Dialog Box – Composition Page

Use the Spectrum Composition page of the Display Options dialog box to calculate elemental compositions and to add columns containing the results to your Spectrum List. The data system determines which chemical formulas have a m/z value most like that of the experimental spectrum peaks. It displays a preview of the results for the current settings in the graphic on the right side of the page.

For more information, see [Setting the Spectrum Composition Options](#).

[Table 62](#) describes the parameters on the Display Options – Composition page for the spectrum view.

Table 62. Spectrum Composition page parameters (Sheet 1 of 2)

Parameter	Description
Label with	
Elemental Comp.	Select whether the data system displays the chemical formula labels at the top of spectrum peaks. The application determines which chemical formulas have a m/z value most like that of the spectrum peaks. To turn on elemental composition labeling, select the Elemental Comp. check box. If the data system displays the elemental composition values in light gray, close Qual Browser and choose Xcalibur Roadmap > Tools > Configuration to display the Configuration page. Click the Fonts tab and set all font sizes to a minimum of 10 points.
Formulae	Type a number that specifies how many of the most likely chemical formulas you want the data system to display at the top of spectrum peaks in the Formulae box.
Theo. Mass	View the theoretical m/z of the chemical formulas that the data system determines. The application displays the theoretical m/z to the right of the formula separated by =.

Table 62. Spectrum Composition page parameters (Sheet 2 of 2)

Parameter	Description
RDB Equiv.	View the value of the ring and double-bond equivalents that the data system calculates for the chemical formulas. The application displays the ring and double-bond equivalent value under the chemical formula. Ring and double-bond equivalents measure the number of unsaturated bonds in a compound—and limit the calculated formulas to only those that make sense chemically. You can specify limits in a range from –100.0 to +100.0. The value is calculated by the following formula: $D = 1 + \frac{\sum_i^{imax} Ni(Vi - 2)}{2}$ where D is the value for the RDB $imax$ 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 results in an exact integer such as 3.0, indicating an odd-electron ion, or an integer with a remainder of 0.5, indicating an even-electron ion. A value of –0.5 is the minimum value and corresponds to a protonated, saturated compound (for example, H_3O^+).
Delta	Label the peak with the difference between the theoretical and experimental m/z .
Delta units	
Specify the units used to calculate the difference between the theoretical and experimental m/z . Select from these options: amu, mmu, or ppm.	

Map or Ion Map View – Display Options Dialog Box – Axis Page

Use the Axis page of the Display Options dialog box to modify the appearance of your map or ion map view. The data system displays the results of the current settings in the graphic on the right side of the page.

For more information, see [Setting the Map Axis Options](#).

[Table 63](#) describes the parameters on the Display Options – Axis page for the map or ion views.

Table 63. Axis page parameters for the map or ion map view (Sheet 1 of 2)

Parameter	Description
X	
Name	View or change the current axis names for the X, Y, and Z axes, as appropriate for the active chromatogram, spectrum, or map. To change an axis name, type the new name in the Name box. The data system displays the results of the current settings in the adjacent graphic. The default axis names are as follows: • X: Time • Y: Relative Abundance • Z: <i>m/z</i>
Show	View or change when the data system should display the axis name next to the corresponding axis. The data system can display the axis label displayed in the axis Name box at the following times: • Never: The data system does not display the axis label when the graphic is displayed or printed. • On Print: The application displays the axis label whenever the graphic is printed as a report. • Always: The application displays the axis label whenever the graphic is displayed or printed. The current option is displayed in the list. To change when the data system displays the axis label, select Never, On Print, or Always in the Show Name list. Since standard reports are not displayed on the screen, the On Print and Always selections for standard reports are identical.

Table 63. Axis page parameters for the map or ion map view (Sheet 2 of 2)

Parameter	Description
Offset	Set the location for the displayed plot at a specified distance from the x and/or y axes. The x-axis offset moves the y axis slightly above the x axis so that you can see baseline details. The y-axis offset moves the x axis slightly to the right of the y axis so that you can see plot details at low x-axis values. The amount of the offset is specified in the Size box.
Y	
Source	Specify that the data system apply either a custom (user-defined) label or a label from the detector to the Y axis of a map plot. When you specify a custom label in Qual Browser, the application retrieves the parameters from a layout (.lyt) file. If no.lyt file exists, the application retrieves the parameters from the default values you specified on the Labeling And Scaling Page of the Xcalibur Configuration dialog box.
Units	Apply absolute or relative scaling to the y axis of a map plot.
Other	
Grid Lines	Determine whether to display lines from major tic marks on the axis scale.
Split Time Range	Split the time scale of the active chromatogram into two or more divisions. To split the time scale, select the Split Time Range check box. The divisions box becomes available so that you can select the number of divisions. If you want to display only one time range, clear the Split Time Range check box.
Divisions	View or change the current number of divisions for a map plot with a split time range. This box becomes available when you select the Split Time Range check box. The number of divisions can be two, three, or four. To change the number of divisions, type the new number in the Divisions box. The data system displays the multiple map plots in the adjacent graphic.

Map or Ion Map View – Display Options Dialog Box – Bandwidth Page

Use the Bandwidth page of the Display Options dialog box to modify the appearance of a map or ion map view. The band width value specifies the bandwidth in amu units.

[Table 64](#) describes the Band Width parameter on the Display Options – Band Width page for the map or ion map views in Qual Browser.

Table 64. Band Width page parameter

Parameter	Description
<i>m/z</i> Band Width (amu)	View or change the current value for the map view bandwidth. The range of acceptable values is from 0.001 to 50.0, with a default value of 1.0. Increasing the bandwidth decreases the resolution.

Map or Ion Map View – Display Options Dialog Box – Color Page

Use the Color page of the Display Options dialog box to modify the appearance of a Map or Ion Map view. The data system displays the results of the current settings in the graphic on the right side of the page.

For more information, see [Setting the Map Color Options](#).

[Table 65](#) describes the parameters on the Display Options – Color page for the map or ion map views.

Table 65. Map or Ion Map Color page parameters (Sheet 1 of 2)

Parameter	Description
Line	Change the color of framing lines for the active map. The current color is displayed to the right of the Line button. To change the color of the framing lines, click Line . The Color Dialog Box opens with a color palette where you can select a preset color or customize a color. The application displays the results of the current settings in the adjacent graphic.
Fill Solid	Change the color of the solid fill for the active map. The current color is displayed to the right of the Fill solid button. To change the color of the solid fill, click Fill Solid . The Color Dialog Box opens with a color palette where you can select a preset color or customize a color. The application displays the results of the current settings in the adjacent graphic.

Table 65. Map or Ion Map Color page parameters (Sheet 2 of 2)

Parameter	Description
Backdrop	Change the color of the backdrop (background) of a map view, overlaid (3D) spectrum view, or overlaid (3D) chromatogram view. Click Backdrop to display a background. The application displays the current plot color to the right of the Backdrop button. To select the color of the backdrop, click Backdrop. The Color Dialog Box opens with a color palette where you can select a preset color or customize a color. The application displays the results of the current settings in the adjacent graphic.
Gray Scale	Turn off all color choices and display the map as a gray scale.
Log Scale	Display the color of the map in a logarithmic scale. The factor width that you set in the Factor box determines the scaling between color bands.
Factor	View or change the Factor that determines the scaling between color bands. The valid values are 1.1 to 20. Selecting the Log scale check box activates the Factor box.
Shade	
Shade (%)	Change the color of the map at 0%, 20%, 40%, 60%, 80%, and 100% relative abundance. To change the color, click a (%) button. The Color Dialog Box opens with a color palette where you can select a preset color or customize a color.

Map or Ion Map View – Display Options Dialog Box – Normalization Page

Use the Normalization page of the Display Options dialog box to modify the appearance of a Map or Ion Map view. The data system displays the results of the current settings in the graphic on the right side of the page.

For more information, see [Setting the Map Normalization Options](#).

[Table 66](#) describes the parameters on the Display Options – Normalization page for the map or ion map views.

Table 66. Normalization page parameters for the map or ion map views (Sheet 1 of 2)

Parameter	Description
Mass grouping	
Specify the mass grouping compression method. Mass grouping describes how the data system compresses mass data to form the colored bands in the 3D plot. Masses from a scan are compressed for each colored band using one of two methods: Base peak or Sum.	
Base Peak	Use the largest peak within each band (mass range) to determine the intensity of the band.
Sum	Use the sum of the intensities within each band (mass range) to determine the intensity of the band.
Normalize to Entire File	Select this check box to have the data system normalize the map to the largest peak in the raw data file.
Fix Scale	Select this check box to have the data system normalize the map to a fixed intensity value. Type an intensity value between 0.01 and 1e+20 in the Fix scale box.
Normalize method	
Auto Range	Select the Auto range normalization method for chromatograms. The data system reviews the chromatogram data, detects the minimum and maximum signal data points, and assigns these values to the extremes on the y axis. The entire dynamic range of the chromatogram is then displayed in the active view, normalized over the full range of the y axis.

Table 66. Normalization page parameters for the map or ion map views (Sheet 2 of 2)

Parameter	Description
Intensity Range	Display the relative abundance range of mass peaks that the Xcalibur system includes in the current Map or Ion Map view. The valid range must fall between –200.000 and 200.000 percent. To change the range of relative abundances, type the minimum and maximum relative abundance you want to display in the Intensity Range box, separated by a dash. For example, to display all peaks in a mass spectrum with relative abundances ranging from 50 to 100 percent, type 50.000–100.000. The data system then excludes spectrum peaks with relative abundances that range from 0.000 to 49.999 from the displayed map or ion map view.
Normalize each mass to	
Largest Peak in Subsection	Set the <i>y</i> -axis maximum for each subsection (division) equal to the largest peak in the subsection (division). Set the number of subsections on the Axis page.
Largest Peak in Time Range	Set the <i>y</i> -axis maximum equal to the largest peak in the time range. The time range is the sum of all subsections (divisions). Each subsection has the same <i>y</i> -axis maximum. Set the number of subsections on the Axis page.
Largest Peak in All Times	Set the <i>y</i> -axis maximum equal to the largest peak in all times. Each subsection (division) has the same <i>y</i> -axis maximum. Set the number of divisions on the Axis page.
Normalize mass plots	
Individually	Normalize mass plots individually.
All the Same	Normalize all mass plots equally.

Map or Ion Map View – Display Options Dialog Box – Style Page

Use the Style page of the Display Options dialog box to modify the appearance of a Map or Ion Map view. The data system displays the results of the current settings in the graphic on the right side of the page.

For more information, see [Setting the Map Style Options](#).

[Table 67](#) describes the parameters on the Display Options – Style page for the map or ion map views.

Table 67. Style page parameters for the map or ion map views

Parameter	Description
Stack	Stack plots vertically, with no overlap, for plots in the active cell.
Overlay (3D)	Overlay plots vertically with optional elevation and horizontal skew (time offset) for the active map.
Density Map	Display a density map that shows different shades for each intensity for the active map.
3D	
This area becomes available when you select the Overlay (3D) option.	
Elevation	Set the elevation angle (amount of overlay) to a value of 0 to 60 degrees for an overlay arrangement of plots in the active cell. To set the elevation angle, either drag the Elevation slider or click the Elevation slider left or right arrow until you reach the desired angle. The data system displays the current angle setting below the scroll box.
Skew	Set the skew angle (time offset) to a value of 0 to 45 degrees for an overlay arrangement of plots in the active cell. To set the skew, either drag the Skew slider or click the Skew slider left or right arrow until you reach the desired angle. The data system displays the current angle setting below the scroll box.
Fill	View or change the current fill option for the active map. The data system fill options are Plain Lines, Colored Lines, None, Solid color, Intensity shaded, and Shaded with frame.
Draw Backdrop	Select a graphic style that includes a drawn perspective backdrop for an overlay arrangement of plots in the active cell.

Spectrum List View – Display Options Dialog Box – Normalization Page

Use the Spectrum List Normalization page of the Display Options dialog box to modify the appearance of your Spectrum List. The data system displays the results of the current settings in the graphic on the right side of the page.

For more information, see [Setting the Spectrum List Normalization Options](#).

[Table 68](#) describes the parameters on the Display Options – Normalization page for the spectrum list view.

Table 68. Normalization page parameters for the spectrum list view

Parameter	Description
Intensity Range	View or change the relative abundance range of mass spectrum peaks that the data system includes in the current Spectrum List view. The valid range must fall within 0.000 to 200.000 percent. To change the range of relative abundances, type the minimum and maximum relative abundance you want to display in the Intensity range box, separated by a dash. For example, to display all peaks in a mass spectrum with relative abundances ranging from 50 to 100 percent, type 50.000–100.000 . The data system then excludes spectrum peaks with relative abundances that range from 0.000 to 49.999 from the displayed Spectrum List.
Normalize list to	
Largest Peak in Subsection	Set the value listed in the Relative column equal to a percentage of the largest peak in the subsection (division).
Largest Peak in (mass) Range	Set the value listed in the Relative column equal to a percentage of the mass-to-charge ratio of the largest peak in the mass range. (The mass range is the sum of all subsections [divisions].)
Largest Peak in Scan	Set the value listed in the Relative column equal to a percentage of the largest peak in the full mass range.

Spectrum List View – Display Options Dialog Box – Style Page

Use the Spectrum List Style page of the Display Options dialog box to modify the appearance of a Spectrum view. The data system displays the results of the current settings in the graphic on the right side of the page.

For more information, see [Setting the Spectrum List Style Options](#).

[Table 69](#) describes the parameters on the Display Options – Style page for the spectrum list view.

Table 69. Spectrum List Style page parameters (Sheet 1 of 4)

Parameter	Description
Display	
Select the All Peaks check box or type the number of peaks that you want to display in the Top box.	
All Peaks	Specifies whether the Spectrum List view displays all of the mass spectrum peaks in a selected scan. By default, the Spectrum List view displays the m/z value, intensity, and relative intensity of each mass spectrum peak (in the range specified in the Spectrum List Ranges dialog box or as specified in the active scan filter). To display all of the mass spectrum peaks, select the All Peaks check box. When you select this check box, the Top box becomes unavailable.
Top	Specifies the maximum number of peaks to include in the Spectrum List. This box is only active if the All peaks check box is clear. The valid range is 1 to 1000. If you order the list by mass (m/z), the data system displays the specified number of peaks having the greatest intensity in ascending mass (m/z) order. For example, if you type the value 10 in the Top box, the application displays a Spectrum List with the 10 greatest intensity peaks sorted in ascending order by m/z. If you order the list by intensity, the data system displays the specified number of peaks having the greatest intensity in descending intensity order. For example, if you type the value 10 in the Top box, the data system displays a spectrum list with the 10 greatest intensity peaks sorted in descending order by intensity.

Table 69. Spectrum List Style page parameters (Sheet 2 of 4)

Parameter	Description
Flags	Specifies whether the data system displays letters in the Flags column of the Spectrum List view to provide supplemental information about the peak data. The possible flags are as follows: • S—Saturated peaks are peaks with a signal too large to measure (over range from A to D converter). • R—Reference peaks are peaks from a reference compound used for an internal recalibration of a scan (for example, in MAT95 series). • L—Lock peaks are local references used to calculate accurate mass of nearby peaks (for example, in Quantum AM). • E—Exception peaks are also peaks from a reference compound, but not used for recalibration. These are typically small isotopes or fragments of the main references. • #—Mathematically modified peaks are peaks where the peak mass was recalculated by the instrument, usually due to a calibration process. • M—Merged peaks are peaks where the centroider combined two nearby peaks. • F—Fragmented peaks are peaks separated into multiple peaks by the centroiding activity.
Label Data	This check box is only available for the raw data files acquired with a Thermo Scientific mass spectrometer that provides label stream data. Label stream data includes the resolution, charge state, baseline, Selecting this check box activates the following check boxes: Resolution, Charge, Baseline, and Noise.
Resolution	Specifies whether the Spectrum List view displays the resolution information provided by the mass spectrometer for each centroid in the Spectrum List view. Selecting the Label Data check box activates this check box. The Label Data check box is only available for raw data files acquired with a mass spectrometer that provides label stream data.

Table 69. Spectrum List Style page parameters (Sheet 3 of 4)

Parameter	Description
Charge	Specifies whether the Spectrum List view displays the charge state information provided by the mass spectrometer for each centroid in the spectrum list. Selecting the Label Data check box activates this check box. The Label Data check box is only available for raw data files acquired with a mass spectrometer that provides label stream data.
Baseline	Specify whether the Spectrum List view displays baseline information provided by the mass spectrometer in the spectrum list. Selecting the Label Data check box activates this check box. The Label Data check box is only available for raw data files acquired with a mass spectrometer that provides label stream data.
Noise	Specifies whether the Spectrum List view displays noise information provided by the mass spectrometer for each centroid in the Spectrum List. Selecting the Label Data check box activates this check box. The Label Data check box is only available for raw data files acquired with a mass spectrometer that provides label stream data.
Centroid	This check box is only available for scan data acquired in the profile mode with a Thermo Scientific LCQ™, TSQ Quantum™, DSQ™, Polaris, or GCQ mass spectrometer. Selecting the Centroid check box activates the Resolution check box and the Choose Algorithm button.
Choose Algorithm	Opens the Choose Centroiding Algorithm dialog box, where you can select a centroiding algorithm. ❖ To activate the Choose Algorithm button 1. Open a raw data file that was acquired in the profile mode with one of the following mass spectrometers: LCQ, TSQ Quantum, DSQ, Polaris, or GCQ. 2. Select the Centroid check box.

Table 69. Spectrum List Style page parameters (Sheet 4 of 4)

Parameter	Description
Order by	
You can order the mass spectrum peak list by mass or intensity.	
Mass	Selecting this option orders the Spectrum List in ascending m/z value order. Sort by mass to ensure that the highest intensity peak (with relative intensity 100.00) is always in the list, but not necessarily the first entry in the list.
Intensity	Selecting this option orders the Spectrum List in descending intensity order. Sort by intensity to ensure that the highest intensity peak (with relative intensity 100.00) is always the first entry in the list.
Precision	
Decimals	Specifies the number of places after the decimal point that the data system uses to process MS data. Specify from 0 to 5 decimal places. The number of decimal places applies to the MS data in the Qual Browser window.

Spectrum List View – Display Options Dialog Box – Composition Page

Use the Spectrum List Composition page of the Display Options dialog box to calculate elemental compositions and to add columns containing the results to your spectrum list. The data system determines which chemical formulas have a m/z value most like that of the experimental spectrum peaks. It displays a preview of the results for the current settings in the list on the right side of the page.

For more information, see [Setting the Spectrum List Composition Options](#).

[Table 70](#) describes the parameters on the Display Options – Composition page for the spectrum list view.

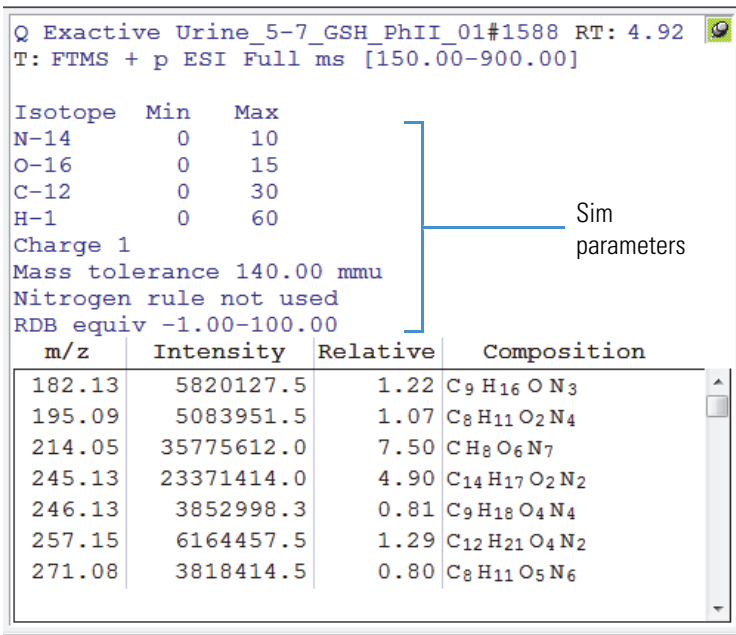
Table 70. Spectrum List Composition page parameters (Sheet 1 of 3)

Parameter	Description
Label with	
Elemental Comp.	Select whether the application displays the Composition column. The application determines which chemical formulas have a m/z value most like that of the spectrum peaks. To turn on elemental composition labeling, select the Elemental Comp. check box.
Formulae	Type a number that specifies how many of the most likely chemical formulas you want the application to display in the Formulae box.
Theo. Mass	The Theo. mass column lists the theoretical m/z of the chemical formulas that the data system determines.

Table 70. Spectrum List Composition page parameters (Sheet 2 of 3)

Parameter	Description
RDB Equiv.	Select whether the application displays the value of the ring and double-bond equivalents that the application calculates for the chemical formulas. The application displays the ring and double-bond equivalent value under the chemical formula. Ring and double-bond equivalents measure the number of unsaturated bonds in a compound—and limit the calculated formulas to only those that make sense chemically. You can specify limits in a range from –100.0 to +100.0. The value is calculated by the following formula: $D = 1 + \frac{\sum_i^{imax} Ni(Vi - 2)}{2}$ where D is the value for the RDB $imax$ 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 results in an exact integer such as 3.0, indicating an odd-electron ion, or an integer with a remainder of 0.5, indicating an even-electron ion. A value of –0.5 is the minimum value and corresponds to a protonated, saturated compound (for example, H₃O⁺).

Table 70. Spectrum List Composition page parameters (Sheet 3 of 3)

Parameter	Description
Sim Parameters	Select whether the data system displays the settings in the Limits area of the Qual Browser – Elemental Composition page.
	
Delta	In the Delta column, display the difference between the theoretical and experimental m/z .
Delta units	
Specify the units used to calculate the difference between the theoretical and experimental m/z values. Select from these options: amu, mmu, or ppm.	

Global Mass Options Dialog Box

IMPORTANT Use the Global Mass Options dialog box to specify tolerance and precision settings for the mass data displayed in the chromatogram, spectrum, map, and ion map plots in the Qual Browser window.

You can also specify the global default values for tolerance and precision on the Mass Options page of the Xcalibur Configuration dialog box.

For more information, see [Setting the Global Mass Options for the Qual Browser Window](#).

Table 71 describes the parameters in the Global Mass Options dialog box.

Table 71. Global Mass Options dialog box parameters

Parameter	Description
Options	
Apply to Current Cell	Apply the settings in this dialog box to the currently pinned cell.
Apply to All Cells in Current Window	Apply the settings in this dialog box to all cells in the current file window in Qual Browser.
Apply to All Cells in All Windows	Apply the settings in this dialog box to all cells in all open file windows in Qual Browser.
Set Mass Tolerance	
Use User Defined	Specify a custom mass tolerance. If you do not specify a user defined tolerance, Qual Browser will use tolerance values recorded by the mass spectrometer in the raw data file.
Mass Tolerance	Specify the value for mass tolerance. Enter a value in the range of 0.1 to 50 000, and then select units to apply to the value. The data system uses the tolerance value to create the limits of a range of masses.
Units	Specify the unit of measurement for processing your data. Select mmu (millimass units) or ppm (parts per million).
Set Mass Precision	
Decimals	Specify the number of decimal places (mass precision) that the data system uses to display mass values. You can specify from 0 to 5 decimal places. The number of decimal places applies to the mass data in a window.

Heading Editor Dialog Box

Use the Heading Editor dialog box to edit the heading above the raw data graphical views in the Qual Browser window. The heading contains information about the raw data file whose chromatogram, mass spectrum, or map views are displayed. This figure shows an example of a heading.

File name: C:\Xcalibur\examples\data\drugx_23	Sample type: QC
Path: C:\LCQ\DATA\mrw_27417\Sat_0504_WD1	Inj vol: 50.000000
Created: 05/05/1996 03:50:49 AM	Comment: QC=400 pg/ml,IS=100 pg/ml

Table 72 describes the parameters in the Heading Editor dialog box.

Table 72. Heading Editor dialog box parameters (Sheet 1 of 6)

Parameter	Description
Heading Table	Enter labels and values to be displayed above the graphical views. The data system arranges the heading information into one, two, or three columns of label/value pairs (Label1, Value1; Label2, Value2; Label3, Value3).
Label Columns	Type in a label or enter an asterisk (*) to accept the default label. The Label column uses these default values: File Name: File Name Time Stamp: Created Sample Name: Sample Name Comment: Comment Sequence Row: Sequence Row Sample Type: Sample Type Calibration Level: Cal Level Sample ID: Sample ID Instrument Method: Inst Meth Processing Method: Proc Meth Path: Path Calibration File: Cal File Position: Position Injection Volume: Inj Vol

Table 72. Heading Editor dialog box parameters (Sheet 2 of 6)

Parameter	Description
	Sample Weight: Sample Weight
	Sample Volume: Sample Volume
	Internal Standard Amount: ISTD Amount
	CD Factor: CD Factor
	Bar Code: Bar Code
	Bar Code Status: Bar Code Status
	Tray Index: Tray Index
	Vial Index: Vial Index
	Vials Per Tray: Vials Per Tray
	Vials Per Tray X: Vials Per TrayX
	Vials Per Tray Y: Vials Per TrayY
	Tray Shape: Tray Shape
	Tray Name: Tray Name
	Instrument Name: Inst Name
	Instrument Model: Inst Model
	Instrument Serial Number: Inst Serial #
	Instrument Software Version: Inst Software Version
	Instrument Hardware Version: Inst Hardware Version
	Flags: Flags
	User Text 1: Study
	User Text 2: Client
	User Text 3: Laboratory
	User Text 4: Company
	User Text 5: Phone
	Mass Tolerance: Mass Tolerance

Table 72. Heading Editor dialog box parameters (Sheet 3 of 6)

Parameter	Description
Value Columns	Select the values from a dropdown list. You display the dropdown list by clicking a Value field in the Label/Value grid. For the Values column, you can choose from these values: File Name: The name and path of the file storing the displayed data. Time Stamp: The date and time the data system acquired the displayed data. Sample Name: The sample name specified in the Sample Name column in the sequence row corresponding to the displayed data. Comment: The comment specified in the Comment column in the sequence row corresponding to the displayed data. Sequence Row: The number of the sequence row corresponding to the displayed data. Sample Type: The type of sample selected in the Sample Type column in the sequence row corresponding to the displayed data. Calibration Level: The calibration level specified in the Level column in the sequence row corresponding to the displayed data. Sample ID: The unique identification (ID) number specified in the Sample ID column in the Sequence Setup view. Instrument Method: The path and file name of the instrument method specified in the Inst Method column in the Sequence Setup view. Processing Method: The path and file name of the processing method specified in the Proc Method column in the Sequence Setup view. Path: The path where you had the data system save the raw data file(s) specified in the Path column in the Sequence Setup view. Calibration File: The path and file name of the Calibration File specified in the Calibration File column in the Sequence Setup view. Position: The position of the sample in the autosampler specified in the Position column in the Sequence Setup view.

Table 72. Heading Editor dialog box parameters (Sheet 4 of 6)

Parameter	Description
	Injection Volume: The injection volume in microliters of sample specified in the Inj Vol column in Sequence Setup.
	Sample Weight: The amount of a component specified in the Sample Weight column in Sequence Setup.
	Sample Volume: The volume of a component specified in the Sample Vol column in Sequence Setup.
	Internal Standard Amount: The internal standard correction amount specified in the ISTD Corr Amt column in Sequence Setup.
	CD Factor: The concentration/dilution factor set in Sequence Setup.
	Bar Code: The bar code information number from the autosampler.
	Bar Code Status: Indicates whether the bar code has been read by the autosampler.
	Tray Index: A combination of letters and numbers that identifies the autosampler tray.
	Vial Index: A combination of letters and numbers that identifies the autosampler vial.
	Vials Per Tray: The number of vials in the autosampler tray.
	Vials Per Tray X: The number of vials across the autosampler tray.
	Vials Per Tray Y: The number of vials that the autosampler is deep.
	Tray Shape: The shape of the autosampler tray (for example, rectangular).
	Tray Name: A name that identifies the type of autosampler tray.
	Instrument Name: The name of the mass spectrometer series (for example, LCQ).
	Instrument Model: The model name of the mass spectrometer (for example, Deca XP Plus).
	Instrument Serial Number: The serial number of the mass spectrometer.

Table 72. Heading Editor dialog box parameters (Sheet 5 of 6)

Parameter	Description
	Instrument Software Version: The version number of the Xcalibur software that is installed on the system. Instrument Hardware Version: The version number of the hardware components that are installed on the mass spectrometer. Flags: Additional information about the mass spectrometer. User Text 1: The text that you entered in the Heading 1 column in the Sequence Setup view. User Text 2: The text that you entered in the Heading 2 column in the Sequence Setup view. User Text 3: The text that you entered in the Heading 3 column in the Sequence Setup view. User Text 4: The text that you entered in the Heading 4 column in the Sequence Setup view. User Text 5: The text that you entered in the Heading 5 column in the Sequence Setup view. Mass Tolerance: The upper and lower mass limits that the data system uses to condense to a single mass value all the scans in the mass range.
Set Label Color	Open the Color dialog box to select the color that you want to use for all labels in the heading.
Set Value Color	Open the Color dialog box to select the color that you want to use for all values in the heading.
Column Position Editor	
Column Position Editor	Set the absolute horizontal position of the columns of labels and values in the header.
Auto Value Position	Determine the spacing between a label and its corresponding value automatically.

Table 72. Heading Editor dialog box parameters (Sheet 6 of 6)

Parameter	Description
Label	Specify the absolute position of each column of labels. The value must be between 0 and 2000. However, for a screen resolution of 1152 by 864, position values larger than about 75 place the label off the screen.
Value	Specify the absolute position of each column of values. These settings are unavailable if you select the Auto Value Position check box. The value must be between 0 and 2000. However, for a screen resolution of 1152 by 864, position values larger than about 75 place the value off the screen.

Peak Purity Dialog Box

Use the Peak Purity dialog box to specify the values of the peak purity parameters to be applied to PDA raw data in an active chromatogram view.

The Peak Purity command in the Actions menu becomes active only when you open a raw data file that contains scan data (for example, PDA data) in Qual Browser and select the PDA Detector Type from the [Chromatogram Display Options Dialog Box](#).

[Table 73](#) describes the parameters in the Peak Purity dialog box.

Table 73. Peak Purity dialog box parameters (Sheet 1 of 2)

Parameter	Description
Enable	Turn on Peak Purity parameters for PDA chromatograms in an active chromatogram cell and calculate peak purity results by selecting the Enable check box. Peak detection occurs automatically before the peak purity calculation.
Scan Threshold	Specify a minimum value of intensity for wavelength scans in microabsorbance units (μ AU). Peak Purity computation using scan threshold starts with the scan at the apex of the peak and collects wavelength data from scans on both sides of the apex until the scan threshold is reached. Use scan threshold for either symmetrical or asymmetrical peaks. The default value for scan threshold is 3000 μ AU. The range of possible values is 0 to 1 000 000 μ AU (or 1 AU). In a sample with high background or noise, you might start with a value for scan threshold of 40 000 μ AU.

Table 73. Peak Purity dialog box parameters (Sheet 2 of 2)

Parameter	Description
Peak Coverage	Specify a maximum percent value of the width of the integrated peak. Peak Purity computation using peak coverage starts with the scan at the apex of the peak and collects wavelength data from scans on both sides of the apex until the percent peak coverage is reached. Use peak coverage for symmetrical peaks. The default value for peak coverage is 95% of the integrated peak width.
Limit Scan Wavelength	Activate the Wavelength Range box. Select this check box to limit the number of wavelengths to include in the Peak Purity computation. Then, enter a range in the Wavelength Range box.
Wavelength Range	Specify a range of UV scans (in nanometers) that include the wavelengths of your peak(s) of interest. Peak Purity computation using wavelength range starts with the scan at the apex of a peak; and then collects wavelength data from scans on both sides of the apex until all the wavelengths in the range are included. Use wavelength range for either symmetrical or asymmetrical peaks. The default wavelength range is the full width of the scan. This box is available only if you select the Limit Scan Wavelength check box.
Apply to All Traces	Compute peak purity for all the peak traces in a cell. If the check box is empty, the data system computes peak purity for the selected trace only.

Print Dialog Box

Use the Print dialog box in the Qual Browser window to specify what to print and how to print it.

Table 74 describes the parameters in the Print dialog box.

Table 74. Print dialog box parameters

Parameter	Description
Print What	
All Cells in the Selected Window	Print all of the cells in the selected window. Before opening the Print dialog box, select the window by clicking its title bar.
Selected Cell Only	Print a selected cell. Before opening the Print dialog box, select the cell by clicking its cell pin icon,  .
Print How	
One Page	Print cells on a single page. To make sure the area selected for printing prints on only one page, this option might delete some of the information contained in a cell or cells displaying text. For example, the data system might print only a partial spectrum list or method.
Each Cell on a Separate Page	Print cells with each cell on a separate page. To print each cell on a separate page, select the Each Cell On Separate Page option. To make sure all information in all cells is printed, this option can print more than one page per cell when one or more cells display text. For example, a spectrum list or method can require multiple pages.

Ranges Dialog Boxes

Use the Ranges dialog boxes to define the range parameters for the views.

- [Chromatogram Display Options Dialog Box](#)
- [Spectrum Ranges Dialog Box](#)
- [Map Ranges Dialog Box](#)
- [Scan Filter Range Dialog Box](#)
- [Scan Header Range Dialog Box](#)
- [Spectrum List Ranges Dialog Box](#)
- [Status Log Range Dialog Box](#)
- [Tune Method Range Dialog Box](#)

Chromatogram Display Options Dialog Box

Use the Chromatogram Display Options dialog box to view and edit the mass range, time range, and other properties of a chromatogram plot:

- In Qual Browser, for all plots in the active chromatogram view.
- On the home page, for the active chromatogram plot in Real Time Plot mode.

You can also apply automatic processing options such as smoothing and background subtraction.

The dialog box consists of two pages:

- [Automatic Processing Page – Chromatogram Display Options Dialog Box](#)
- [Ranges Page – Chromatogram Display Options Dialog Box](#)

Automatic Processing Page – Chromatogram Display Options Dialog Box

Use the Automatic Processing page of the Chromatogram Display Options dialog box to apply automatic processing options such as smoothing and baseline subtraction to all plots in the active cell. You can also specify values for Mass Tolerance and Mass Precision that are applied to the raw data display in the active chromatogram view.

Table 75 describes the parameters on the Chromatogram Display Options – Automatic Processing page.

Table 75. Chromatogram Display Options – Automatic Processing page parameters (Sheet 1 of 3)

Parameter	Description
Smoothing	
Smoothing	Apply smoothing to all chromatogram plots in the active view.
Enable	Turn on chromatogram smoothing for all the chromatograms in the active view. Define the type of smoothing in the Chromatogram Smoothing Type list. Define the degree of smoothing in the Smoothing Points box. To smooth all active chromatograms, select the Enable check box in the Smoothing area.
Type	View the current type of smoothing that the data system applies to the active chromatogram. To make this list active, select the Enable check box in the Smoothing area. To change the current setting, open the list and select Boxcar or Gaussian.
Points	View or change the number of points that the data system uses for chromatogram smoothing. The type of smoothing is defined in the Type list. This list is only active when you select the Enable check box in the Smoothing area. The valid range for smoothing points is 3 for minimum smoothing to 15 for maximum smoothing. To change the number of smoothing points, type an odd integer from 3 to 15 in the Points box.
Baseline Subtraction	
Baseline Subtraction	Apply baseline subtraction to all chromatogram plots in the active view. This algorithm fits a smooth curve through the noise in the chromatogram, then subtracts this curve from the chromatogram, leaving the peaks on a flat baseline.

Table 75. Chromatogram Display Options – Automatic Processing page parameters (Sheet 2 of 3)

Parameter	Description
Enable	Activate Baseline Subtraction to chromatograms in the active cell. To turn on baseline subtraction, select the Enable check box.
Polynomial Order	Specify the degrees of freedom allowed to the fitted curve. With polynomial order set to 0, a horizontal straight line is fitted. With polynomial order set to 1, a sloping straight line is fitted. The further the background is from a straight line, the higher you must set the polynomial order control. Too high a value will cause the fitted curve to begin to follow the peak shapes. Normal operating range for this parameter is 3 to 20. With higher order polynomials, background subtract will sometimes have difficulty converging on a solution. There is a pre-set upper limit of 300 iterations. If background subtract does not seem to be making progress, press the Cancel button in the status box and try again with a lower-order polynomial.
Below Curve	Move the background curve up and down in the noise. The curve fit is constrained to place the specified percentage of data points beneath the fitted background curve. Normal operating range for this parameter is 5% to 30%, depending on the abundance and width of peaks in the chromatogram. For more or wider peaks, increase the value.
Tolerance	View the precision level for performing internal arithmetic. It should not normally be altered from its default value of 0.01.
Flatten Edges	Select the Flatten Edges check box to apply the polynomial so that the beginning and end of the chromatogram plot are horizontal.
Overlay Graph of Fitted Polynomial	Display the polynomial as an graphic overlay on the chromatogram plot.
Include Peaks	
Include Peaks	Include or exclude the reference peaks (R) and exception peaks (E) for the MS data in a Qual Browser window.
Reference and Exception Peaks	Include or exclude the reference peaks (R) and exception peaks (E) for the MS data in a Qual Browser window.
Mass Tolerance	
Mass Tolerance	Specify a value for mass tolerance to affect the display of the MS data in a Qual Browser window.

Table 75. Chromatogram Display Options – Automatic Processing page parameters (Sheet 3 of 3)

Parameter	Description
Use User Defined	Specify the values for mass tolerance and mass units for the MS data in a Qual Browser window. To change the parameter values, select the Use User Defined check box. If you clear the check box, the data system uses the values for mass tolerance and units that are stored in the raw data file.
Mass Tolerance	Specify the value for mass tolerance. Enter a value in the range from 0.1 to 50 000 and select units to apply to the value. For a mass range chromatogram, the data system uses the tolerance value to create the limits of a range of masses. The central mass of the range is the one specified on the Ranges Page – Spectrum Ranges Dialog Box. If a single mass is entered for a mass chromatogram, the data from each (filtered) scan is analyzed in the chromatogram from mass – tolerance to mass + tolerance. If a range of masses is entered, the limits are considered precise, and no tolerance is applied. Therefore, a mass1–mass2 range causes data to be analysed between the exact masses entered. Use the mass precision setting if more decimals are needed to specify masses. For base peak chromatogram, the largest mass in the range is selected, and for mass chromatogram, the data in the specified range is summed.
Units	Specify the default units that are used in processing MS data in the Qual Browser window. To change the user-defined settings, select the Use User Defined check box. Select either the mmu (millimass units) option or the ppm (parts per million) option. To turn off the user-defined units, clear the Use User Defined check box.
Mass Precision	
Mass Precision	Apply mass precision to the MS data in a Qual Browser window.
Decimals	Specify the number of decimal places (significant digits after the decimal point) that the data system uses to process MS data. Specify from 0 to 5 decimal places. The number of decimal places applies to the mass spectral data in a Qual Browser window.

Ranges Page – Chromatogram Display Options Dialog Box

Use the Ranges page of the Chromatogram Display Options dialog box to view and edit the mass range, time range, and other properties of a chromatogram plot.

Table 76 describes the parameters on the Ranges page of the Chromatogram Ranges dialog box.

Table 76. Ranges page parameters (Sheet 1 of 4)

Parameter	Description
Range	
Time Range	View or change the time range in minutes for the active chromatogram. The valid range is 0.00 to 9999.00 minutes. To select a time range, type the lower and upper time limits in minutes, separated by a dash (no spaces) in the Time Range box. For example, to select a time range from 0.10 to 9.10 minutes, type 0.10–9.10 .
Fixed Scale	Define the maximum range for the y axis of the active chromatogram by selecting the Fixed Scale check box.
Plot Properties Table	
Enable check boxes	View or hide the display of a chromatogram plot. The plot is defined by its position in the list and is described by the settings in the Plot Properties box. Select the Type check box to display the chromatogram.
Plot Properties	
Raw File	View or change the path and filename of the raw data file used to generate the highlighted plot in the Ranges list on the Ranges page of the Chromatogram Ranges dialog box. Open the Raw File list to see a list of all the files active in the current cell. You can change the source of the active plot in one these ways: • Select a file from the list. • Click Browse adjacent to the box and browse to the required file. • Type the full path and filename of the required file into the box.
Scan Filter	View the scan filter used for the active chromatogram. To select a filter, open the Scan Filter list to display the scan filters that are stored in the raw data file. Select the desired filter. The data system displays the selected filter. You can also use the scan filter format to type a scan filter the Scan Filter box.

Table 76. Ranges page parameters (Sheet 2 of 4)

Parameter	Description
Plot Type	Specify the type of chromatogram you want to view in the active plot. You can select: 1. A basic chromatogram type, for example, TIC, from the first list. 2. A logical operator: + or – from the second list. Your selection of an operator activates. 3. The third list for you to select a second chromatogram type to add to, or subtract from, the first type. For example, Mass Range. The list includes the valid remaining trace types. You can use trace combinations for subtracting contributions to a chromatogram from a solvent or other noise. Combinations are limited to traces of the same type. For MS scans, valid trace types are TIC, Mass Range and Base Peak. For MS/MS scans, valid trace types are TIC, Mass Range, Base Peak, and Neutral Fragment. For Analog data, up to four channels are supported (labeled Analog 1-4). For data from an A/D Card, four channels are supported (labeled A/D Card Ch 1-4). For PDA data, valid trace types are Wavelength Range, Total Scan, or Spectrum Maximum. See these topics for valid trace types: • MS Trace Combinations • Analog Trace Combinations • A/D Card Trace Combinations • PDA Trace Combinations • UV Trace Combinations

Table 76. Ranges page parameters (Sheet 3 of 4)

Parameter	Description
Range(s)	Specify the range of the selected chromatogram plot type. For an MS detector type, the Ranges box displays the current mass range of the active chromatogram if you select a Mass Range or Base Peak plot type. Two Ranges boxes are displayed if you select one of these plot combinations: • Mass Range $\pm$ Mass Range • Base Peak $\pm$ Mass Range • Mass Range $\pm$ Base Peak Use the Ranges boxes to specify the ranges of the two plot types. For a PDA detector type, the Ranges box displays the current wavelength range if you select a Wavelength Range or plot type. Two Ranges boxes are displayed if you select one of these plot combinations: • Wavelength Range $\pm$ Wavelength Range • Wavelength Range $\pm$ Spectrum Maximum • Spectrum Maximum $\pm$ Wavelength Range Use the Ranges boxes to specify the ranges of the two plot types. For other detector types, the parameter is unavailable. To change a range or to add a new range, type the range in the box. The valid range is dependent upon the configured detector. The format is as follows: <i>Low Mass/Wavelength–High Mass/Wavelength.</i> For example, for the range m/z 123 through 234, type the following: 123–234 To enter multiple ranges, separate each range with a comma, for example: 100–120, 130–150, 200–220, 300, 302–310

Table 76. Ranges page parameters (Sheet 4 of 4)

Parameter	Description
Mass	The neutral fragment mass. This box is displayed only when you select the MS detector and Neutral Fragment plot type.
Detector	View the currently selected detector data type: • MS • Analog • A/D Card • PDA • UV ❖ To change the detector data type 1. Open the Detector list. 2. Select the required detector type. The data system extracts the data type from the raw data file.
Peak Algorithm	Select one of the peak detection algorithms. The algorithm use is active for the currently selected file. When you select an algorithm, the data system changes the default parameters for peak detection and integration to those specific to that algorithm. If a raw data file is open, you can select a peak detection algorithm from the list and click OK to recalculate the data using that algorithm.
Delay	View or change the delay time between when a component peak is detected by the mass spectrometer and the same peak is detected by a UV or analog detector. The valid time range is -5.0 to $+5.0$ minutes. To change the value, enter the new delay time in the Delay box. You can acquire data from more than one detector during a sample run. Use this parameter to visually align the chromatograms from different detectors.
Fix Scale To	View or change the current maximum range for the y axis of the active chromatogram. This box is only active when you select the Fixed Scale check box. The maximum y-axis value can range from 0.01 to 10^{10}. To change the value, input the new maximum y-axis value in the Fix Scale To box.

These topics describe the valid trace combinations:

- [MS Trace Combinations](#)
- [Analog Trace Combinations](#)
- [A/D Card Trace Combinations](#)
- [PDA Trace Combinations](#)
- [UV Trace Combinations](#)

MS Trace Combinations

This table lists the valid trace combinations available in the Trace lists. Your choice of combination affects other controls on the page as described in the resulting controls column.

[Table 77](#) describes the MS trace combinations.

Table 77. MS trace combinations parameters

Trace 1	Operator	Trace 2	Resulting controls
Mass Range	[blank]	[unavailable]	Mass (m/z) box
Mass Range	–	Mass Range	Mass1 (m/z) box 2 text box
Mass Range	+	Mass Range	Mass1 (m/z) box 2 text box
TIC	[blank]	[unavailable]	none
TIC	–	Mass Range	Mass (m/z) box
TIC	–	Base Peak	Mass (m/z) box
Base Peak	[blank]	[unavailable]	Mass (m/z) box
Base Peak	–	Mass Range	BP box MR text box
Base Peak	+	Mass Range	BP box MR text box
Neutral Fragment (MS/MS data only)	[unavailable]	[unavailable]	Mass

Analog Trace Combinations

This table lists the valid trace combinations available in the Trace lists. The Mass Range/Wavelength Range control is unavailable.

Table 78 describes the analog trace combinations.

Table 78. Analog trace combinations parameters

Trace 1	Operator	Trace 2	Resulting controls
Analog n ($1 \leq n \leq 4$)	[blank]	[unavailable]	None
Analog n ($1 \leq n \leq 4$)	–	Analog m ($1 \leq m \leq 4, m \neq n$)	None
Analog n ($1 \leq n \leq 4$)	+	Analog m ($1 \leq m \leq 4, m \neq n$)	None

A/D Card Trace Combinations

This table lists the valid trace combinations available in the Trace lists when you have selected an A/D Card detector type. The Mass Range/Wavelength Range control is unavailable.

Table 79 describes the trace combinations for an A/D card.

Table 79. A/D card trace combinations parameters

Trace 1	Operator	Trace 2	Resulting controls
A/D Card Channel n ($1 \leq n \leq 4$)	[blank]	[unavailable]	None
A/D Card Channel n ($1 \leq n \leq 4$)	–	A/D Card Channel m ($1 \leq m \leq 4, m \neq n$)	None
A/D Card Channel n ($1 \leq n \leq 4$)	+	A/D Card Channel m ($1 \leq m \leq 4, m \neq n$)	None

PDA Trace Combinations

This table lists the valid trace combinations available in the Trace lists when you have selected a PDA detector type in the Type list on the Identification page of Qual or Quan views. Your choice of combination affects other controls on the page as described in the Resulting Controls column.

Table 80 describes the trace combinations for a PDA detector.

Table 80. PDA trace combinations parameters

Trace 1	Operator	Trace 2	Resulting controls
Wavelength Range	[blank]	[unavailable]	Wavelength (nm) box
Wavelength Range	+	Wavelength Range	Wavelength1 (nm) box 2 text box
Wavelength Range	–	Wavelength Range	Wavelength1 (nm) box 2 text box
Wavelength Range	+	Spectrum Maximum	Wavelength1 (nm) box 2 text box
Wavelength Range	–	Spectrum Maximum	Wavelength1 (nm) box 2 text box
Total Scan	[blank]	[unavailable]	None
Total Scan	–	Wavelength Range	Wavelength (nm) box
Total Scan	–	Spectrum Maximum	Wavelength (nm) box
Spectrum Maximum	[blank]	[unavailable]	Wavelength (nm) box
Spectrum Maximum	+	Wavelength Range	Wavelength1 (nm) box 2 text box
Spectrum Maximum	–	Wavelength Range	Wavelength1 (nm) box 2 text box

UV Trace Combinations

This table lists the valid trace combinations available in the Trace lists for UV detectors. The Mass Range/Wavelength Range control is unavailable.

Table 81 describes the UV trace combinations.

Table 81. UV trace combinations parameters

Trace 1	Operator	Trace 2	Resulting controls
Channel n ($A \leq n \leq D$)	[blank]	[unavailable]	None
Channel n ($A \leq n \leq D$)	–	Channel m ($A \leq m \leq D, m \neq n$)	None
Channel n ($A \leq n \leq D$)	+	Channel m ($A \leq m \leq D, m \neq n$)	None

Spectrum Ranges Dialog Box

Use the Spectrum Ranges dialog box to view and edit the mass range, time, and other properties of a spectrum plot:

- In Qual Browser, for all plots in the active spectrum view.
- On the home page, for the active spectrum plot in Real Time Plot mode.

You can also apply automatic processing options such as smoothing and background subtraction. The dialog box consists of two pages:

- [Automatic Processing Page – Spectrum Ranges Dialog Box](#)
- [Ranges Page – Spectrum Ranges Dialog Box](#)

Automatic Processing Page – Spectrum Ranges Dialog Box

Use the Automatic Processing page of the Spectrum Ranges dialog box to set spectrum Smoothing or Refine enhancement parameters. These are applied to all spectra in the active view.

Table 82 describes the parameters on the Spectrum Ranges – Automatic Processing page.

Table 82. Automatic Processing page parameters – Spectrum Ranges dialog box (Sheet 1 of 3)

Parameter	Description
Smoothing	
Enable	Turn on the smoothing. Define the type of smoothing in the Type list. Define the degree of smoothing in the Points box.
Type	View or select the current type of smoothing. To make this list active, select the Enable check box in the Smoothing area. To change the current setting, open the Type list and select Boxcar or Gaussian . The data system displays your new selection in the Type box.
Points	View or change the number of points that the data system uses for smoothing. The type of smoothing is defined in the Type list. This list is only active when you select the Enable check box in the Smoothing area. The valid range for smoothing points is the set of odd integers from 3 for minimum smoothing to 15 for maximum smoothing. To change the number of smoothing points, type an odd integer from 3 to 15 in the Points box.

Table 82. Automatic Processing page parameters – Spectrum Ranges dialog box (Sheet 2 of 3)

Parameter	Description
Refine	
	Apply the Refine spectrum enhancement to all the spectra displayed in the active spectrum view. Refine requires two parameters: Window Size (sec) and Noise Threshold. The Refine algorithm examines the mass chromatogram of each ion contributing to the mass spectrum at the apex of a chromatographic peak: 1. It discards masses without a peak maximum within ± 1 scan of the defined chromatogram peak apex. 2. It then searches for a minimum within the specified Window Size range either side of the peak apex. These points define the peak start and peak end. 3. Using scans at and beyond the chromatographic peak start and peak end, Refine measures the background noise level in the mass chromatogram. 4. Refine uses extrapolation to estimate the contribution of noise to the scan at the peak apex. Refine adjusts the mass intensity of the apex scan accordingly. 5. Finally, Refine uses the Noise Threshold parameter to determine whether the adjusted intensity is significant in comparison to the background noise. If the following is true: $\text{Adjusted Intensity} < \text{Noise Threshold} \times \text{Background Noise}$ the mass is discarded from the final mass spectrum.
Enable	Turn on Refine spectrum enhancement for all the spectra in the active view. To apply Refine to the active spectrum view, select the Enable check box in the Refine area.
Window Size	Enter a time window for the Refine spectrum enhancement method. The Refine algorithm applies the window across a chromatogram peak apex and uses it to search for the peak start and peak end and to estimate the background noise. Set this parameter to the peak width.
Noise Threshold	Enter a value for the Noise Threshold parameter. The Refine algorithm uses the Noise Threshold parameter to determine whether adjusted ion intensities are significant in comparison to the background noise. The parameter is actually a factor rather than a threshold. For example, with a Noise Threshold value of 2, ions are discarded from the enhanced spectrum unless their intensities are twice the measured background noise.

Table 82. Automatic Processing page parameters – Spectrum Ranges dialog box (Sheet 3 of 3)

Parameter	Description
Include Peaks	
Reference and Exception Peaks	Include or exclude the reference peaks (R) and exception peaks (E) for the mass data in a Qual Browser window.
Mass Tolerance	
Specify a value for mass tolerance to affect the display of the MS data in a Qual Browser window.	
Use User Defined	Specify the values for mass tolerance and mass units for the MS data in a Qual Browser window. To change the parameter values, select the Use User Defined check box. If you clear the check box, the data system uses the values for mass tolerance and units that are stored in the raw data file.
Mass Tolerance	Specify the value for mass tolerance. Type a value from of 0.1 to 50000 , and then select units. The data system uses the tolerance value to create the limits of a range of values. Specify up to eight spectral ranges on the Ranges Page – Spectrum Ranges Dialog Box .
Units	Specify the default units that are used in processing MS data in the Qual Browser window. To change the user-defined settings, select the Use User Defined check box. Select either the mmu (millimass units) option or the ppm (parts per million) option.
Mass Precision	
Apply mass precision to the MS data in a Qual Browser window.	
Decimals	Specify the number of decimal places (significant digits after the decimal point) that the data system uses to display mass values. You can specify from 0 to 5 decimal places. The number of decimal places applies to the MS data in a Qual Browser window.

Ranges Page – Spectrum Ranges Dialog Box

Use the Ranges page of the Spectrum Ranges dialog box to set the mass and time ranges and other parameters for a spectrum plot.

Table 83 describes the parameters on the Ranges page of the Spectrum Ranges dialog box.

Table 83. Ranges page parameters – Spectrum Ranges dialog box (Sheet 1 of 3)

Parameter	Description
Range	
Mass/Wavelength Range	- Detector = MS View or change the current mass range of the active spectrum. To change the mass range, input the first mass and last mass of the scan in the Mass Range box. The format is <i>First Mass–Last Mass</i>. For example, to display mass/charge 100 through 200, type 100–200. - Detector = PDA View or change the current wavelength range in nanometers. To change the wavelength range, input the short wavelength and long wavelength of the scan in the Wavelength Range box. The format is <i>Short Wavelength–Long Wavelength</i>. For example, to display a wavelength range of 195 through 795 nanometers, type 195–795.
Average	Turn on the data system spectrum averaging. To average all scans defined by the mass range, time range, and filter settings in the Spectrum Ranges dialog box, select the Average check box.
Fix Scale	Turn on the fix scale setting displayed in the Spectrum Fix Scale box. To change the maximum range for the y axis of the active spectrum, select the Fix Scale check box. Then, type a value in box to the right of the check box. The valid range is 10 to 10 000 000 000.
Plot Properties Table	
Enable check boxes	Turn on the display of a spectrum plot. The plot is defined by its position in the list and is described by the settings in the Plot Properties box. To display the chromatogram, select the check box to the left of the Time column.

Table 83. Ranges page parameters – Spectrum Ranges dialog box (Sheet 2 of 3)

Parameter	Description
Plot Properties	
Detector	View the currently selected detector data type: • MS • Analog • A/D Card • PDA • UV ❖ To change the detector data type 1. Click the arrow to display the list of detector types. 2. Click the required detector type. Qual Browser extracts the data type from the raw data file.
Time	View or change the time range in minutes for the active spectrum in minutes. The valid range is 0.00 to 200.00 minutes. To select a time range, type the lower and upper time limits in minutes, separated by a dash (no spaces) in the Time box. For example, to select a time range from 0.10 to 9.10 minutes, type the following: 0.10–9.10.
Filter	View the scan filter used for the active spectrum. ❖ To select a different scan filter 1. Open the Filter list to display the scan filters stored in the raw data file. 2. Select the filter of interest from the list or type a scan filter in the box using the scan filter format (see Scan Filter Format). Not all MSⁿ detectors provide the MSⁿ Browser feature. If your MSⁿ detector provides the MSⁿ Browser feature, you can display either the scan filters by selecting the Scan option or you can display the processing filters by selecting the Process option. The processing filters display the average spectra and composite spectra builds using the data in the file displayed in the Raw File list. The Filter list is available only for MS detectors.

Table 83. Ranges page parameters – Spectrum Ranges dialog box (Sheet 3 of 3)

Parameter	Description
Raw File	View the path and filename of the current raw data file. Open the Raw File list to display the active files. To change the current raw data file, do one of the following: • Select a file from the list. • Click Browse adjacent to the list and browse to the required file. • Type the full path and filename of the required file into the box.
Formula	Enter a formula to simulate. This box is only available when you select the Simulation check box.
Background Subtraction	
Time Range 1	View whether background subtraction has been performed for the active spectrum. When the check box is selected, the data system displays the first time range used for background subtraction in the Time Range 1 box. In Qual Browser, the data system enters these settings automatically when you perform a background subtraction by choosing Actions > Subtract Spectra from the menu bar.
Time Range 2	View whether background subtraction has been performed for the active spectrum. When the check box is selected, the data system displays the second time range used for background subtraction in the Time Range 2 box. In Qual Browser, the data system enters these settings automatically when you perform a background subtraction by choosing Actions > Subtract Spectra from the menu bar.
Simulation	View whether the selected plot contains simulated data.

Map Ranges Dialog Box

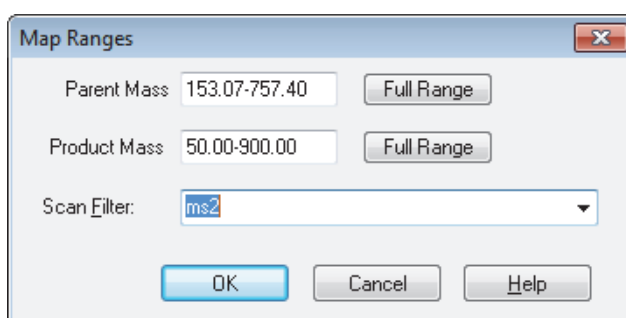
The Map Ranges dialog box consists of two pages:

- [Map Ranges Dialog Box for the Ion Map View](#)
- [Map Ranges Dialog Box for the Map View](#)

Map Ranges Dialog Box for the Ion Map View

Use the [Ion] Map Ranges dialog box ([Figure 72](#)) to set the mass ranges for the precursor (parent) and product masses.

Figure 72. Map Ranges dialog box for the ion map view



[Table 84](#) describes the parameters on the Map Ranges dialog box for the ion map view.

Table 84. Map Ranges dialog box parameters for the ion map view (Sheet 1 of 2)

Parameter	Description
Parent Mass	View or change the precursor (parent) mass coordinates for the Ion Map pane in the Parent Mass box. To display the precursor (parent) mass coordinates, drag the cursor in the Ion Map pane along the Parent m/z axis. The data system displays the precursor (parent) mass coordinates in the Parent Mass box. You can also enter the precursor (parent) mass coordinates in the Parent Mass box. The valid range is m/z 0.00 to 100 000.00.
Product Mass	View or change the product mass coordinates for the Ion Map pane in the Product Mass box. To display the product mass coordinates, drag the cursor in the Ion Map pane along the Product m/z axis. The data system displays the product mass coordinates in the Product Mass box. You can also enter the product mass coordinates in the Product Mass box. The valid range is m/z 0.00 to 100 000.00.

Table 84. Map Ranges dialog box parameters for the ion map view (Sheet 2 of 2)

Parameter	Description
Full Range	To reset the mass coordinates to the full range of the Ion Map, click Full Range .
Scan Filter	View the scan filters available for the data and edit the scan filters as text. ❖ To edit a scan filter 1. Open the Scan Filter list. 2. Select one of the scan filters and edit the text (see Scan Filter Format).

Map Ranges Dialog Box for the Map View

Use the Map Ranges dialog box to set the mass and time range for a map. For more information, see [Setting Map Ranges](#).

[Table 85](#) describes the parameters in the Map Ranges dialog box for the map view.

Table 85. Map Ranges dialog box (map) parameters (Sheet 1 of 2)

Parameter	Description
Detector	View the currently selected detector data type: • MS • Analog • A/D Card • PDA • UV ❖ To change the detector data type 1. Open the Detector list. 2. Select the detector type of interest. Qual Browser extracts the data type from the raw data file.
Mass	View or change the current mass range of the active map. To change the mass range, input the first mass and last mass of the scan in the Mass Range box. The format is as follows: <i>First Mass–Last Mass</i> For example, to display mass/charge 100 through 200, type 100–200 .

Table 85. Map Ranges dialog box (map) parameters (Sheet 2 of 2)

Parameter	Description
Time	View or change the time range in minutes for the active map. The valid range is set by the current data. To select a time range, type the lower and upper time limits in minutes, separated by a dash (no spaces) in the Time box. For example, to select a time range from 0.10 to 9.10 minutes, type: 0.10–9.10 .
Scan Filter	View the scan filter used for the active map. ❖ To select a different scan filter 1. Open the Scan Filter list to display the scan data that is stored in the raw data file. 2. Select the filter of interest from the list or type a scan filter in the box using the scan filter format (see Scan Filter Format).

Scan Filter Range Dialog Box

Use the Scan Filter Range dialog box to set the scan filter time.

[Figure 73](#) shows the ToolTip for a raw data file with a 10 min data acquisition time.

Figure 73. Scan Filter Range dialog box

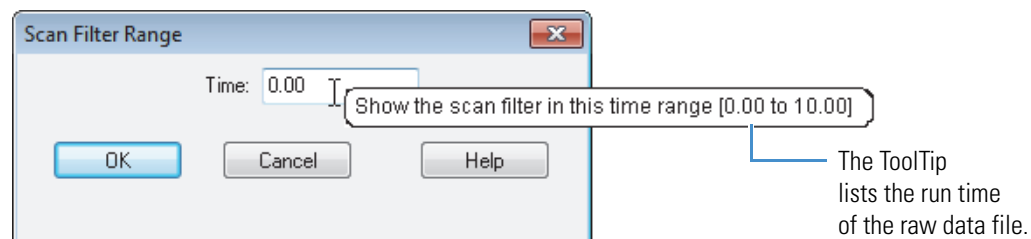


Table 86 describes the parameter in the Scan Filter Range dialog box.

Table 86. Scan Filter Range dialog box parameter

Parameter	Description
Time	View or change the time range in minutes for the active scan filter. The valid range is 0.00 to the acquisition time in minutes of the raw data file. The ToolTip for this parameter lists the lower and upper time limits for the raw data file. To select a time range, type the lower and upper time limits in minutes, separated by a dash (no spaces) in the Time box. For example, to select a time range from 0.10 to 9.10 minutes, type 0.10–9.10.

Scan Header Range Dialog Box

Use the Scan Header Range dialog box to set the scan header time.

Table 87 describes the parameter in the Scan Header Range dialog box.

Table 87. Scan Header Range dialog box parameter

Parameter	Description
Time	View or change the time range in minutes for the active scan header. The lower time limit depends on the acquisition instrument: typically 0.01 or 0.00 minutes. The upper time limit is the acquisition time in the raw data file. To specify a time range, type the lower and upper time limits in minutes, separated by a dash (no spaces) in the Time box. For example, to select a time range from 0.00 to 9.10 minutes, type: 0.00–9.10.

Spectrum List Ranges Dialog Box

Use the Spectrum List Ranges dialog box (Figure 74) to set up the mass range, time, detector type, and scan filter for an active spectrum list view. You can also apply the Smoothing, Refine, and Background Subtraction algorithms, change the mass tolerance and mass precision, and include reference and exception peaks.

Figure 74. Spectrum List Ranges dialog box

Spectrum List Ranges

Mass: 50.00-900.00 Detector: MS

Time: 3.85

Scan filter: FTMS + p ESI Full ms [150.00-900.00]

Smoothing

☒ Enable:

Type: Gaussian

Points: 7

Refine

☒ Enable

Window size (sec.): 6.00

Noise threshold: 3

Background subtraction

☐ Time range 1: 0.00

☐ Time range 2: 0.00

Mass tolerance

☒ Use user defined

Mass tolerance: 500.0

Units: ☒ mmu ☐ ppm

Include peaks

☐ Reference and exception peaks

Mass Precision

Decimals: 2

OK Cancel Help

Figure 88 describes the parameters in the Spectrum List Ranges dialog box.

Table 88. Spectrum List Ranges dialog box parameters (Sheet 1 of 4)

Parameter	Description
Mass	View or change the current mass range of the active spectrum list. To change the mass range, in the Mass Range box, type the first mass and last mass of the scan that you want to view, separated by a hyphen. The format is First Mass–Last Mass. For example, to display mass/charge 100 through 200, type 100–200.
Detector	This drop-down list displays the currently selected detector data type: • MS • Analog • A/D Card • PDA • UV To change the detector data type, open the Detector list and select the required detector type. Qual Browser extracts the data type from the raw data file.
Time	View or change the time range in minutes for the active spectrum list. The valid range is 0.00 to 200.00 minutes. To select a time range, in the Time box, type the lower and upper time limits in minutes, separated by a dash (no spaces). For example, to select a time range from 0.10 to 9.10 minutes, type: 0.10–9.10.
Scan Filter	View the scan filter used for the active spectrum list. ❖ To select a different scan filter 1. Open the Scan Filter list to display the scan data that is stored in the raw data file. 2. Select the filter of interest from the list or type a scan filter in the box using the scan filter format (see Scan Filter Format).
Smoothing	
Enable	Turn on smoothing. When you select the Enable check box, the Type list and the Points box become available. Select the smoothing algorithm in the Type list. Define the degree of smoothing in the Smoothing Points box.

Table 88. Spectrum List Ranges dialog box parameters (Sheet 2 of 4)

Parameter	Description
Type	Specifies the smoothing algorithm. ❖ To enable smoothing 1. In the Smoothing area, select the Enable check box. 2. Select one of the smoothing algorithms: Boxcar or Gaussian. 3. In the Points box, type the number of points for degree of smoothing. The valid range is 3 to 15.
Points	View or change the number of points that the data system uses for spectrum list smoothing. The valid range for smoothing points is 3 for minimum smoothing to 15 for maximum smoothing. To change the number of smoothing points, type an integer from 3 to 15 in the Points box.
Refine Apply the Refine spectrum enhancement to the spectrum described in the spectrum list view. Refine requires two parameters: Window Size (sec) and Noise Threshold. The Refine algorithm examines the mass chromatogram of each ion contributing to a chromatogram peak apex scan: 1. Refine discards masses without a peak maximum within ± 1 scan of the defined chromatogram peak apex. 2. Refine then searches for a minimum within the specified Window Size range either side of the peak apex. These points define the peak start and peak end. 3. Using scans at and beyond the peak start and peak end, Refine measures the background noise level in the mass chromatogram. 4. Refine uses extrapolation to estimate the contribution of noise to the scan at the peak apex. Refine adjusts the mass intensity of the apex scan accordingly. 5. Finally, Refine uses the Noise Threshold parameter to determine whether the adjusted intensity is significant in comparison to the background noise. If: $\text{Adjusted Intensity} < \text{Noise Threshold} \times \text{Background Noise}$ the mass is discarded from the final spectrum.	
Enable	Turn on Refine spectrum enhancement for the spectrum listed in the active spectrum list view. To apply Refine, select the Enable check box.

Table 88. Spectrum List Ranges dialog box parameters (Sheet 3 of 4)

Parameter	Description
Window Size	Enter a time window for the Refine spectrum enhancement method. The Refine algorithm applies the window across a chromatogram peak apex and uses it to search for the peak start and peak end and to estimate the background noise. Set this parameter to the peak width.
Noise Threshold	Enter a value for the Noise Threshold parameter. The Refine algorithm uses the Noise Threshold parameter to determine whether adjusted ion intensities are significant in comparison to the background noise. The parameter is actually a factor rather than a threshold. For example, with a Noise Threshold value of 2, ions are discarded from the enhanced spectrum unless their intensities are twice the measured background noise.
Background Subtraction	
Background Subtraction	These settings display the background subtraction time regions applied to the spectrum described in the spectrum list view. You can adjust these values or type your own.
Time Range 1	View whether background subtraction has been performed for the spectrum described in the active spectrum list. When you select the check box, the data system displays the first time range used for background subtraction in the Time Range 1 box. The application enters these settings when you perform a background subtraction by choosing Actions > Subtract Spectra from the menu bar.
Time Range 2	View whether background subtraction has been performed for the spectrum described in the active spectrum list. When you select the check box, the data system displays the second time range used for background subtraction in the Time Range 2 box. The application enters these settings when you perform a background subtraction by choosing Actions > Subtract Spectra from the menu bar.
Mass Tolerance	
Mass Tolerance	Specify a value for mass tolerance. Settings in this box affect the display of MS data in a Qual Browser window.

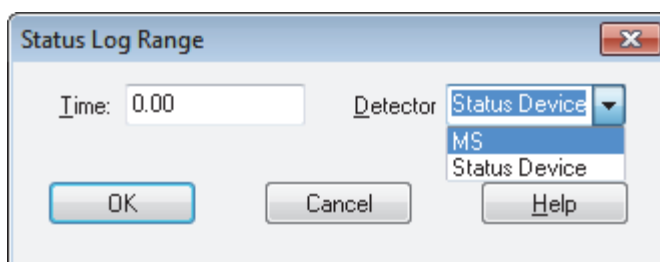
Table 88. Spectrum List Ranges dialog box parameters (Sheet 4 of 4)

Parameter	Description
Use User Defined	Specify the values for mass tolerance and mass units for the MS data in a Qual Browser window. To change the parameter values, select the Use User Defined check box. If you clear the check box, the data system uses the values for mass tolerance and units that are stored in the raw data file.
Mass Tolerance	Specify the value for mass tolerance. In the Mass Tolerance box, type a value in the range from 0.1 to 50 000 , and then select units to apply to the value. The data system uses the tolerance value to create the limits of a range of masses.
Units	Specify the default units that are used in processing MS data in the Qual Browser window. To change the user-defined settings, select the Use User Defined check box. Select either the mmu (millimass units) option or the ppm (parts per million) option. To turn off the user-defined units, clear the Use User Defined check box.
Include Peaks	
Reference and Exception Peaks	Include or exclude the reference peaks (R) and exception peaks (E) for the mass data in a Qual Browser window.
Mass Precision	
Decimals	Specify the number of decimal places (significant digits after the decimal point) that the data system uses to process MS data. Specify from 0 to 5 decimal places. The number of decimal places applies to the MS data in a Qual Browser window.

Status Log Range Dialog Box

Use the Status Log Range dialog box (Figure 75) to set the time range and the device that you want to be displayed in the status log view.

Figure 75. Status Log Range dialog box



❖ **To select a time range**

1. In the Time box, type the lower and upper time limits in minutes, separated by a dash (no spaces). For example, to select a time range from 0.10 to 9.10 minutes, type: **0.10–9.10**.
2. Click **OK**.

❖ **To change the detector data type**

1. In the Detector list, select the device of interest (MS, PDA, UV, and so on).
2. Click **OK**.

Figure 89 describes the parameters in the Status Log Range dialog box.

Table 89. Status Log Range dialog box parameters

Parameter	Description
Time	View or change the time range in minutes for the active status log view. The valid range is 0.00 to 200.00 minutes.
Detector	This drop-down list displays the currently selected detector data type: • MS • Analog • A/D Card • PDA • UV ❖ To change the detector data type In the Detector list, select the detector of interest. Qual Browser extracts the data type from the raw data file.

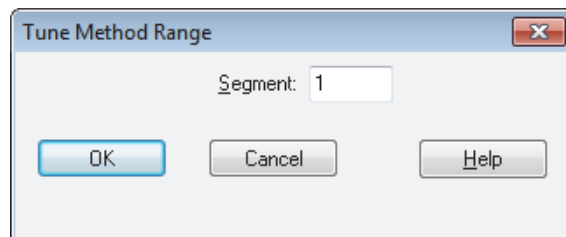
Tune Method Range Dialog Box

Use the Tune Method Range dialog box to select the tune method for a specific run segment.

❖ **To display the tune method for a specific run segment**

1. In the Qual Browser window, make the tune method view the active view.
2. Right-click the view and choose **Ranges** from the shortcut menu.
The Tune Method Range dialog box opens.
3. In the Segment box, type the segment number (Figure 76).

Figure 76. Tune Method Range dialog box



4. Click **OK**.

Table 90 describes the parameter in the Tune Method Range dialog box.

Table 90. Tune Method Range dialog box parameter

Parameter	Description
Segment	View or change the current run segment. The active Qual Browser window cell displays the tune method for that segment.

Search Properties Dialog Box

Use the Search Properties dialog box to select and prioritize the libraries used during library searching. You can also change the way that the search is carried out. The dialog box consists of two pages:

- [Search List Page – Search Properties Dialog Box](#)
- [Search Parameters Page – Search Properties Dialog Box](#)

For more information about using the Search Properties dialog box, refer to the *Xcalibur Library Browser User Guide*.

Search List Page – Search Properties Dialog Box

Use the Search List page to select the libraries and search order for library searches of spectra from Qual Browser.

Table 91 describes the parameters on the Search Properties – Search List page.

Table 91. Search List page parameters – Search Properties dialog box (Sheet 1 of 2)

Parameter	Description
Library Lists	
Available Libraries	View the libraries that are currently excluded from searching during processing. The data system regenerates this list when you open the dialog box.

Table 91. Search List page parameters – Search Properties dialog box (Sheet 2 of 2)

Parameter	Description
Selected Libraries	View the libraries that are currently included in searches during processing. The order of the libraries defines the order in which they are searched by the data system.
Buttons	
Add	Transfer a library from the Available Libraries list box to the Selected Libraries list box. This appends the library in the search list.
Remove	Transfer a library from the Selected Libraries list box to the Available Libraries list box.
Top	Move a library in the Selected Libraries list box to the top of the list (first in the search order).
Up	Move a library in the Selected Libraries list box up one position (earlier in the search order).
Down	Move a library in the Selected Libraries list box down one position (later in the search order).
Bottom	Move a library in the Selected Libraries list box to the final position (last in the search order).

Search Parameters Page – Search Properties Dialog Box

Use the Search Parameters page of the Search Properties dialog box to select the type of library search, limit the search by a molecular weight constraint, and determine how the results of the search are returned.

Table 92 describes the parameters on the Search Properties – Search Parameters page.

Table 92. Search Parameters page parameters – Search Properties dialog box (Sheet 1 of 3)

Parameter	Description
Search Type	
Use the settings in this group box to choose the type of library search applied to spectra. There are two main options: Identity and Similarity. The difference between the two search types is primarily in the weightings of the spectrum as a function of mass.	
Identity	Apply an Identity search algorithm for library matching of spectra. A Normal Identity search is the default option.
Normal	Apply a Normal Identity search algorithm for library matching of spectra. This is the default option. A Normal Identity search is suited to low quality or unusual spectra. The search algorithm uses a standard pre-screen search filter.

Table 92. Search Parameters page parameters – Search Properties dialog box (Sheet 2 of 3)

Parameter	Description
Quick	Apply a Quick Identity search algorithm for library matching of spectra. Use this option when you are sure the spectrum or compound exists in the library. The search algorithm uses a fast pre-screen search filter.
Penalize Rare Compounds	Limit the impact of rare compounds by reducing the match factor. This option is effective only when you have selected one or more of the NIST databases (such as MAINLIB). It has no effect on spectra in user libraries or other commercial libraries. Each reference spectrum in a NIST library contains a record of other commercial databases containing information about the compound. A compound is considered rare if it is present in a limited number of these databases. If you select the Penalize Rare Compounds option, hit (matching) compounds that are present in few, or no other databases other than the NIST libraries, will have their match factors reduced (the maximum penalty is 50 out of 1000). This, in effect, leads to a relative increase in the match factors of common compounds, placing them higher in the hit list than exotic isomers with near identical spectra. This roughly adjusts for the so-called “a priori probabilities” of finding a compound in an analysis.
Similarity	Apply a Similarity search algorithm for library matching of spectra.
Simple	Select this option button if you want to apply a Simple Similarity search algorithm for library matching of spectra. This option finds a large set of spectra to compare with the submitted spectrum, and is generally slower than an Identity search. A Simple Similarity search should be used if: • You know that the unknown spectrum is not in the library. • The spectrum is of poor quality, which makes a reliable match is unlikely.
Hybrid	Select this option button if you want to apply a Hybrid Similarity search algorithm for library matching of spectra. This option uses a combination of the Simple and Neutral Loss search strategies. As for the neutral loss search, an estimate of the unknown’s molecular weight is required. If the unknown compound contains chemical structures that generate both characteristic ions and neutral loss patterns, these structures can be identified from the hit list produced by this search.

Table 92. Search Parameters page parameters – Search Properties dialog box (Sheet 3 of 3)

Parameter	Description
Neutral Loss	Select this option if you want to apply a Neutral Loss Similarity search algorithm for library matching of spectra. The neutral losses in a spectrum are the mass differences between the molecular ion and other major ions in the spectrum. For certain classes of compound, neutral losses can be very characteristic spectral features. In a Neutral Loss search, the data system examines the submitted spectrum and identifies the molecular ion. The application submits the mass value of the molecular ion to the search along with the spectrum. The search algorithm calculates the significant neutral losses and compares them with library data. Hits are returned according to matches of the molecular ion and its neutral losses.
Options	
Search With MW=	Select this check box if you want to restrict the search to library entries with a particular molecular weight. Use the associated text box to enter the molecular weight.
Reverse Search	Select this check box to sort matching library spectra by the Reverse Search Match Factor. By default, the data system sorts matches by the Forward Match Factor.
Mass Defect	
This area contains the parameters used in library searches that allow you to correct for the differences between the actual masses and the nominal integer masses of the atoms in a molecule. Assign a larger value (in millimass units) for mass defect to larger molecules because, in general, they are composed of more atoms than smaller molecules; larger molecules need a larger correction factor to approximate the linear function that the data system uses to calculate masses. When you enable mass defect, the data system uses the parameters in library searches of spectra that you export from the spectrum view of Qual Browser.	
Enable	Include mass defect values for library searches in a processing method.
Defect	Specify values (in millimass units) for mass defect. Specify a smaller value for lower mass ranges in the first text box, and specify a larger value for higher mass ranges in the second text box.
At Mass	Specify the masses at which the data system applies specified mass defect values to calculations of mass. Specify a smaller mass value in the first text box, and specify a larger mass value in the second text box.

Select Isotopes Dialog Box

Use the Select Isotopes dialog box to display the isotopes of each element and select one or more isotopes to include in the calculation of chemical formulas (Figure 77).

Figure 77. Select Isotopes dialog box

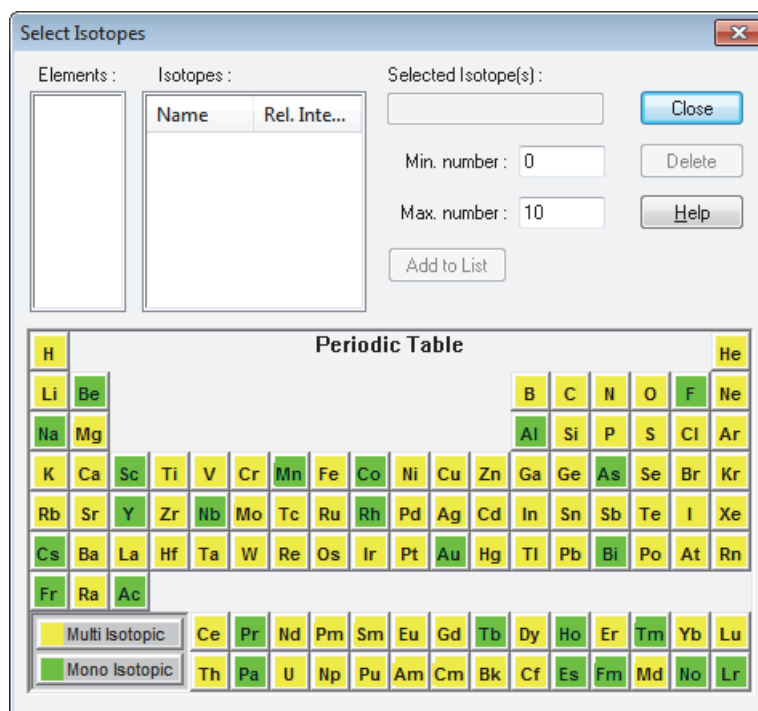


Table 93 describes the parameters in the Select Isotope dialog box.

Table 93. Select Isotopes dialog box parameters (Sheet 1 of 2)

Parameter	Description
Elements	View the chemical elements. Click an element in the Periodic Table to add it to the Elements list. Click the element in the Elements list to display isotopes for that element. The isotopes appear in the Isotopes list.
Isotopes	View the name and relative intensities of the isotopes for the current element you selected from the Elements list. Select an isotope from the list. The data system displays it in the Selected Isotope box.
Selected Isotopes	View the isotope you select from the Isotopes list.
Min. Number	View or change the minimum number of occurrences of the selected isotope in the formula that Qual Browser calculates. To change the minimum number of occurrences, type a number from 0–10 000 in the box.

Table 93. Select Isotopes dialog box parameters (Sheet 2 of 2)

Parameter	Description
Max. Number	View or change the maximum number of occurrences of the selected isotope in the formula that Qual Browser calculates. To change the maximum number of occurrences, type a number from 0–10 000 in the box.
Periodic Table	Click an element in the Periodic Table to add that element to the Elements list. ❖ To change the color of the multi-isotopic or monoisotopic elements 1. Click the Multi Isotopic or Mono Isotopic in the lower left corner of the periodic table. The Color dialog box opens. 2. Select a new color.
Buttons	
Add to List	Add the isotopes listed in the Selected Isotopes list to the Elements in Use list of the Elemental Composition Page .
Delete	Remove an element from the list. To remove an element from the list, select the element in the Elements list and click Delete .
Close	Close the Select Isotopes dialog box.

Specify Mixture for Simulation Dialog Box

Use the Specify Mixture for Simulation dialog box to specify the compounds and amounts to include in the mixture so that the data system can simulate a spectrum.

Table 94 describes the parameters in the Specify Mixture for Simulation dialog box.

Table 94. Specify Mixture for Simulation dialog box parameters

Parameter	Description
Formula	Enter the chemical formula of a compound in the mixture in the Formula column. You can enter both upper and lower case letters, however the data system interprets all lower case input as two-letter symbols. For example, the string <i>inau</i> will be parsed as <i>In Au</i>. You can force other interpretations by being more specific in capitalization, namely <i>INAu</i> or <i>INaU</i>. The application interprets all upper case input as single-letter element names. For example, <i>COSI</i> is interpreted as <i>C O S I</i>. You can specify a specific isotope by naming it in the following fashion: $[13]C$. (That is, square brackets about the isotope mass number.) You can specify mixtures of substances by using additional symbols + (addition) and * (multiplication). Both will be required to specify a mixture. A valid mixture has the format substance*quantity + substance* quantity, for example, C4H8*2+H2O*5. Parentheses are allowed in the formula input edit field to specify repeating moieties such as found in polymers, for example, $HO(C_2H_4O)_5H$.
Amount	Enter the percentage of the compound in the mixture in the Amount column.
Color	Select one of 48 basic colors or 16 (maximum) preselected custom colors. The Color column becomes active when you select the Also Show Separate Traces for Each Compound check box. Click a color in the Color column for the selected trace.
Also Show Separate Traces for Each Compound	Select this check box to display a trace for each compound. Use the Color box to select the color for each trace. To select a color for the trace, select the trace, and then select the color.

Toolbars Dialog Box

Use the Toolbars dialog box to show or hide the Main and Amplify toolbars. You can also choose to display ToolTips and determine whether the toolbars display large or small buttons.

Table 95 describes the parameters in the Toolbars dialog box.

Table 95. Toolbars dialog box parameters

Parameter	Description
Main and Amplify check boxes	List the toolbars available in Qual Browser: Main and Amplify. To display a toolbar, select its check box. To hide the toolbar, clear its check box.
Show ToolTips	Show or hide ToolTips. To display ToolTips, select the ToolTips check box. If you do not want to display ToolTips, clear the ToolTips check box.
Large Buttons	Display the toolbars with large or small buttons. To display large buttons on the toolbar, select the Large Buttons check box. To display small buttons in the toolbar, clear the Large Buttons check box.

Subtract Background Window

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 (Figure 78). You can use this utility to subtract a background spectrum from a raw data file or deconvolute merged or overlapping component peaks.

Figure 78. Subtract Background window

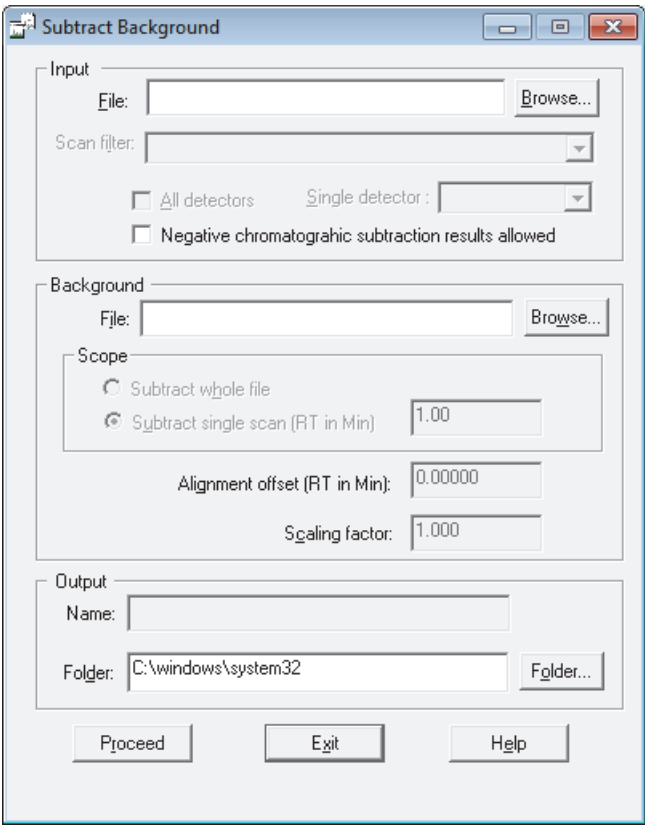


Table 96 describes the parameters in the Subtract Background window.

Table 96. Subtract Background window parameters (Sheet 1 of 3)

Parameter	Description
Input	
File	View or change the path name of the input raw data file. You can change the source of the input file in one of these ways: - Click Browse adjacent to the box and browse to the required file - Type the full path and filename of the required file into the box.

Table 96. Subtract Background window parameters (Sheet 2 of 3)

Parameter	Description
Scan Filter	View the selected scan filter to be applied to the input file. You can also use the scan filter format to type a scan filter into the Filter box. ❖ To select a scan filter 1. Open the Scan Filter list to display the scan filters that are stored in the raw data file. 2. Select the filter of interest.
All Detectors	Specify that all detector data sources should be used to produce the input chromatogram. The check box is unavailable for single source raw data files.
Single Detector	Select a data source for the input chromatogram from the chosen raw data file. The box lists the detector sources recorded in the raw data file.
Negative Chromatographic Subtraction Results Allowed	Background subtraction normally enforces a rule that chromatogram data cannot be less than zero. Normally, if background subtraction results in a negative value, it is set to zero. However, select this check box to prevent this action from happening.
Background	
File	View or change the path name of the raw data file to be subtracted from the input file. You can change the source of the background file in one of these ways: - Click Browse adjacent to the box and browse to the required file - Type the full path and filename of the required file into the box.
Scope	
Subtract Whole File	Specify that the whole of the background file is to be subtracted from the input file.
Subtract Single Scan (RT)	Specify that a single scan from the background file is to be subtracted from each scan of the input file. Type the number of the scan in the adjacent box.
Alignment Offset (RT)	Specify how much time, in minutes, to offset the background subtraction file. A positive alignment offset implies that the peaks in the background subtraction file have larger retention times than the peaks in the file it is subtracted from.

Table 96. Subtract Background window parameters (Sheet 3 of 3)

Parameter	Description
Scaling Factor	Specify a scaling factor for the subtract background file operation. Type the factor you want to apply to the background file before its subtraction from the input file.
Output	
Name	View the filename for the output file resulting from the subtraction of the background file from the input file. The data system uses the input filename with a BG_ prefix.
Folder	View or change the folder to store the output file after the subtract background file operation. To change the folder, do one of the following: - Click Folder adjacent to the box and browse to the required folder. - Type the full path of the folder into the box.
Buttons	
Proceed	Start the Subtract Background file operation using the settings in the dialog box.
Exit	Exit the window and stop the Subtract Background file operation.

Qual Browser Result File Window

You can open a raw data file (RAW file type), a result file (RST file type), or a sequence file (SLD file type) in the Qual Browser window.

❖ To open a result file (RST) in the Qual Browser window

Do one of the following:

- From the Qual Browser menu bar, choose **File > Open Result File**.

—or—

- On the Main toolbar, click the **Open Result File** icon, .

A result file contains a list of detected peaks from the chromatogram, and the processing results associated with each peak including any library search results.

Qual Browser displays the result file in a fixed, two cell arrangement:

- A chromatogram plot in the upper cell with the detected peaks highlighted.
- The spectrum plot associated with the currently selected chromatogram peak in the lower cell.

Note Many of Qual Browser's features are not available for use with a result file because the raw data file is not directly available for processing.

It is not possible to submit the spectrum from the results display for a library search. If a library search has been carried out during processing (when the result file was created), search results will be stored in the result file and displayed for each detected peak. To submit a spectrum for library searching or to export a spectrum to the Library Browser, you must open the raw data file.

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