

Thermo

XReport

Reporting Tool for the Xcalibur Data System

User Guide

Software Version 4.5

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

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Preface

Thermo XReport is the custom reports application for the Thermo Xcalibur™ mass spectrometry data system. Use XReport to create custom reports.

Contents

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

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 and the XReport application

❖ **To view the product manuals**

- To access the Xcalibur manual set, do one of the following:
 - From the computer taskbar, choose **Start > Thermo Scientific Xcalibur Manuals**.
 - From the Xcalibur home page – Roadmap view, choose **Help > Manuals**.
- To access the manual set for the Thermo Scientific mass spectrometers from the computer taskbar, choose **Start > Thermo Instruments > *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 product-name 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 Helpful information that can make a task easier.

Contacting Us

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U.S. Technical Support	us.techsupport.analyze@thermofisher.com	(U.S.) 1 (800) 532-4752	
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Introduction to XReport

The XReport application is the custom reports feature of the Xcalibur data system. Use XReport to create customized reports containing all of the results and important information produced with the application. In addition, use XReport to format a report to a style, print the report, and save the report in text (TXT), Microsoft™ Word document (DOC), Microsoft Excel™ workbook (XLS), rich text (RTF), portable display (PDF), or web page (HTM or HTML) formats. Use these options to email reports or display them on the Internet.

Create Xcalibur reports containing the following:

- Textual information (for example, sample information)
- Tabulated information (for example, a calibration file table)
- Graphical information (for example, a spectrum or a chromatogram)

Contents

- [The XReport Window](#)
- [Report Templates Overview](#)
- [Configuring XReport Objects Overview](#)
- [Using XReport](#)

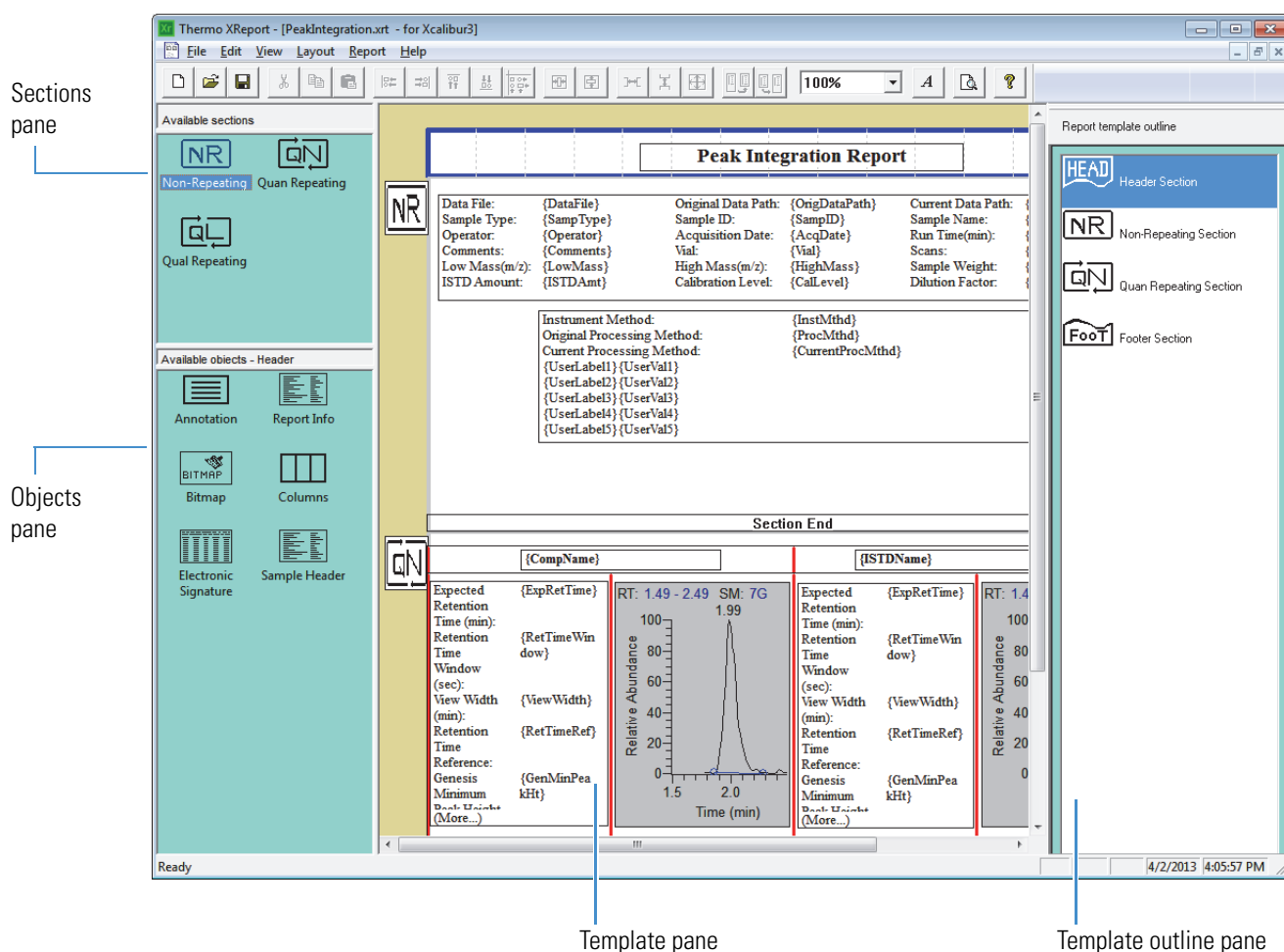
The XReport Window

The XReport window is split in four different panes:

- Sections pane
- Objects pane
- Template pane
- Report Template Outline pane

See [Figure 1](#) for the location of the panes.

Figure 1. XReport window



The Sections pane lists the available sections for the selected application (for example, the Xcalibur data system). To add a section to a report, drag it from the Sections pane to the Template pane.

The Objects pane lists the objects that are available for the currently selected section. To add an object to a report, drag it from the Objects pane to the currently selected section in the Template pane.

Use the Template pane to configure a report layout by dragging and arranging objects.

- To configure a report object, right-click it and choose **Properties** from the shortcut menu.
- To configure a repeating section, right-click the **QL** or **QN** icon in the left margin of the page at the top of the sections pane and choose **Properties** from the shortcut menu. The size of the page in this pane corresponds to the size of a standard 8.5 × 11 in. piece of paper in either portrait or landscape mode.
- Adjust the height of sections by dragging the bottom border of the section downward. A selected section has a bright blue border around it.

The **Report Template Outline pane** lists the sections that are in the current report. You can move or delete sections from this pane, as well as undock, reposition, or close it.

- To undock the pane, drag the top gray portion away from the pane.
- To redisplay the pane, choose **View > Report Template Outline pane**.
- To delete a section from a template, click it in the Report Template Outline pane and press DELETE.
- To move a section, drag it up or down in the Report Template Outline pane list. You cannot move the header and footer sections.
- To select and scroll to a section, double-click it.

Report Templates Overview

This section defines the basic terminology used throughout the software and this manual for new users of the XReport application and the Xcalibur data system. This section defines the following key terms:

- [Report Template](#)
- [Report Sections](#)
- [Report Objects](#)
- [Data Source Files](#)
- [Report](#)

Report Template

An XReport template is an XReport document (XRT file) that defines the content, layout, and style of a report. Use the template to include sections and report objects (for example, graphs, tables, annotation text, or graphics) in a report template. The software generates an Xcalibur report after combining a report template with Xcalibur data source files.

XReport provides several example report templates for you to use. These are located in the Xcalibur\Templates folder. For details about the preconfigured report templates, see [Appendix A, “Sample XReport Template Files.”](#)

Report Sections

Divide the report template in sections to hold report objects. Add sections to a report template using the Sections pane in the XReport window.

The basic types of section used in XReport are as follows:

- [Header or Footer Sections](#)
- [Repeating Sections](#)
- [Nonrepeating Sections](#)

A report object that is placed in a repeating section can behave differently from the same report object placed in a nonrepeating section when the software combines a report template with data. For information on how a report object functions when it is placed inside or outside a repeating section, see [Appendix B, “Types of Report Objects.”](#)

Header or Footer Sections

A header or footer section is a section of the report that is automatically repeated at the top and bottom of each page in the resolved report. Header and footer sections can contain objects such as a company logo, report information, page numbers, and date stamps.

Repeating Sections

A repeating section is a section of a report template that is automatically repeated for every component or peak in a resolved document. Change the properties of a repeating section to customize its behavior.

Two types of repeating section can be used in an XReport template:

Qual repeating section	Use a Qual repeating section to display details relating to a single Qual peak within some data. The section is repeated for all Qual peaks found.
Quan repeating section	Use a Quan, or component, repeating section to display details relating to a single Quan peak in some data or a component configured in a processing method. The section is repeated for all Quan peaks or components.

Nonrepeating Sections

A nonrepeating section usually displays static details associated with data or methods that apply once and globally within the system (for example, processing method settings, instrument method settings, filename, confirmation ion information, and so on).

Report Objects

Report objects are customized tables, graphics, or text that indicate what kind of data appears in the report. When the Xcalibur data system combines a report template with data, it replaces the report objects in the report template with data to generate a report. See [Report Objects](#) for more information.

Report objects include the following:

- [Text Objects](#)
- [Table Objects](#)
- [Graphic Objects](#)
- [Formatting Objects](#)

For a descriptive listing of XReport objects, see [Appendix B, “Types of Report Objects.”](#)

Text Objects

Text objects contain static text labels and associated customized data fields. To customize the specific fields to display, right-click the object and choose **Properties** from the shortcut menu. The Configuration dialog box opens. When the software combines a template with data to generate a report, it replaces the text object fields with textual information (static text). See [Text Objects](#) for more information.

The following Xcalibur text objects are available in XReport:

- Annotation
- Component Ident/Detect/Cal Settings
- Component ISTD Settings Summary
- Component Settings Summary
- Component Sys Suit/Flags Settings
- Instrument Method
- Processing Method – General
- Processing Method – Qual
- Quan ISTD Peak Summary
- Quan Peak Summary
- Report Info
- Sample Header

Table Objects

When the Xcalibur data system combines a template with data, it replaces table objects with tabulated information (creates a populated data table). Configure or change the properties of a table object to customize its output.

XReport provides the following table objects:

- Avalon Qual Events Table
- Avalon Quan Events Table
- Calibration File Table
- Component Cal Level Table
- Component QC Level Table
- Component Spectrum Table
- Dilution Factor Table
- Electronic Signature
- Ion Ratio Confirmation Results Table
- IRC Settings Table
- IRC Summary Table
- Lib. Search Graph Table
- Lib. Search Results Table
- Proc. Method Programs Table
- Proc. Method Sample Reports Settings Table
- Proc. Method Summary Reports Settings Table
- Qual Peak Table
- Qual Summary Table
- Quan Peak Table
- Quan Summary Table
- Sample Table (Quan Results)
- Sequence Table
- Spectrum Candidate Results Table
- Spectrum List Table

Graphic Objects

When XReport combines a report template with data, it replaces graphic objects with graphical information. Configure or change the properties of a graphic object to customize its output. See [Graphic and Formatting Objects](#) for more information.

The following graphic objects are available in XReport:

- Bitmap
- Chromatogram
- Component Cal (Calibration) Curve
- Spectrum

Formatting Objects

These objects, which only format the report, are available in XReport:

- Columns
- Page Break

Data Source Files

Data source files are files that contain acquired data. For example, there are five types of Xcalibur data source files:

- Processing method (PMD file)
- Raw data file (RAW file)
- Result (RST file)
- Sequence (SLD file)
- Calibration (XCAL file)

Report

Generate a report (or resolved document) using a report template. In an Xcalibur report, the software combines the report objects in the report template with Xcalibur data. Save and display reports in any of these formats:

- Microsoft Word document (DOC file)
- Text (TXT file)
- Microsoft Excel workbook (XLS file)
- Rich text (RTF file)
- PDF (PDF file)
- Web page (HTM or HTML file)

Configuring XReport Objects Overview

Use the Template pane of the XReport window to configure objects by right-clicking them and choosing Properties from the shortcut menu. Set parameters in the configuration dialog box that opens.

You can configure nearly all items in XReport, including the following:

- Repeating sections
- Tables
- Chromatograms
- Spectra
- Component calibration curves
- Text objects

For specific information on configuring each object, see [Chapter 4, “Configuring Objects and Sections.”](#)

Configuring a Repeating Section Overview

Use the Repeating Section Properties dialog box to specify the following:

- Whether to exclude Internal Standards or Target Compounds from a Quan repeating section
- The order in which peaks and components are repeated
- Any limit on number of peaks to be reported
- How the individual peaks or components are split across pages in the final report

For information about the parameters in the Repeating Section Properties dialog box, see [Repeating Section Properties Dialog Box](#).

Configuring a Table Overview

Use the *Table Properties* wizard to do the following:

- Specify the columns to be included in the table
- Define and customize table columns
- Specify an order for the table

For information about the parameters in the *Table Properties* wizard, see [Table Properties Wizard](#).

Using the Chromatogram Wizard Overview

Use the Chromatogram wizard to do the following:

- Select chromatogram type and peak type
- Use a demonstration (demo) file
- Select plot details
- Select smoothing parameters
- Use MS Quan traces
- Configure the Chromatogram display, style, labeling, axes, and normalization methods

For information about the parameters in the Chromatogram wizard, see [Chromatogram Properties Dialog Box and Wizard](#).

Configuring a Component Calibration Curve Overview

Use the Component Calibration Curve wizard to specify the name of the component plotted for a nonrepeating Component Cal Curve report object in a report.

For information about the parameters in the Component Calibration Curve dialog box, see [Component Calibration Curve Dialog Box](#).

Using the Data Source Browser Overview

Use the Data Source Browser to select data files that can be used to generate reports from within XReport.

For information about the parameters in the Data Sources dialog box, see [Data Sources Dialog Box](#).

Sample XReport Templates Overview

An XReport template is an XReport document (XRT file) with XReport objects embedded within it. You do not have to create personal XReport templates. XReport provides customized report templates for you to use with your data. For full details of these report templates, see [Appendix A, "Sample XReport Template Files."](#)

Using XReport

To use the XReport application, follow these topics:

- [Starting XReport](#)
- [Selecting a Report Template](#)
- [Creating and Generating Reports with XReport](#)
- [Exiting XReport](#)

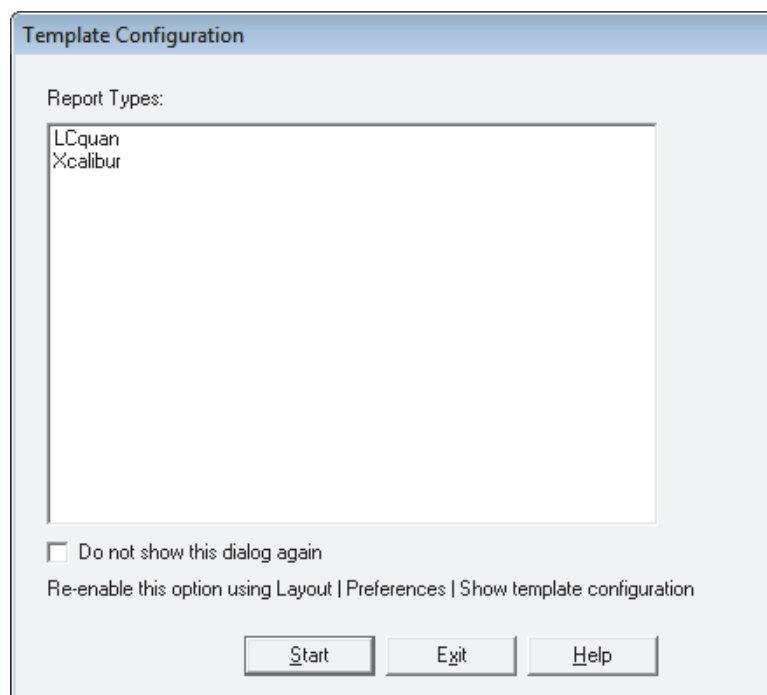
Starting XReport

❖ To start XReport

1. From the data system computer, double-click the **XReport** icon, , on the desktop, or choose **All Programs** (or **Programs**) > **Thermo Xcalibur** > **XReport** from the Windows Start menu.

When more than one application is installed that uses XReport for reporting, the Template Configuration dialog box opens ([Figure 2](#)).

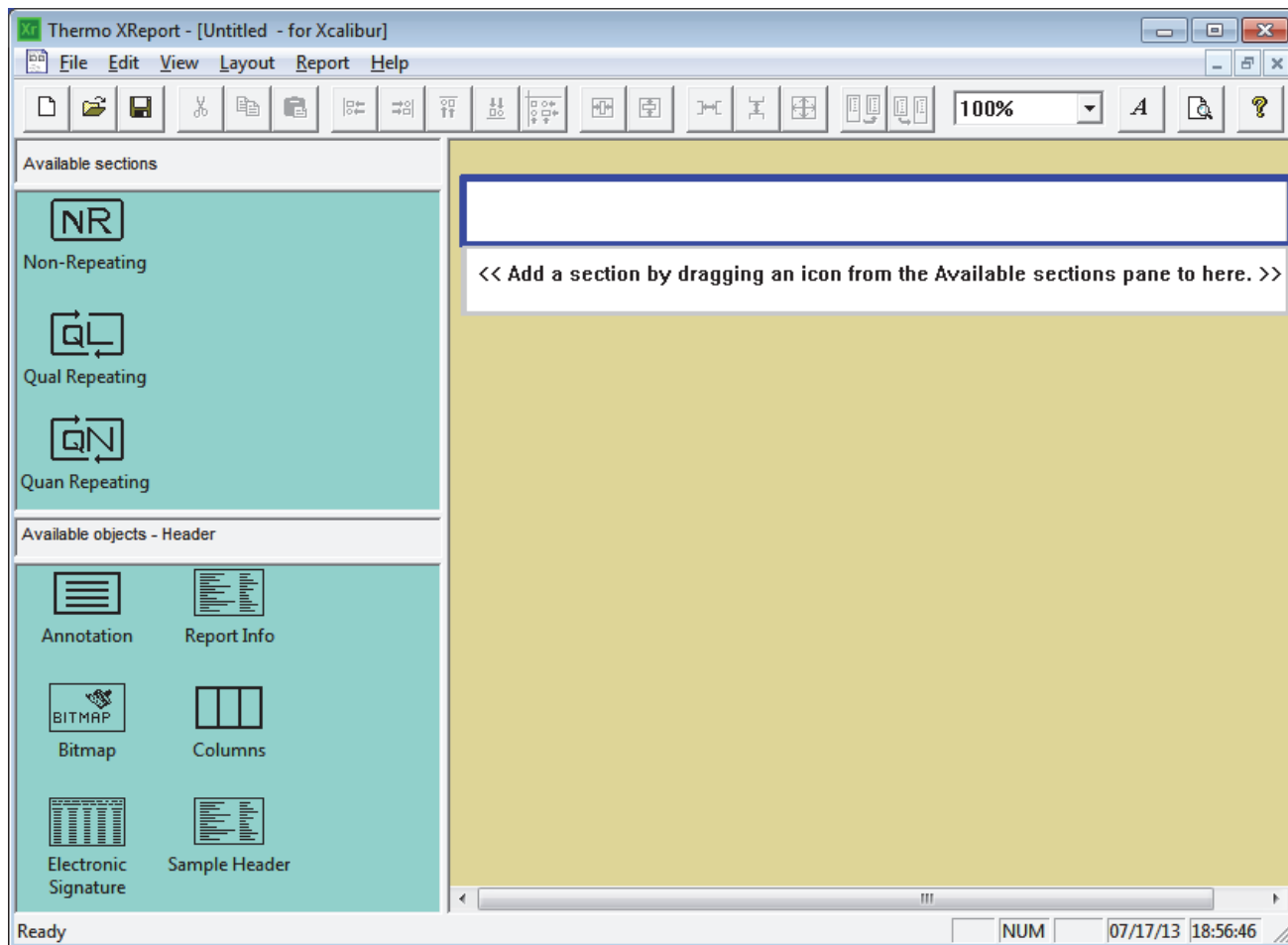
Figure 2. Template Configuration dialog box



2. Select the application for the report template and click **OK**.

XReport opens and creates a new template (Figure 3).

Figure 3. XReport window, showing a new template



Selecting a Report Template

❖ To select a report template

1. In the Reports view, choose **File > Open**. A browse dialog box opens.
2. To select the required report template, click the template name. If the name does not appear, browse to the correct folder.

The template name appears in the File name box.

3. To view the report template and close the dialog box, click **Open**.

Creating and Generating Reports with XReport

There are two distinct stages in the process of producing a customized Xcalibur report using XReport:

- [Creating a Report Template](#)
- [Generating a Report Using a Report Template](#)

These stages are discussed in more detail in these chapters: [Creating a Template](#) and [Generating a Report](#). The Xcalibur data system provides sample XReport templates for you to use. These are XRT files with XReport objects embedded within them and are located in the Xcalibur\templates folder. For details on these report templates, see [Appendix A, “Sample XReport Template Files.”](#)

Creating a Report Template

Use XReport to create a customized report template (.xrt file) that defines how the final report looks and defines the specific information in the report.

❖ To create a report template

1. Click the **XReport** icon, , on the desktop to start XReport.

A new XReport document appears in the report window (see [Figure 3](#) on [page 12](#)).

2. Add sections and report objects to the report template by dragging items from the Available Sections and Available Objects panes to the report preview pane.
3. Configure the sections and report objects included in the report template to adjust their properties and customize their output.

Right-click objects and sections to configure and choose **Properties** from the shortcut menu. Set parameters in the configuration dialog boxes. Use the menus, toolbars, or mouse to align, resize, and reposition objects.

4. Save the report template.

For more detailed information on how to create and configure a report template, see [Chapter 2, “Creating a Template,”](#) and [Chapter 4, “Configuring Objects and Sections.”](#)

Generating a Report Using a Report Template

After creating a report template, generate a report (or resolved document) by combining a report template with one or more data source files (for example, an Xcalibur processing method [PMD], raw data file [RAW], result file [RST], sequence file [SLD], and calibration file [XCAL]).

For detailed information on how to generate a report from within the Xcalibur data system, see [Chapter 3, “Generating a Report.”](#)

There are three ways to generate a report:

- From a report template open in XReport: Search for the required data source files and combine the data with the template to generate a report. Preview, print, and save the report as a text file (TXT), Word document file (DOC), Excel spreadsheet file (XLS), rich text format file (RTF), portable document format file (PDF), or web page (HTM or HTML).
- From a data processing application (for example, the Xcalibur data system): Associate the data you produce in the application with a report template (for example, do this in Quan Browser) and combine the data with the template to generate a single report.
- From a data processing application (for example, the Xcalibur data system): Insert the name of the template to a processing method (such as Processing Setup) and generate reports automatically when you batch process data (such as in Sequence Setup).

Exiting XReport

❖ To save the report template or report and XReport

Complete or cancel any active dialog boxes and choose **File > Exit**.

Creating a Template

This chapter explains how to create a custom report template. When you create a custom report template, you can save the template and use it to generate an Xcalibur report. For more information about generating a report, see [Chapter 3](#).

Contents

- [Opening a New or an Existing XReport Template](#)
- [Adding, Ordering, and Configuring Sections](#)
- [Adding and Configuring Report Objects](#)
- [Previewing and Saving the Template](#)

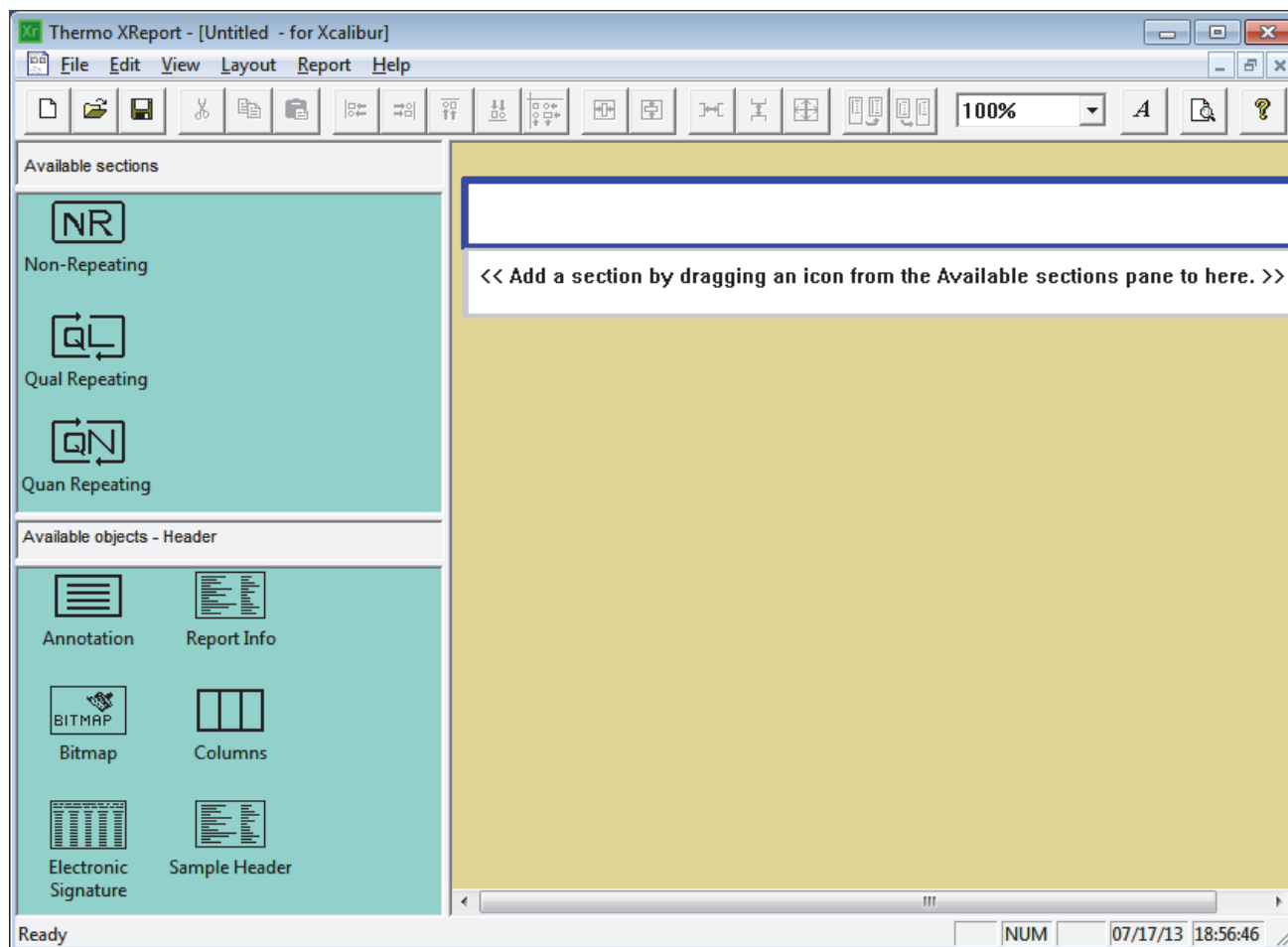
2 Creating a Template

Opening a New or an Existing XReport Template

Opening a New or an Existing XReport Template

When you start XReport, XReport creates a new template that includes header and footer sections (Figure 4). Either work with this new template, or choose **File > Open** to open an existing template and select an XReport template (XRT) file.

Figure 4. XReport window, showing a new template



Adding, Ordering, and Configuring Sections

To begin creating a template, select sections to include in the report template. Choose to include Quan-based or Qual-based repeating sections or nonrepeating sections in your report template. For a description of the different section types and how repeating sections work, see [Configuring a Repeating Section](#).

This section contains the following topics:

- [Adding, Deleting, or Reordering Sections](#)
- [Resizing Sections](#)
- [Configuring a Qual or Quan Repeating Section](#)

Adding, Deleting, or Reordering Sections

Follow these procedures.

❖ To add a section to the report

Drag it from the Sections pane (upper left) to the Template pane (center).

Add only one section to the template at a time.

❖ To delete a section from the report

1. Do one of the following:

- Click the section in the Report Template Outline pane (far right) and press DELETE. The system prompts you to confirm the deletion. You cannot delete the header or footer sections.

—or—

- When the Report Template Outline pane is not visible, choose **View > Report Template Outline** or right-click a section and choose **Delete Section** from the shortcut menu.

❖ To change the order of the sections in the template

Drag the sections in the Report Template Outline pane. Header and footer sections must remain at the top and bottom of the list, respectively.

Resizing Sections

To resize a section, follow these procedures.

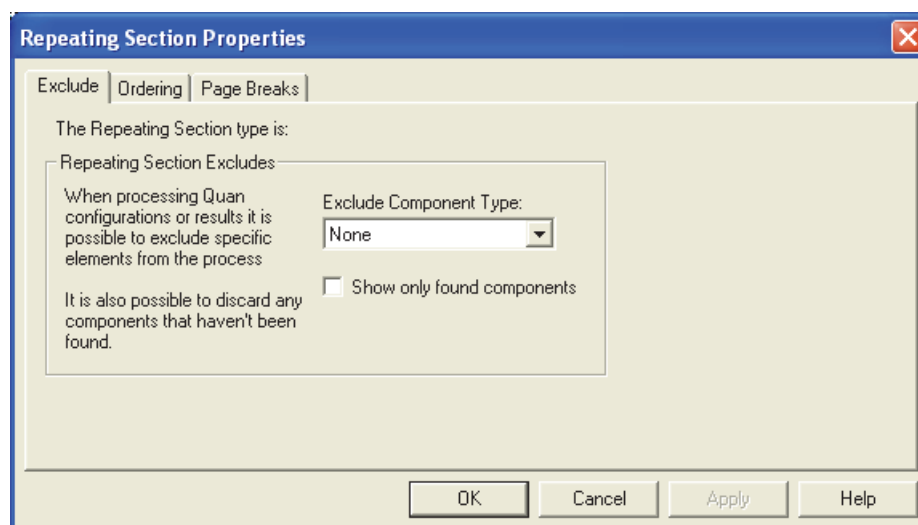
- ❖ **To automatically remove the extra space at the top and bottom of a section**
Select the section and choose **Layout > Shrink Wrap**.
- ❖ **To automatically add a half page of extra space at the bottom of a section**
Select the section and choose **Layout > Expand**.
- ❖ **To manually add or remove extra space at the bottom of a section**
Drag the bottom border of a section up or down.

Configuring a Qual or Quan Repeating Section

For more information about the Repeating Section Properties dialog box, see [Repeating Section Properties Dialog Box](#).

- ❖ **To configure a Qual or Quan repeating section**
 1. Scroll to where you can see the QL or QN icon at the top left side of a section in the Template pane.
 2. Right-click the icon and choose **Properties** from the shortcut menu. The Repeating Section Properties dialog box opens ([Figure 5](#)).

Figure 5. Repeating Section Properties dialog box



3. Set the parameters and click **OK**.

Adding and Configuring Report Objects

After adding and configuring sections, select the report objects you want to include in a specified section of the report template. Select from these options: text objects, table objects, graphic objects, and text, depending on the selections you made in [Configuring a Qual or Quan Repeating Section](#).

XReport displays the objects that are available for the currently selected section in the Objects pane (lower left). The contents of this pane change when you select different sections.

To add and configure report objects, follow these procedures:

- [Adding, Deleting, Repositioning, and Resizing Objects](#)
- [Aligning Objects](#)
- [Centering Objects](#)
- [Using the Report Template Grid](#)
- [Using Columns](#)
- [Using Page Breaks](#)
- [Configuring Objects](#)
- [Adding User Text to a Text Object](#)
- [Adding a Formula to a Table](#)
- [Changing Font Settings](#)
- [Changing the Page Layout](#)

Adding, Deleting, Repositioning, and Resizing Objects

You can add, delete, reposition, and resize objects in a report template.

❖ To add an object to the report

Drag an object from the Objects pane (lower left) to the currently selected section (in blue) in the Template pane (center). Add only one object to the template at a time.

❖ To delete an object from the report

1. Select the object in the Template pane (center). Blue handlebars on each side and at each corner become visible.
2. Press DELETE.

❖ To reposition an object

Drag the object to the preferred location.

❖ **To resize an object**

Drag the object by one of the corner handles (small blue squares) until the object is the preferred size.

❖ **To make two or more objects the same size**

1. Select the first object to size.

The size of the first object selected determines the size of subsequent objects.

2. Hold down the SHIFT key and select other objects to resize.
3. Click the icon in the toolbar that corresponds to the dimension you want to resize:



Same Width



Same Height



Same Width and Height

❖ **To resize the columns in a table object**

1. Double-click the table.

Handles (small blue boxes) appear on the interior column borders.

2. Drag the handles to resize the columns.

Aligning Objects

❖ **To align one or more objects**

1. Select the first object to align. The position of the first object selected determines how subsequent objects are aligned.
2. Hold down the SHIFT key and select each object to align.
3. Click the toolbar icon that corresponds to the edge to align.

Left Align icon



Right Align icon



Top Align icon



Bottom Align icon



Or click the **Auto Align** icon, , to snap all objects to the nearest grid line.

4. Choose **View > Report Template Grid** to view the grid lines. To adjust the grid settings, choose **Layout > Preferences**. The Preferences dialog box opens (Figure 6).

Centering Objects

❖ To center one or more objects

1. Select the first object to center. Then, hold down the SHIFT key and select each object to center with respect to the first object.
2. To center the objects on the page, do the following:
 - Click the **Center Horizontally** icon, .
 - Click the **Center Vertically** icon, .

Using the Report Template Grid

The Template pane has a built-in grid.

❖ To view the grid lines

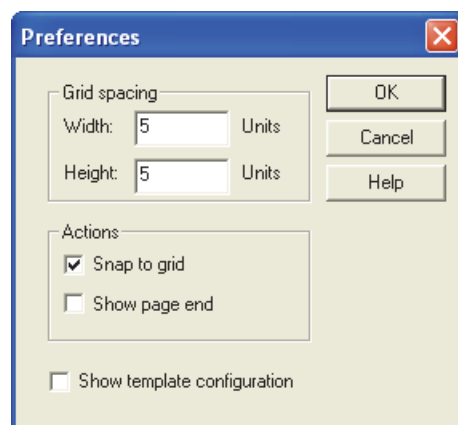
Choose **View > Report Template Grid**.

❖ To adjust the grid settings

1. Choose **Layout > Preferences**.

The Preferences dialog box opens (Figure 6). For more information about the Preferences dialog box, see [Preferences Dialog Box](#).

Figure 6. Preferences dialog box



2. Set the spacing between grid lines and whether to snap objects to the grid as they are added to the Template pane.

Using Columns

Add columns to arrange other reporting objects so that they appear in columns. To add a column to the template, drag the column object from the Objects pane to the Template pane.

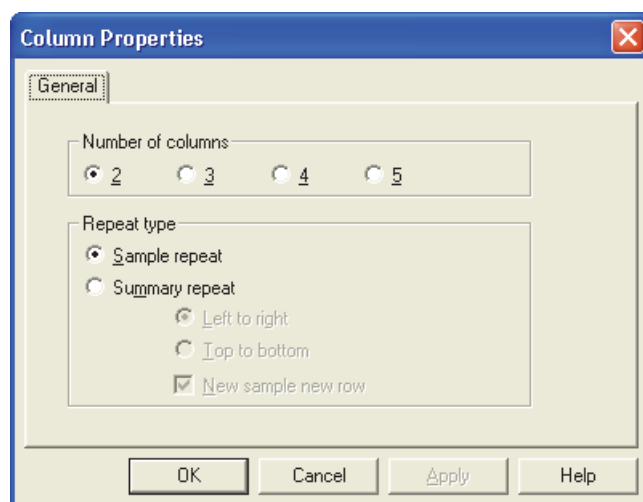
After adding a column object to the template, you can resize, reposition, and configure it.

❖ To configure a column object

1. Right-click the column object.
2. Choose **Properties** from the shortcut menu.

The Column Properties dialog box opens ([Figure 7](#)). To learn how to configure columns and how columns work with different repeat types, see [Configuring Columns](#).

Figure 7. Column Properties dialog box



You can resize the entire column object (select it and drag the corner handles), but the columns within the column object remain equal in size.

After you have finished configuring the columns, drag objects to the columns.

Using Page Breaks

If you do not manually insert page breaks, objects automatically shift to a new page when there is not enough room on the current page.

❖ To preview automatic page breaks

1. Choose **Layout > Preferences**.

The Preferences dialog box opens (see [Figure 6](#) on [page 21](#)).

2. Select the **Show Page End** check box.

❖ **To add a page break to the template**

1. Drag the **Page Break** object from the Objects pane to the Template pane.
2. After adding a page break to the template, drag the page break to reposition it.
3. Right-click the **Page Break** object and choose Properties from the shortcut menu.

The Page Setup dialog box opens. See [Page Setup Dialog Box](#).

4. Choose the paper source and page orientation.
5. Click **OK** to return to the template pane.

The Page Break object displays the page orientation.

Configuring Objects

For information about the XReport objects, see [Report Objects](#).

❖ **To configure an object**

1. Right-click the object.
2. Choose **Properties** from the shortcut menu.

The Properties dialog box opens.

For information about configuring each of the specific objects, see [Chapter 4](#). For a description of each object, including which sections each object can be used in, see [Appendix B, “Types of Report Objects.”](#)

Adding User Text to a Text Object

To add additional customized text headings to text objects, use the [<Blank Line >](#) and [<User Text> Data Items](#). These items are available for all text objects except the [Annotation Object](#) and the [Instrument Method Object](#).

For more information, see [Adding Custom Text Fields](#) and [Text Objects](#).

❖ **To add custom text to a text object**

1. Right-click the text object and choose **Properties** from the shortcut menu.

The [Data Page](#) of the *Text Object* dialog box opens.

2. To add a text item to the Selected list, do the following:
 - a. Select **<User Text>** in the Available Items list.
 - b. Click **Add**.

3. To position the <User Text> item where you want your text displayed, click **Move Up** or **Move Down**.
4. In the Selected list, select the <User Text> item.
The User Text box appears.
5. In the User Text box, type the appropriate text.
6. Click **Apply**.

The text you entered replaces the <User Text> item in the Selected list.

❖ To edit a <User Text> item

1. In the Selected list, select the <User Text> item of interest.
2. In the User Text box, type the appropriate text.
3. Click **Apply**.

Adding a Formula to a Table

You can create custom formulas in XReport to perform mathematical operations on table data and display the result in a table column.

❖ To add a formula to a table

1. In your XReport template, right-click a table object and choose **Properties**.

The Select Table Fields page opens ([Figure 8](#)). For information about the parameters on this page, see [Select Table Fields Page](#). The available parameters depend on the selected table object. The screen captures in this procedure show the parameters for a Spectrum List table object.

Figure 8. Select Table Fields dialog box for a Quan Repeating – Spectrum List Table

2. Select one of the User Columns fields in the Available Columns list: [User Column 1], [User Column 2], [User Column 3], [User Column 4], or [User Column 5].

For the five User Column fields available, you can create up to five separate formulas for a single table.

3. Click **Next** to go to the Configure User Column Parameters Page (Figure 9).

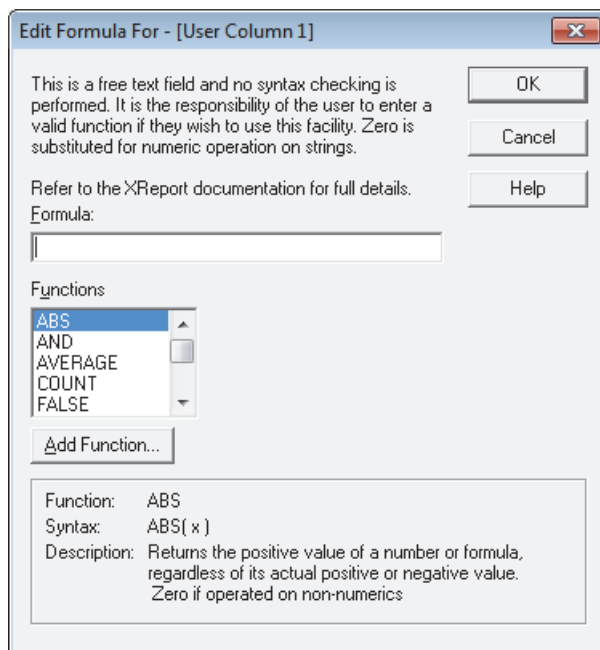
For information about the parameters on this page, see [Configure User Column Parameters Page](#).

Figure 9. Configure User Column Parameters dialog box for the Spectrum List Table

4. Type a title for this column in the User Column Title box.
5. Click **Edit Formula**.

The Edit Formula For Dialog Box opens (Figure 10). For information about the parameters on this page, see [Edit Formula For Dialog Box](#).

Figure 10. Edit Formula For dialog box



6. Enter a formula in the Formula box. Formulas can be entered in one of several ways:
 - Type formulas directly in the box. Formulas obey the following syntax rules:
 - The formula must begin with an equals sign (=).
 - Each table column is represented by an alphabetic letter identifier (A, B, C, and so on), displayed beneath the column title in the Table object.
 - Type simple mathematical expressions (A+B, A-B, A*B, and A/B), as well as any of the functions listed in the Functions list.

Mathematical formulas are computed on a row-by-row basis. That is, if you type =A+B as a formula in a User Column, the results are computed as follows:

- The value in the first row of column A is added to the value in the first row of column B, and the result appears in the first row of the User Column.
- The value in the second row of column A is added to the value in the second row of column B, and the result appears in the second row of the User Column.
- This process is continued until all rows of the table have been completed.

- Select a function from the Functions list and click **Add Function**. The [Configure Function Dialog Box](#) opens. Select the columns to be used with the function. When you configure your function and click OK, XReport enters the configured function in the Formula box.
7. When you have entered your formula, click **OK** to close the Edit Formula For dialog box and return to the Table Properties wizard. Continue through the remaining pages of the wizard to finish configuring your table.

Changing Font Settings

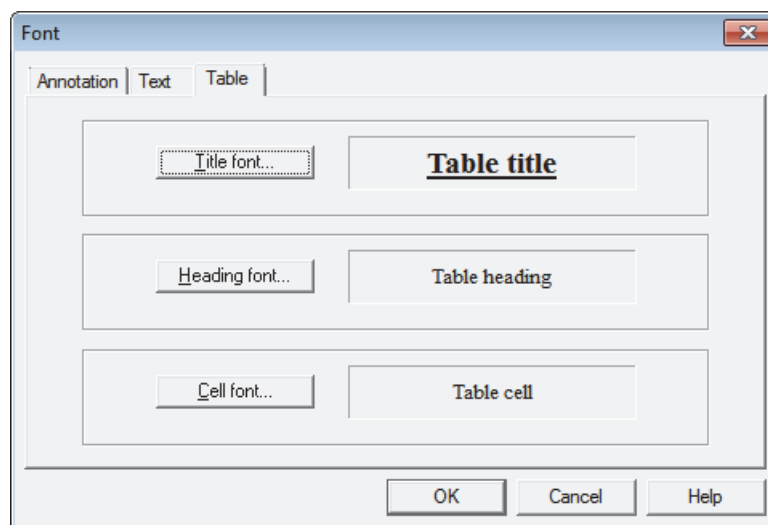
In the XReport application, you can change font settings globally or locally for text and table objects. When you change the font settings globally, each object added from that point forward appears in the new fonts (objects that are already in the template are not updated). When you change font settings locally, only the selected objects reflect the new font settings.

❖ To change the font settings for a single object

1. Do one of the following:
 - Select the object and click  in the toolbar.

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

Figure 11. Font dialog box for a table object



—or—

- a. Right-click the object and choose **Properties** from the shortcut menu. For some objects, the *object type* Properties dialog box opens. For table objects, a wizard opens.
 - b. Click the **Font** tab of the Properties dialog box or click Next in the table wizard until a Fonts page opens.
2. Update the settings and click **OK**.

❖ **To change the font settings for more than one text or table object at a time**

1. Select the first object.
2. Hold down the SHIFT key while you select the other objects.
3. Click  in the toolbar.

The Font dialog box opens.

4. Update the settings and click **OK**.

❖ **To globally change the font settings used for all new objects to add to the template**

1. Click any section and confirm that no objects are selected.
2. Click  in the toolbar.

The Font dialog box opens.

3. Update the settings and click **OK**.

Changing the Page Layout

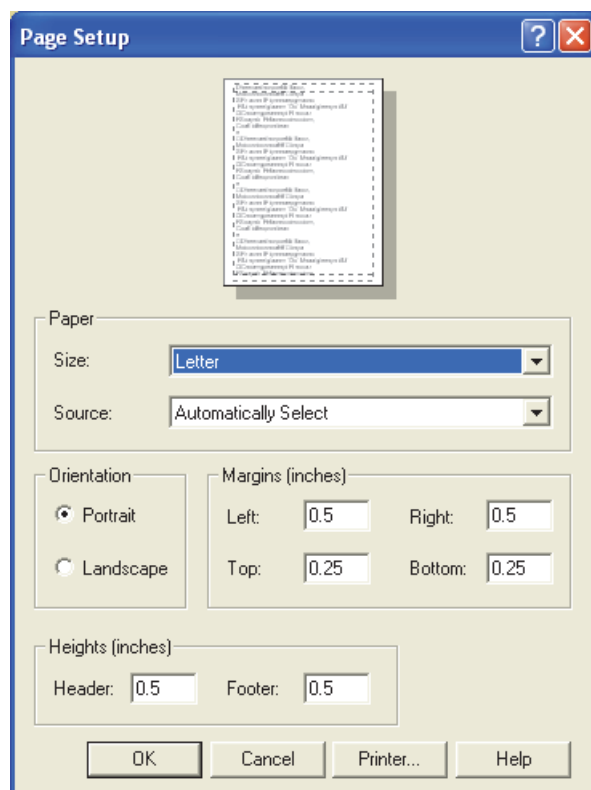
You can change the page layout for your XReport templates by using the Page Setup dialog box.

❖ **To change the page layout**

1. Do one of the following:
 - Choose **File > Page Setup**.
- or–
 - Right-click a **Page Break** object in the template pane and choose **Properties**.

The Page Setup dialog box opens ([Figure 12](#)).

Figure 12. Page Setup dialog box



2. Change any of the following: header and footer section heights, portrait or landscape page orientation, or margins.
3. Click **OK** to change the page layout.

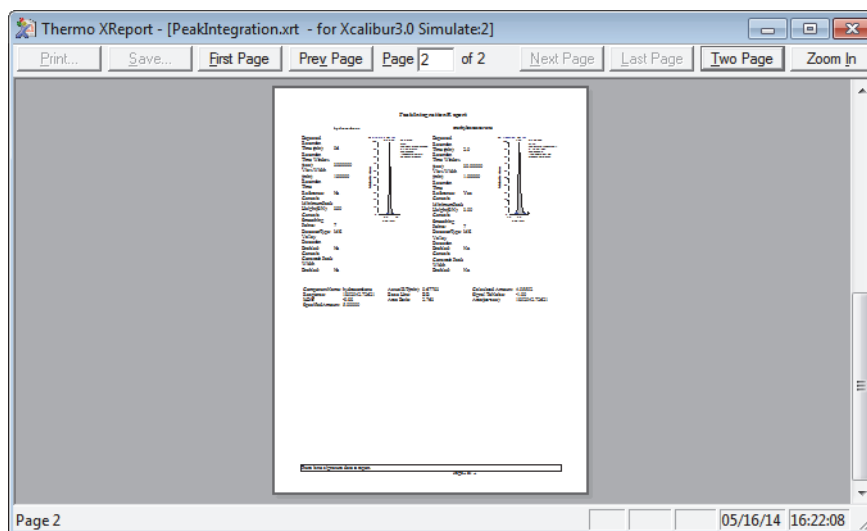
Previewing and Saving the Template

Before you use a template to print reports, preview the template with the example data provided with the Xcalibur data system or with a representative data file.

❖ To preview the appearance of the template

1. Choose **Report > Simulate Report**. The Preview window opens (Figure 13). The Preview window shows the report with the default data.

Figure 13. Preview window



2. When the report is correct, click **Close** to close the preview window.
3. To save the template, choose **File > Save**. To save changes to a locked template choose **File > Save As** and rename the file.

XReport uses the steroid example data that is provided with the Xcalibur data system as the default data set. It consists of the following files:

- steroid.pmd
- steroids02.raw
- steroids02.rst
- steroid.sld

When your template is designed for a very different type of data set than the default data, you might not see the results you expect when you preview the template. In that case, choose appropriate data sources for the template and create the report as described in [Creating a Report Within XReport](#).

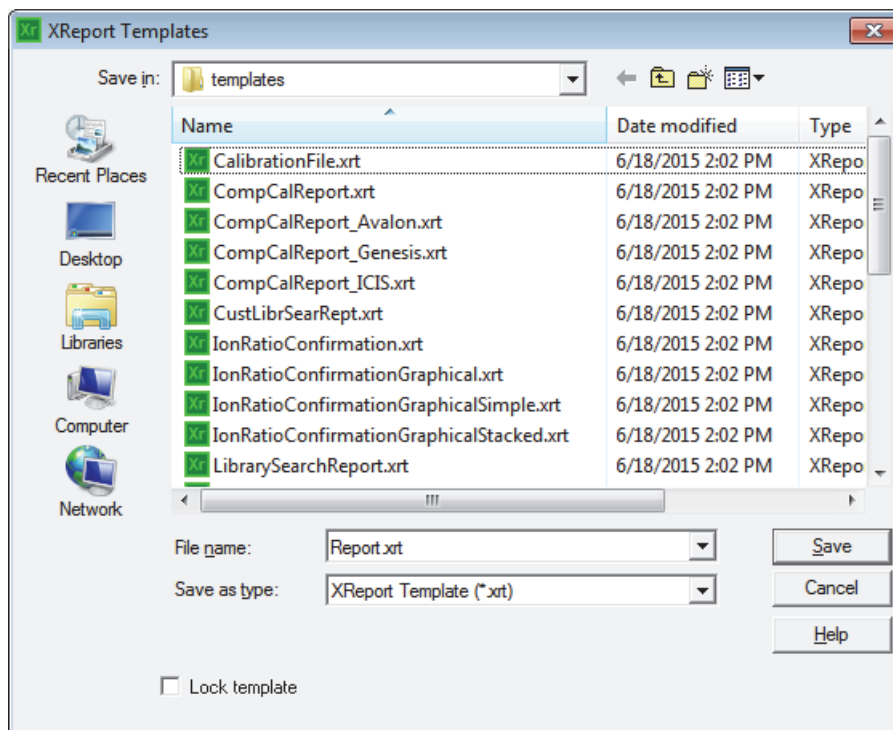
Use XReport to lock a template so that it can never be modified and saved with the same filename. To modify a locked template, save it with a different filename. Choose **File > Open** to open a locked template the same way you open any other template.

❖ **To lock the template**

1. Choose **File > Save As**.

The Save As dialog box opens (Figure 14).

Figure 14. Save As dialog box for XReport Templates



2. Give the report template an appropriate name and save it in the Xcalibur\templates folder with the templates that ship with the Xcalibur data system.
3. Select the **Lock Template** check box and click **Save**.

2 Creating a Template

Previewing and Saving the Template

Generating a Report

To generate an Xcalibur report (resolved document), combine a report template with one or more Xcalibur data source files (processing methods [PMD], raw data files [RAW], result files [RST] sequence files [SLD], and calibration files [XCAL]).

There are two ways to generate reports:

- Use the XReport Data Source Browser to automatically search for the required data source files and combine the data with a template to generate a report. This method generates a single report.
- Associate the data you produced in the Xcalibur data system with a report template and combine the data with the template to generate a report. This method generates multiple reports from the data system.

Contents

- [Creating a Report Within XReport](#)
- [Creating a Report from the Xcalibur Data System](#)

Creating a Report Within XReport

To create a report within XReport, use these procedures:

- [Choosing Data Sources for a Template](#)
- [Generating, Saving, and Printing a Report](#)

Choosing Data Sources for a Template

The process of generating a report from an XReport template involves using the [Data Sources Dialog Box](#) to search for the required data source files. The data source files required to generate a report depend on the content (sections and report objects) of the report template. To learn which data files are needed for each type of report object, see [Appendix B, “Types of Report Objects.”](#)

❖ **To resolve a template with data**

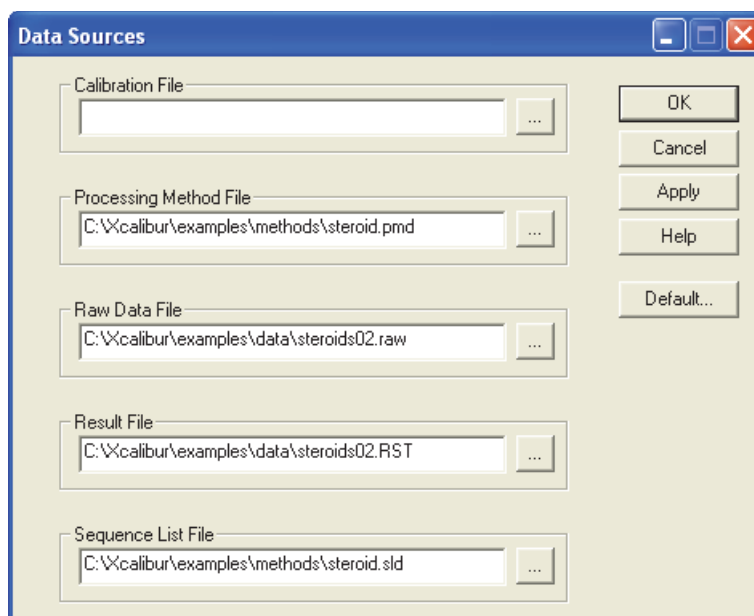
1. To open the template (XRT file), choose **File > Open** in XReport.

The XReport Templates dialog box opens.

2. Select the template and click **Open**.
3. Choose **Report > Data Sources**.

The Data Sources dialog box opens ([Figure 15](#)).

Figure 15. Data Sources dialog box



4. In each box, enter or search for a data file.

If you specify a result file (RST) that references a raw data file (RAW) and that raw data file does not exist or is in the wrong folder, XReport sends an error message. Make sure the raw data file is in the correct folder.

5. Click **OK**.

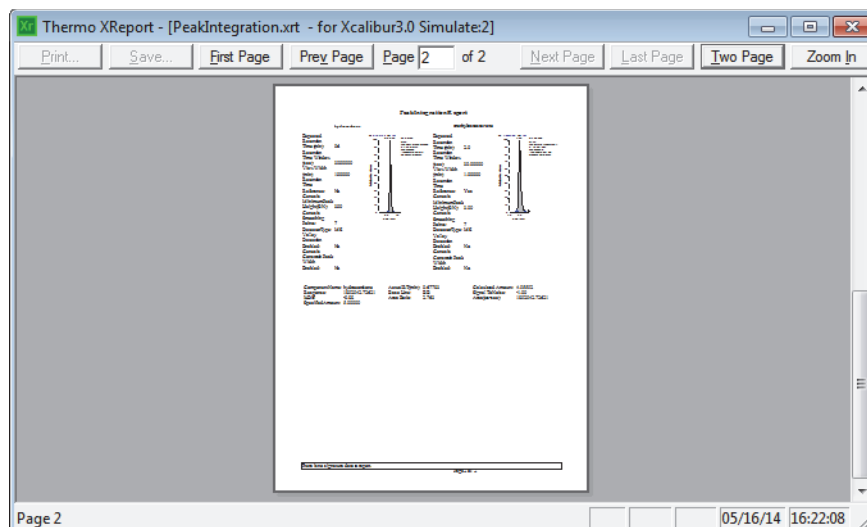
Generating, Saving, and Printing a Report

❖ **To create a report using selected data sources**

1. Select the appropriate data sources as described in [Choosing Data Sources for a Template](#).
2. Choose **Report > Resolve Report** in XReport.

The Preview window opens ([Figure 16](#)). The Preview window shows a report combined with selected data sources.

Figure 16. Preview window



3. Click **Save** to save the report in the following file formats: Microsoft Word (DOC), Microsoft Excel (XLS), web page (HTM or HTML), rich text (RTF), PDF (PDF), or text (TXT).
4. To print the report, click **Print**.
5. To return to the XReport window, click **Close**.

Creating a Report from the Xcalibur Data System

When generating a report, the data system combines the data that you produced in the data system with a report template. You can generate multiple reports from the data system. To proceed, you must have a basic understanding of the Xcalibur data system. Refer to the *Xcalibur Getting Started Guide* for more information.

Generate a report from the following areas of the application:

- See [Generating a Report From Sequence Setup](#) when running a sample or sequence and batch processing.
- See [Generating a Report From Quan Browser](#) when using the Reports dialog box.

In addition, when generating reports from the Xcalibur data system, create reports containing electronic signature information.

Always save and close the report template in XReport before using it to generate a report from the Xcalibur data system.

Sample Reports and Summary Reports

To set up reporting options in the data system in Processing Setup or Quan Browser, select two types of reports:

- Sample reports to print reports that give information about individual samples
- Summary reports to print reports that give summary information about an entire sequence or set of samples

The example template files included with XReport indicate the specific templates to use to generate sample reports or summary reports. For descriptions of sample files, see [Sample XReport Template Files](#).

Generating a Report From Sequence Setup

To generate reports from the Sequence Setup window, create a processing method that includes the necessary report options on the Reports page of the method.

Use the Sequence Setup window to generate reports when running a sample or sequence or batch processing a sequence.

See these topics for more information:

- [Setting Report Options in a Processing Method](#)
- [Generating Reports when Running a Sequence](#)
- [Generating Reports when Batch Processing a Sequence](#)

Setting Report Options in a Processing Method

To automated reporting, set up the appropriate report templates in your processing methods.

❖ To set up reports in a processing method

1. Open the Processing Setup window and set up a processing method. For more information, refer to the *Xcalibur Data Acquisition and Processing User Guide*.
2. Choose **View > Reports**.

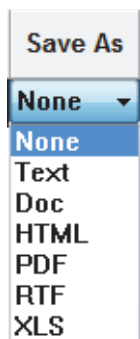
The Reports view opens.

3. To add one or more reports to either the sample or summary report tables, do the following:

The sample table lists the reports to be produced for processed samples in a sequence. The Summary table lists the reports to be produced for sequences or brackets.

- a. Click the **Enable** column to display a check box and select the check box to enable the report.
- b. To create a sample table, select the **Std**, **QC**, **Unk**, and **Other** check boxes.

- c. Select the output for the report in the Save As column. Choose from **None** (this prints the report, but does not save it), **Text**, **Doc**, **HTML**, **PDF**, **RTF**, or **XLS** (select one of these options to save the report in the selected format).



The Xcalibur data system saves reports created from the processing method in the same directory as the source data files and names files. The reports use this format:

data file name template name.xxx

where

data file name is the name of the data file from which the report was generated

template name is the name of the template used to generate the report

xxx is the suffix [for example, (.doc) or (.pdf)] indicating the file type

When more than one report is generated from the same data file and template, XReport adds a date stamp before the suffix.

- d. Double-click the Report Name column to select an XReport template (XRT file) to use for this report.
4. Save the processing method.

Generating Reports when Running a Sequence

You must create a sequence to run either a single sample or multiple samples from the Sequence Setup window. When you click the Run Sample icon in the Sequence Editor toolbar, the data system automatically selects the first row of the sequence. When you click the Run Sequence icon, the data system automatically selects the entire sequence if you have not already selected a subset of sequence rows.

❖ To generate reports when running a sequence

1. Set up the report options in a processing method as described in [Setting Report Options in a Processing Method](#).
2. In the Xcalibur Sequence Setup window, open the sequence that you want to run.
3. Specify the processing method that includes all of the report options in the Proc Meth column.

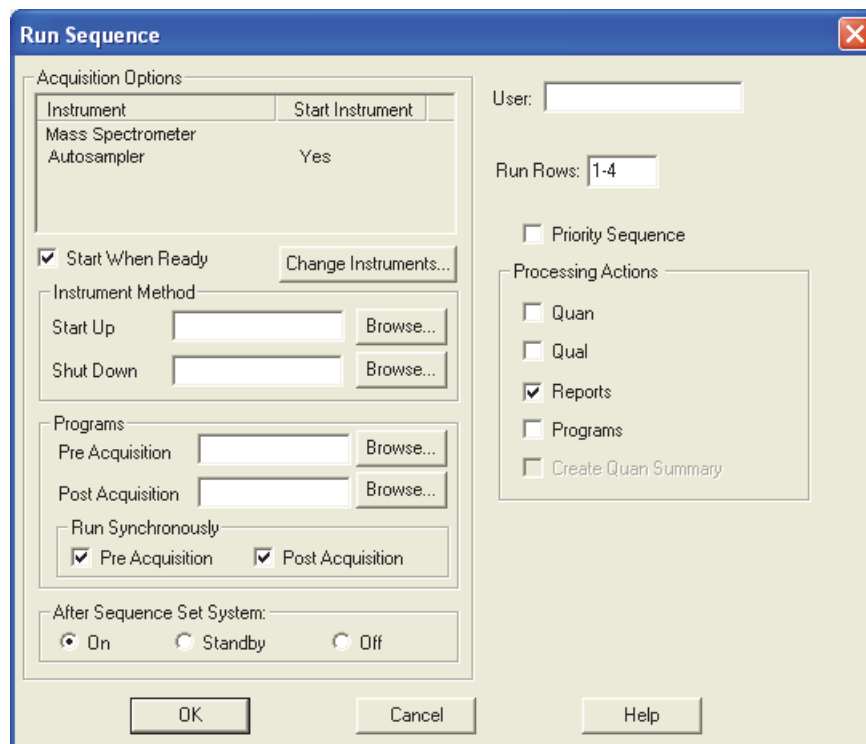
3 Generating a Report

Creating a Report from the Xcalibur Data System

4. To run a subset of the sequence, select the sequence rows that you want to run.
5. Choose **Actions > Run This Sequence** or **Actions > Run This Sample**.

The Run Sequence dialog box opens (Figure 17). The Run Rows box lists the row selection.

Figure 17. Run Sequence dialog box



6. Select the **Reports** check box in the Processing Actions area.
7. Set all of the other parameters.
8. Click **OK**.

The data system submits the selected sample or samples to the acquisition queue.

Generating Reports when Batch Processing a Sequence

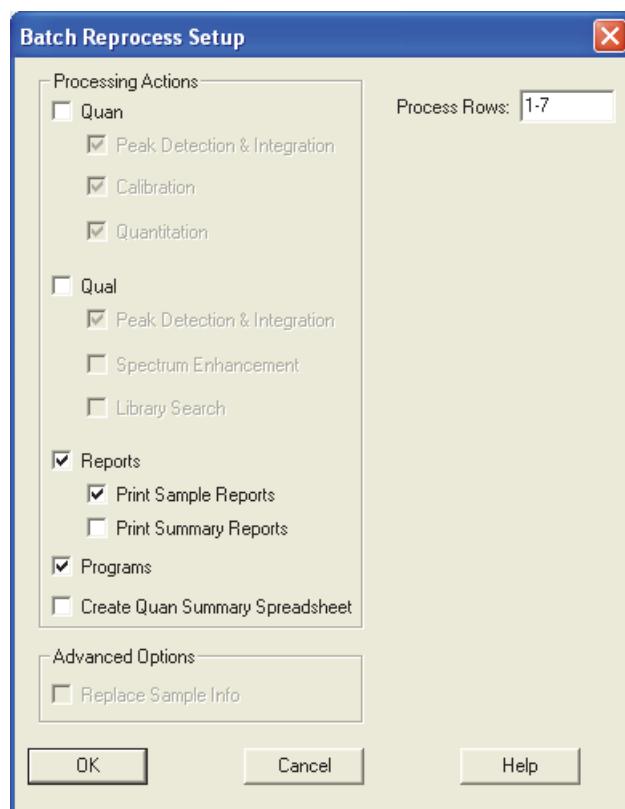
You can set up a batch processing job to print reports.

❖ To generate reports when batch processing a sequence

1. Set report parameters in the processing method as described in [Setting Report Options in a Processing Method](#).
2. In the Xcalibur Sequence Setup window, open the sequence that you want to batch reprocess.
3. Enter the processing method that includes all of the report options in the Proc Meth column.
4. Select the rows that you want to process.
5. Choose **Actions > Batch Reprocess**.

The Batch Reprocess Setup dialog box opens ([Figure 18](#)). The Process Rows box lists the selected sequence rows.

Figure 18. Batch Reprocess Setup dialog box



6. If necessary, change the rows to be processed by entering the first and last row to be processed in the Process Rows box. The format is either *nRow* for one sample or *First Row#–Last Row#* for multiple samples.
7. Select **Quan** or **Qual** processing actions and select from active options.

8. Select from these XReport processing options:
 - To create reports while batch processing, select the **Reports** check box.
 - To print reports for the samples displayed in the Process Rows box, select the **Print Sample Reports** option. You defined the Sample report parameters in the Reports view of the Processing Setup window.
 - Select the **Print Summary Reports** option to print reports for the samples that are displayed in the Process Rows box. You defined the summary report parameters in the Reports view of the Processing Setup window.
 - Select programs, spreadsheet, and advanced options.
9. Click **OK**.

The data system initiates batch processing of the selected samples.

Generating a Report From Quan Browser

You can print reports for a sample set from the Quan Browser window.

❖ To generate a report from the Quan Browser window

1. Open the Quan Browser window.

The Open dialog box opens.
2. To select a sequence, select an SLD file with samples to use in the reports. Then, click **Open**.
3. Choose **View > Reports Dialog**.

The Reports dialog box opens ([Figure 19](#)).

Figure 19. Reports dialog box in the Quan Browser window

Sample Reports - 0 selected samples

	Enabled	Std	QCs	Unks	Other	Save As	Report Template Name
1	Yes	Yes	Yes	Yes	Yes	PDF	C:\Xcalibur\templates\PeakIntegration.xrt
*		Yes	Yes	Yes	Yes	None	

Summary Reports

	Enabled	Save As	Report Template Name
1	Yes	PDF	C:\Xcalibur\templates\QuantifySampleReport.xrt
*		None	

☒ Include Sample Reports ☒ Include Summary Report

Select Samples... Print Reports OK Cancel Help

4. To make a row of the Sample Reports area active, do the following:
 - a. Click the **Enable** box in the first row and click the **Enable** box again.
A check box appears in the box.
 - b. Click the check box.
When you click the check box again, the word Yes appears in the Enable box to indicate that the entire row of options is selected.
5. To select the report type to print for the sample, do the following:
 - a. Click one of the following boxes: **Std**, **QC**, **Unk**, or **Other**.
A check box control appears.
 - b. Click the check box.
When you click the check box again, the word Yes appears in the Enable box to indicate that reports are to be printed for all selected samples of this sample type.
6. Repeat [step 4](#) and [step 5](#) to print reports for needed sample types.
7. To display the Open Report Template dialog box, double-click the Report Template Name box. Select the previously prepared report template document and click **Open**.
The full path and the file name of the report template (XRT) document appear in the Report Template Name box.

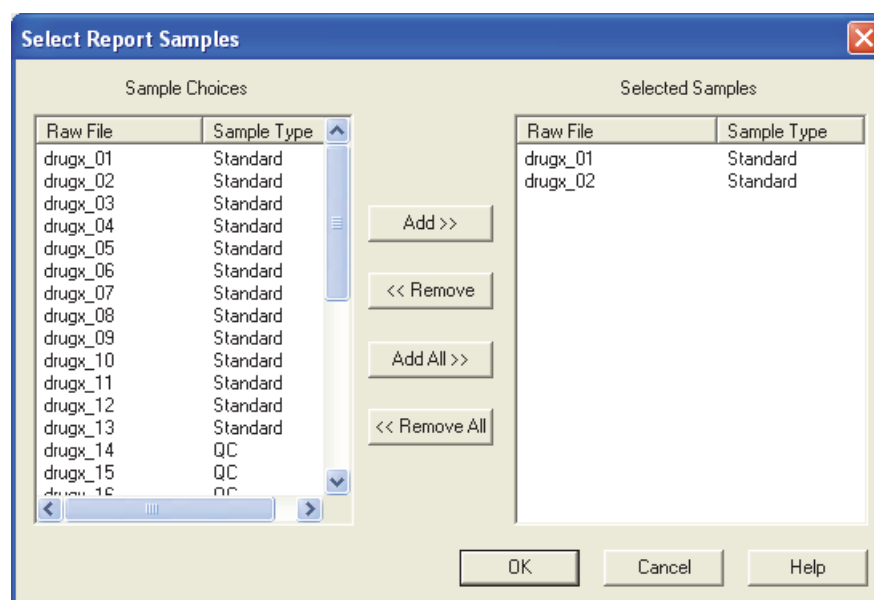
3 Generating a Report

Creating a Report from the Xcalibur Data System

8. To print reports for each report template document, repeat steps 4 through 7 for the next row.
9. To make all of the sample reports you have selected for printing available, click the **Include Sample Reports** check box at the bottom of the Reports dialog box. Click the **Include Summary Report** check box to make summary reports available.
10. To select the samples for the report, do the following:
 - a. Click **Select Samples** to open the Select Report Samples dialog box.

The samples available from the sequence file opened in [step 2](#) appear in the Sample Choices box ([Figure 20](#)).

Figure 20. Select Report Samples dialog box



- b. Select the samples:
 - For a group of contiguous samples, click the first of the sequence, scroll until you see the last sample in the sequence and, while holding down the SHIFT key, click the last sample in the sequence. The data system highlights the selected sequence.
 - For a group of non-contiguous samples, hold down the CTRL key while you click each sample to select or clear it. The data system highlights the selected samples.
 - c. To copy the selected samples to the Selected Samples area, click **Add**.
 - d. To return to the Reports dialog box, click **OK**.

11. To print reports, click **Print Reports**.

Prior to printing reports, the data system does the following:

- Displays the Printer Activity icon at the bottom of the Quan Browser window.
- Combines the data in the sample file with the selected Report Template document.
- Adds the report printing tasks to the processing queue and displays the Printing message box.

After printing the reports, the data system returns you to the Quan Browser window.

The application saves reports created from the processing method in the same directory as the source data files and names files. The reports use this format:

data file name template name.xxx

where

data file name is the name of the data file from which the report was generated,

template name is the name of the template used to generate the report, and

xxx is the suffix [for example, (.doc) or (.pdf)] indicating the file type.

When more than one report is generated from the same data file and template, XReport adds a date stamp before the suffix.

Creating a Signed Report

When generating reports from Quan Browser or by batch processing in Sequence Setup, you can create signed reports containing electronic signatures.

❖ To create a signed report

1. Create a report template containing the Electronic Signature table object or choose one of the preconfigured templates supplied with XReport.

All of the preconfigured templates contain the Electronic Signature table object in the footer.

2. Confirm that the Xcalibur Authorization Manager settings are set to require electronic signatures at the report generating step.

See [Configuring Authorization Manager Settings for Signed Reports](#) for that process.

3. Generate the report.

Configuring Authorization Manager Settings for Signed Reports

To produce signed reports with electronic signatures, configure the Xcalibur Authorization Manager Settings to require signatures. The Xcalibur data system administrators must perform this configuration before setting permissions in either Quan Browser or Sequence Setup.

❖ To set permissions for producing signed reports from Sequence Setup

1. Choose **Start > Thermo Scientific Foundation x.x > Authorization Manager**.

The Authorization Manager window opens (Figure 21).

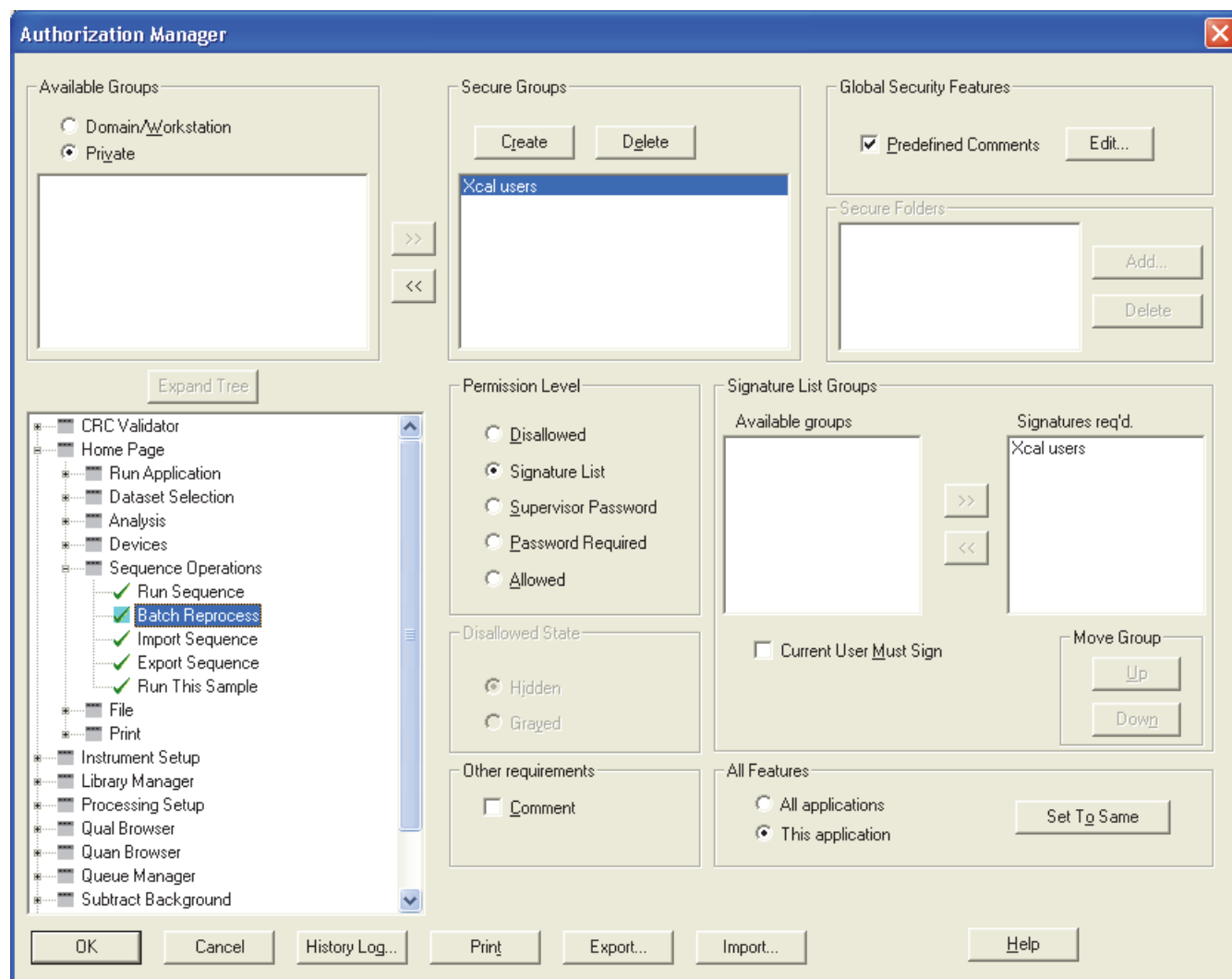
2. Expand the Home Page entry. In the directory tree, expand the Sequence Operations entry in the permission level pane.
3. Select **Batch Reprocess** from the list of operations below Sequence Operations.
4. Select **Signature List** in the Permission Level area.
5. In the Signature List Groups area, select a group from the Available groups list and click >> to move it to the Signatures Req'd list. The members of this group must type their login names and passwords to electronically sign the report when it is generated. Repeat this step for each group that you want to add to the Signatures Req'd list.

Note If you do not have any groups available or if the groups do not contain the correct members, refer to the *Foundation Administrator Guide* or the Foundation Help for information on how to create and modify groups.

6. To require a signature from the current user when the report is generated, select the **Current User Must Sign** check box.

At this point, the settings should be similar to the settings in Figure 21.

Figure 21. Sequence Setup settings for producing signed reports



❖ **To set permissions for producing signed reports from Quan Browser**

1. Choose **Start > Thermo Scientific Foundation x.x > Authorization Manager**.

The Authorization Manager window opens (Figure 22).

2. In the tree directory, expand the Quan Browser entry and expand the Print entry.
3. Select **Print Reports**.
4. In the Permission Level area, select **Signature List**.

3 Generating a Report

Creating a Report from the Xcalibur Data System

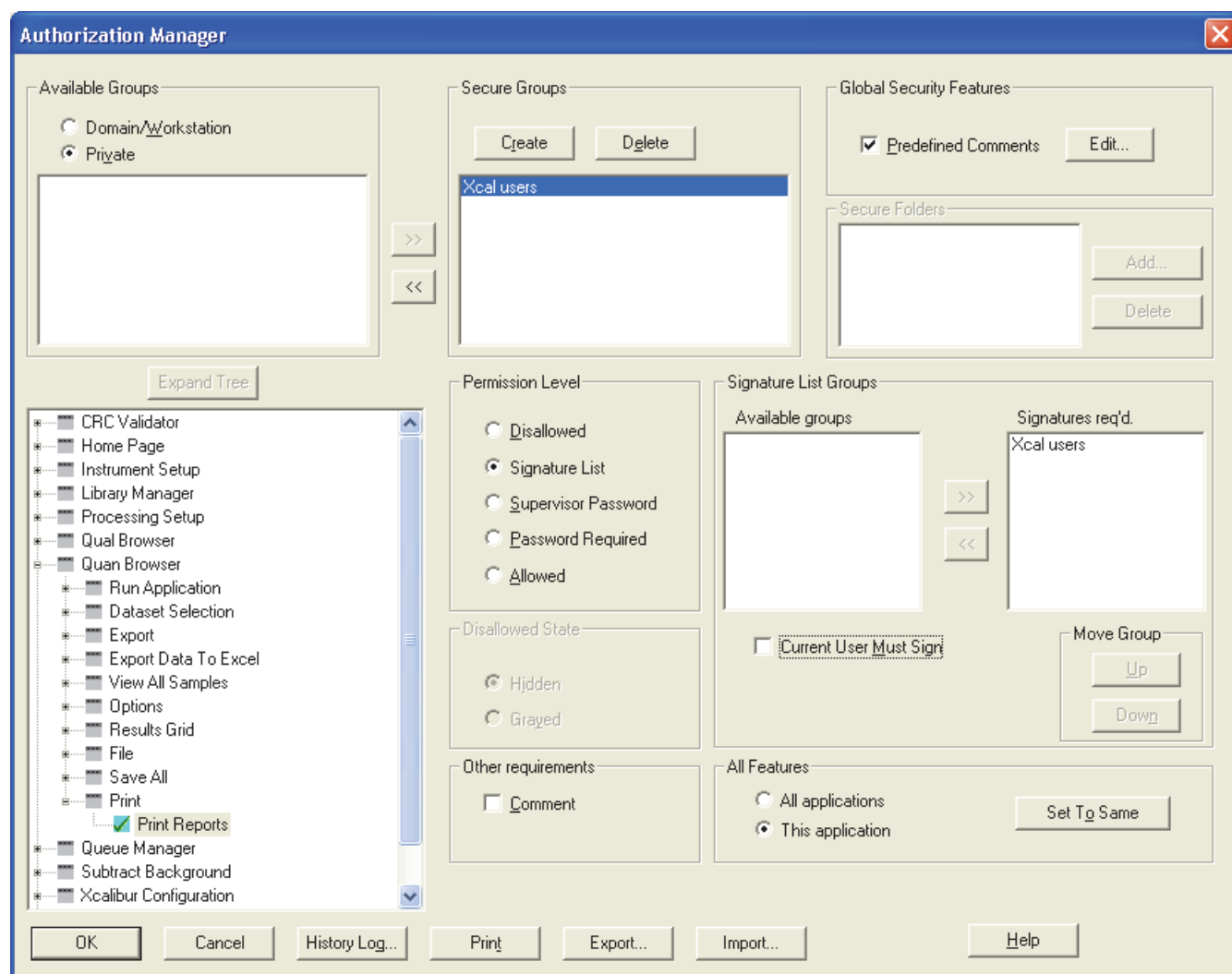
5. In the Signature List Groups area, select a group from the Available groups list and click >> to move it to the Signatures Req'd list. The members of this group are required to type their log on names and passwords to electronically sign the report when it is generated. Repeat this step for each group that you want to add to the Signatures Req'd list.

Note If you do not have any groups available or if the groups do not contain the correct members, refer to the *Foundation Administrator Guide* for information on how to create and modify groups.

6. To require a signature from the current user when the report is generated, select the **Current User Must Sign** check box.

At this point, the settings should be similar to the settings in [Figure 22](#).

Figure 22. Quan Browser settings for producing signed reports



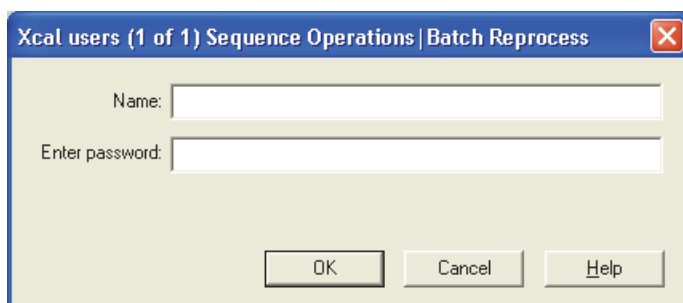
7. Click **OK** to save the settings and close the Authorization Manager dialog box.

Generating Signed Reports

Once you have a template containing an Electronic Signatures object, generate the report as described in [Generating Reports when Batch Processing a Sequence](#) or in [Generating a Report From Quan Browser](#). The Xcalibur data system prompts you to type signature information when the report is generated. Each user whose signature is required must type their log on name and password to sign the report.

[Figure 23](#) displays an example of a signature dialog box.

Figure 23. Example of a signature dialog box



3 Generating a Report

Creating a Report from the Xcalibur Data System

Configuring Objects and Sections

You can configure the following objects and sections in XReport. When you configure an object, you can change or edit only the individual properties of that specific object. When you add another object of the same type to the report, XReport inserts it with the default settings.

Contents

- [Configuring a Repeating Section](#)
- [Configuring a Text Object](#)
- [Configuring an Annotation Object](#)
- [Configuring a Table Object](#)
- [Configuring a Bitmap Object](#)
- [Configuring a Chromatogram Object](#)
- [Configuring a Component Calibration Curve](#)
- [Configuring a Spectrum Object](#)
- [Configuring Columns](#)

Configuring a Repeating Section

There are two different types of repeating sections in XReport:

Qual repeating section	Displays details related to a single Qual peak in some data. The section is repeated for all Qual peaks found.
Quan repeating section	Displays details related to a single Quan peak in some data or a component configured in a processing method. The section is repeated for all Quan peaks or components.

In the Repeating Section Properties dialog box, specify these parameters:

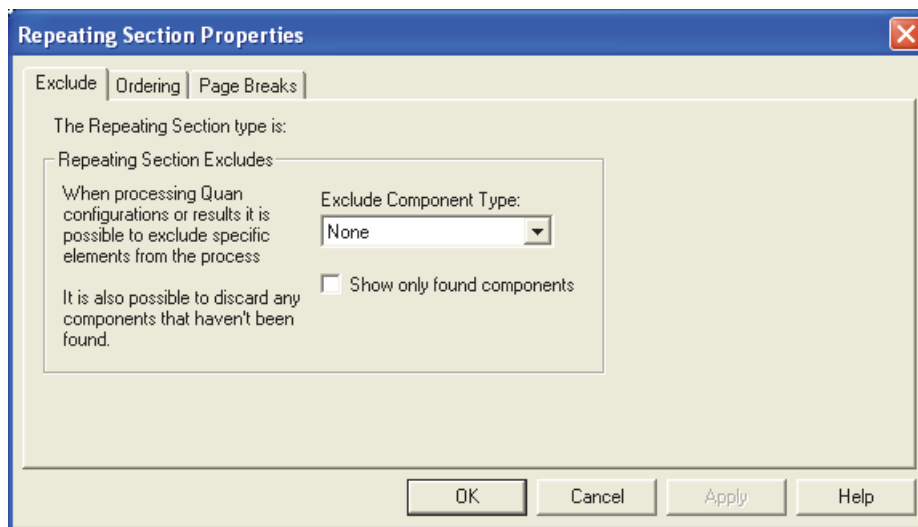
- Whether to exclude internal standards or target compounds from a Quan repeating section
- The repeat order for peaks and components
- Any limit on the number of peaks to be reported
- How the individual peaks or components are split across pages in the final report

❖ **To configure a Qual or Quan repeating section**

1. Scroll to where you can see the QL or QN icon at the top left side of the template pane and right-click the icon.
2. Choose **Properties** from the shortcut menu.

The Repeating Section Properties dialog box opens (Figure 24). This dialog box has three pages: Exclude (available for a Quan repeating section only), Ordering, and Page Breaks.

Figure 24. Exclude page in the Repeating Section Properties dialog box



3. When configuring a Quan repeating section, use the Exclude page to exclude specific elements from the process and discard any components that have not been found.
 - a. From the Exclude Component Type list, define the exclusions for the Quan repeating section by selecting one of the following:
 - None (no exclusions)
 - Internal Standards (excludes internal standard compounds from the report)
 - Target Compounds (excludes target compounds from the report)

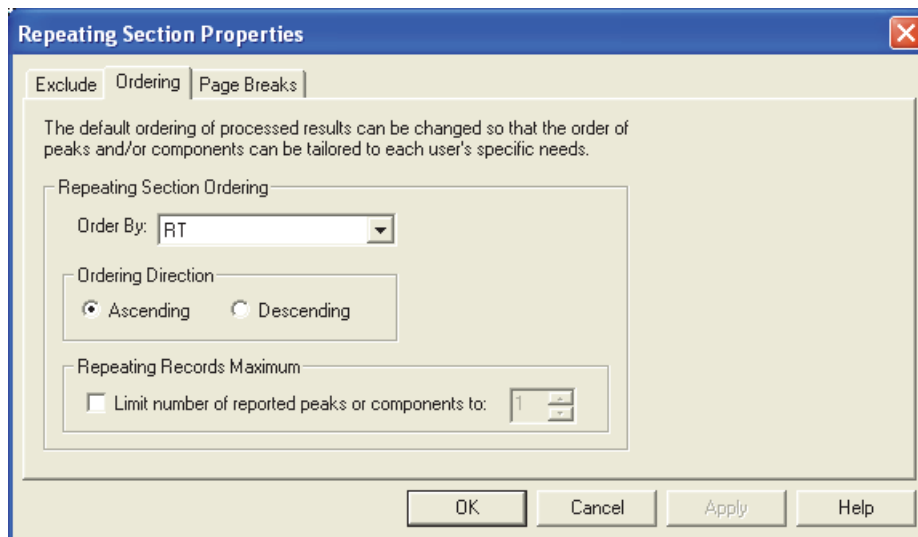
The default selection is None.

- b. To discard any components that have not been found, select the **Show Only Found Components** check box.

For more information about the parameters on the Exclude page, see [Exclude Page](#).

4. Click the **Ordering** tab to display the Ordering page ([Figure 25](#)). Use this page to change the default ordering of processed results, defining the order of peaks and components in either a Qual or Quan repeating section.

Figure 25. Ordering page in the Repeating Section Properties dialog box



5. To specify the order for the repeating section in the Repeating Section Ordering area, select one of the following from the Order By list:
 - RT (retention time)
 - Component Name (Quan only)
 - Peak Height Intensity
 - Peak Area Intensity
 - Peak Response Intensity (Quan only)
 - Component Concentration (Quan only)

The default selection is RT.

6. To define the direction for the ordering in the Ordering Direction area, select one of these options:
 - Ascending: Sort data in ascending order
 - Descending: Sort data in descending order

4 Configuring Objects and Sections

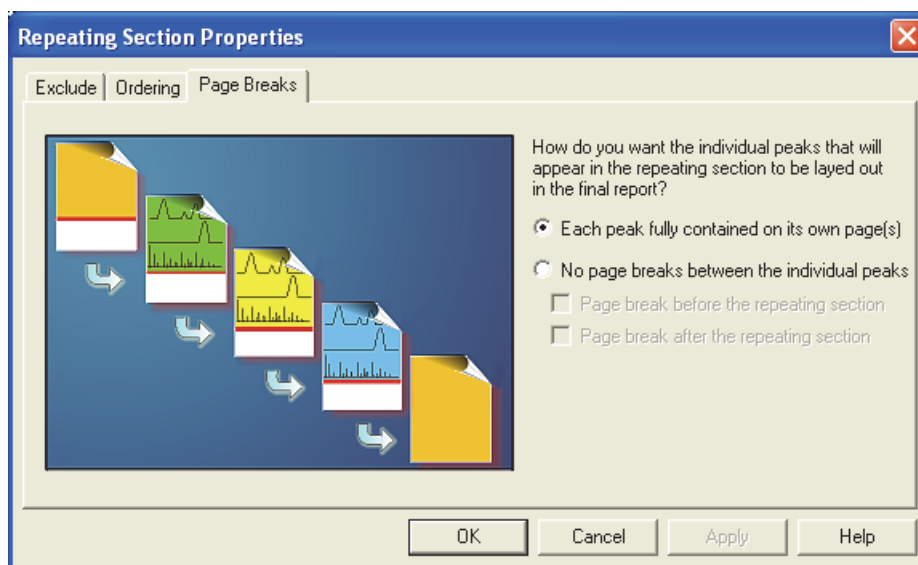
Configuring a Repeating Section

7. To set a maximum number of peaks or components to order (up to 999) in the Repeating Records Maximum area, select the **Limit Number of Reported Peaks or Components** check box and select a value from the active box.

For more information about the parameters on the Ordering page, see [Ordering Page](#).

8. Click the **Page Breaks** tab to display the Page Breaks page. Use this page to define the layout for the individual peaks that appear in the Qual or Quan repeating section in the final report ([Figure 26](#)).

Figure 26. Page Breaks page in the Repeating Section Properties dialog box



Select the option either to print each peak on its own pages or to avoid page breaks between the individual peaks.

For more information about the parameters on the Page Breaks page, see [Page Breaks Page](#).

9. When you have made selections in the Repeating Sections Properties dialog box, click **OK**.
10. Choose **File > Save** to save any changes.

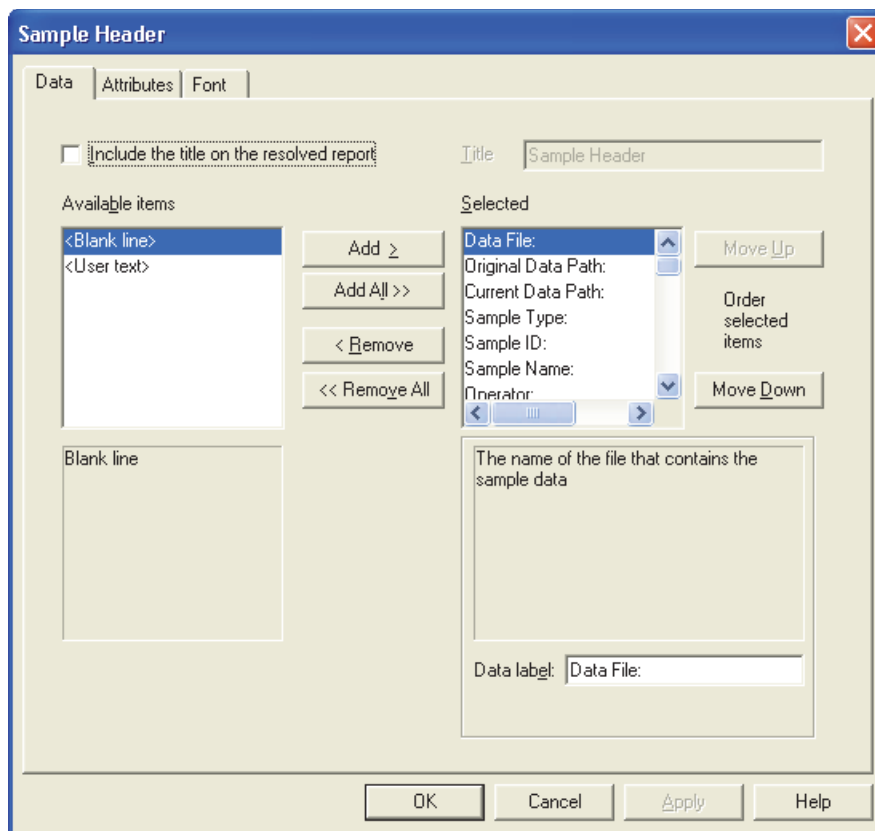
Configuring a Text Object

Use the *Text Object* dialog box to configure a text object within the report.

To configure a text object, right-click the object and choose **Properties**. A dialog box opens (Figure 27), named for the type of object you chose.

For a description of each text object, including which section each object is in, see [Appendix B, “Types of Report Objects.”](#)

Figure 27. Data page in the Sample Header dialog box



Use the *Text Object* dialog box for these tasks:

- [Configuring Text Fields](#)
- [Adding Custom Text Fields](#)
- [Configuring Text Attributes](#)
- [Setting Text Fonts](#)

Configuring Text Fields

Use the Data page of the *Text Object* dialog box to set up the text fields.

❖ To configure the text fields

1. In the template pane, open the *Text Object* dialog box by right-clicking a text object and selecting **Properties** from the shortcut menu.

The *Text Object* dialog box opens to the Data page.

2. To include a custom title for the object, do the following:
 - a. Select the **Include the Title on the Resolved Report** check box.

The Title box appears.

- b. Type a name in the Title box.
3. Select the items to include from the Available Items list.
 - Select an item and click **Add**.
 - Double-click an item.
 - To move all available fields, click **Add All**.

The fields you have chosen appear in the selected list.

4. Select the fields in the Selected list that you do not want to include and click **Remove**.
5. To change the order of the selected items in the Selected list box, select an item and click **Move Up** or **Move Down**.
6. To edit a data label, select it in the Selected list and edit its text in the Data label box. Headings cannot be edited. However, use User Text items to add custom Headings to a text object. See the next topic, [Adding Custom Text Fields](#).
7. Click **OK** to save your changes and close the dialog box.

Adding Custom Text Fields

Add a custom text field to the text object to use as a heading or annotation. For more information about the parameters on the Data page, see [Data Page](#).

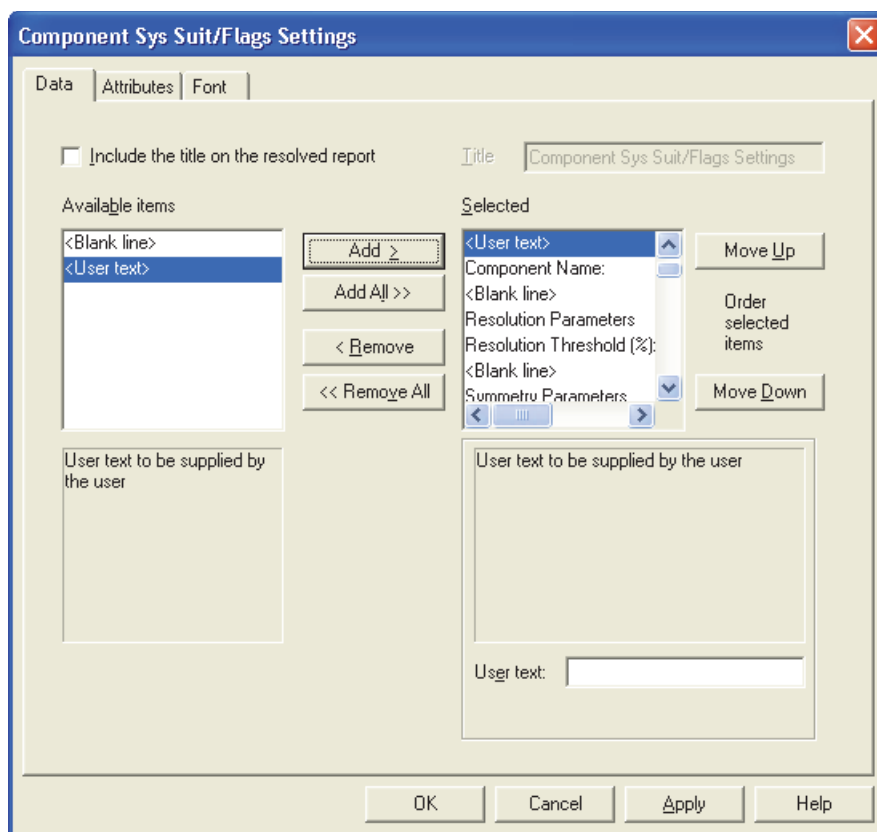
❖ To add a custom text field

1. In the template pane, right-click a text object and choose **Properties** from the shortcut menu.

The *Text Object* dialog box opens to the Data page.

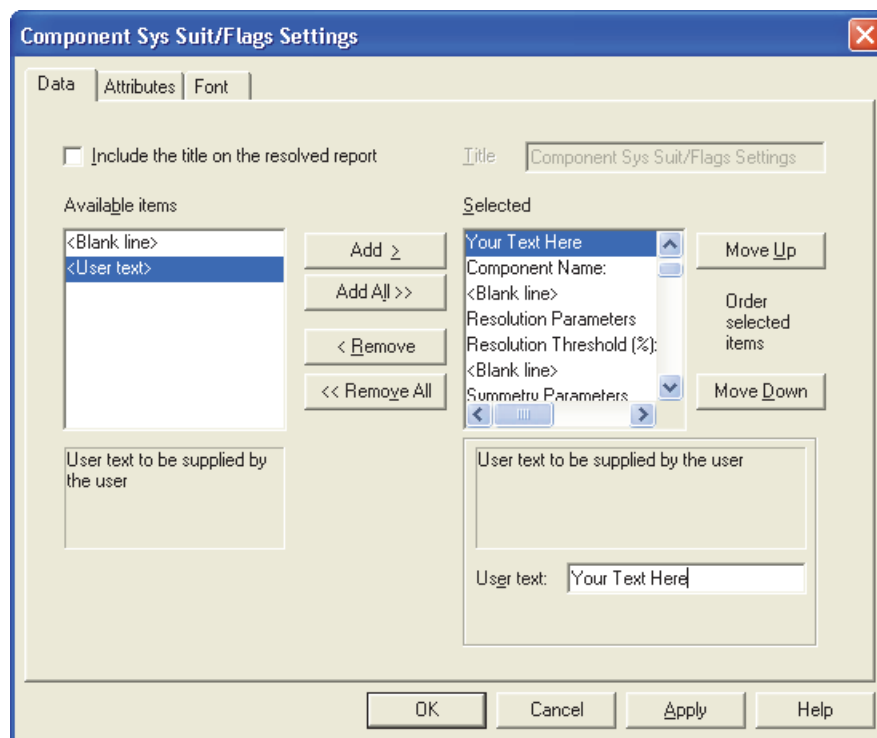
2. On the Data page of the *Text Object* dialog box, select **<User Text>** in the Available Items list and click **Add** ([Figure 28](#)).

Figure 28. Adding a custom text field



3. Select **<User Text>** in the Selected list.
4. Type the text in the User Text box and click **Apply** ([Figure 29](#)).

Figure 29. Customizing a text field

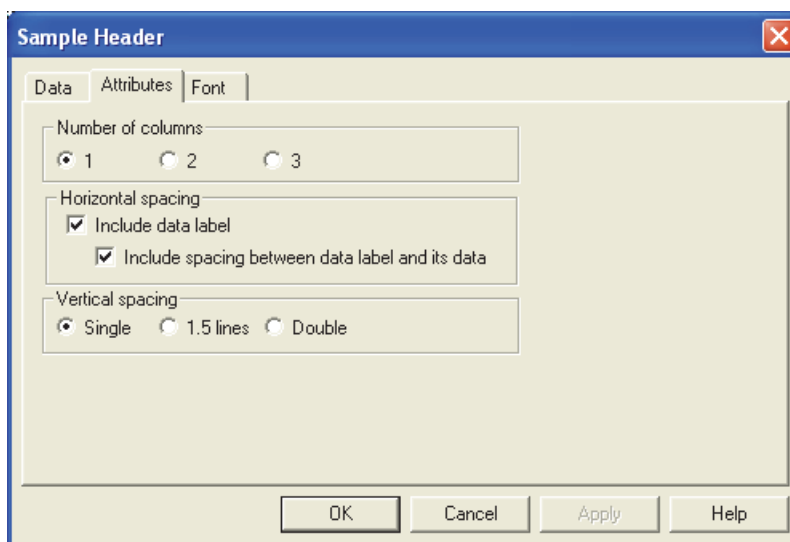


5. Click **OK** to save your changes.

Configuring Text Attributes

To configure text attributes, use the Attributes page of the *Text Object* dialog box (Figure 30). For information about the parameters on the Attributes page, see [Attributes Page](#).

Figure 30. Attributes page in the Sample Header (text object) dialog box



❖ **To configure attributes**

1. On the template pane, right-click a text object and choose **Properties** from the shortcut menu.

The *Text Object* dialog box opens.

2. Click the **Attributes** tab.
3. To format the text in columns, select the number of columns in the Number of Columns area.
4. To include data labels in the object in the Horizontal Spacing area, select the **Include Data Label** check box.
5. To add extra space between data labels and data, select the **Include Spacing Between a Label and Its Data** check box.
6. Select a line spacing option in the Vertical Spacing area.
7. Click **OK** to save your changes.

Setting Text Fonts

Use the Fonts page of the *Text Object* dialog box to set the text fonts. You can select a font type for the title, heading, data label, and data. For more information about the parameters on the Fonts page for a text object, see [Font Page](#).

❖ **To open the Fonts page**

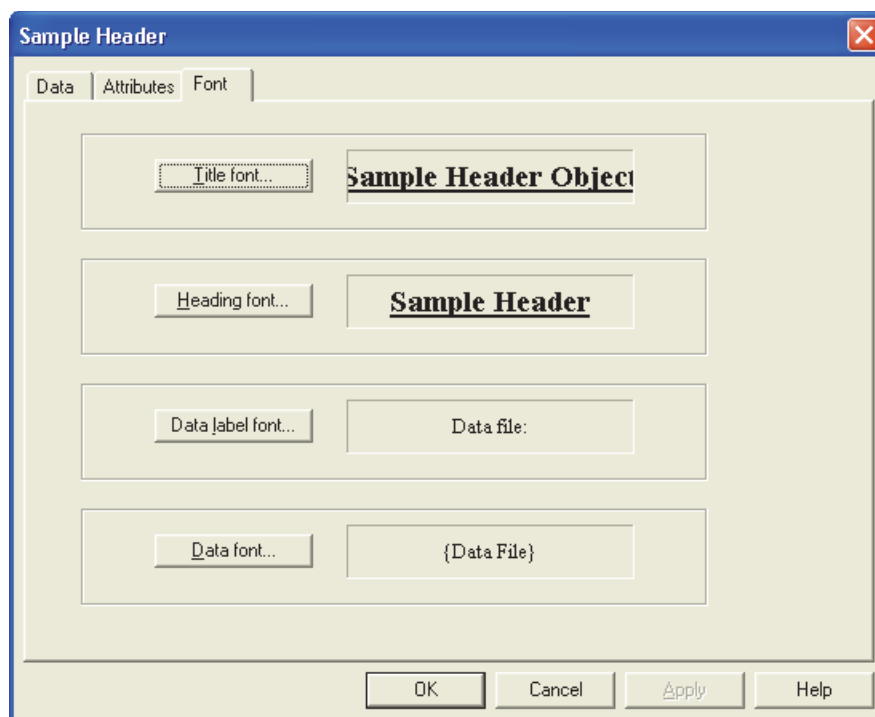
1. On the template pane, right-click a text object and choose **Properties** from the shortcut menu.

The *Text Object* dialog box opens.

2. Click the **Font** tab.

The Font page opens ([Figure 31](#)).

Figure 31. Font page for a text object

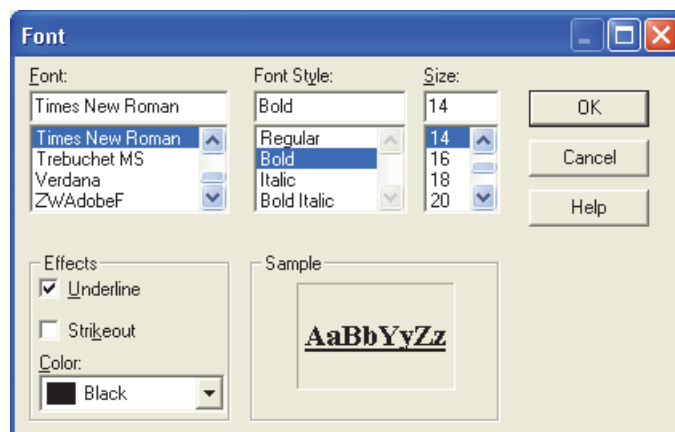


❖ **To set the font for a specific text item**

1. Click a text type button.

The Font dialog box opens (Figure 32).

Figure 32. Font dialog box



2. Make the font selections and click **OK**.

Note The Heading Font selection is also used for User Text. See [Adding Custom Text Fields](#).

Configuring an Annotation Object

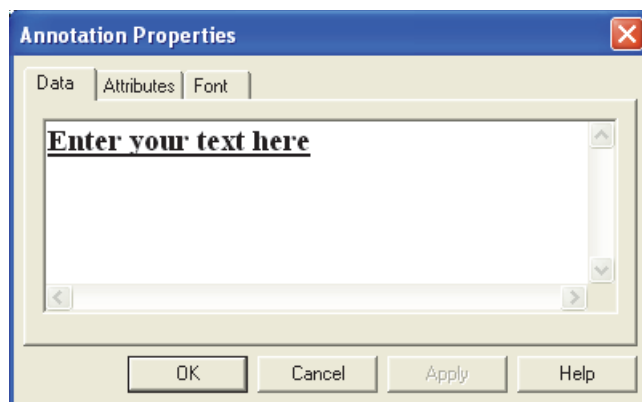
You can include an annotation object in any section type.

❖ To configure the Annotation object

1. On the template pane, right-click the annotation object in the template and choose **Properties** from the shortcut menu.

The Annotation Properties dialog box opens (Figure 33).

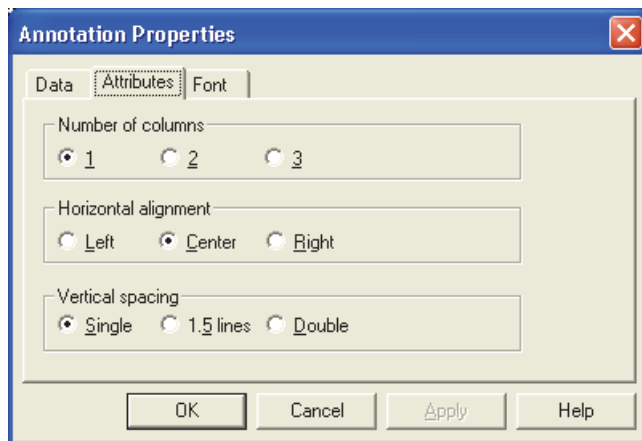
Figure 33. Data page in the Annotation Properties dialog box



2. On the Data page, click the box on the Annotation Properties dialog box to get a cursor. Delete the words *Enter your text here* and type annotation text.
3. On the Attributes page, select the number of columns to display annotation text in the Number of Columns area (Figure 34).

For information about the parameters on the Annotation Properties – Attributes page, see [Attributes Page](#).

Figure 34. Attributes page in the Annotation Properties dialog box



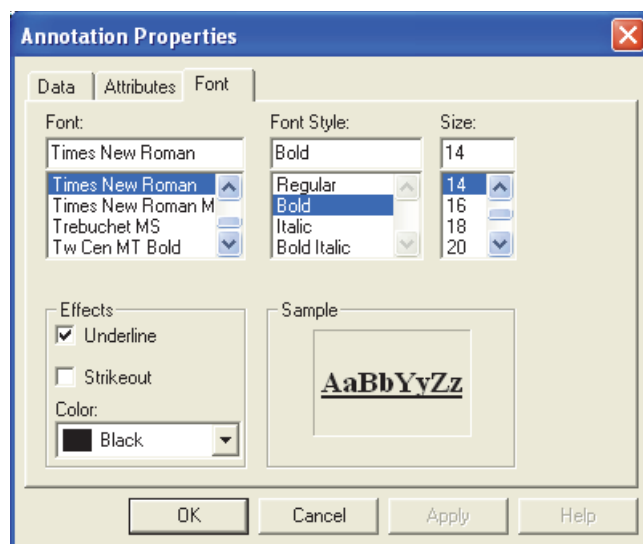
4. In the Horizontal Alignment area, select an alignment option for the annotation text: **Left**, **Center**, or **Right**.

4 Configuring Objects and Sections

Configuring an Annotation Object

5. In the Vertical Spacing area, select a spacing option for the annotation text line: **Single**, **1.5 lines**, or **Double**.
6. On the Font page, configure the font by setting the font parameters (Figure 35).

Figure 35. Font page in the Annotation Properties dialog box



7. Click **OK** to save your changes.

Configuring a Table Object

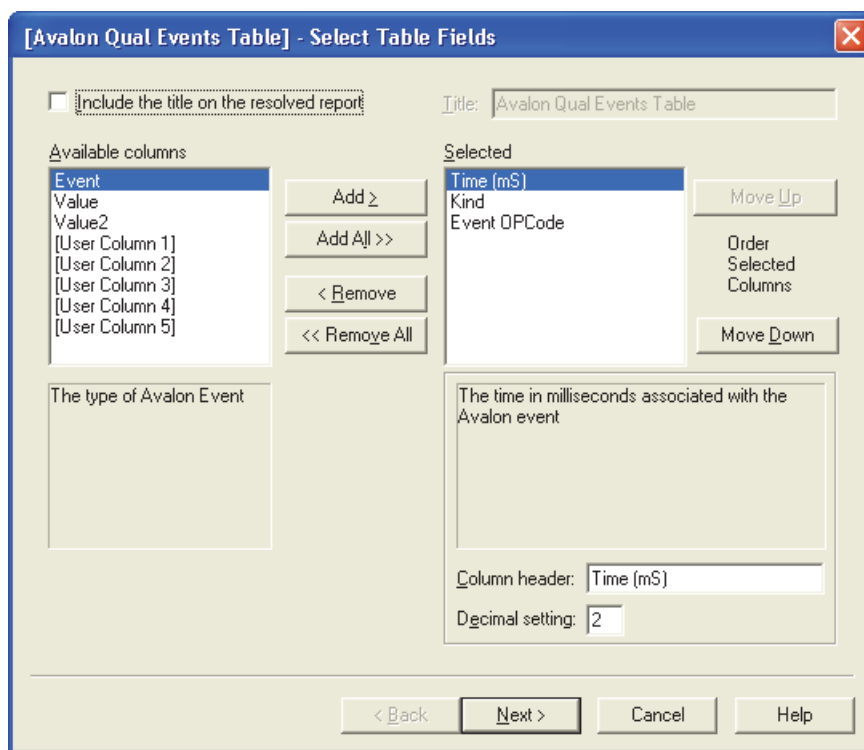
Use the *Table Object* wizard to configure a table object.

❖ To configure a table object

On the template pane, right-click a table object and choose **Properties** from the shortcut menu.

The *Table Object* wizard opens (Figure 36), named for the type of table you selected. For a description of each table, including the sections where a table can appear, see [Appendix B](#), “Types of Report Objects.”

Figure 36. Select Table Fields page of the Avalon Qual Events Table object wizard



Using the *Table Object* wizard, configure a table object included in the report template by changing its properties. Use the wizard for the following:

- [Choosing Table Columns](#)
- [Configuring Custom \(User\) Columns](#)
- [Specifying Table Sort Order](#)
- [Setting Table Fonts](#)
- [Setting Additional Table Properties](#)

Choosing Table Columns

To select the columns to include in the table, use the Select Table Fields page of the *Table Object* wizard. The columns available for a table appear in alphabetical order, but can be added to a report template in any order. Your column options to select depend on the type of table object you are configuring.

For more information about the parameters on this page, see [Select Table Fields Page](#).

❖ To select and arrange table columns

1. On the template pane, right-click a table object and choose **Properties** from the shortcut menu.

The *Table Object* – Select Table Fields page opens.

2. To include a custom title for the table, type the title in the Title box and select the **Include the Title on the Resolved Report** check box.
3. To select the columns to include in the table from the Available Columns list, do one of the following:
 - Select an item and click **Add**.
 - Double-click an item.
 - To move all available fields, click **Add All**.

The fields you have chosen appear in the selected list.

Note All table objects have user columns available for selection. Use the user columns to define formulas for calculating table data and to display the results in the table. For more information on user columns, see [Configuring Custom \(User\) Columns](#).

4. Type the column heading text in the Column Header box.
5. To arrange the order of the selected columns in the Selected Columns list, click **Move Up** or **Move Down**.
6. Click **Next** to go to the next page of the wizard.

Configuring Custom (User) Columns

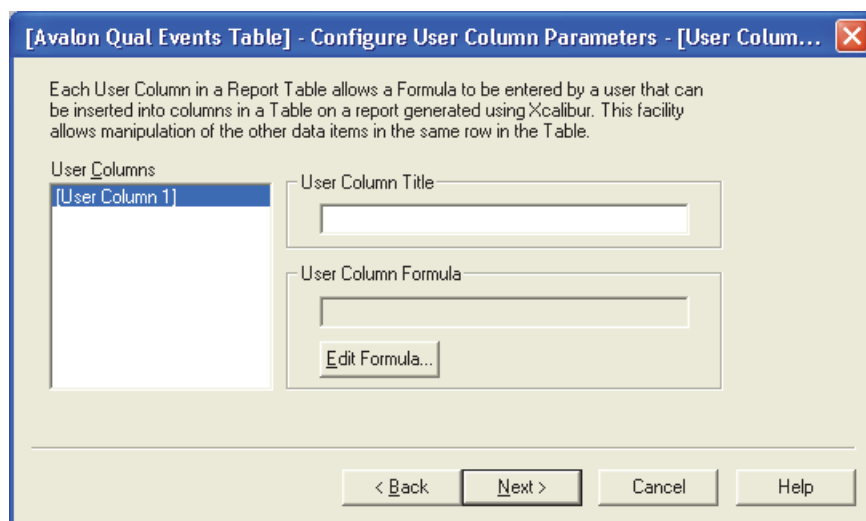
The Configure User Column Parameters page of the *Table Object* wizard appears only if you chose to include custom User Columns in the table (on the Select Table Fields page). Use this page to define parameters for each User Column in the table.

For more information about the parameters on this page, see [Configure User Column Parameters Page](#).

You can use the User Columns to define mathematical formulas for calculating table data. Formulas obey the following syntax rules:

- The formula must begin with an equals sign (=).
- Each table column is represented by an alphabetic letter identifier (A, B, C, and so on) that appears beneath the column title in the Table object.
- The mathematical expressions are kept simple, for instance, type A+B, A-B, A*B, or A/B. This is true as well for any of the functions listed in the Functions list of the Edit Formula dialog box. Formulas are computed on a row-by-row basis. That is, if you type =A+B as a formula in a User Column, the results are computed as follows:
 - a. The Xcalibur data system adds the value in the first row of column A to the value in the first row of column B and displays the result in the first row of the User Column.
 - b. The data system adds the value in the second row of column A to the value in the second row of column B and displays the result in the second row of the User Column.
 - c. The data system continues this process until all rows of the table have been completed.

Figure 37. Configure User Column Parameters page



The data system displays the User Columns you have selected for the table in the User Columns list.

❖ **To define each user column**

1. On the template pane, right-click a table object and choose **Properties** from the shortcut menu.

The *Table Object – Select Table Fields* page opens.

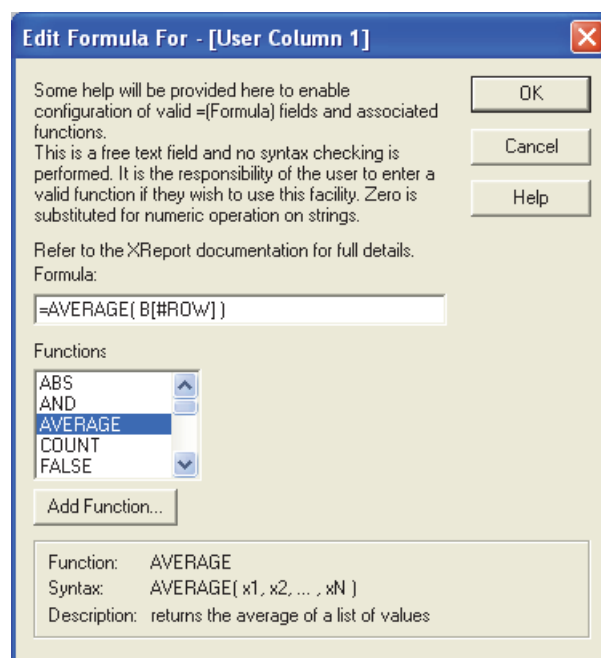
2. Add a User Column to the table and then click **Next**.

The Configure User Column Parameters page appears.

3. Select a user column in the User Columns list.
4. Type a title for the user column in the User Column Title box.
5. Click **Edit Formula** in the User Column Formula area.

The Edit Formula dialog box opens ([Figure 38](#)). For more information about the creating formulas, see [Edit Formula For Dialog Box](#) and [Adding a Formula to a Table](#).

Figure 38. Edit Formula For dialog box



6. For the selected column, edit a formula for the user column and configure valid fields and associated functions. Below the functions list is a brief description of each function at the bottom of the dialog box.
7. To enter a formula in the Formula box, select a function from the Functions list and click **Add Function** or type directly in the box.

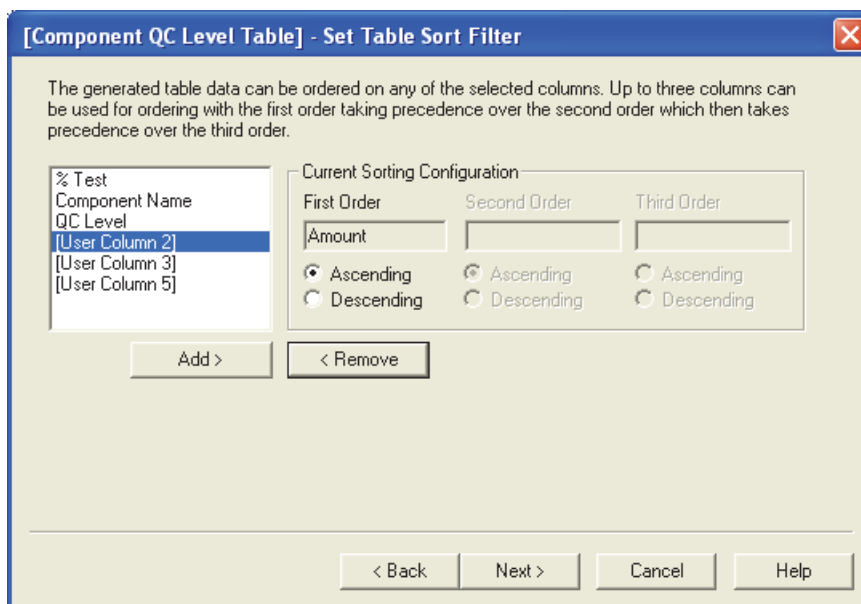
When you click **Add Function**, a configuration dialog box opens for that function. For example, for the Average function, choose the column to average.

8. To return to the Configure User Column Parameters page, click **OK**.
9. Click **Next** to go to the next page of the wizard.

Specifying Table Sort Order

Use the Set Table Sort Filter page of the *Table Object* wizard to define a method for sorting table data when you generate a report (Figure 39).

Figure 39. Set Table Sort Filter page



XReport displays the columns selected for the table in a list on the left side of the dialog box. Set the order for the table using any of the selected columns. Use up to three columns for ordering the table: The first order takes precedence over the second order, which takes precedence over the third order.

❖ To define a method for ordering data in the table

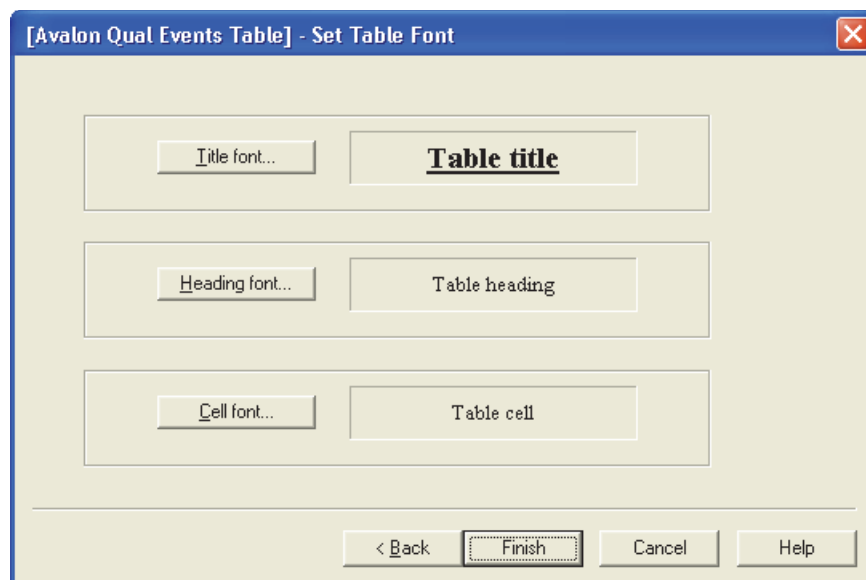
1. On the template pane, right-click a table object and choose **Properties** from the shortcut menu.
The *Table Object* dialog box opens.
2. Click **Next** until the Set Table Sort Filter page opens.
3. To select a variable to provide the first level of sorting for the table, double-click the item in the column list to move it to the First Order box.

4. To define how to sort the First Order column data in the Current Sorting Configuration area, select one of the following options:
 - Ascending: Sort data in ascending order.
 - Descending: Sort data in descending order.
5. To define the second and the third variable used to order table columns, repeat the first two steps.
6. To move to the Font page, click **Next**.

Setting Table Fonts

Use the final page of the *Table Object* wizard, the Set Table Font page, to set the font type for elements in the table (Figure 40).

Figure 40. Set Table Font page



❖ To define the font for a specific element

1. On the template pane, right-click a table object and choose **Properties** from the shortcut menu.

The *Table Object* dialog box opens.

2. Click **Next** until the Set Table Fonts page opens.
3. Click the appropriate button.

The Font dialog box opens.

4. Select font options and click **OK**.

Repeat [step 3](#) and [step 4](#) as needed for other table elements.

Setting Additional Table Properties

After completing the *Table Object* wizard, additional Properties dialog boxes appear for the following table objects:

- [Library Search Graphics Table Properties](#)
- [Library Search Results Table Properties](#)
- [Sample Table Properties](#)
- [Spectrum List Table Properties](#)
- [Electronic Signature Table Properties](#)

Library Search Graphics Table Properties

Use the Library Search Graphics Table Properties dialog box to set the number of hits to be displayed. For more information about the parameters in this dialog box, see [Library Search Graphics Table Properties Dialog Box](#).

❖ To open the Library Search Graphics Table Properties dialog box

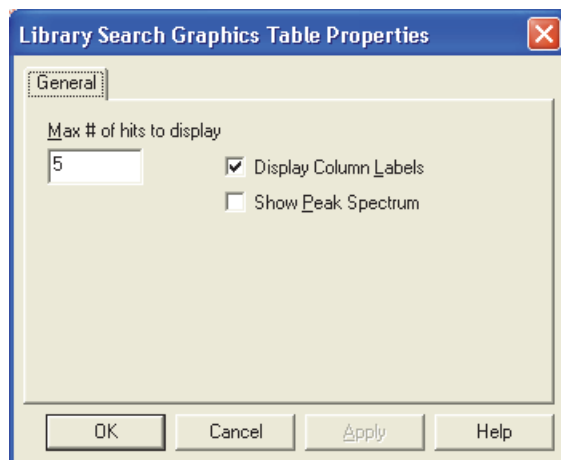
1. On the template pane, right-click the Library Search Graphic Table object and choose **Properties** from the shortcut menu.

The Library Search Graphics Table – Select Table Fields page opens.

2. Make changes as necessary.
3. Click **Finish**.

The Library Search Graphics Table Properties dialog box opens ([Figure 41](#)).

Figure 41. Library Search Graphics Table Properties dialog box



❖ To set the parameters in the Library Search Graphics Table Properties dialog box

1. Type the total number of search results to display in the table in the Max # of hits to display box.
2. To display column labels, select the **Display Column Labels** check box.
3. To show the peak spectrum, select the **Show Peak Spectrum** check box.
4. Click **OK**.
5. Choose **File > Save** to save any changes made.

Library Search Results Table Properties

Use the Library Search Results Table Properties dialog box to specify the maximum number of hits to be displayed. For more information about the parameters in this dialog box, see [Library Search Results Table Properties Dialog Box](#).

❖ To open the Library Search Results Table Properties dialog box

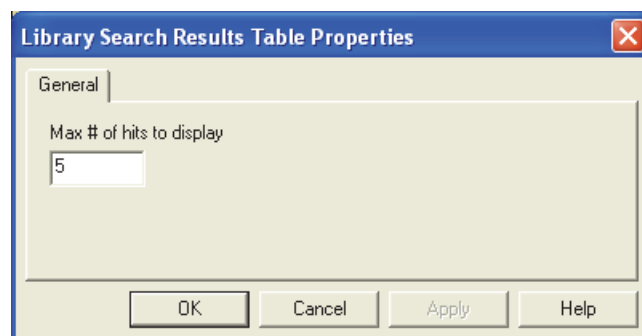
1. On the template pane, right-click the Library Search Results Table object and choose **Properties** from the shortcut menu.

The Library Search Results Table wizard opens to the Select Table Fields page.

2. Make the necessary changes.
3. Click **Finish**.

The Library Search Results Table Properties dialog box opens ([Figure 42](#)).

Figure 42. Library Search Results Table Properties dialog box



❖ To set the parameters in the Library Search Results Table Properties dialog box

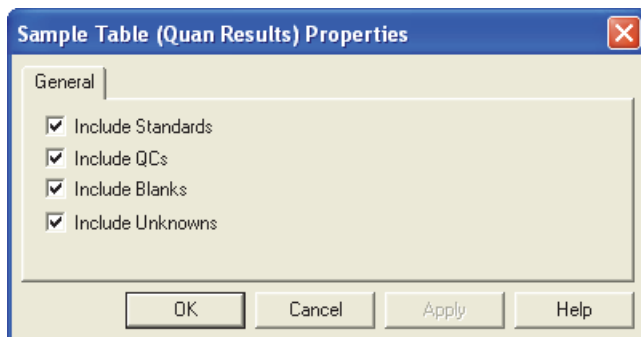
1. Type the total number of search results to display in the table in the Max # of hits to display box.
2. Click **OK**.

Sample Table Properties

When you click Finish on the last page of the Sample Table object wizard (in a Quan Repeating section), the Sample Table (Quan Results) Properties dialog box opens (Figure 43).

For more information about the parameters in the Sample Table Properties dialog box, see [Sample Table Properties Dialog Box](#).

Figure 43. Sample Table Properties dialog box



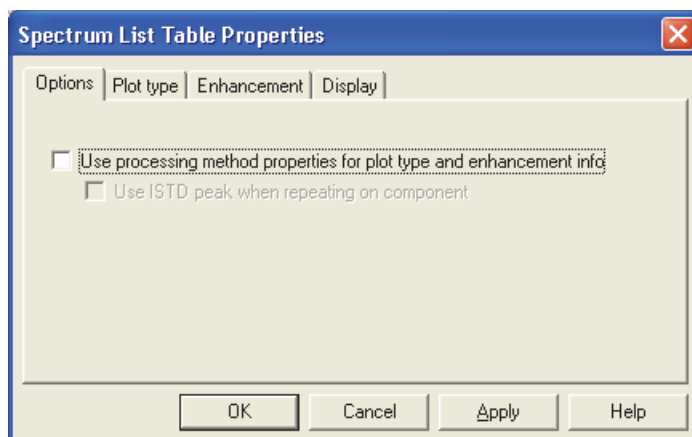
❖ To set parameters in the Sample Table Properties dialog box

1. In the template pane, open the Sample Table (Quan Results) Properties dialog box as follows:
 - a. In a Quan Repeating section, right-click a **Sample Table** object and choose **Properties**.
The Sample Table wizard opens.
 - b. Complete the wizard and click **Finish**.
2. To include standards, QCs, blanks, or unknowns in the Sample table, select the corresponding check boxes.
3. Click **OK**.

Spectrum List Table Properties

When you click Finish on the last page of the Spectrum List Table object wizard (in a Quan or Qual Repeating section), the Spectrum List Table Properties dialog box opens ([Figure 44](#)).

Figure 44. Options page in the Spectrum List Table Properties dialog box



This dialog box has four pages:

- [Options Page](#)
- [Plot Type Page](#)
- [Enhancement Page](#)
- [Display Page](#)

Options Page

For information about the parameters on the Spectrum List Table Properties – Options page, see [Options Page for a Spectrum Object](#).

❖ To set the parameters on the Options page

1. Open the Options page of the Spectrum List Table Properties dialog box as follows:
 - a. Right-click a Spectrum List Table object and choose **Properties**.
 - b. Complete the wizard and click **Finish**.
 - c. Click the **Options** tab.
2. Select or clear the **Use Processing Method Properties for Plot Type and Enhancement Info** check box ([Figure 44](#)).

When you select this check box, the application hides the parameters on the Plot Type and Enhancement pages.

3. To use the ISTD peak when repeating on a component, select the corresponding check box. You must select the Use Processing Method Properties for Plot Type check box to activate the ISTD peak option. (This option only applies when this object is used in a Quan repeating section. It is not available when the Spectrum List Table is used in a Qual Repeating Section.)
4. Click **OK**.

Plot Type Page

For information about the parameters on the Spectrum List Table Properties – Plot Type page, see [Plot Type Page for a Spectrum Object](#).

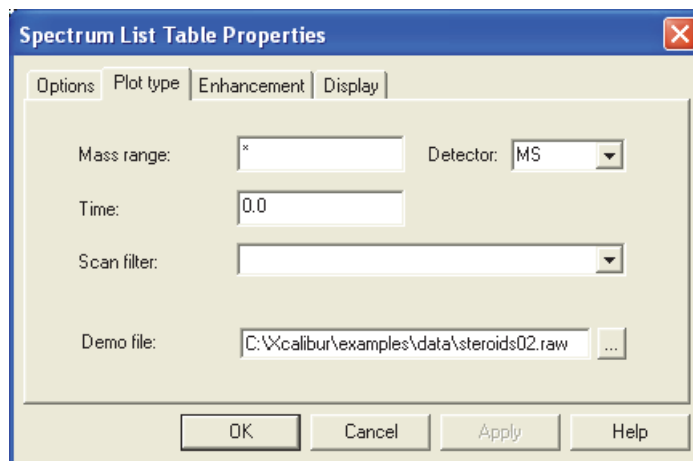
❖ To set parameters on the Plot Type page

1. Open the Plot Type page of the Spectrum List Table Properties dialog box as follows:
 - a. On the template pane, right-click a Spectrum List Table object and choose **Properties**.
 - b. Complete the wizard and click **Finish**.

The Spectrum List Table Properties dialog box opens to the Options page.

- c. Clear the **Use Processing Method Properties for Plot Type and Enhancement Info** check box.
 - d. Click the **Plot Type** tab.
2. Type the mass range to display in the Mass range box. Separate the values by a dash: *lowmass–highmass*. Type * to display the entire range ([Figure 45](#)).

Figure 45. Plot Type page in the Spectrum List Table Properties dialog box



3. Select the type of detector that you are using from the Detector list: **MS** or **PDA**.
4. Type the time range to display in minutes in the Time box. Type the values separated by a dash: *firsttime–secondtime*. Type * to display the entire range.

5. Enter the scan filter to use with the data in the Scan Filter list.
6. Type or search in the Demo File box for the name of the file you to use as a demonstration file for the settings in the template.
7. Click **OK**.

Enhancement Page

For information about the parameters on the Spectrum List Table Properties – Enhancement page, see [Enhancement Page for a Spectrum List Table](#).

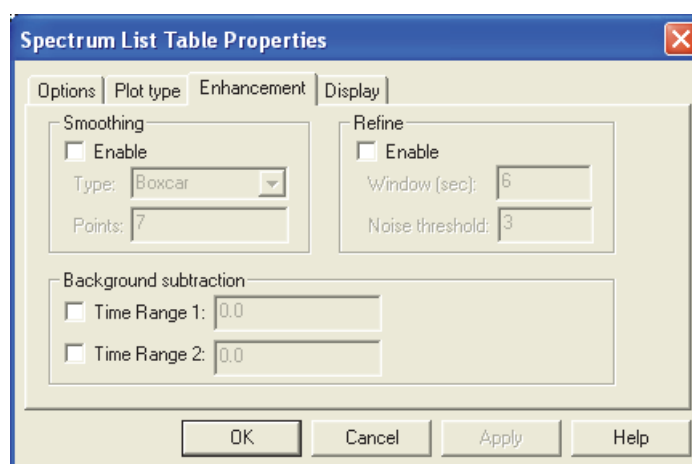
❖ To set parameters on the Enhancement page

1. Open the Plot Type page of the Spectrum List Table Properties dialog box as follows:
 - a. On the template pane, right-click a Spectrum List Table object and choose **Properties**.
 - b. Complete the wizard and click **Finish**.

The Spectrum List Table Properties dialog box opens to the Options page.

 - c. Clear the **Use Processing Method Properties for Plot Type and Enhancement Info** check box.
 - d. Click the **Enhancement** tab.
2. To add smoothing to the data, select the **Enable** check box in the Smoothing area ([Figure 46](#)).

Figure 46. Enhancement page in the Spectrum List Table Properties dialog box



3. To select a type of smoothing, select **Boxcar** or **Gaussian** from the Type list.
4. Select the number of smoothing points (odd numbers from 3 to 15) to be used in the Points list.
5. To refine the data, select the **Enable** check box in the Refine area.

6. To define an area for drawing a peak, type the number of seconds on either side of the specified point. A reasonable initial value for the window is the peak width in seconds.
7. Type the cutoff point for peaks in the Noise Threshold box. To show all peaks in the spectrum, type **0**. Return to this box to eliminate more noise. Slowly increase the value until the noise peaks are eliminated. Use this setting to eliminate peaks generated from baseline noise.
8. To turn on a first baseline region that is used for assessing background subtraction, select one or both of the **Time Range** check boxes. Type the time range to use in the box.

The Background Subtraction area shows details of background subtraction if applied to the spectrum. The background contribution is determined by averaging the scans from one or two baseline regions.

9. Click **OK**.

Display Page

For information about the parameters on the Spectrum List Table Properties – Display page, see [Display Page for a Spectrum List Table](#).

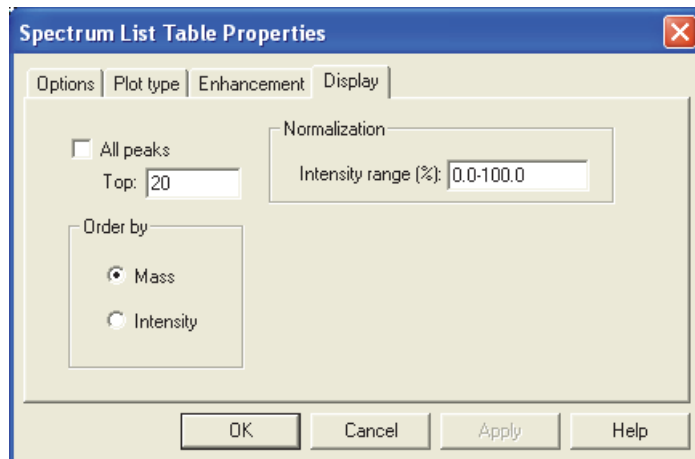
❖ To set parameters on the Display page

1. Open the Plot Type page of the Spectrum List Table Properties dialog box as follows:
 - a. On the template pane, right-click a Spectrum List Table object and choose **Properties**.
 - b. Complete the wizard and click **Finish**.

The Spectrum List Table Properties dialog box opens to the Options page.

 - c. Click the **Display** tab.
2. To display all peaks in the spectrum, select the **All Peaks** check box or, to limit the display to the strongest peaks, type a value in the Top box ([Figure 47](#)).

Figure 47. Display page in the Spectrum List Table Properties dialog box



3. To order the data by mass or by intensity, select the appropriate option in the Order By area.
4. Type a value representing the relative abundance range of mass peaks to include in the table in the Normalization area.
5. Click **OK**.

Electronic Signature Table Properties

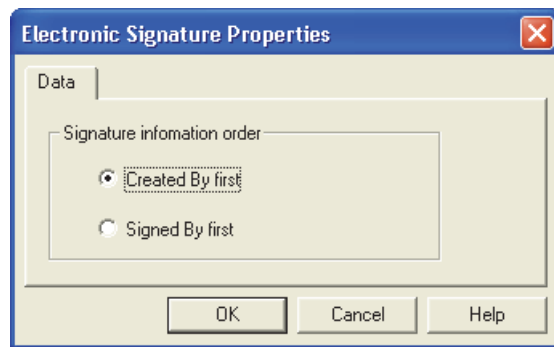
Use the Electronic Signature table object to specify whether the Created By signature block appears before or after the Signed By signature block. For more information about the parameters in the Electronic Signature Properties dialog box, see [Electronic Signature Properties Dialog Box](#).

❖ To configure the Electronic Signature table object

1. On the template pane, right-click the **Electronic Signature** table object and choose Properties from the shortcut menu.

The Electronic Signature Properties dialog box opens ([Figure 48](#)).

Figure 48. Electronic Signature Properties dialog box



2. To display the Created By signature block before the Signed By signature block, select the **Created By First** option in the Signature Information Order area or, to display the Signed By block before the Created By block, select the **Signed By First** option.
3. Click **OK**.

Configuring a Bitmap Object

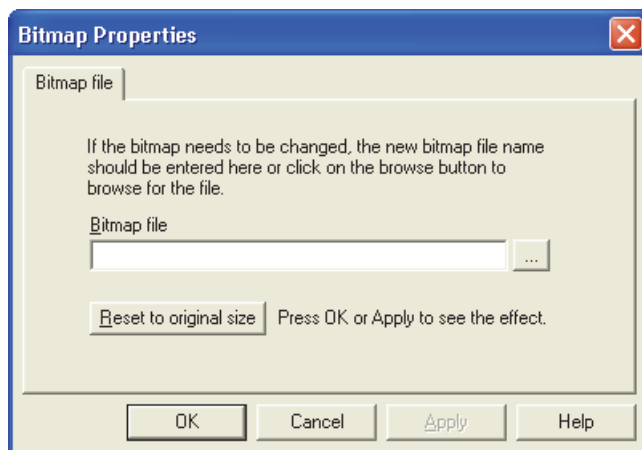
For information about the parameters on the Bitmap file page of the Bitmap Properties dialog box, see [Bitmap Properties Dialog Box](#).

❖ To configure the bitmap object

1. On the template pane, right-click the bitmap object and choose **Properties** from the shortcut menu.

The Bitmap Properties dialog box opens ([Figure 49](#)).

Figure 49. Bitmap Properties dialog box



2. Enter the name of the image file. Choose one of the following image file formats: BMP, DIB, GIF, JPG, or ICO.
3. To set the size of the bitmap image to the size of the original file, click **Reset to Original Size**.
4. Click **OK**.

Configuring a Chromatogram Object

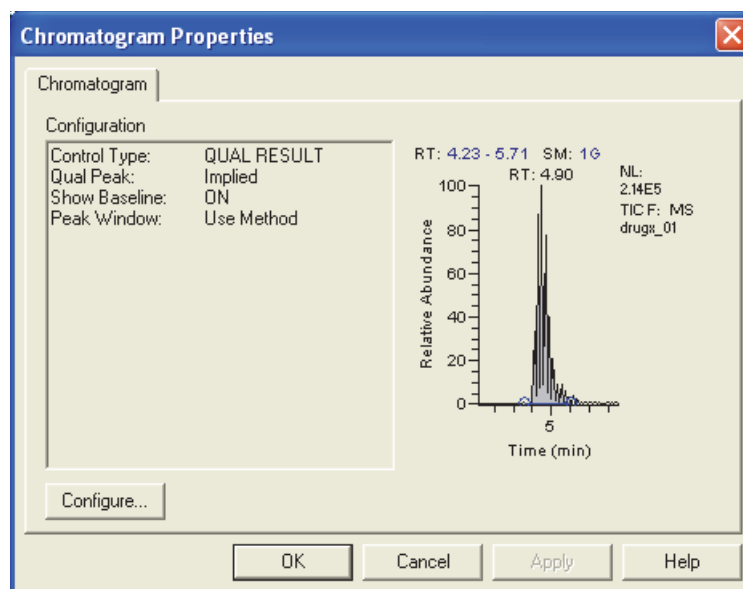
For information about the parameters in the Chromatogram Properties dialog box, see [Chromatogram Properties Dialog Box and Wizard](#).

❖ To configure a chromatogram report object

1. On the template pane, right-click the object and choose **Properties** from the shortcut menu.

The Chromatogram Properties dialog box opens ([Figure 50](#)).

Figure 50. Chromatogram Properties dialog box



2. Click **Configure**.

The Chromatogram wizard opens.

The Chromatogram wizard guides you through the process of changing the properties of a chromatogram report object contained in the report template.

The XReport Chromatogram wizard displays different pages and contains different options depending on the type of section containing the chromatogram and the selections for the Chromatogram Type and Peak Type properties.

Table 1 lists the wizard pages and their order. Each wizard page is described in a topic below. See the appropriate topic to learn how to complete each wizard page.

Table 1. Possible Chromatogram wizard pages, given the section type, in order of appearance

Page in the XReport Chromatogram wizard	Nonrepeating section (Chromatogram Type)			Repeating section	
	Raw	Quan	Qual	Quan	Qual
Use Container Supplied Quan Peak Page				X	
Use Container Supplied Qual Peak Page					X
Select Chromatogram Type Page	X	X	X	X ^a	X ^b
Select Demo File Page	X	X	X	X	X
Select the Quan Peak Page		X		X ^a	X ^b
Select Component				X ^c	
Select the Qual Peak Page			X	X ^a	X ^b
Select Mass Spectrum Quan Traces to Display Page		X		X ^a	X ^b
Configure How the Peak Window Will Look Page		X	X	X	X
Select Plot Details Page	X			X ^d	X ^e
Select Enhance Details Page	X			X ^d	X ^e
Select Chromatogram Style Page	X	X	X	X	X
Select the Peak Labeling Page	X	X	X	X	X
Select How the Chromatogram Axes Will Be Configured Page	X	X	X	X	X
Configure Normalization for the Chromatogram Page	X	X	X	X	X

^a This page is only displayed when you select the Explicitly Specify the Chromatogram's Behavior check box on the Use Container Supplied Quan peak page.

^b This page is only displayed when you select the Explicitly Specify the Chromatogram's Behavior check box on the Use Container Supplied Qual peak page.

^c This page is only displayed when you select the Explicitly Specify the Chromatogram's Behavior check box on the Use Container Supplied Quan peak page and the Quan Results Based Chromatogram option on the Select Chromatogram Type page.

^d This page is only displayed when you select the Explicitly Specify the Chromatogram's Behavior check box on the Use Container Supplied Quan peak page and the Raw File Based Chromatogram option on the Select Chromatogram Type page.

^e This page is only displayed when you select the Explicitly Specify the Chromatogram's Behavior check box on the Use Container Supplied Qual peak page and the Raw File Based Chromatogram option on the Select Chromatogram Type page.

Note When you select the All Qual Peaks option for a Qual Result Based Chromatogram, the wizard page order is the same as for the Qual Result Based Chromatogram Type without the Select Qual Peak page.

When the chromatogram report object to be configured is contained in a Quan or Qual repeating section, the default Chromatogram Type is Quan or Qual Result Based with no explicit Peak Type set. The next page of the wizard (Use Container Supplied Quan (or Qual) asks you to confirm this.

Use Container Supplied Quan Peak Page

Use the Use Container Supplied Quan Peak page of the Chromatogram wizard to display the details of the internal standard associated with the implicit Quan peak or ignore the implicit Quan peak and explicitly configure the chromatogram type.

For more information about the parameters on this page, see [Use Container Supplied Quan Peak](#). For more information about the Chromatogram wizard, see [Configuring a Chromatogram Object](#).

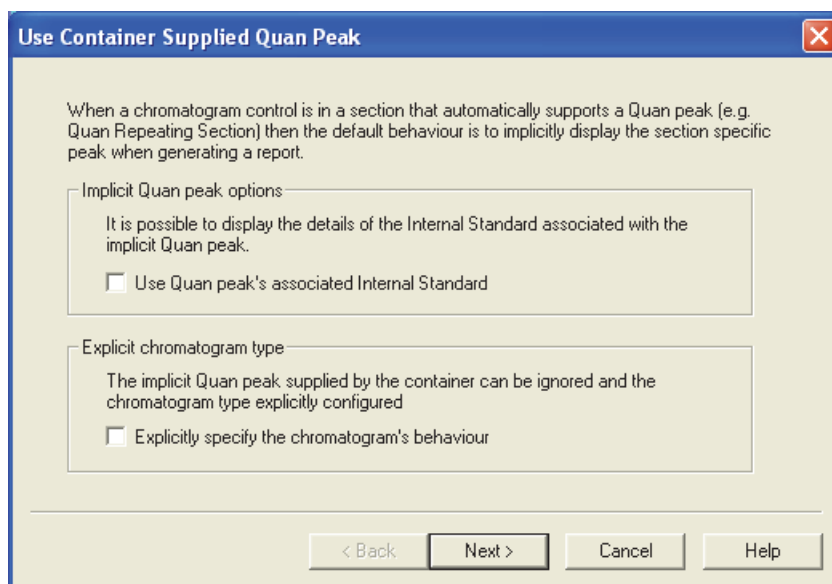
❖ To explicitly configure a chromatogram type in a Quan repeating section

1. In a Quan repeating section, do the following:
 - a. Right-click a **Chromatogram** object and choose **Properties**.
 - b. Click **Configure**.

The Use Container Supplied Quan Peak page of the Chromatogram wizard opens. By default, the Use Quan Peak's Associated Internal Standard and Explicitly Specify check boxes are clear.

2. To display the details of the internal standard associated with the implicit Quan peak, select the **Use Quan Peak's Associated Internal Standard** check box in the Implicit Quan Peak Options area ([Figure 51](#)).

Figure 51. Use Container Supplied Quan Peak page



3. To ignore the implicit Quan peak supplied by the container and explicitly configure the chromatogram type, select the **Explicitly Specify the Chromatogram's Behaviour** check box in the Explicit Chromatogram Type area.
4. Click **Next** to go to the next page of the wizard.

Use Container Supplied Qual Peak Page

Use the Use Container Supplied Qual Peak page of the Chromatogram wizard to ignore the implicit Qual peak and explicitly configure the chromatogram type.

For information about the parameters on the Use Container Supplied Qual Peak page, see [Use Container Supplied Qual Peak](#). For more information about the Chromatogram wizard, see [Configuring a Chromatogram Object](#).

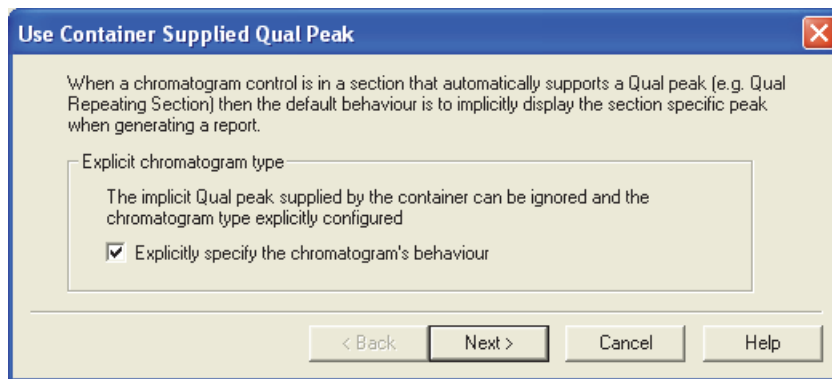
❖ To explicitly configure a chromatogram type in a Qual repeating section

1. In a Qual repeating section, do the following:
 - a. Right-click a **Chromatogram** object and choose **Properties**.
 - b. Click **Configure**.

The Use Container Supplied Qual Peak page of the Chromatogram wizard opens. By default, the Explicitly Specify the Chromatogram's Behaviour check box is clear.

2. To ignore the implicit Qual peak supplied by the container and explicitly configure the chromatogram type, select the **Explicitly Specify the Chromatogram's Behaviour** check box in the Explicit Chromatogram Type area ([Figure 52](#)).

Figure 52. Use Container Supplied Qual Peak page



3. Click **Next** to go to the next page of the wizard.

One of these pages opens:

- The Select Chromatogram Type page opens if you selected the Explicitly Specify the Chromatogram's Behaviour check box.
- The Select Demo File page opens if you left the Explicitly Specify the Chromatogram's Behaviour check box clear.

Select Chromatogram Type Page

Use the Select Chromatogram Type page of the Chromatogram wizard to set the chromatogram type for the chromatogram report object being configured in the report template.

For information about the parameters on the Select Chromatogram Type page, see [Select Chromatogram Type](#). For more information about the Chromatogram wizard, see [Configuring a Chromatogram Object](#).

❖ To open the Select Chromatogram Type page

1. Right-click a **Chromatogram** object and choose **Properties**.
2. Click **Configure**.

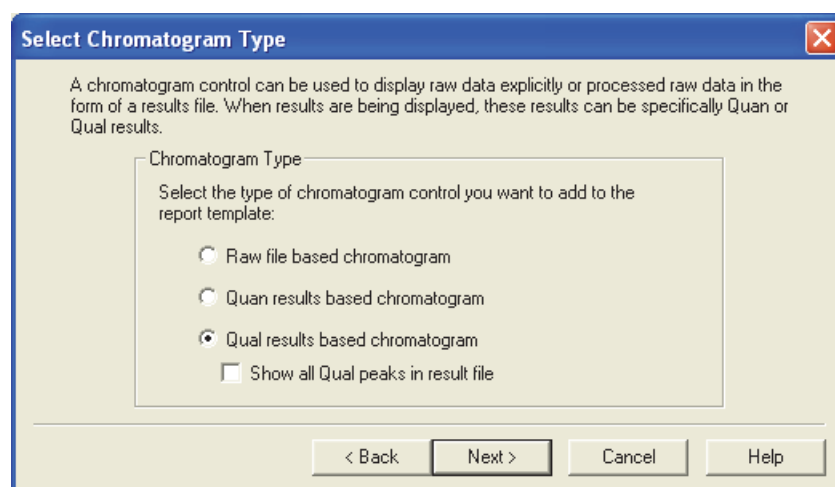
In a non-repeating section, the Select Chromatogram Type page opens. In a Qual or Quan repeating section, the Use Container Supplied Qual or Quan Peak page of the Chromatogram wizard opens.

3. In the Use Container Supplied Qual or Quan Peak page, select the **Explicitly Specify the Chromatogram's Behaviour** check box. Then click **Next**.

The Select Chromatogram Type page opens.

4. Define the chromatogram type in the Chromatogram Type area ([Figure 53](#)) by selecting one of the following options:
 - Raw file based chromatogram
 - Quan results based chromatogram
 - Qual results based chromatogram

Figure 53. Select Chromatogram Type page



When you select the Qual Results Based Chromatogram option, the Show All Qual Peaks in Result File check box becomes available.

5. If you select a Qual results based chromatogram in [step 4](#), select the **Show All Qual Peaks in Result File** check box to display all Qual peaks in a resolved Xcalibur report. This is a Peak Type setting.
6. Click **Next** to go to the next page of the wizard, the Select Demo File Page.

Select Demo File Page

Use the Select Demo File page of the Chromatogram wizard to associate a demonstration file (RAW or RST file) with a chromatogram report object. A demo file shows how the chromatogram report object appears in the report template and in wizard page previews with its current settings when applied to real Xcalibur data.

For information about the parameters on the Select Demo File page of the Chromatogram wizard, see [Select Demo File](#).

❖ To open the Select Demo File page of the Chromatogram wizard

1. In a Qual, Quan, or non-repeating section, right-click a **Chromatogram** object and choose **Properties**.
2. Click **Configure**.
 - In a non-repeating section, the Select Chromatogram Type page opens. Go to [step 4](#).
 - In a Qual or Quan section, the Use Container Supplied Qual or Quan Peak page of the Chromatogram wizard opens.
3. On the Use Container Supplied Qual or Quan page, do one of the following:
 - a. Select the **Explicitly Specify the Chromatogram's Behaviour** check box. Click **Next**.

The Select Chromatogram Type page opens.
 - b. Go to [step 4](#).

—or—

 - Leave the **Explicitly Specify the Chromatogram's Behaviour** check box clear. Click **Next**.

The Select Demo File page opens.
4. For an explicit chromatogram type, select one of the options in the Chromatogram Type area and click **Next**.

The Select Demo File page opens.

The appearance of the Select Demo File page depends on the chromatogram type and the peak type settings chosen in the Chromatogram Type page of the wizard.

- [Raw File Based Chromatogram](#)
- [Quan Result Based Chromatogram](#)
- [Qual Result Based Chromatogram – Explicit Peak](#)
- [Qual Result Based Chromatogram – All Available Peaks](#)

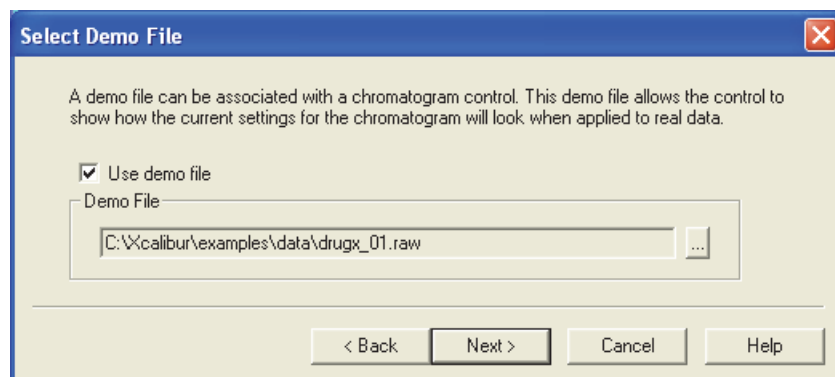
Raw File Based Chromatogram

When configuring a chromatogram report object based on a raw data file, use this procedure to select a file.

❖ To select a demo file for a raw file-based Chromatogram

1. To associate a demo file with the chromatogram report object, select the **Use Demo File** check box on the Select Demo File page ([Figure 54](#)).

Figure 54. Select a raw data file based chromatogram



2. To search for the required demo file (RAW file), click the browse button in the Demo File area.

The Select Raw Data File dialog box opens.

3. Select a demo file and click **Open**.
4. Click **Next** to go to the next page of the wizard.

Quan Result Based Chromatogram

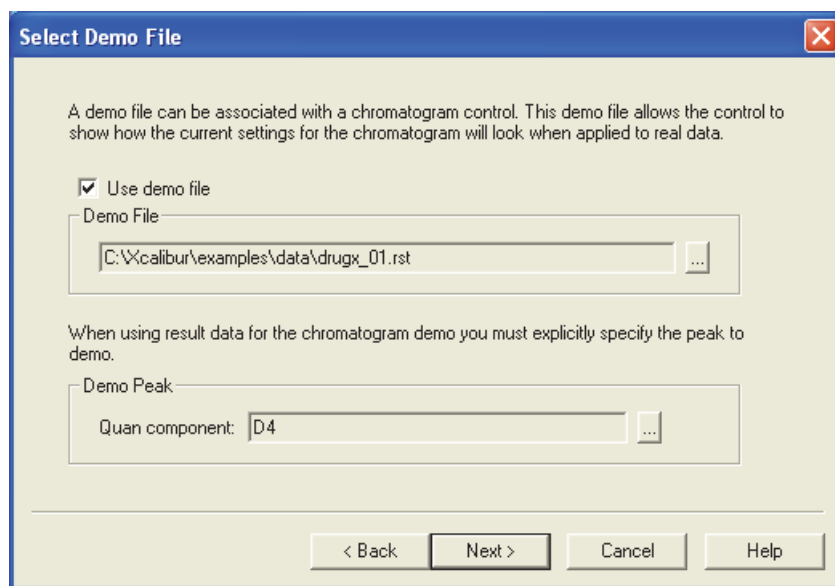
When configuring a chromatogram report object based on Quan results, use this procedure to select a file.

For information about the parameters on the Select Demo File page of the Chromatogram wizard, see [Select Demo File](#).

❖ To select a demo file for a Quan-based chromatogram

1. To associate a demo file with the chromatogram report object, select the **Use Demo File** check box on the Select Demo File page (Figure 55).

Figure 55. Selecting a Quan result based chromatogram



2. To search for the required demo file (RAW file), click the browse button in the Demo File area.

The Select Raw Data File dialog box opens.

3. Select a demo file and click **Open**.
4. To specify the peak to demo, click the browse button in the Demo Peak area.

The Select a Peak dialog box opens.

5. Select a peak from the list located in the result file.
6. Click **OK** to apply the selection and return to the wizard.
7. Click **Next** to go to the next page of the wizard.

Qual Result Based Chromatogram – Explicit Peak

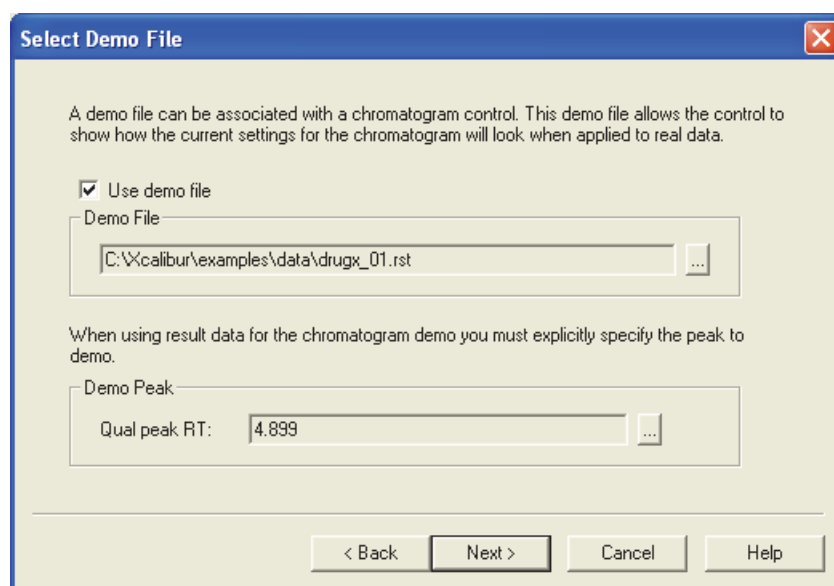
When configuring a chromatogram report object based on Qual Results with an explicit Peak Type required, use this procedure to select a file.

For information about the parameters on the Select Demo File page of the Chromatogram wizard, see [Select Demo File](#).

❖ To select a demo file for a Qual-based chromatogram

1. Select the **Use Demo File** check box on the Select Demo File page to associate a demo file with the chromatogram report object ([Figure 56](#)).

Figure 56. Selecting an explicit peak in a Qual result based chromatogram



2. To search for the required demo file (RAW file), click the browse button in the Demo File area.

The Select Raw Data File dialog box opens.

3. Select a demo file and click **Open**.
4. To specify the peak to demo, click the browse button in the Demo Peak area.

The Select a Peak dialog box opens.

5. Select a peak from the list located in the result file.
6. Click **OK** to apply the selection and return to the wizard.
7. Click **Next** to go to the next page of the wizard.

Qual Result Based Chromatogram – All Available Peaks

When configuring a chromatogram report object that is Qual result based with Show all Qual peaks set (peak type setting), use this procedure to select a file.

For information about the parameters on the Select Demo File page of the Chromatogram wizard, see [Select Demo File](#).

❖ To select a demo file for all available peaks

1. To associate a demo file with the chromatogram report object, select the **Use Demo File** check box on the Select Demo File page.
2. To search for the required demo file (RAW file), click the browse button in the Demo File area.

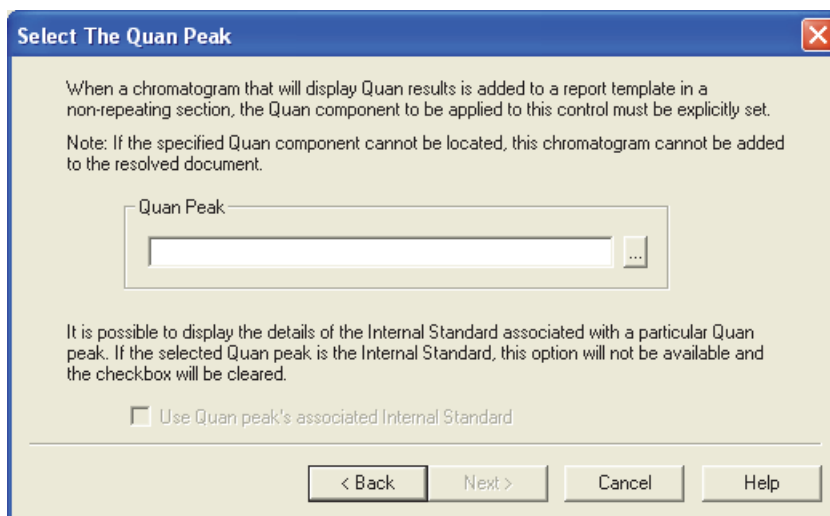
The Select Raw Data File dialog box opens.

3. Select a demo file and click **Open**.
4. Click **Next** to go to the next page of the wizard.

Select the Quan Peak Page

Use the Select The Quan Peak page ([Figure 57](#)) of the Chromatogram wizard to explicitly specify the Quan peak (component) for a Quan results based chromatogram report object.

Figure 57. Select the Quan Peak page



For more information about the parameters on this page, see [Select the Quan Peak](#). For more information about the Chromatogram wizard, see [Configuring a Chromatogram Object](#).

❖ **To specify a Quan peak**

1. Open the Select the Quan Peak page of the Chromatogram wizard as follows:
 - a. In a Qual, Quan, or non-repeating section, right-click a **Chromatogram** object and choose **Properties**.
 - b. Click **Configure**.
 - In a non-repeating section, the Select Chromatogram Type page opens. Go to [step 1e](#).
 - In a Qual or Quan section, the Use Container Supplied Qual or Quan Peak page of the Chromatogram wizard opens.
 - c. On the Use Container Supplied Qual or Quan Peak page, select the **Explicitly Specify the Chromatogram's Behaviour** check box.
 - d. Click **Next**.

The Select Chromatogram Type page opens.
 - e. Select the **Quan Results Based Chromatogram Option** and click **Next**.

The Select Demo File page opens.
 - f. Follow the instructions in [Quan Result Based Chromatogram](#). Then click **Next**.
2. To specify the Quan peak, do one of the following:
 - Type the text name of the component in the Quan Peak box.

—or—

 - Select the Quan peak from the component list of a processing method as follows:
 - i. Click the browse button.

The Select Processing File dialog box opens.
 - ii. Select a processing method file.

The Select Component dialog box opens. For more information about this dialog box, see [Select Component](#).
 - iii. Select a component. The list includes the components defined in the selected processing method.
 - iv. Click **OK** to return to the wizard. The Next button is active only after you have entered a component.
3. To use the associated internal standard of the Quan peak instead of the Quan peak, select the **Use Quan Peak's Associated Internal Standard** check box.

Note Select a valid peak for XReport to resolve the report correctly. If the file used to resolve the report does not contain the specified peak, the Xcalibur data system removes the chromatogram from the resolved report.

4. Click **Next** to go to the next page of the wizard, the Select Mass Spectrum Quan Traces To Display page.

Select the Qual Peak Page

Use the Select the Qual Peak page of the Chromatogram wizard to explicitly specify the Qual peak for a Qual Results Based chromatogram report object.

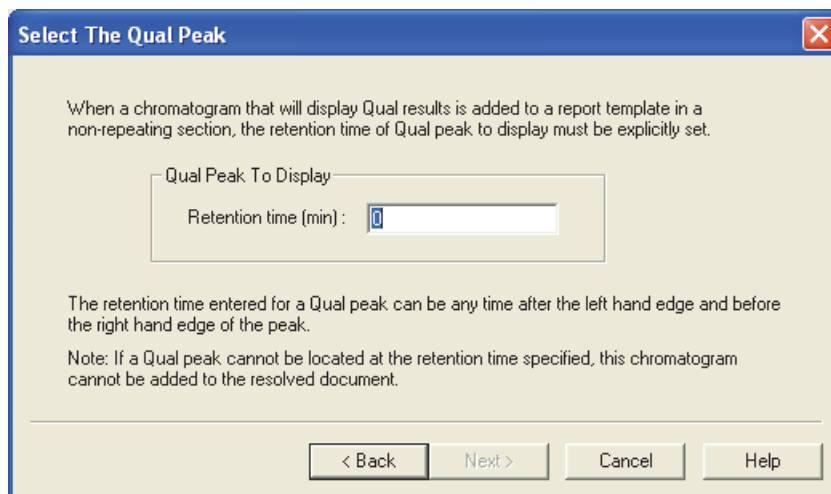
❖ To specify a Qual peak

1. Open the Select the Qual Peak page of the Chromatogram wizard as follows:
 - a. In a Qual, Quan, or non-repeating section, right-click a **Chromatogram** object and choose **Properties**.
 - b. Click **Configure**.
 - In a non-repeating section, the Select Chromatogram Type page opens. Go to [step 1e](#).
 - In a Qual or Quan section, the Use Container Supplied Qual or Quan Peak page of the Chromatogram wizard opens.
 - c. On the Use Container Supplied Qual or Quan Peak page, select the **Explicitly Specify the Chromatogram's Behaviour** check box.
 - d. Click **Next**.
The Select Chromatogram Type page opens.
 - e. Select the **Qual Results Based Chromatogram Option**, leave the **Show All Qual Peaks in Result File** clear, and click **Next**.
The Select Demo File page opens.
 - f. Follow the instructions in [Qual Result Based Chromatogram – Explicit Peak](#). Then click **Next**.
The Select The Qual Peak page of the Chromatogram wizard opens.
2. To specify the Qual peak in the Qual Peak To Display area, type the appropriate retention time in the Retention time box ([Figure 58](#)).

The Next button is active only after you have selected a component in the Retention time box. Set the retention time to any time within the start and end peak boundaries.

Note Select a valid retention time for XReport to resolve the report correctly. If the file used to resolve the report does not contain the specified retention time, the chromatogram is removed from the resolved report.

Figure 58. Select the Qual Peak page



3. Click **Next** to go to the next page of the wizard, the Configure How The Peak Window Will Look page.

Select Mass Spectrum Quan Traces to Display Page

Use the Select Mass Spectrum Quan Traces to Display page of the Chromatogram wizard to configure the Quan Traces property for MS data. (This page is only applicable to MS data and is inactive for other detector types.)

When a chromatogram report object displays a Quan component, there are potentially six traces associated with the component, as follows:

- Quan Mass (QM) Trace (the actual component peak)
- Up to five Confirmation Ions

Note The Ion Ratio Confirmation settings on this page apply only to GC-MS data.

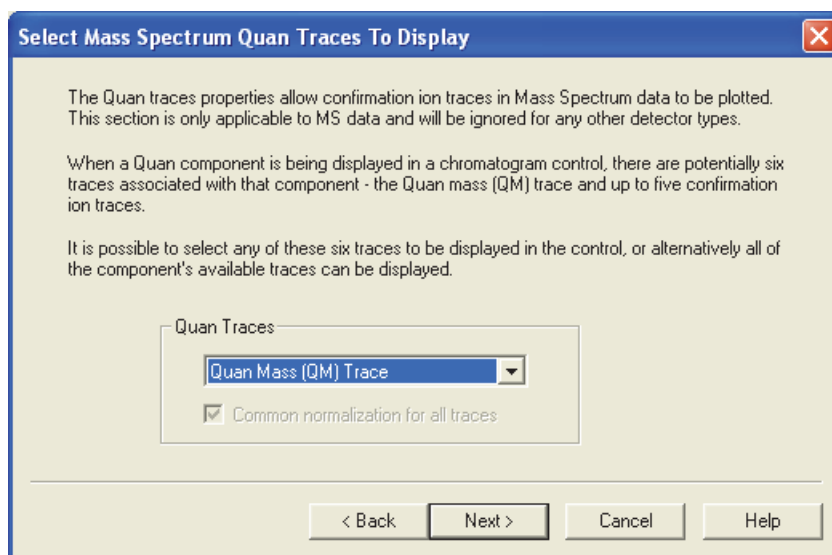
Select any of these possible six traces to be displayed in the Chromatogram or display all available traces of the component.

For parameter information, see [Select Mass Spectrum Quan Traces to Display](#).

❖ **To specify a Quan trace**

1. Select one of the following from the Quan Traces list (Figure 59):
 - Quan Mass (QM Trace)
 - First Qualifier Ion
 - Second Qualifier Ion
 - Third Qualifier Ion
 - Fourth Qualifier Ion
 - Fifth Qualifier Ion
 - All Quan Traces

Figure 59. Select Mass Spectrum Quan Traces To Display page



2. To normalize all the traces the same way, select the **Common Normalization for All Traces** check box.
3. Click **Next** to go to the next page of the wizard.

Configure How the Peak Window Will Look Page

Use the Configure How the Peak Window Will Look page of the Chromatogram wizard to control the display of the baselines (Quan and Qual peaks) and the peak window width (active for Qual peak and Quan peak in some cases) when a peak from a result file is set to display in a Chromatogram.

❖ To open the Configure How the Peak Window Will Look page

1. Right-click a **Chromatogram** object and choose **Properties**.
2. Click **Configure**.

Depending on the section type, one of these pages opens.

- In a Quan repeating section, the Use Container Supplied Quan Peak page opens. Go to [step 3](#).
 - In a Qual repeating section, the Use Container Supplied Qual Peak page opens. Go to [step 3](#).
 - In a non-repeating section, the Select Chromatogram Type page opens. Go to [step 4](#).
3. Make the appropriate selection and click **Next**.

If you selected the Explicitly Specify the Chromatogram's Behaviour check box, the Select Chromatogram Type page opens. Otherwise, the Select Demo File page opens.

4. Depending on whether the Select Demo File page or the Select Chromatogram Type page opens, do one the following:

If the Select Demo File page opens, do the following:

- a. Follow the instructions in [Select Demo File Page](#). Then click **Next**.

The Select Mass Spectrum Quan Traces To Display page opens.

- b. Select the appropriate trace. Then click **Next**.

The Configure How the Peak Window Will Look page opens.

If the Select Chromatogram Type page opens, select either the Quan or Qual Results Based Chromatogram option:

- a. Select the Quan Results Based Chromatogram option. Then click **Next**.

The Select Demo File page opens.

- b. Follow the instructions in [Select Demo File Page](#). Then click **Next**.

The Select The Quan Peak page opens.

- c. Follow the instructions in [Select the Quan Peak Page](#). Then click **Next**.

The Select Mass Spectrum Quan Traces To Display page opens.

- d. Follow the instructions in [Select Mass Spectrum Quan Traces to Display Page](#). Then click **Next**.

The Configure How The Peak Window Will Look page opens.

–or–

- a. Select the Qual Results Based Chromatogram option. Then click **Next**.

The Select Demo File page opens.

- b. Follow the instructions in [Select Demo File Page](#). Then click **Next**.

If you left the Show All Qual Peaks in Result File check box clear, the Select The Qual Peak page opens. Otherwise, the Configure How the Peak Window Will Look page opens.

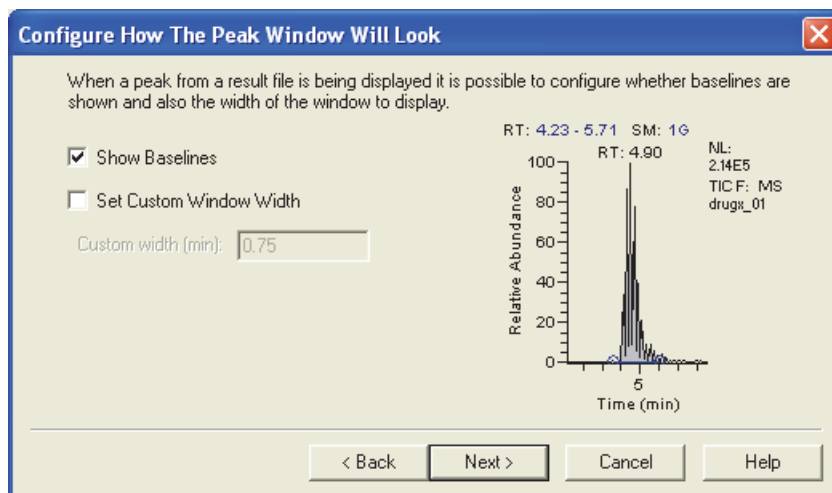
- c. Follow the instructions in [Select the Qual Peak Page](#). Then click **Next**.

The Configure How The Peak Window Will Look page opens.

❖ **To specify the width of the peak window and whether the peak window shows an integrated peak**

1. Select the **Show Baselines** check box to display the baselines for a Chromatogram peak (Quan or Qual) ([Figure 60](#)). When you clear this check box, the XReport application does not display the baselines, peak tracing, or full peak annotation.

Figure 60. Configure How the Peak Window Will Look page



2. To manually override the default value of the peak window width (the default is peak width plus 1 min), select the **Set Custom Window Width** check box. Use the Custom width edit box to type a value for the window width (min). The default value for this field is 0.75 min.

The Set Custom Window Width check box is unavailable if you selected the Show All Qual Peaks in Result File check box in the Select Chromatogram Type page.

3. Click **Next** to go to the next page of the wizard.

Select Plot Details Page

Use the Select Plot Details page of the Chromatogram wizard to configure how the plot is drawn when raw data is being displayed in a chromatogram report object.

For more information about the parameters on this page of the wizard, see [Select Plot Details](#).

❖ To configure a plot on a raw file-based chromatogram

1. Open the Select Plot Details page as follows:
 - a. Right-click a **Chromatogram** object and select **Properties**.
 - b. Click **Configure**.
 - In a Qual repeating section, the Use Container Supplied Qual Peak page opens.
 - In a Quan repeating section, the Use Container Supplied Quan Peak page opens.
 - In a non-repeating section, the Select Chromatogram Type page opens.
 - c. In a Qual or Quan repeating section, do the following:
 - i. Select the **Explicitly Specify the Chromatogram's Behaviour** check box on the Use Container Supplied Qual Peak page or the Use Container Supplied Quan Peak page, respectively. Then click **Next**.

The Select Demo File page opens.
 - ii. Follow the instructions in [Select Demo File Page](#). Then click **Next**.

The Select Chromatogram Type page opens.
 - d. For a Qual, Quan, or non-repeating section, select the **Raw File Based Chromatogram** option on the Select Chromatogram Type page.

The Select Plot Details page opens.
2. Select the type of detector used to generate the raw data file from the Detector list in the Plot Type area ([Figure 61](#)). The type of detector determines the available traces.

Figure 61. Select Plot Details page

3. Type in the offset of the start of a chromatogram trace in the Delay box. This box is available only when you select a non-MS detector type, such as UV or PDA.
4. From the Filter list, select the processing applied to a subset of the scans in a raw data file.

This option is available only when you select MS detectors. The list displays scan filter options stored in the selected demo RAW file. If no demo file is selected, type a valid filter string.

5. From the Trace lists, select the following:
 - a. From the first list, select a basic chromatogram type, for example, **TIC**.
 - b. From the second list, select a logical operator: + or -. Selecting an operator makes the third list active.
 - c. From the third list, select a second chromatogram type to add to, or subtract from, the first trace (for example, **Mass Range**). The list features valid plot types.

The list of valid traces depends on the detector used to generate the data as follows.

Detection	Valid traces
MS	Mass Range, TIC, and Base Peak
Analog	Analog 1–4
A/D card	A/D Card Ch 1–4
PDA	Wavelength Range, Total Scan, and Spectrum Maximum
UV	Channel A–D

6. Depending on the type of chromatogram you select, do the following:
 - a. If you choose MS detector types, specify the mass or mass range for Mass Range or Base Peak Traces in the Mass list as follows:

If you choose Base Peak $\pm$ Mass Range or Mass Range $\pm$ Mass Range plot combinations in step 4 above, the identification page displays a Mass (m/z) field for each trace type.
 - b. If you choose other detector types, use this field to specify the wavelength or wavelength range for the chromatogram. If you use a plot combination such as Wavelength Range + Wavelength Range, an additional Wavelength (nm) box appears for you to specify the second wavelength range.

The valid range depends on the configured detector. The format is *Low Mass/Wavelength–High Mass/Wavelength*. Separate entries by a dash with no spaces. For example, for the range m/z 123 through 456, type: **123–456**.
7. Specify the lower and upper time limits for the plot (in minutes to 1 decimal place) in the Time Range box. Separate entries by a dash with no spaces.

Type * (the default setting) to display the complete time range for the plot.
8. Select the **Fixed Scale** check box to set the y -axis maximum to a specific value.

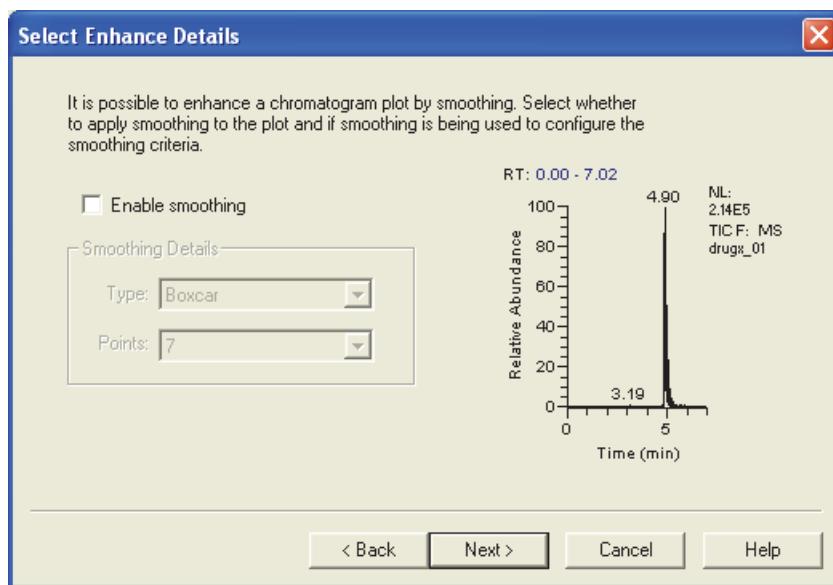
Selecting the Fixed Scale check box activates the Normalize To area on the final page of the wizard and the box where you type the maximum y -axis value on the current page.
9. Select the **Autofilter** check box to repopulate a chromatogram view with the following:
 - A plot showing the chromatogram without any scan filters
 - Plots for each scan filter applied to the chromatogram
10. Click **Next** to go to the next page of the wizard.

Select Enhance Details Page

Use the Select Enhance Details page of the Chromatogram wizard to enhance a chromatogram plot by applying smoothing (Figure 62).

For more information about the parameters on this wizard page, see [Select Enhance Details](#).

Figure 62. Select Enhance Details page



❖ To enhance a chromatogram

1. To open the Select Enhance Details page, open the Select Plot Details page as described in [step 1 of To configure a plot on a raw file-based chromatogram](#). Then click **Next**.
2. To apply smoothing to the chromatogram, select the **Enable Smoothing** check box.
3. To select a type of smoothing, select **Boxcar** or **Gaussian** from the Type list in the Smoothing Details area.
4. Select the number of smoothing points (odd numbers from 3 to 15) to use in the Points list.
5. Click **Next** to go to the next page of the wizard.

Select Chromatogram Style Page

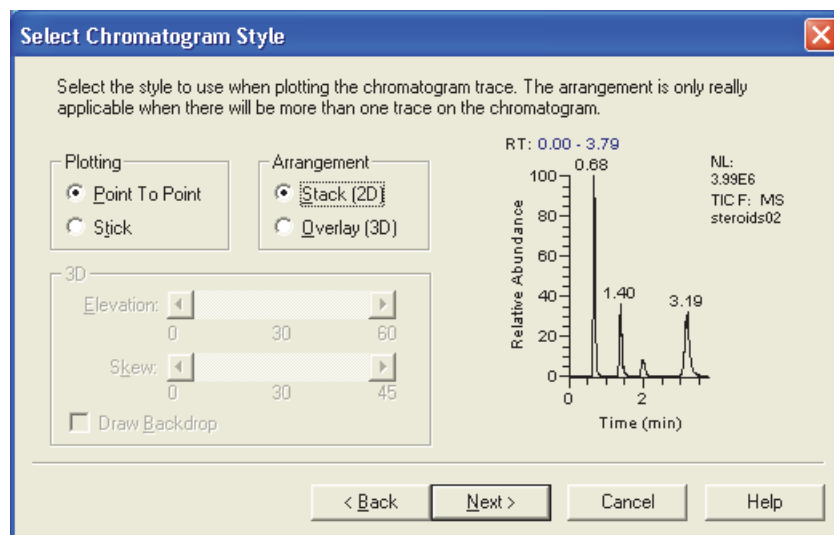
Use the Select Chromatogram Style page of the Chromatogram wizard to determine the appearance of the chromatogram. For more information about the parameters on this page of the wizard, see [Select Chromatogram Style](#).

This page of the Chromatogram wizard is available for all of the report sections and for all of the chromatogram types whether implicit or explicit.

❖ To define styles for a chromatogram

1. To define the plotting style, select one of the following options in the Plotting area (Figure 63):
 - **Point To Point**: Display point-to-point peak profiles.
 - **Stick**: Display the chromatogram as vertical lines.

Figure 63. Select Chromatogram Style page



2. To define the plotting arrangement, select one of the following options in the Arrangement area:
 - **Stack (2D)**: Stack plots vertically (same x axis) with no overlap (own y axis).
 - **Overlay (3D)**: Overlay plots vertically (same x axis). Use the 3D arrangement when you selected Multiple Quan Traces on the Select Mass Spectrum Quan Traces page of the wizard.
3. When you select an Overlay (3D) arrangement, set the following in the active 3D area:
 - a. To set the Elevation angle (from 0 to 60 degrees) for the 3D plot style, adjust the **Elevation** slider bar. Either drag the Elevation slider bar or click the Elevation slider left or right arrows until you reach the desired angle.
 - b. To set the skew angle for the 3D plot style, adjust the **Skew** slider bar. 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).
 - c. To add a backdrop to 3D plots, select the **Draw Backdrop** check box.
4. Click **Next** to go to the next page of the wizard.

Select the Peak Labeling Page

Use the Select the Peak Labeling page of the Chromatogram wizard to choose the type and style of peak labels. From this page, click **Advanced** to open a dialog box where you set advanced labeling options.

This page of the Chromatogram wizard is available for all of the report sections and for all of the chromatogram types whether implicit or explicit.

To label peaks in reports, see these topics:

- [Basic Peak Labeling Options](#)
- [Advanced Labeling Options for a Quan Peak](#)
- [Advanced Labeling Options for a Qual Peak](#)

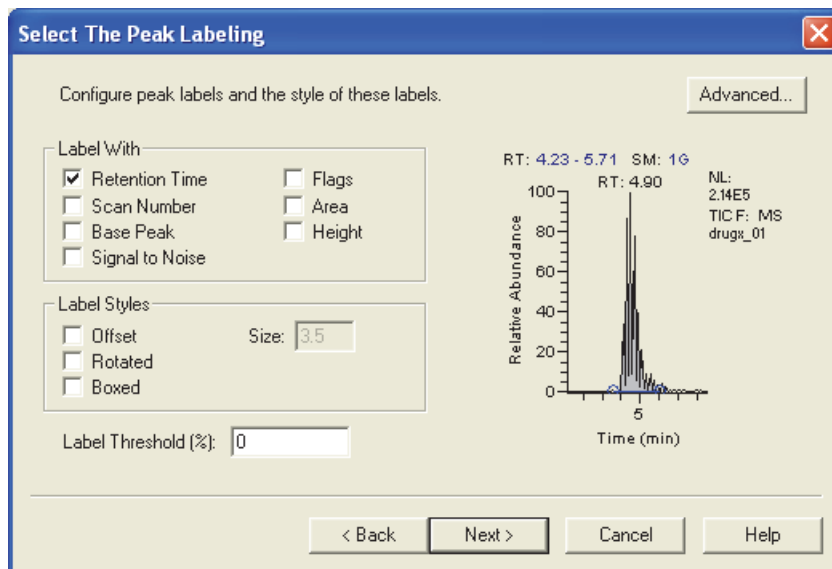
Basic Peak Labeling Options

To set up the basic peak labeling options, follow this procedure.

❖ To select peak labeling options

1. To label peaks with the time in minutes in the chromatogram plot, select the **Retention Time** check box in the Label With area (Figure 64). The data system displays **RT** before the label.

Figure 64. Select the Peak Labeling page



2. To label peaks with the number of mass scans at peak maximum, select the **Scan Number** check box. The data system displays **S#** before the label.
3. To label the base peak in the mass spectrum of the chromatogram peak, select the **Base Peak** check box. The data system displays **BP** before the label.

4. To label peaks with the signal-to-noise ratio at the peak maximum, select the **Signal-to-Noise** check box. The data system displays **SN** before the label.
5. To label peaks with flags providing supplemental information about the peak data, select the **Flags** check box. When a peak is saturated, the data system displays an **S** above the peak.
6. To label peaks with the integrated area of the peaks, select the **Area** check box. The data system displays **AA** before the label when detected automatically or **MA** when detected manually.
7. To label peaks with the apex height, select the **Height** check box. The data system displays **AH** before the label when detected automatically or **MH** when detected manually.
8. To offset a label from its normal position to avoid conflict with another label, select the **Offset** check box in the Label Styles area. Type the number for the offset (for the number of characters) in the Size box.
9. To use vertical, rather than horizontal, labels, select the **Rotated** check box.
10. To place a rectangular outline around each peak label, select the **Boxed** check box.
11. To limit the labeling of peaks to those exceeding the specified percentage of the base peak, set the Label threshold box to a percent value between 100 and 0.
12. To open the Advanced Quan Peak Annotation Options dialog box or the Advanced Qual Peak Annotations dialog box, click **Advanced**.
 - If you are configuring a Quan peak, see the next topic [Advanced Labeling Options for a Quan Peak](#).
 - If you are configuring a Qual peak, see [Advanced Labeling Options for a Qual Peak](#).
13. Click **Next** to go to the next page of the wizard, the Select How the Chromatogram Axes Will Be Configured page.

Advanced Labeling Options for a Quan Peak

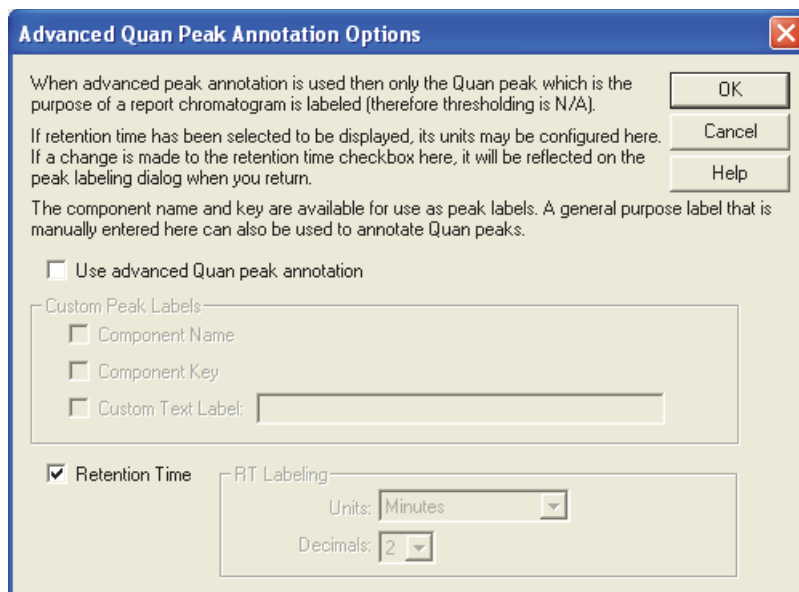
If are configuring a Quan peak in any of the report sections, the Advanced Quan Peak Annotation Options dialog box opens when you click Advanced on the Select The Peak Labeling page of the Chromatogram wizard. When you set Advanced Labeling options, the data system labels only the Quan peak.

For more information about the parameters in this dialog box, see [Advanced Quan Peak Annotation Options](#). For information about the Select Peak Labeling page of the Chromatogram wizard, see [Select the Peak Labeling Page](#).

❖ **To set advanced Quan peak annotation options**

1. To activate advanced Quan peak options, select the **Use Advanced Quan Peak Annotation** check box (Figure 65).

Figure 65. Advanced Quan Peak Annotation Options dialog box



2. To label the Quan peak with the component name, select the **Component Name** check box in the Custom Peak Labels area.
3. To label the Quan peak with the component key, select the **Component Key** check box.
4. To specify a custom label, select the **Custom Text Label** check box. Type a custom label for the Quan peak in the active box.
5. To label the Quan peak with the retention time, select the **Retention Time** check box.

If you selected Retention Time check box in the Label With area on the Select The Peak Labeling page of the Chromatogram wizard, this check box is already selected. Clearing the Retention Time check box in the Advanced Quan Peak Annotation Options dialog box also clears the Retention Time check box on the Select The Peak Labeling page.

6. In the RT Labeling area, select the unit for the retention time from the Units list: **Minutes** or **Seconds**.
7. Select the number of decimal places to be displayed in the retention time label from the Decimals list: **1**, **2**, or **3**.
8. Click **OK** to save the changes and close the dialog box.
9. To continue configuring the properties of the Chromatogram object, click **Next** on the Select the Peak Labeling page of the Chromatogram wizard.

Advanced Labeling Options for a Qual Peak

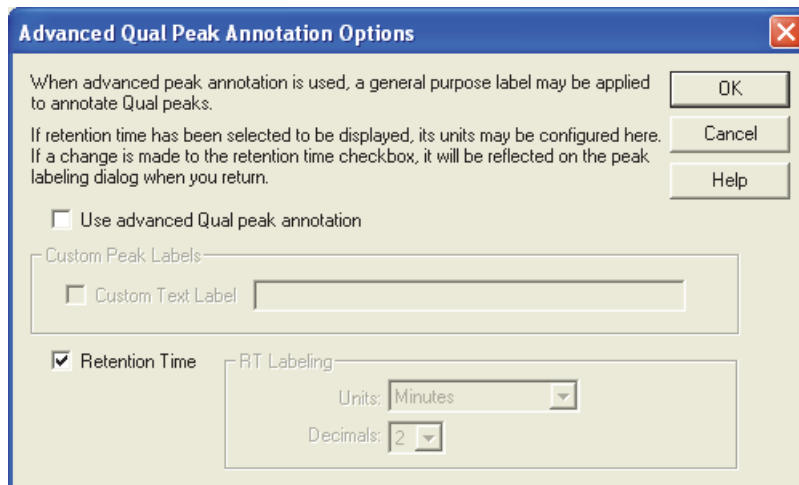
If you are configuring a Qual peak in any of the report sections, the Advanced Qual Peak Annotation Options dialog box opens when you click Advanced on the Select The Peak Labeling page of the Chromatogram wizard. When you set Advanced Labeling options, the data system labels only the Qual peak.

For more information about the parameters in this dialog box, see [Advanced Qual Peak Annotation Options](#). For information about the Select Peak Labeling page of the Chromatogram wizard, see [Select the Peak Labeling Page](#).

❖ To set advanced Qual peak annotation options

1. To activate the advanced Qual peak options, select the **Use Advanced Qual Peak Annotation** check box (Figure 66).

Figure 66. Advanced Qual Peak Annotation Options dialog box



2. To specify a custom label, select the **Custom Text Label** check box in the active Custom Peak Labels area. Type a custom label for the Qual peak in the box.
3. To label the Qual peak with the retention time, select the **Retention Time** check box.

If you selected Retention Time check box in the Label With area on the Select The Peak Labeling page of the Chromatogram wizard, this check box is already selected. Clearing the Retention Time check box in the Advanced Qual Peak Annotation Options dialog box also clears the Retention Time check box on the Select The Peak Labeling page.

4. In the RT Labeling area, select the type of unit for the retention time from the Units list.
5. Select the number of decimal places to be displayed in the retention time label from the Decimals list.
6. Click **OK** to save the changes and close the Advanced Qual Peak Annotation Options dialog box.

7. To continue configuring the properties of the Chromatogram object, click **Next** on the Select the Peak Labeling page of the Chromatogram wizard.

Select How the Chromatogram Axes Will Be Configured Page

Use the Axes page of the Chromatogram wizard to set chromatogram axes label and display options. For more information about the parameters on this page, see [Select How the Chromatogram Axes Will Be Configured](#).

This page of the Chromatogram wizard is available for all of the report sections and for all of the chromatogram types whether implicit or explicit. For information about the Chromatogram wizard, see [Configuring a Chromatogram Object](#).

❖ To specify the appearance for chromatogram axes

1. To set the name of the x axis in the X Axis area, type it in the Name box ([Figure 67](#)).

Figure 67. Select How the Chromatogram Axes Will Be Configured page

2. To offset the axis label from the chromatogram, select the **Offset** check box.
3. To split the chromatograms into two or more separate graphs with equal time ranges, select the **Split Time Range** check box.
4. Type the number of split time range graphs displayed for each chromatogram in the Divisions box. This box is active only when you select the **Split Time Range** check box.
5. In the Y Axis area, select either the **From Detector** option in the Label area to use the detector-specific label for the y axis (stored in the RAW file) or the **Custom** option to use your own label.
6. To specify the setting for the y -axis units, select either **Absolute** or **Relative** in the Units area.

7. If you have chosen to use a Custom label for the y axis, type a y -axis name in the Name box.
8. To offset the axis label from the chromatogram, select the **Offset** check box.
9. To go to the next page of the wizard, click **Next**.

Configure Normalization for the Chromatogram Page

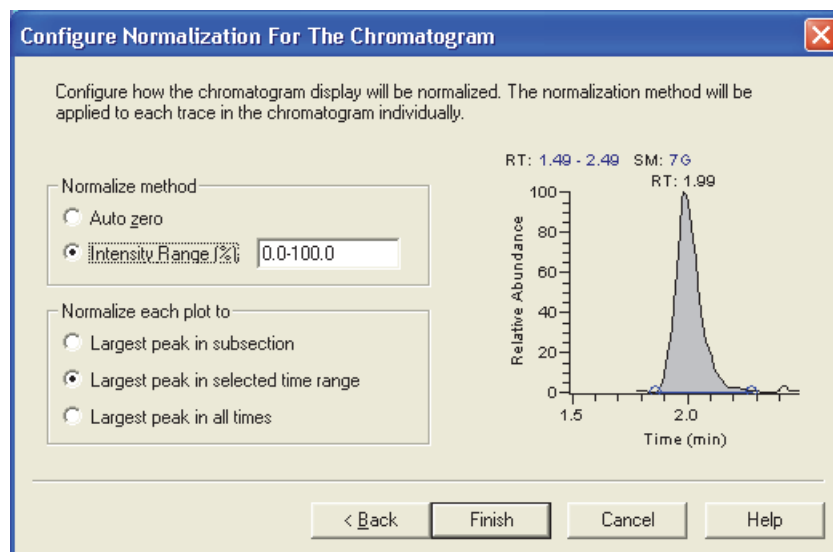
Use the Normalization page of the Chromatogram wizard to select the normalization (y -axis scaling) method used for the chromatogram. For more information about the parameters on this page, see [Configure Normalization For The Chromatogram](#).

This page of the Chromatogram wizard is available for all of the report sections and for all of the chromatogram types whether implicit or explicit. For information about the Chromatogram wizard, see [Configuring a Chromatogram Object](#).

❖ To specify normalization options

1. Define the normalizing method in the Normalize Method area ([Figure 68](#)) by selecting one of the following options:
 - **Auto Zero:** Optimize the y axis automatically for each chromatogram.
 - **Intensity Range (%):** Set the range manually. Type the minimum and maximum intensity required for the y axis. The valid range is -200.00 to $+200.00\%$.

Figure 68. Configure Normalization for the Chromatogram page



2. Define a peak to use for normalization in the Normalize Each Plot area by selecting one of the following options:
 - **Largest Peak in Subsection:** Normalize each split time range to the largest peak in the division.
 - **Largest Peak in Selected Time Range:** Normalize the spectrum to the largest peak in the displayed time range.
 - **Largest Peak in All Times:** Normalize the spectrum to the largest peak in the entire chromatogram.

The Normalize Each Plot area is active when you select a raw file-based chromatogram and you have selected the Fixed Scale check box on the Plot Type Page (see [Plot Type Page](#)).

Finishing the Chromatogram Wizard

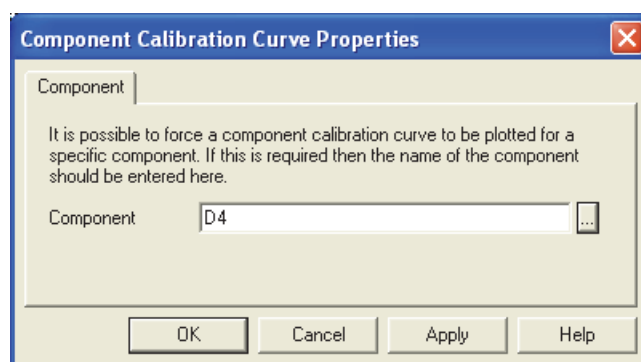
To change selections in the Chromatogram wizard, click **Back** to go back through the previous pages. When the page is done, click **Finish**.

For more information about the Chromatogram wizard, see [Configuring a Chromatogram Object](#).

Configuring a Component Calibration Curve

To configure a Component Calibration Curve object, right-click it and choose **Properties** from the shortcut menu. The Component Calibration Curve Properties dialog box opens ([Figure 69](#)).

Figure 69. Component Calibration Curve Properties dialog box



If your report has a nonrepeating Component Cal Curve report object, use the Component Calibration Curve wizard to specify the name of the component.

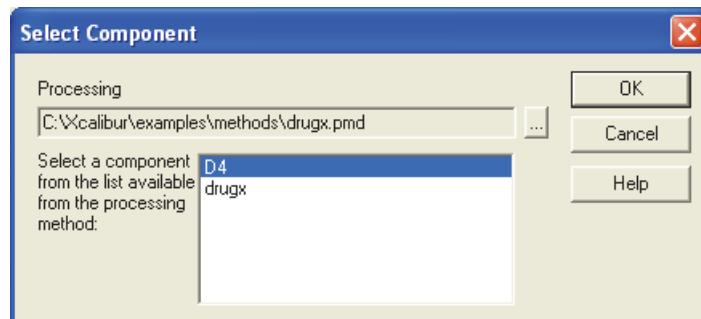
❖ To specify the name of the component

1. To search for the required processing method file (PMD), click the browse button. A dialog box opens. By default, the wizard searches in the Xcalibur\methods folder.

2. To open a file, select it and click **Open**.

The Select Component dialog box opens (Figure 70).

Figure 70. Select Component dialog box



3. Select the required component from the list available for the chosen processing method and click **OK**. The Component Name page opens, displaying the specified name of the component in the box.
4. Click **OK**.

Configuring a Spectrum Object

Use the Spectrum Properties dialog box to configure a Spectrum object in an XReport template. Use the XReport Spectrum Properties pages to do the following:

- [Configure Options](#)
- [Configure Plot Types](#)
- [Enhance Spectra](#)
- [Configure Spectrum Style](#)
- [Configure Spectrum Peak Labels](#)
- [Configure Axes](#)
- [Select Normalization Options](#)
- [Specify a Peak](#)

To configure the Spectrum report object, make selections on each page based on these corresponding procedures.

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

❖ To open the Spectrum Properties dialog box

Right-click a Spectrum object and choose **Properties** from the shortcut menu.

Configure Options

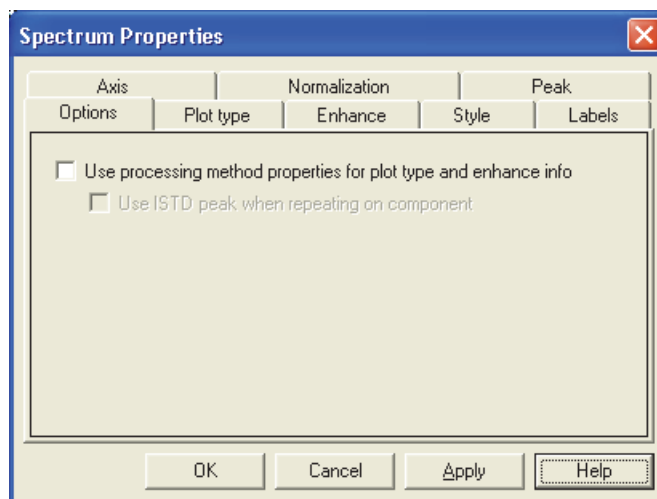
To configure Spectrum options, use the Options page of the Spectrum Properties dialog box. For information about the parameters on this page, see [Options Page for a Spectrum Object](#).

❖ To configure Spectrum options

1. In the template pane, right-click a Spectrum object and choose **Properties**.

The Spectrum Properties dialog box opens to the Options page ([Figure 71](#)).

Figure 71. Options page



2. To use processing method properties for Plot type and Enhance information, select the **Use Processing Method Properties for Plot Type and Enhance Info** check box.

When you select this check box, the options on the Plot type and Enhance pages are not available.

3. To use the Internal Standard peak when repeating on a component, select the **Use ISTD Peak When Repeating on Component** check box. This option is only available when you select the Use processing method properties for plot type and enhance info check box.

Configure Plot Types

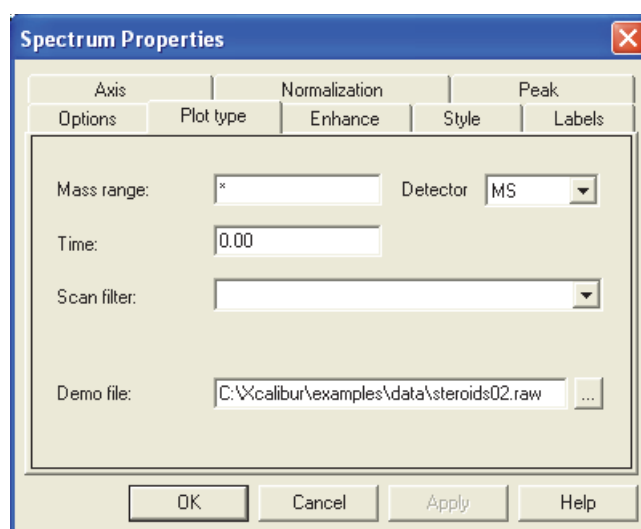
When raw data is being displayed in a Spectrum report object, use the Plot Type page of the Spectrum Properties dialog box to configure how the plot is drawn. For more information about the parameters on this page, see [Plot Type Page for a Spectrum Object](#).

If you selected the Use processing method properties for plot type and enhance info check box on the Options page, this page is blank.

❖ To configure plot types

1. In the template pane, right-click a Spectrum object and choose **Properties**.
The Spectrum Properties dialog box opens.
2. Click the **Plot Types** tab.
3. Specify the mass or mass range for MS detector types in the Mass Range box ([Figure 72](#)).

Figure 72. Plot type page



For PDA detector types, use this parameter to specify the wavelength or wavelength range (nm). Type the lower and upper limits for the plot. Separate entries by a dash (no spaces). To use the entire mass/wavelength range, type an asterisk:*

4. Select the type of detector used to generate the raw data file from the Detector list. Valid types are **MS** and **PDA**. The type of detector determines the available Plot types.
5. Select the time of the mass scan in the host chromatogram in the Time box. Type a new value or range as required.
6. From the Scan Filter list, select a filter or type a new one in the box using the scan filter format.
7. Click the browse button in the Demo File box and select the file. This box shows the path and filename of the demo file (RAW) used to generate the selected plot.

Enhance Spectra

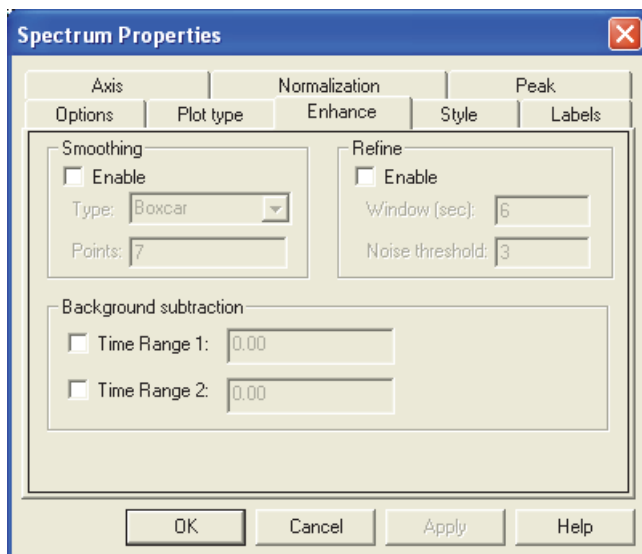
Use the Enhance page of the Spectrum Properties dialog box to apply smoothing (the refine algorithm) to the spectrum and set background subtraction time ranges. For information about the parameters on this page, see [Enhance Page for a Spectrum Object](#).

If you selected the Use processing method properties for plot type and enhance info check box on the Options page, this page is blank.

❖ To define spectrum enhancement options

1. To turn on spectrum smoothing, select the **Enable** check box in the Smoothing area ([Figure 73](#)).

Figure 73. Enhance page



2. To select a type of smoothing, select **Boxcar** or **Gaussian** from the Type list.
3. Type the number of points for spectrum smoothing in the Points list. Type an odd number from **3** (minimum smoothing) to **15** (maximum smoothing).
4. To turn Refine spectrum enhancement on or off, select the **Enable** check box in the Refine area.
5. To apply the refining algorithm and specify a length of time for mass chromatograms, type a value in the Window box indicating the number of seconds on either side of the specified point. A reasonable initial value is the peak width in seconds.
6. To eliminate peaks generated from baseline noise, type **0** (this shows all peaks in the spectrum) in the Noise threshold box. After you close this box to display the results, you can open the box again to increase the value until noise peaks are eliminated.

7. To specify the first baseline region used for assessing the background, select the **Time Range 1** check box in the Background Subtraction area. Type the time range in the box.

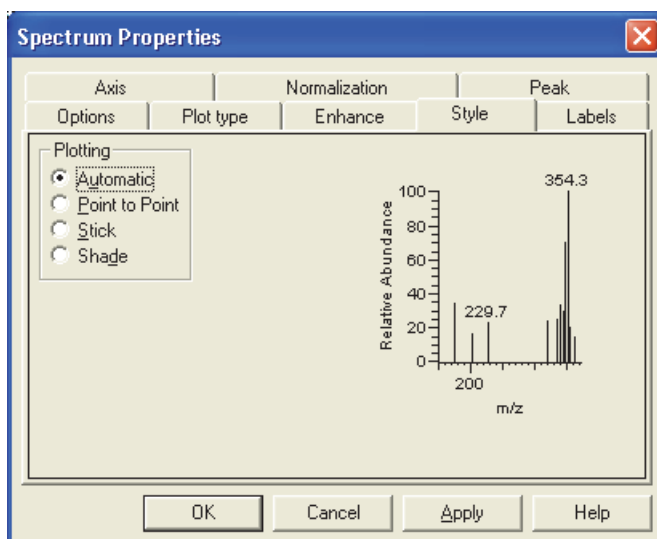
The Background Subtraction area shows details of background subtraction when this value has been applied to the spectrum. The background contribution is determined by averaging the scans from one or two baseline regions.

8. To specify the second baseline region used for assessing the background, select the **Time Range 2** check box. Type the time range in the box.

Configure Spectrum Style

To set parameters that determine the appearance of the spectrum, use the Style page of the Spectrum Properties dialog box (Figure 74). For information about the parameters on this page, see [Style Page for a Spectrum Object](#).

Figure 74. Style page



❖ To set plotting options

To define the plotting style, select one of the following options in the Plotting area:

- **Automatic:** Choose the graphic style based on the data acquisition method used for the active spectrum.
- **Point to Point:** Display a point-to-point peak profile.
- **Stick:** Display spectral mass peaks as vertical lines.
- **Shade:** Display the spectrum as a shaded representation of intensity in each amu band for the active spectrum.

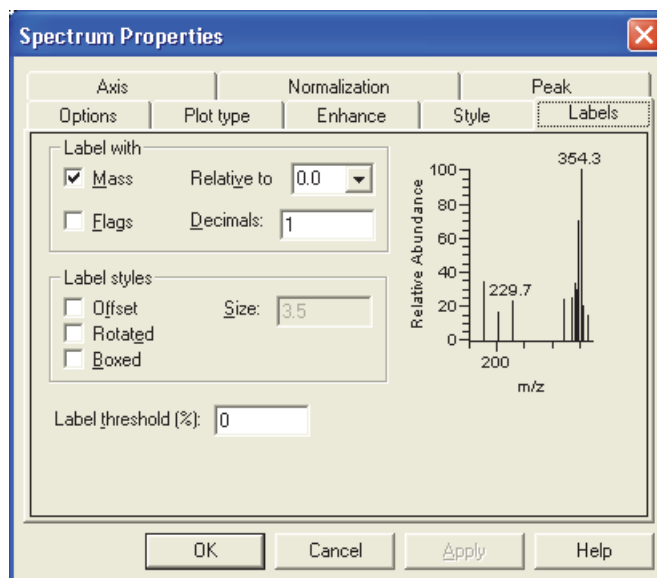
Configure Spectrum Peak Labels

To choose the type and style of peak labels, use the Labels page of the Spectrum Properties dialog box. For information about the parameters on this page, see [Labels Page for a Spectrum Object](#).

❖ To configure spectrum peak labels

1. To label spectrum peaks with m/z value, select the **Mass** check box ([Figure 75](#)) in the Label With area.

Figure 75. Labels page



2. To label spectrum peaks with flags, select the **Flags** check box. Flags provide supplemental information about the peak data. For example, when a peak is saturated, the Xcalibur data system displays an **S** above the peak.
3. To specify that other spectrum peaks are labeled relative to that value, type a value in the Relative to box.
4. Type the number of decimal places to be used in the labels in the Decimals box.
5. To move a label from its normal position to avoid conflict with another label, select the **Offset** check box in the Label Styles area. Choose the number for the offset (for the number of characters) in the Size box.
6. To use vertical, rather than horizontal, labels, select the **Rotated** check box.
7. To place a rectangular outline around each peak label, select the **Boxed** check box. This option does not apply to flags.
8. To limit the labeling of peaks to those exceeding the specified percentage of the base peak, type a percent in the Label Threshold% box.

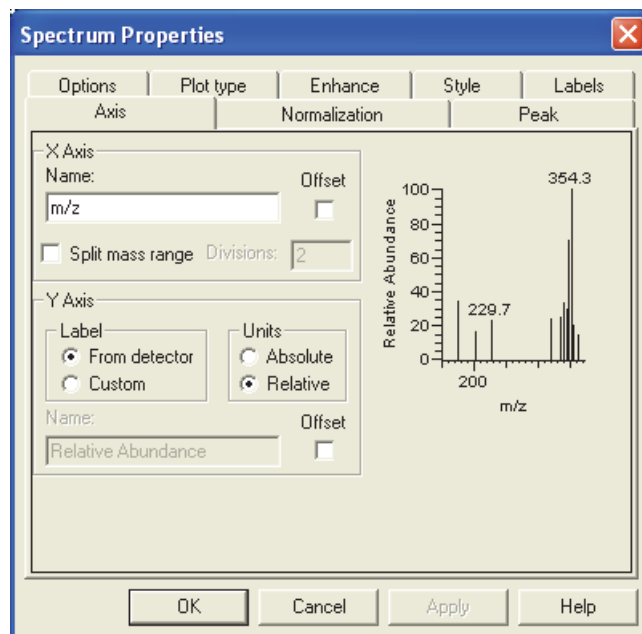
Configure Axes

To set spectrum axis labels and display options, use the Axis page of the Spectrum Properties dialog box. For information about the parameters on this page, see [Axis Page for a Spectrum Object](#).

❖ To configure axis options

1. Type the x -axis name in the Name box in the X Axis area ([Figure 76](#)).

Figure 76. Axis page in the Spectrum Properties dialog box



2. To offset the axis label from the spectrum, select the **Offset** check box.
3. To split the spectra into two or more separate graphs with equal ranges, select the **Split Mass Range** check box. Type the number of split range graphs displayed for each spectrum in the Divisions box.
4. Select one of the following options in the Y Axis area under Label:
 - **From Detector:** Use the detector-specific label for the y axis (stored in the RAW file).
 - **Custom:** Use your own label.
5. To specify the setting for the y -axis units, select the **Absolute** or the **Relative** option.
6. Type a y -axis name in the Name box.
7. To move the axis label away from the spectrum, select the **Offset** check box.

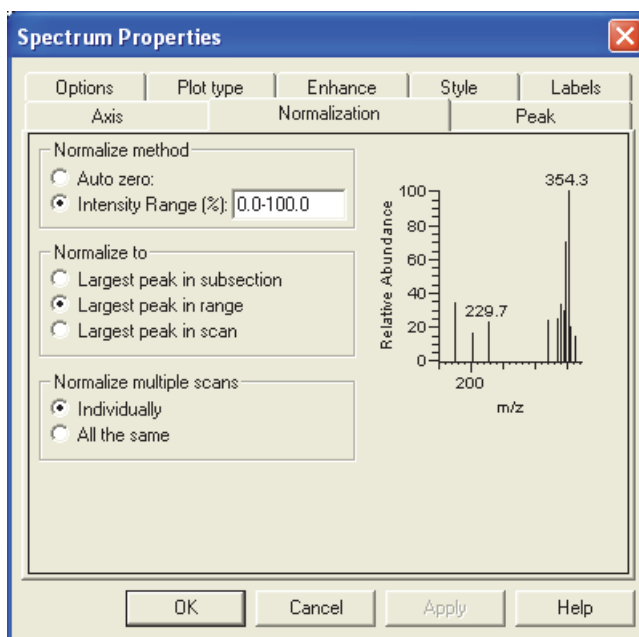
Select Normalization Options

Use the Normalization page of the Spectrum Properties dialog box to select normalization options for spectrum plots. For information about the parameters on this page, see [Normalization Page for a Spectrum Object](#).

❖ To select normalization options

- To define the normalization method, select one of the following options in the Normalize Method area ([Figure 77](#)).
 - Auto Zero:** Automatically optimize the y axis.
 - Intensity Range (%):** Set the y -axis range. Use the box to type the minimum and maximum intensity. The valid range is -200.00 to $+200.00\%$.

Figure 77. Normalization page



- To define the peak that the spectrum is normalized to, select one of the following options in the Normalize To area:
 - Largest Peak in Subsection:** Normalize each split mass range to the largest peak in the division.
 - Largest Peak in Mass Range:** Normalize the spectrum to the largest peak in the displayed mass range.
 - Largest Peak in Scan:** Normalize the spectrum to the largest peak in the entire spectrum.

- To define how multiple scans are normalized, select one of the following options in the Normalize Multiple Scans area:
 - Individually:** Normalize each mass plot individually.
 - All the Same:** Normalize all mass plots equally.

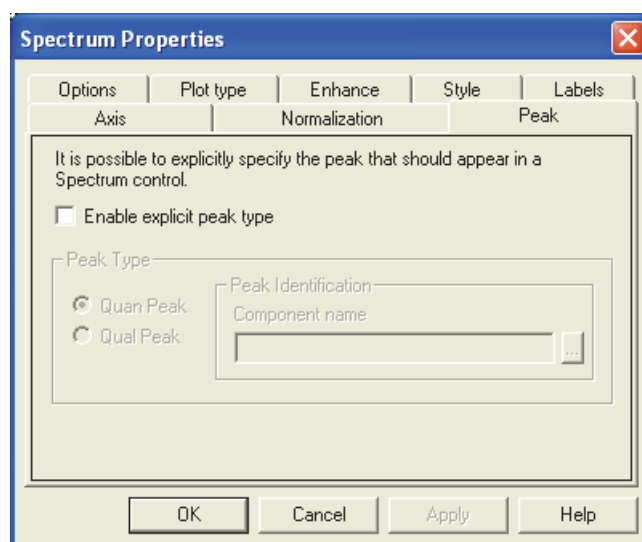
Specify a Peak

To explicitly specify the peak to display in the Spectrum report object, use the Peak page of the Spectrum Properties dialog box. For information about the parameters on this page, see [Peak Page for a Spectrum Object](#).

❖ To specify a peak

- To specify a specific type of peak to appear in the spectrum, select the **Enable Explicit Peak Type** check box ([Figure 78](#)).

Figure 78. Peak page



- To specify the peak type to appear in the Spectrum, do one of the following:
 - To specify a Quan peak, select the **Quan Peak** option.
 - To specify a Qual peak, select the **Qual Peak** option.
- Depending on the peak type, do one of the following:
 - For a Quan peak, type a name for the component in the Peak Identification area.
 - For a Qual peak, type the retention time (any time between the start time and end time of the peak) or click the browse button.

The Select a Peak dialog box opens.

- Select a peak and click **OK** to close the dialog box.

Configuring Columns

Use the Column Properties dialog box to configure a column object.

For information about the parameters in this dialog box, see [Column Properties Dialog Box](#). For information about the column objects in the XReport application, see [Columns Object](#).

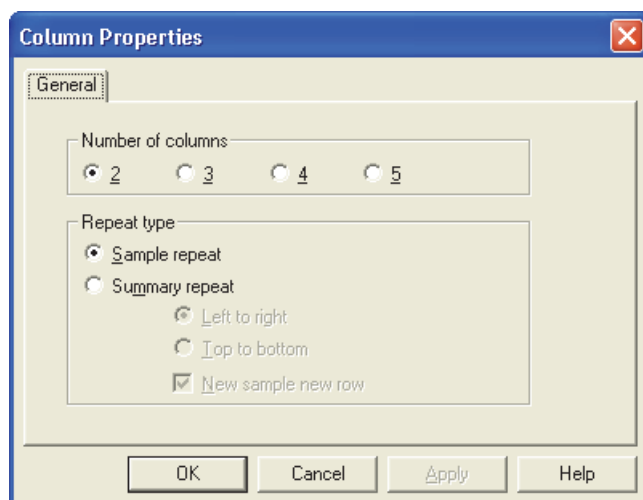
After you have configured a column object, drag objects to the columns.

❖ To configure a column object

1. To configure a column object, right-click it and choose **Properties** from the shortcut menu.

The Column Properties dialog box opens ([Figure 79](#)).

Figure 79. Column Properties dialog box



2. Select the number of columns to use in the Number of Columns area.
3. If the column object is in a nonrepeating section, configure the options in the Repeat type area. Select **Sample Repeat** or **Summary Repeat** by clicking the appropriate option. For an example of using these options, see [Set Sample Repeat Options](#) and [Set Summary Repeat Options](#).

The Repeat type options are not available in Quan repeating or Qual repeating sections.

4. If you selected Summary repeat, select whether you would like to repeat from **Left to Right** or from **Top to Bottom** by clicking the appropriate option.
5. To start each sample on a new row, select the **New Sample New Row** check box.

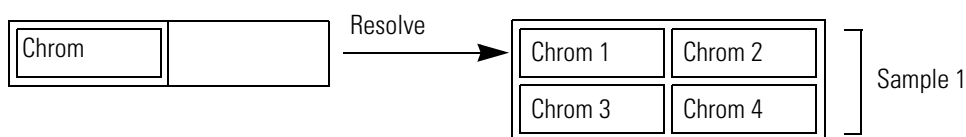
Set Sample Repeat Options

Use the Sample repeat option to present information relating to a raw data file of a single sample and the results created when processing it. Use this repeat type as a layout tool to indicate where objects are placed on the page of the resolved report.

Note The Sample repeat and Summary repeat options are applicable only in nonrepeating report sections. These options are not available in other types of report sections.

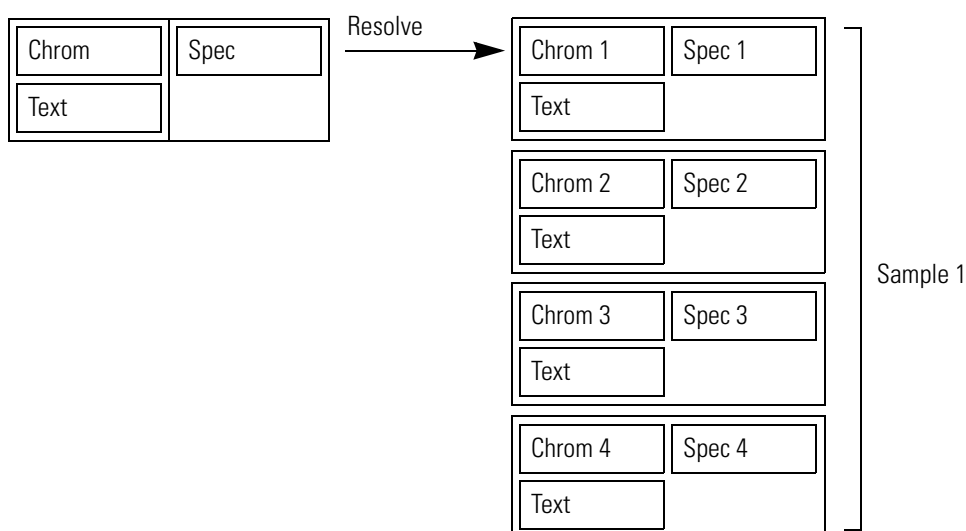
For example, when you place a 2-column object in a nonrepeating section, add a Quan-based chromatogram to the left column and combine or resolve the template using data of 1 sample with 4 components, the report appears as in [Figure 80](#).

Figure 80. 2-column object behavior in a nonrepeating section, with a chromatogram object



In another example, place a 2-column object in a nonrepeating section and add a chromatogram and a text object to the left column and a spectrum to the right column. Combine (resolve) the template using data of 1 sample with 4 components. All objects in the column are repeated for a single sample, and the report appears as in [Figure 81](#).

Figure 81. 2-column object behavior in a nonrepeating section, with chromatogram and spectrum objects



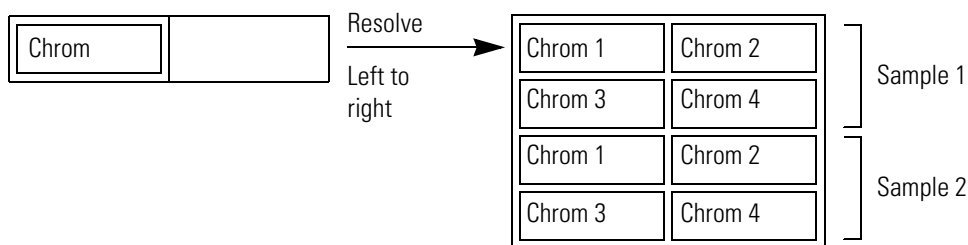
Set Summary Repeat Options

Use the Summary repeat option to present information relating to all of the samples in an Xcalibur sequence and the results created when processing them.

Note The Sample repeat and Summary repeat options are applicable only in nonrepeating report sections. These options are not available in other types of report sections.

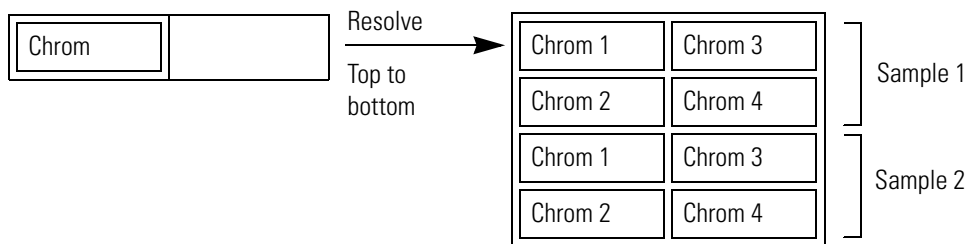
For example, when you place a 2-column object in a nonrepeating section, add a chromatogram (in either column), and combine (resolve) the template using data of 2 samples with 4 components each, the report appears as in [Figure 82](#).

Figure 82. 2-column object behavior in a nonrepeating section, with a chromatogram, Left to right option



If you choose instead the Top To Bottom option, the report appears as in [Figure 83](#).

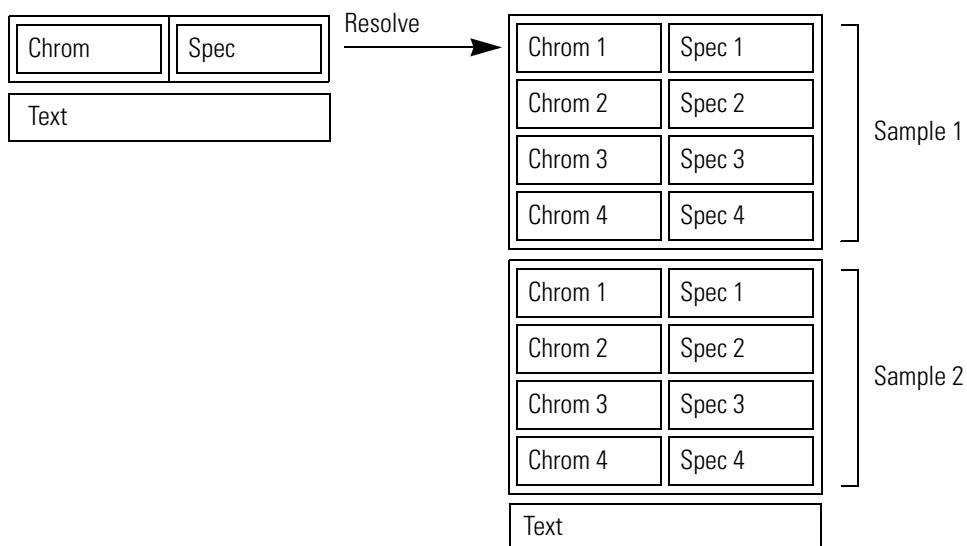
Figure 83. 2-column object behavior in a nonrepeating section, with a chromatogram, Top to bottom option



If you place an object in the right column and leave the left column empty, XReport combines the data as if the object is placed in the left column, as illustrated above.

If you place an object in each column, the Xcalibur data system ignores the Top to bottom and Left to right options. The report appears as in [Figure 84](#).

Figure 84. 2-column object behavior in a nonrepeating section, with chromatogram and spectrum objects



Sample XReport Template Files

The Xcalibur data system provides several sample XReport templates for you to use when creating your own reports. This appendix provides details of these report templates stored at the following location:

Xcalibur\templates

Table 2 describes the standard report templates.

Table 2. Sample XReport template files (Sheet 1 of 2)

Report template file name	Data source files	Description/Use
CalibrationFile.xrt	raw data file (RAW) calibration file (XCAL)	Generates sample reports with calibration data.
CompCalReport.xrt	result file (RST)	Generates summary reports showing processing method details, calibration curve, and sample table (Quan results). Can be used from Batch Processing and Quan Browser in the Xcalibur data system.
CompCalReport_Avalon.xrt	raw data file (RAW)	
CompCalReport_Genesis.xrt	processing method (PMD)	
CompCalReport_ICIS.xrt	sequence file (SLD)	
CustLibrSearRept.xrt	result file (RST)	Generates Qual sample reports that display Qual peaks and library search details. Use from Batch Processing in the Xcalibur data system.
LibrarySearchReport.xrt	raw data file (RAW)	
IonRatioConfirmation.xrt	result file (RST) raw data file (RAW) processing method (PMD)	Generates a Quan sample report containing non-graphical ion ratio confirmation results.
IonRatioConfirmationGraphical.xrt	result file (RST)	Generates Quan sample reports containing graphical ion ratio confirmation results. These report templates take advantage of the explicit confirmation ion settings available when using the XReport Chromatogram wizard.
IonRatioConfirmationGraphicalSimple.xrt	raw data file (RAW) processing method (PMD)	
IonRatioConfirmationGraphicalStacked.xrt		

Table 2. Sample XReport template files (Sheet 2 of 2)

Report template file name	Data source files	Description/Use
PeakIntegration.xrt	result file (RST) raw data file (RAW) processing method (PMD)	Generates a Quan sample report containing peak integration data generated using Genesis.
ProcessingMethod.xrt	processing method (PMD)	Generates processing method sample reports. Use from Processing Method Setup in the Xcalibur data system.
ProcessingMethod_Avalon.xrt		
ProcessingMethod_Genesis.xrt		
ProcessingMethod_ICIS.xrt		
QualPeakReport.xrt	result file (RST) raw data file (RAW)	Generates a simple Qual sample report. Use for data from Batch Processing in the Xcalibur data system.
QuanPeakResults_ESTD.xrt	result file (RST) raw data file (RAW)	Generates Quan sample reports. Can be used from Batch Processing or Quan Browser in the Xcalibur data system.
QuanPeakResults_ISTD.xrt	processing method (PMD)	
QuanResults.xrt		
QuanSimple.xrt		
QuantifySampleReport.xrt	result file (RST) raw file (RAW) processing method (PMD) sequence file (SLD)	Generates a Quan summary report containing chromatograms and a Quan summary table.
SequenceReport.xrt	sequence file (SLD)	Generates a summary report showing the sequence being processed. Use for batch processing in the Xcalibur data system. Refer to the <i>Xcalibur Data Acquisition and Processing User Guide</i> .
SpectrumCandidates.xrt	result file (RST) raw data file (RAW)	Generates a Quan summary report (only applicable to GC/MS). Use from batch processing or Quan Browser in the Xcalibur data system.

Types of Report Objects

The following tables list the report objects you can place onto a report template: text objects, table objects, graphic objects, and formatting objects. The tables briefly describe an object and indicate in which sections the object is available.

Contents

- [Text Object Descriptions](#)
- [Table Object Descriptions](#)
- [Graphic Object Descriptions](#)
- [Formatting Object Descriptions](#)

Text Object Descriptions

[Table 3](#) describes the text objects.

Table 3. Text objects (Sheet 1 of 3)

Text object	Data source file	Description	Section placement
Annotation	none	Displays static text. Use this object for adding headings or comments.	Any
Component Ident/Detect/Cal Settings	PMD	Displays the peak detection, calibration, and integration parameters for a single component.	Quan repeating
Component ISTD Settings Summary	PMD	Displays a summary of the configuration details for each component's ISTD configuration in the Quantitation section of a processing method.	Quan repeating
Component Settings Summary	PMD	Displays a short list of peak detection and integration parameters for a specified component.	Quan repeating

Table 3. Text objects (Sheet 2 of 3)

Text object	Data source file	Description	Section placement
Component Sys Suit/Flags Settings	PMD	Displays Calibration, Quantitation, and Detection flags and system suitability parameters to specify automatic chromatographic checks that assign a pass/fail qualification to a target peak.	Quan repeating
Instrument Method	RAW	Displays general instrument method parameters. This text object does not have any editable properties.	Nonrepeating
Processing Method – General	PMD	Displays general processing method parameters, including date created, date modified, baseline definition, chromatography type (LC/GC).	Nonrepeating
Processing Method – Qual	PMD	Displays Qual processing method parameters, including the following: • Identification • Spectrum Enhancement • Detection Options • Advanced Detection Options • Library Search Constraints • Library Search Options	Nonrepeating
Quan ISTD Peak Summary	RST or PMD	Displays summary parameters for a Quan component's associated ISTD peak. For example: • ISTD NameBase Line • Actual RTSIGNAL To Noise • Response Expected RT	Quan repeating
Quan Peak Summary	RST or PMD	Displays Component Peak summary parameters, for example: • Actual RT% Diff • Calculated AmountArea Ratio • Response Area ISTD • Base Line Specified Amount • Signal To Noise	Quan repeating, header or footer

Table 3. Text objects (Sheet 3 of 3)

Text object	Data source file	Description	Section placement
Report Info	none	Displays general information about the report itself.	Header or footer
Sample Header	RAW or SLD	Displays general information about a sample, for example: • Sample Name • Operator • Sample Type • Run Time • Acquisition Date	Nonrepeating, header or footer

Table Object Descriptions

Table 4 describes the table objects.

Table 4. Table objects (Sheet 1 of 3)

Table object	Data source file	Description	Section placement
Avalon Qual Events Table	PMD	Displays details of the Avalon peak detection algorithm events configured in the Qual section of a processing method.	Nonrepeating
Avalon Quan Events Table	PMD	Displays details of the Avalon peak detection algorithm events configured for a component in the Quan section of a processing method.	Quan repeating
Calibration File Table	XCAL, SLD, RAW	Displays component names, response factors, and %RSD of standards.	Nonrepeating
Component Cal Level Table	PMD	Shows the calibration levels, amounts, and acceptance test values defined for a specific component.	Quan repeating, or Nonrepeating
Component QC Level Table	PMD	Shows the QC levels, amounts, and percent test values defined for a specific component.	Quan repeating
Component Spectrum Table	PMD	Displays m/z and intensity data for up to fifty spectrum peaks. The data system uses this data to identify components when the Spectrum Peak Identification Method is specified in the processing method. This object is used only for GC chromatography.	Quan repeating

Table 4. Table objects (Sheet 2 of 3)

Table object	Data source file	Description	Section placement
Dilution Factor Table	RST	Displays the names of calibration levels and dilution factors for components that are not internal standards.	Nonrepeating
Electronic Signature	none	Displays up to five electronic signatures in table format. This object is not editable in XReport.	Any
Ion Ratio Confirmation Results Table	RST	Displays the following data about each qualifier ion, based on search criteria specified in the processing method: • Mass • Coelution test pass/fail • Ion Ratio Test Target (%) • Ion Ratio Test Window (%)	Quan repeating
IRC Settings Table	PMD	Displays up to five qualifier ions within tolerance limits to confirm the detection of a target analyte. The ions are specified in the processing method.	Quan repeating
IRC Summary Table	RST	Displays all of the information for the confirmation ion for each component. Most useful when the Name column is the first column.	Nonrepeating
Lib. Search Graph Table	RST, RAW	Displays the graphical results from a library search on a Qual peak (for example, Hit Spectrum, Delta, and Compound Structure).	Qual repeating
Lib. Search Results Table	RST, RAW	Displays the results of a Library Search on a Qual peak (for example, Name, Probability, RSI, SI, CAS#, Area).	Qual repeating
Proc. Method Programs Table	PMD	Displays a list of programs to be run by the Xcalibur data system after the sample has been analyzed and the data has been processed. The data system runs the programs in the order listed.	Nonrepeating
Proc. Method Sample Reports Table	PMD	Displays Sample Report information for each sample in a sequence, including Template name and the Report file name. Specify Sample Type in the processing method.	Nonrepeating

Table 4. Table objects (Sheet 3 of 3)

Table object	Data source file	Description	Section placement
Proc. Method Summary Reports Table	PMD	Displays Summary Reports to be issued after processing the samples in a bracketed or non-bracketed sequence.	Nonrepeating
Qual Peak Table	RST	Displays information specific to chromatogram peaks detected by qualitative analysis for a single sample.	Nonrepeating
Qual Summary Table	SLD, RST	Displays information specific to chromatogram peaks detected by qualitative analysis for all samples in a sequence.	Nonrepeating
Quan Peak Table	RST, PMD	Displays information specific to component peaks detected by quantitative analysis for a single sample.	Nonrepeating
Quan Summary Table	SLD, RST, PMD	Displays information specific to component peaks detected by quantitative analysis for all samples in a sequence.	Nonrepeating
Sample Table (Quan Results)	SLD	Displays system suitability and flag processing results for each component in a sample, and repeats this information for every sample in a sequence.	Quan repeating
Sequence Table	SLD	Displays the contents of the sequence file.	Nonrepeating
Spectrum Candidate Results Table	RST	Displays the results of spectrum candidate processing for GC/MS data on a per component basis. Parameters include the following: • Forward fitStart RT • Reverse fitEnd RT • MatchArea • Found RTHeight	Nonrepeating
Spectrum List Table	RST, RAW	Displays the text equivalent of the Spectrum graphic object. The Spectrum List Table contains a header and lists values for the <i>m/z</i> , intensity, and relative intensity.	Qual or Quan repeating

Graphic Object Descriptions

Table 5 describes the graphic objects.

Table 5. Graphic objects

Graphic object	Data source file	Description	Section placement
Bitmap	BMP, DIB, GIF, JPG, or ICO	Displays a graphical image, for example, a company logo.	Any
Chromatogram	RAW, RST	Displays a graphical trace that can show either raw data or processed data for any acquisition device supported by the data system (MS, Analog, A/D Card, PDA, UV).	Qual or Quan repeating and nonrepeating sections
Component Cal Curve	RST, PMD	Shows the calibration curve used to quantify a specified component. The curve is specified in the processing method as response versus amount of standard.	In a Quan repeating section, the Component Cal Curve object repeats on the component peaks. In a Nonrepeating section, the Component Cal Curve object uses the specified component.
Spectrum	RAW, RST	Displays a graphical spectrum that can show either raw data or processed data for any acquisition device supported by the data system (mass spectrometer, PDA detector).	Qual or Quan repeating and nonrepeating sections

Formatting Object Descriptions

Table 6 describes the formatting objects.

Table 6. Formatting objects

Graphic object	Data source file	Description	Section placement
Columns	none	Specify the layout and repeating properties of graphic and text objects.	Any
Page Break	none	Insert a manual page break in the report.	Qual or Quan repeating and nonrepeating sections

Sample Report

This appendix contains a sample Xcalibur report that is generated when you use PeakIntegration.xrt (located in the Xcalibur\templates folder) to generate a Quan sample report that contains certain peak integration data. The sample report uses the steroids02.rst data file from the Xcalibur\examples\data folder.

Contents

- [Peak Integration Report, Page 1](#)
- [Peak Integration Report, Page 2](#)
- [Peak Integration Report, Page 3](#)
- [Peak Integration Report, Page 4](#)

Peak Integration Report, Page 1

Peak Integration Report

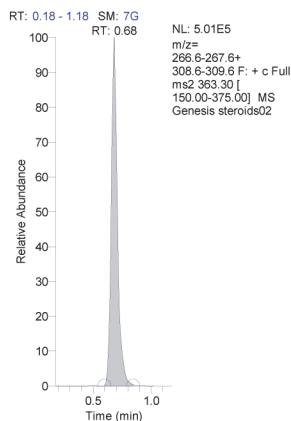
Data File:	steroids02	Original Data Path:	C:\pitcon\trial2	Current Data Path:	C:\Xcalibur\examples\data
Sample Type:	Std Bracket Start	Sample ID:	Sample02	Sample Name:	
Operator:	jackc	Acquisition Date:	02/28/96 11:20:31 AM	Run Time(min):	3.79
Comments:		Vial:	1	Scans:	336
Low Mass(m/z):	100.00	High Mass(m/z):	375.00	Sample Weight:	0.00
ISTD Amount:	0.000	Calibration Level:	3	Dilution Factor:	1.00
Instrument Method:		C:\pitcon\trial2\steroidMSMSis			
Original Processing Method:		C:\pitcon\trial2\steroidmsmsIS			
Current Processing Method:		C:\Xcalibur\examples\methods\steroid			

Peak Integration Report, Page 2

Peak Integration Report

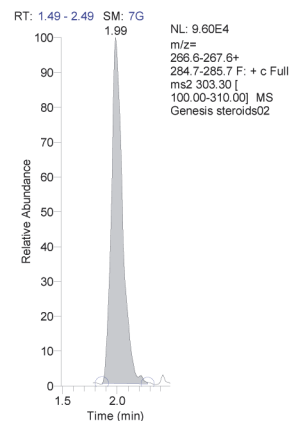
hydrocortisone

Expected
Retention
Time (min): 0.6
Retention
Time Window
(sec): 30.00000
View Width
(min): 1.00000
Retention
Time
Reference: No
Genesis
Minimum Peak
Height (S/N): 3.00
Genesis
Smoothing
Points: 7
Detector Type: MS
Valley
Detection
Enabled: No
Genesis
Constrain Peak
Width Enabled: No



methyltestosterone

Expected
Retention
Time (min): 2.0
Retention
Time Window
(sec): 30.00000
View Width
(min): 1.00000
Retention
Time
Reference: Yes
Genesis
Minimum Peak
Height (S/N): 3.00
Genesis
Smoothing
Points: 7
Detector Type: MS
Valley
Detection
Enabled: No
Genesis
Constrain Peak
Width Enabled: No



Component Name: hydrocortisone

Actual RT(min): 0.67783

Calculated Amount: 4.95592

Response: 1892942.72621

Base Line: BB

Signal To Noise: 707.56

%Diff: -0.88

Area Ratio: 2.763

Area(cts-sec): 1892942.72621

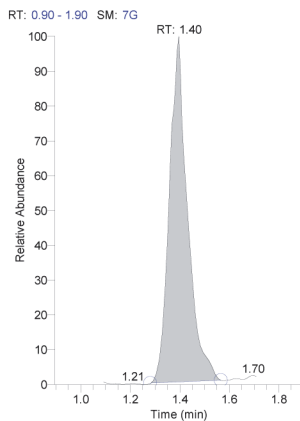
Specified Amount: 5.00000

Peak Integration Report, Page 3

Peak Integration Report

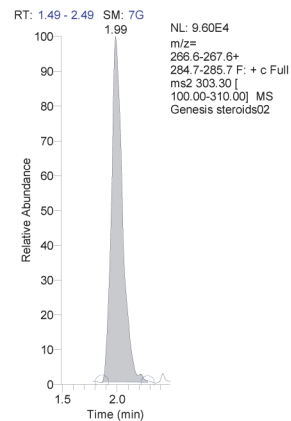
deoxycorticosterone

Expected Retention Time (min): 1.4
Retention Time Window (sec): 30.00000
View Width (min): 1.00000
Retention Time Reference: No
Genesis Minimum Peak Height (S/N): 3.00
Genesis Smoothing Points: 7
Detector Type: MS
Valley Detection Enabled: No
Genesis Constrain Peak Width Enabled: No



methyltestosterone

Expected Retention Time (min): 2.0
Retention Time Window (sec): 30.00000
View Width (min): 1.00000
Retention Time Reference: Yes
Genesis Minimum Peak Height (S/N): 3.00
Genesis Smoothing Points: 7
Detector Type: MS
Valley Detection Enabled: No
Genesis Constrain Peak Width Enabled: No



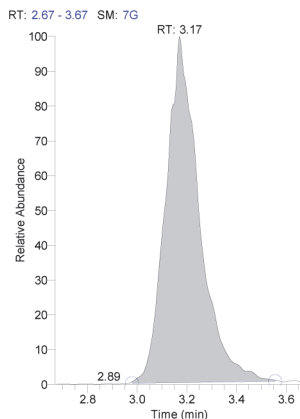
Component Name:	deoxycorticosterone	Actual RT(min):	1.39533	Calculated Amount:	5.10841
Response:	1040530.60245	Base Line:	BB	Signal To Noise:	148.23
%Diff:	2.17	Area Ratio:	1.519	Area(cts-sec):	1040530.60245
Specified Amount:	5.00000				

Peak Integration Report, Page 4

Peak Integration Report

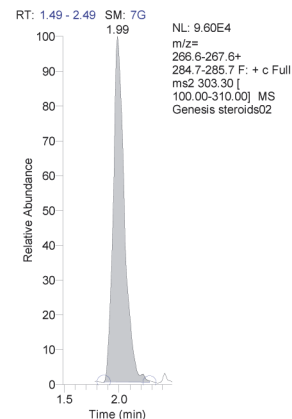
progesterone

Expected Retention Time (min): 3.2
Retention Time Window (sec): 30.00000
View Width (min): 1.00000
Reference: No
Genesis Minimum Peak Height (S/N): 3.00
Genesis Smoothing Points: 7
Detector Type: MS
Valley Detection Enabled: No
Genesis Constrain Peak Width Enabled: No



methyltestosterone

Expected Retention Time (min): 2.0
Retention Time Window (sec): 30.00000
View Width (min): 1.00000
Reference: Yes
Genesis Minimum Peak Height (S/N): 3.00
Genesis Smoothing Points: 7
Detector Type: MS
Valley Detection Enabled: No
Genesis Constrain Peak Width Enabled: No



Component Name: progesterone

Actual RT(min): 3.16867

Calculated Amount: 4.94898

Response: 2995893.97127

Base Line: BB

Signal To Noise: 344.16

%Diff: -1.02

Area Ratio: 4.373

Area(cts-sec): 2995893.97127

Specified Amount: 5.00000

XReport Application Features

This appendix provides reference material about the XReport application, including the XReport window and dialog boxes.

Contents

- [Reports View](#)
- [XReport Dialog Boxes](#)
- [Report Sections](#)
- [Report Objects](#)
- [Report Templates](#)

Reports View

Use the XReport application or the Reports view of the Processing Setup window to specify how the Xcalibur data system produces reports for samples and sequences. The data system provides several standard report formats. You can export results in a number of file formats including spreadsheet documents (XLS) and web pages (HTM or HTML).

For more information about the Reports view of the Processing Setup window, refer to the *Xcalibur Data Acquisition and Processing User Guide*.

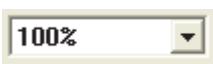
XReport Toolbar Buttons

Table 7 describes the XReport toolbar icons.

Table 7. Toolbar buttons (Sheet 1 of 2)

Icon	Description
	New Create a new report template for the program you select.
	Open Find and open XRT files.
	Save Save the current template as an XRT file. This option is not available if you are using a locked template. In this case, choose File > Save As and save the template with a different name.
	Cut Remove the currently selected objects and place them on the clipboard.
	Copy Copy the currently selected objects to the clipboard.
	Paste Insert the contents of the clipboard in the currently selected section.
	Align Left Align the left edges of the currently selected objects to the left edge of the first selected object. To select more than one object, click and drag a selection box around the objects or hold down the SHIFT key and click each object.
	Align Right Align the right edges of the currently selected objects to the right edge of the first selected object. To select more than one object, click and drag a selection box around the objects or hold down the SHIFT key and click each object.
	Align Top Align the top edges of the currently selected objects to the top edge of the first selected object. To select more than one object, click and drag a selection box around the objects or hold down the SHIFT key and click each object.

Table 7. Toolbar buttons (Sheet 2 of 2)

Icon	Icon	Description
	Align Bottom	Align the bottom edges of the currently selected objects to the bottom edge of the first selected object. To select more than one object, click and drag a selection box around the objects or hold down the SHIFT key and click each object.
	Auto Align	Snap all objects (selected or not) in the current section to the nearest upper and right grid lines.
	Center Horizontally	Center the current object on the page so that it is an equal distance from the left and right sides of the page.
	Center Vertically	Center the current object on the page so that it is an equal distance from the top and bottom sides of the page.
	Make Same Height	Enlarge all selected objects (except for the first selected) to match the height of the first selected object.
	Make Same Width	Enlarge all selected objects (except for the first selected) to match the width of the first selected object.
	Make Same Height and Width	Enlarge all selected objects (except for the first selected) to match the height and the width of the first selected object.
	Shrink Wrap	Shrink the template workspace to remove all unused workspace at the bottom of the section.
	Expand	Enlarge the template workspace to the full height of the section size.
	Zoom	Increase or decrease the magnification of the template display.
	Font	Change the font that is used in the currently selected object or change the global font settings if no object is selected.
	Resolve Report	Combine your report template with your data and view, save, and print your report.
	Help	Open Xcalibur Help.

XReport Menus

The XReport window has the following menus:

- [XReport File Menu](#)
- [XReport Edit Menu](#)
- [XReport View Menu](#)
- [XReport Layout Menu](#)
- [XReport Report Menu](#)
- [XReport Help Menu](#)

XReport File Menu

[Table 8](#) describes the File menu commands for the XReport application.

Table 8. File menu commands

Command	Description
New	Create a new template.
Open	Open a previously saved template.
Save	Save the current template. Note This option is not available if you are using a locked template. In this case, choose File > Save As and give the template a different name.
Save As	Save the current template with a different file name.
Page Setup	Define page layout and margin settings.
<i>Recently Used Files</i>	View the most recently opened template files. To open the template, select a filename in the list.
Close	Close the current template.
Exit	Close XReport.

XReport Edit Menu

Table 9 describes the Edit menu commands for the XReport application.

Table 9. Edit menu commands

Command	Description
Cut	Remove the currently selected objects and place them on the clipboard.
Copy	Copy the currently selected objects to the clipboard.
Paste	Insert the contents of the clipboard in the currently selected section.
Clear	Delete the currently selected objects.
Select All	Select all of the objects in the currently selected section.
Edit Object	Change the current object. For example, to enable resizing of columns in the table object.
Properties	Configure the current object. For example, for a bitmap object, you can select the source file.
Delete Section	Delete the currently selected section. This option is not available when objects are selected.

XReport View Menu

Table 10 describes the View menu commands for the XReport application.

Table 10. View menu commands

Command	Description
Report Template Grid	View or hide the grid in the current section. To change your grid settings, choose Layout > Preferences .
Report Template Outline	View or hide the Report Template Outline pane. This pane displays an overview of all sections and objects in your report template and opens at the right side of the XReport window.
Toolbars	View or hide the toolbars.
Status Bar	View or hide the status bar at the bottom of the XReport window.

XReport Layout Menu

Table 11 describes the Layout menu commands for the XReport application.

Table 11. Layout menu commands (Sheet 1 of 2)

Command	Description
Align > Left	Align the left edges of the currently selected objects to the left edge of the first selected object. To select more than one object, click and drag a selection box around the objects or hold down the SHIFT key and click each object.
Align > Right	Align the right edges of the currently selected objects to the right edge of the first selected object. To select more than one object, click and drag a selection box around the objects or hold down the SHIFT key and click each object.
Align > Top	Align the top edges of the currently selected objects to the top edge of the first selected object. To select more than one object, click and drag a selection box around the objects or hold down the SHIFT key and click each object.
Align > Bottom	Align the bottom edges of the currently selected objects to the bottom edge of the first selected object. To select more than one object, click and drag a selection box around the objects or hold down the SHIFT key and click each object.
Align > Auto	Snap all objects (selected or not) in the current section to the nearest upper and right grid lines.
Make Same Size > Width	Enlarge all selected objects (except for the first selected) to match the width of the first selected object.
Make Same Size > Height	Enlarge all selected objects (except for the first selected) to match the height of the first selected object.
Make Same Size > Both	Enlarge all selected objects (except for the first selected) to match the height and the width of the first selected object.
Center In Page > Vertical	Center the current object on the page so that it is an equal distance from the left and right sides of the page.
Center In Page > Horizontal	Center the current object on the page so that it is an equal distance from the top and bottom sides of the page.
Shrink Wrap	Shrink the current section to fit all of the objects that it contains.

Table 11. Layout menu commands (Sheet 2 of 2)

Command	Description
Expand	Enlarges the current section so you can add additional objects.
Preferences	Change grid settings, enable actions, and view or hide template configuration dialog box.

XReport Report Menu

Table 12 describes the Report menu commands for the XReport application.

Table 12. Report menu commands

Command	Description
Data Sources	Specify the data files for the report.
Simulate Report	View your template before adding real data.
Resolve Report	Display the report with data filled in. Select data in the Data Sources dialog box.
Print Report	Print the current report.

XReport Help Menu

Table 13 describes the Help menu commands for the XReport application

Table 13. Help menu commands

Command	Description
Xcalibur Help	View Xcalibur Help.
Glossary	View the glossary.
How to Use Help	View How to Use Help.
About XReport	Open the About XReport dialog box. The About XReport dialog box displays the version number of XReport, along with copyright information.

XReport Dialog Boxes

You can access the following dialog boxes from the XReport application:

- [Repeating Section Properties Dialog Box](#)
- [Chromatogram Properties Dialog Box and Wizard](#)
- [Spectrum Properties Dialog Box](#)
- [Table Properties Wizard](#)
- [Edit Formula For Dialog Box](#)
- [Configure Function Dialog Box](#)
- [Spectrum List Table Properties Dialog Box](#)
- [Average Scan Filter Selection Dialog Box](#)
- [Library Search Graphics Table Properties Dialog Box](#)
- [Library Search Results Table Properties Dialog Box](#)
- [Sample Table Properties Dialog Box](#)
- [Text Object Properties Dialog Box](#)
- [Bitmap Properties Dialog Box](#)
- [Column Properties Dialog Box](#)
- [Component Calibration Curve Dialog Box](#)
- [Data Sources Dialog Box](#)
- [Electronic Signature Properties Dialog Box](#)
- [Font Dialog Box](#)
- [Preferences Dialog Box](#)
- [Preview Window](#)
- [Save As Dialog Box](#)
- [Template Configuration Dialog Box](#)
- [Page Setup Dialog Box](#)

Repeating Section Properties Dialog Box

Use the Repeating Section Properties dialog box to customize the following settings for your repeating section:

- Including or exclude internal standards or target compounds from a Quan repeating section
- Specifying the order in which peaks and components are repeated
- Defining any limit on the number of peaks reported
- Specifying page breaks in the final report

The Repeating Section dialog box has these pages:

- [Exclude Page](#)
- [Ordering Page](#)
- [Page Breaks Page](#)

Exclude Page

Use the Exclude page of the Repeating Section Properties dialog box to indicate components to exclude from a Quan repeating section, and whether to discard any components that have not been found.

For more information, see [Configuring a Repeating Section](#).

[Table 14](#) describes the parameters on the Repeating Section Properties – Exclude page.

Table 14. Exclude page parameters

Parameter	Description
Repeating Section Excludes	
Exclude Component Type	Exclude specific compounds from the Quan configurations: • None • Internal Standards • Target Compounds
Show Only Found Components	Discard any components that have not been found.

Ordering Page

Set parameters on the Ordering page of the Repeating Section Properties dialog box to indicate the order for peaks or components in the repeating section.

Table 15 describes the parameters on the Repeating Section Properties – Ordering page.

Table 15. Ordering page parameters

Parameter	Description
Repeating Section Ordering	
Order By	Choose a value that determines the order for the peaks or components in the section: • RT • Component Name • Peak Height Intensity • Peak Area Intensity • Peak Response Intensity • Component Concentration
Ordering Direction	
Ascending or Descending	Choose an order for the peaks or components in the section by the property in the Order By list from lowest to highest (ascending) or highest to lowest (descending).
Repeating Records Maximum	
Limit number of reported peaks or components to	Limit the total number of peaks or components that are included in the repeating section.

Page Breaks Page

Set parameters on the Page Breaks page of the Repeating Section Properties dialog box to indicate where to apply page breaks in your report.

Table 16 describes the parameters on the Repeating Section Properties – Page Breaks page.

Table 16. Page Breaks page parameters

Parameter	Description
Each peak contained on its own page(s)	Insert a page break before and after each peak in the repeating section.
No page breaks between the individual peaks	Remove page breaks between each peak in the repeating section.
Page break before the repeating section	Insert a page break before the repeating section.
Page break after the repeating section	Insert a page break after the repeating section.

Chromatogram Properties Dialog Box and Wizard

The Chromatogram Properties dialog box displays a preview of the current chromatogram settings.

❖ To change these settings

Click **Configure**.

The Chromatogram Properties wizard opens.

Use the Chromatogram Properties wizard to configure any of these settings for the Chromatogram report object that is contained in your report template:

- Chromatogram and peak type
- Use of a demo file
- Plot details
- Smoothing parameters
- Use of MS Quan traces
- Chromatogram display, style, labeling, axes, and normalization methods

This Chromatogram Properties wizard displays different pages and contains different options, depending on the type of section containing the chromatogram report object and the selections for the chromatogram type and peak type properties.

The Chromatogram Properties wizard can contain the following pages:

- [Advanced Qual Peak Annotation Options](#)
- [Advanced Quan Peak Annotation Options](#)
- [Configure the Look of the Peak Window](#)
- [Configure Normalization For The Chromatogram](#)
- [Select a Peak Dialog Box](#)
- [Select Chromatogram Style](#)
- [Select Chromatogram Type](#)
- [Select Component](#)
- [Select Demo File](#)
- [Select Enhance Details](#)
- [Select How the Chromatogram Axes Will Be Configured](#)
- [Select Mass Spectrum Quan Traces to Display](#)
- [Select Plot Details](#)
- [Select the Peak Labeling](#)
- [Select the Qual Peak](#)
- [Select the Quan Peak](#)
- [Use Container Supplied Qual Peak](#)
- [Use Container Supplied Quan Peak](#)

Advanced Qual Peak Annotation Options

Set advanced Qual peak annotation parameter on the Advanced Qual Peak Annotation Options page of the Chromatogram Properties wizard. When you set advanced labeling options, only the Qual peak is labeled.

Note If you are in a Quan or nonrepeating section, choose a Qual results-based chromatogram.

Table 17 describes the parameters on the Chromatogram Properties – Advanced Qual Peak Annotation Options page.

Table 17. Advanced Qual Peak Annotation Options page parameters

Parameter	Description
Use Advanced Qual Peak Annotation	Turn on the advanced Qual peak options.
Custom Peak Labels	
Custom Text Label	Label the Qual peak with a custom label.
Retention Time	Label the Qual peak with the retention time.
RT Labeling	
Units	Define the units for the retention time.
Decimals	Specify the number of decimal places to be displayed in the retention time label.

Advanced Quan Peak Annotation Options

Set advanced Quan peak annotation parameters on the Advanced Quan Peak Annotation Options page of the Chromatogram Properties wizard. When you set advanced labeling options, only the Quan peak is labeled.

Note If you are in a Qual or nonrepeating section, choose a Quan results-based chromatogram.

Table 18 describes the parameters on the Chromatogram Properties – Advanced Quan Peak Annotation Options page.

Table 18. Advanced Quan Peak Annotation Options page parameters (Sheet 1 of 2)

Parameter	Description
Use Advanced Quan Peak Annotation	Turn on the advanced Quan peak options.
Custom Peak Labels	
Component Name	Label the Quan peak with the component name.
Component Key	Label the Quan peak with the component key.
Custom Text Label	Label the Quan peak with a custom text label.
Retention Time	Label the Quan peak with the retention time.
RT Labeling	
Units	Specify the units for the retention time.

Table 18. Advanced Quan Peak Annotation Options page parameters (Sheet 2 of 2)

Parameter	Description
Decimals	Define the number of decimal places to be displayed in the retention time label.
Overlaid QI Identifier	
Show QI Peak Label	Label overlaid qualifier ion peaks with a label identifying the qualifier ion. This option is only available when you select one of these options: • The All Quan Traces option on the Select Mass Spectrum Quan Traces to Display page. • The Overlay (3D) option on the Select Chromatogram Style page.

Configure the Look of the Peak Window

Set parameters on the Configure How The Peak Window Will Look page of the Chromatogram Properties wizard to control the display of baselines (Quan and Qual peaks) and the peak window width (Qual peak and in some cases Quan peaks) when a peak from a result file is set to display in a chromatogram.

[Table 19](#) describes the parameters on the Chromatogram Properties – Configure How The Peak Window Will Look page.

Table 19. Configure How the Peak Window Will Look page parameters

Parameter	Description
Show Baselines	View the baselines for a chromatogram peak (Quan or Qual). If you do not select this option, the Xcalibur data system hides the baselines, peak tracing, and full peak annotation.
Set Custom Window Width	Override the default value of the peak window width (the default is peak width plus one min) manually. This option is always available for Qual peaks and is sometimes available for Quan peaks.
Custom Width (min)	Define the Custom window width. The default value is 0.75 min.

Configure Normalization For The Chromatogram

Set parameters on the Configure Normalization For The Chromatogram page of the Chromatogram Properties wizard to select the normalization (*y*-axis scaling) method used for the chromatogram.

Table 20 describes the parameters on the Chromatogram Properties – Configure Normalization For The Chromatogram page.

Table 20. Configure Normalization for the Chromatogram page parameters

Parameter	Description
Normalize Method	
Auto Zero	Optimize the <i>y</i> axis automatically for each chromatogram.
Intensity Range	Set the range manually. Type the minimum and maximum intensity required for the <i>y</i> axis. The value can be from –200.0% to +200.0%.
Normalize Each Plot To	
Largest Peak In Subsection	Normalize each split time range to the largest peak in the division.
Largest Peak In Selected Time Range	Normalize the chromatogram to the largest peak in the displayed time range.
Largest Peak In All Times	Normalize the chromatogram to the largest peak in the entire chromatogram.

Select a Peak Dialog Box

Use the Select a Peak dialog box to select a peak in a demo file that opens in the report preview.

Table 21 describes the parameters in the Select a Peak dialog box.

Table 21. Select a Peak dialog box parameters

Parameter	Description
Result File	Select the name of the result file to be the demo file.
Peak Type	Define the peak type (Quan or Qual) in the result file.
Peak List	View the list of peaks that are in the result file.

Select Chromatogram Style

Use the Select Chromatogram Style page of the Chromatogram Properties wizard to determine the appearance of the chromatogram.

Table 22 describes the parameters on the Chromatogram Properties – Select Chromatogram Style page.

Table 22. Select Chromatogram Style page parameters

Parameter	Description
Plotting	
Point-to-Point (see Figure 63)	Display point-to-point peak profiles.
Stick	Display the chromatogram as vertical lines.
Arrangement	
Stack (2D)	Stack plots vertically (same <i>x</i> axis) with no overlap (one <i>y</i> axis for each plot).
Overlay (3D)	Move plots vertically (same <i>x</i> axis) with an optional horizontal skew (<i>y</i> -axis time offset). When selected, the 3D display options are turned on. Use the 3D arrangement if you selected Multiple Quan Traces on the Select Mass Spectrum Quan Traces to Display page.
3D	
Elevation	Set the elevation angle (amount of overlay) from 0 to 60 degrees for the 3D plot style.
Skew	Set the skew angle (time offset) from 0 to 45 degrees for the 3D plot style.
Draw Backdrop	Add a drawn perspective backdrop to 3D plots.

Select Chromatogram Type

Set the chromatogram type for the chromatogram report object being configured in your report template on the Select Chromatogram Type page of the Chromatogram Properties wizard.

[Table 23](#) describes the parameters on the Chromatogram Properties – Select Chromatogram Type page.

Table 23. Select Chromatogram Type page parameters

Parameter	Description
Chromatogram Type	
Raw File Based Chromatogram	Indicate the chromatogram is based on a raw data file (RAW).
Quan Results Based Chromatogram	Indicate the chromatogram is based on Quan results.
Qual Results Based Chromatogram	Indicate the chromatogram is based on Qual results.
Show All Qual Peaks In Result File	Display all Qual peaks in the finished report.

Select Component

Set parameters in the Select Component dialog box of the Chromatogram wizard to select a component to display when configuring a chromatogram.

For information about selecting the component for a Quan peak, where the chromatogram type is a Quan results based chromatogram, see [Select the Quan Peak Page](#).

[Table 24](#) describes the parameters in the Select Component dialog box of the Chromatogram wizard.

Table 24. Select Component page parameters

Parameter	Description
Processing	View the name of the currently selected processing method (PMD) file or select a different processing method file.
Component List	View a list of components found in the processing method file. Select a component from this list.

Select Demo File

Set parameters on the Select Demo File page of the Chromatogram wizard to associate a demo file (RAW or RST) with a chromatogram report object. Use the demo file to see how the chromatogram report object appears with its current settings when applied to real data.

The appearance of the Select Demo File page depends on the chromatogram type and the peak type settings chosen on the Chromatogram Type page.

[Table 25](#) describes the parameters on the Chromatogram wizard – Select Demo File page.

Table 25. Select Demo File page parameters

Parameter	Description
Use Demo File	
Use Demo File	Connect a demo file with the chromatogram report object.
Demo File	Specify the path to the demo file.
Demo Peak	
Quan Component	Specify the Quan peak to use in the demo file. Click the Browse button. The Select a Peak Dialog Box opens. This box appears only if you are configuring a Quan based chromatogram.
Qual Peak RT	Specify the Qual peak to use in the demo file. Click the Browse button. The Select a Peak Dialog Box opens. This box appears only if you are configuring a Qual based chromatogram, and not showing all Qual peaks. Select these options on the Select Chromatogram Type page.

Select Enhance Details

Set parameters on the Select Enhance Details page of the Chromatogram Properties wizard to enhance a chromatogram plot by applying smoothing.

Table 26 describes the parameters on the Chromatogram Properties – Select Enhance Details page.

Table 26. Select Enhance Details page parameters

Parameter	Description
Enable Smoothing	Apply smoothing to the chromatogram.
Smoothing Details	
Type	Define the type of smoothing algorithm applied to the chromatogram, either Boxcar or Gaussian.
Points	Specify the number of smoothing points to use in the smoothing algorithm.

Select How the Chromatogram Axes Will Be Configured

Set chromatogram axes labels and display parameters on the Select How The Chromatogram Axes Will Be Configured page of the Chromatogram Properties wizard.

Table 27 describes the parameters on the Chromatogram Properties – Select How The Chromatogram Axes Will Be Configured page.

Table 27. Select How the Chromatogram Axes Will Be Configured page parameters (Sheet 1 of 2)

Parameter	Description
X axis	
Name	View or change the name of the <i>x</i> axis.
Offset	Move the <i>x</i> -axis label away from the chromatogram.
Split Time Range	Split the chromatogram into two or more separate graphs with equal time ranges.
Divisions	Define the number of split time range graphs to be displayed for each chromatogram.
Y axis	
Label	
From Detector	Use the detector-specific label for the <i>y</i> axis (stored in the RAW file).
Custom	Use your own label for the <i>y</i> axis.
Units	
Absolute	Use absolute units for the <i>y</i> axis.

Table 27. Select How the Chromatogram Axes Will Be Configured page parameters (Sheet 2 of 2)

Parameter	Description
Relative	Use relative units for the <i>y</i> axis.
Name	Define the custom name of the <i>y</i> axis. This box is available only when you click the Custom option in the Label area.
Offset	Move the <i>y</i> axis label away from the chromatogram.

Select Mass Spectrum Quan Traces to Display

Set parameters on the Select Mass Spectrum Quan Traces To Display page of the Chromatogram Properties wizard to configure the Quan Traces property for MS data. Options on this page only apply to MS data and are ignored for other detector types. When a chromatogram report object displays a Quan component, there are potentially six traces associated with the component: the Quan Mass (QM) trace (the actual component peak) and up to five qualifier ions.

Select any of these possible six traces to be displayed in the chromatogram or display all of the available traces of the component.

Table 28 describes the parameters on the Chromatogram Properties – Select Mass Spectrum Quan Traces To Display page.

Table 28. Select Mass Spectrum Quan Traces to Display page parameters

Parameter	Description
Quan Traces	
Quan Traces	Specify the Quan traces to display. Selections:
Common Normalization For All Traces	Normalize all of the traces the same way. This check box is available only when you select All Quan Traces from the Quan Traces list.

Select Plot Details

Set parameters on the Select Plot Details page of the Chromatogram Properties wizard to configure how the plot is drawn when you configure a raw file-based chromatogram.

❖ To configure a plot

1. If you are in a Qual or Quan repeating section, the Use Container Supplied Qual or Quan Peak page opens. Select the **Explicitly Specify the Chromatogram's Behavior** check box and click **Next**.

2. On the Select Chromatogram Type page, select a raw file based chromatogram and follow the pages of the wizard until the Select Plot Details page opens.

Table 29 describes the parameters on the Chromatogram Properties – Select Plot Details page.

Table 29. Select Plot Details page parameters (Sheet 1 of 2)

Parameter	Description
Plot Type	
Detector	View the type of detector used to generate the raw data file.
Delay (min)	Specify the delay for the start of the chromatogram trace.
Filter	View the processing that is applied to a subset of the scans in the RAW file. The list displays scan filter options that are stored in the selected demo RAW file. If no demo file is selected, type a valid filter string. This option is only available when an MS detector is selected.
Trace	The first list indicates the basic chromatogram type, for example, TIC. The second list indicates a logical operator: + or –. The third list indicates a second chromatogram type to add to, or subtract from, the first trace. For example, Mass Range. The list of traces depends on the detector used to generate the data as follows: • Detector Type • Valid Traces • MS • Mass Range, TIC, Neutral Fragment, and Base Peak • Analog • Analog 1–4 • A/D Card • A/D Card Ch. 1–4 • PDA • Wavelength Range, Total Scan, and Spectrum Maximum • UV • Channel A–D

Table 29. Select Plot Details page parameters (Sheet 2 of 2)

Parameter	Description
Mass (m/z)	Define the display for the mass or mass range for Mass Range or Base Peak traces for MS detector types as follows: If you choose Base Peak $\pm$ Mass Range or Mass Range $\pm$ Mass Range plot combinations, the identification page displays a Mass (m/z) field for each trace type. If you use other detector types, use this field to specify the wavelength or wavelength range for the chromatogram. If you use a plot combination such as <i>Wavelength Range + Wavelength Range</i>, an additional Wavelength (nm) box opens. The valid range depends on the configured detector. The format is <i>low mass/wavelength–high mass/wavelength</i>. Separate entries with a dash, no spaces. For example, for the range m/z 123 through 456, type 123–456.
Time Range (min)	Specify the upper and lower time limits for the plot in minutes, to one decimal place. Separate entries by a dash, with no spaces. The default setting is “*”, which means to display the entire time range for the plot.
Fixed Scale	Set the y-axis maximum to a specific value. Clear this check box to activate the Normalize To area on the Configure Normalization For The Chromatogram page.
Autofilter	Repopulate a chromatogram view with • A plot showing the chromatogram without any scan filters • Plots for each scan filter applied to the chromatogram

Select the Peak Labeling

Set parameters on the Select the Peak Labeling page of the Chromatogram Properties wizard to choose the type and style of peak labels.

Table 30 describes the parameters on the Chromatogram Properties – Select the Peak Labeling page.

Table 30. Select the Peak Labeling page parameters

Parameter	Description
Label With	
Retention Time	Label the peaks with the time in minutes, prefixed by RT .
Scan Number	Label the peaks with number of mass scans at peak maximum, prefixed by S# .
Base Peak	Label the base peak in the mass spectrum of the chromatogram peak, prefixed by BP .
Signal To Noise	Label the peaks with the signal-to-noise ratio at the peak maximum, prefixed by SN .
Flags	Label the peaks with flags providing supplemental information about the peak data. For example, if a peak is saturated, the data system displays an S above the peak.
Area	Label the peaks with the integrated area of the peaks, prefixed by AA if detected automatically or MA if detected manually.
Height	Label the peaks with the apex height, prefixed by AH if detected automatically or MH if detected manually.
Label Styles	
Offset	Move a label away from its normal position to avoid conflict with another label.
Size	Specify the offset size, measured in number of characters.
Rotated	Use vertical rather than horizontal mass labels. Flags are always displayed unrotated.
Boxed	Place a rectangular outline around each peak mass label. Flags are not boxed.
Label Threshold	Limit the labeling of peaks to those exceeding the specified percentage of the base peak.
Advanced	Set advanced labeling options. Only the Quan or Qual peak is labeled if you click this option.

Select the Qual Peak

Set the parameter on the Select the Qual Peak page to explicitly specify the Qual peak for a Qual results-based chromatogram report object.

Table 31 describes the parameter on the Chromatogram Properties – Select the Qual Peak page.

Table 31. Select the Qual Peak page parameter

Parameter	Description
Qual Peak To Display	
Retention Time (min)	The retention time of the Qual peak. The retention time can be any time between the start and end peak boundaries. You must select a valid retention time to combine template and data correctly. If the file used to resolve the report does not contain the specified retention time, the Xcalibur data system removes the chromatogram from the report.

Select the Quan Peak

Set parameters on the Select the Quan Peak page of the Chromatogram Properties wizard to explicitly specify the Quan peak (component) for a Quan results-based chromatogram report object.

Table 32 describes the parameters on the Chromatogram Properties – Select the Quan Peak page.

Table 32. Select the Quan Peak page parameters

Parameter	Description
Quan Peak	
Quan Peak	Set the name of the Quan peak. To select a processing method (PMD) file and select a component, click the Browse button. The Select Component dialog box opens.
Use Quan Peak's Associated Internal Standard	Use the associated internal standard of the Quan peak instead of the Quan peak. You must select a valid peak for XReport to resolve the report correctly. If the file used to resolve the report does not contain the specified peak, the chromatogram is removed from the resolved report.

Use Container Supplied Qual Peak

Set the parameter on the Use Container Supplied Qual Peak page of the Chromatogram Properties wizard to ignore the implicit Qual peak and explicitly configure the chromatogram type.

Table 33 describes the parameters on the Chromatogram Properties – Use Container Supplied Qual Peak page.

Table 33. Use Container Supplied Qual Peak page parameter

Parameter	Description
Explicit Chromatogram Type	
Explicitly Specify The Chromatogram's Behaviour	Ignore the implicit Quan peak supplied by the container and explicitly configure the chromatogram type.

Use Container Supplied Quan Peak

Set parameters on the Use Container Supplied Quan Peak page of the Chromatogram Properties wizard to either display the details of the internal standard associated with the implicit Quan peak or ignore the implicit Quan peak and explicitly configure the chromatogram type.

Table 34 describes the parameters on the Chromatogram Properties – Use Container Supplied Quan Peak page.

Table 34. Use Container Supplied Quan Peak page parameters

Parameter	Description
Implicit Quan Peak Options	
Use Quan Peak's Associated Internal Standard	View the details of the internal standard associated with the implicit Quan peak.
Explicit Chromatogram Type	
Explicitly Specify The Chromatogram's Behaviour	Ignore the implicit Quan peak supplied by the container and explicitly configure the chromatogram type.

Spectrum Properties Dialog Box

Use the Spectrum Properties dialog box to configure the settings for your spectrum report object.

Spectrum Properties dialog box pages:

- [Axis Page for a Spectrum Object](#)
- [Enhance Page for a Spectrum Object](#)
- [Labels Page for a Spectrum Object](#)
- [Normalization Page for a Spectrum Object](#)
- [Options Page for a Spectrum Object](#)
- [Peak Page for a Spectrum Object](#)
- [Plot Type Page for a Spectrum Object](#)
- [Style Page for a Spectrum Object](#)

Axis Page for a Spectrum Object

Set spectrum axis labels and display options on the Axis page of the Spectrum Properties dialog box.

[Table 35](#) describes the parameters on the Spectrum Properties – Axis page.

Table 35. Axis page parameters (Sheet 1 of 2)

Parameter	Description
X axis	
Name	View or change the name for the x axis.
Offset	Move the axis label away from the spectrum.
Split Mass Range	Split the spectrum into two or more separate graphs with equal ranges.
Divisions	View the number of split range graphs for each spectrum.
Y axis	
Label	
From Detector	Use the detector-specific label for the y axis (stored in the raw data file).
Custom	Use your own label for the y axis.
Name	Specify the name for the y axis if you selected Custom label above.
Offset	Move the axis label away from the spectrum.

Table 35. Axis page parameters (Sheet 2 of 2)

Parameter	Description
Units	
Absolute	Use absolute units on the <i>y</i> axis.
Relative	Use relative units on the <i>y</i> axis.

Enhance Page for a Spectrum Object

Specify spectrum enhancement details on the Enhance page of the Spectrum Properties dialog box.

Note Clear the Use Processing Method Properties For Plot Type And Enhancement Info check box on the [Options Page for a Spectrum List Table](#) to modify the Enhance page parameters.

[Table 36](#) describes the parameters on the Spectrum Properties – Enhance page.

Table 36. Enhance page parameters (Sheet 1 of 2)

Parameter	Description
Smoothing	
Enable	Turn on spectrum smoothing.
Type	Specify the type of smoothing algorithm to apply to the spectrum. Choose from Boxcar or Gaussian.
Points	Specify the number of points for spectrum smoothing. This must be an odd number from 3 (minimum smoothing) to 15 (maximum smoothing).
Refine	
Enable	Turn on refine spectrum enhancement.
Window	Define an area for drawing a peak by specifying the number of seconds on either side of the specified point. A reasonable initial value is the peak width in seconds.
Noise Threshold	Specify the cutoff point for peaks. Type 0 to show all peaks in the spectrum and slowly increase the value until the noise peaks are eliminated. Use this setting to eliminate peaks generated from baseline noise.

Table 36. Enhance page parameters (Sheet 2 of 2)

Parameter	Description
Background Subtraction	
This area shows details of background subtraction if it was applied to the spectrum. The background contribution is determined by averaging the scans from one or two baseline regions.	
Time Range 1	Add a first baseline region that is used for assessing the background. When you click this option, the Xcalibur data system activates a box. Type the time range to use in the box.
Time Range 2	Add a second baseline region that is used for assessing the background.

Labels Page for a Spectrum Object

Choose the type and style of peak labels on the Labels page of the Spectrum Properties dialog box.

Table 37 describes the parameters on the Spectrum Properties – Labels page.

Table 37. Labels page parameters (Sheet 1 of 2)

Parameter	Description
Label With	
Mass or Wavelength	Label the peaks with m/z values (if MS is selected as the detector on the Plot Type Page for a Spectrum Object) or wavelength values (if PDA is selected as the detector on the Plot Type Page for a Spectrum Object).
Flags	Label spectrum peaks with flags. Flags provide supplemental information about peak data. For example, if a peak is saturated, the Xcalibur data system displays an S above the peak.
Relative To	Move the m/z labels for the peaks away from the peaks by the specified amount.
Decimals	Specify the number of decimal places to be used in mass labels.
Label Styles	
Offset	Move a label from its normal position to avoid conflicts with other labels.
Size	Specify the offset size to use (in number of characters).
Rotated	Use vertical rather than horizontal mass labels. Flags are always displayed unrotated.

Table 37. Labels page parameters (Sheet 2 of 2)

Parameter	Description
Boxed	Place a rectangular outline around each peak mass label. Flags are not boxed.
Label Threshold	Specify a peak height level, in percent of the base peak. Above that level, XReport labels a peak.

Normalization Page for a Spectrum Object

Select normalization options for spectrum plots on the Normalization page of the Spectrum Properties dialog box.

Table 38 describes the parameters on the Spectrum Properties – Normalization page.

Table 38. Normalization page parameters

Parameter	Description
Normalize Method	
Auto Zero	Optimize the y axis automatically.
Intensity Range	Set the y-axis range. Use the box to type the minimum and maximum intensity. The valid range is from –200.00 to 200.00%.
Normalize To	
Largest Peak In Subsection	Normalize each split mass range to the largest peak in the division.
Largest Peak In Range	Normalize the spectrum to the largest peak in the displayed mass range.
Largest Peak In Scan	Normalize the spectrum to the largest peak in the entire spectrum.
Normalize Multiple Scans	
Individually	Normalize each mass plot individually.
All The Same	Normalize all mass plots equally.

Options Page for a Spectrum Object

Set spectrum parameters on the Options page of the Spectrum Properties dialog box.

Table 39 describes the parameters on the Spectrum Properties – Options page.

Table 39. Options page parameters

Parameter	Description
Use Processing Method Properties For Plot Type and Enhance Info	Use properties from the selected processing method to set plot type and enhance information for the spectrum.
Use ISTD Peak When Repeating On Component	Use the selected ISTD (internal standard) peak when repeating on a component. Select the Use Processing Method Properties For Plot Type and Enhance Info option to modify this parameter.

Peak Page for a Spectrum Object

Set parameters on the Peak page of the Spectrum Properties dialog box to explicitly specify the peak to display in the spectrum report object.

Table 40 describes the parameters on the Spectrum Properties – Peak page.

Table 40. Peak page parameters

Parameter	Description
You can explicitly specify the peak that you want to appear in a spectrum control	
Enable Explicit Peak Type	Activate controls so you can specify the type of peak to appear in the spectrum.
Peak Type	
Quan Peak	Specify a Quan peak.
Qual Peak	Specify a Qual peak.
Peak Identification	
Component Name	Define the name of the Quan peak or the retention time of the Qual peak. If you are entering a Qual peak, you can type any time between the start time and end time of the peak.

Plot Type Page for a Spectrum Object

Configure how the spectrum is drawn on the Plot Type page of the Spectrum Properties dialog box.

Note The parameters in the Plot Type page are enabled only when you clear the Use Processing Method Properties For Plot Type And Enhancement Info check box on the [Options Page for a Spectrum List Table](#).

[Table 41](#) describes the parameters on the Spectrum Properties – Plot Type page.

Table 41. Plot Type page parameters

Parameter	Description
Mass Range or Wavelength Range	Specify the mass or mass range for MS detector types. For PDA detector types, use this box to specify the wavelength or wavelength range (nm). Type the upper and lower limits for the plot. Separate entries by a dash, with no spaces. To use the entire mass or wavelength range, type an asterisk (*).
Detector	View the type of detector that was used to generate the raw data file. Valid types are MS and PDA. The type of detector determines the available plot types.
Time	View or change the time of the mass scan in the host chromatogram. Type a new value or range as required.
Scan Filter	Specify the scan filter to apply to your data. Select a filter from the list or type a new filter using the scan filter format.
Demo File	Specify the path and filename of the demo file (raw data file) that is used to generate a preview of the selected plot.

Style Page for a Spectrum Object

On the Style page of the Spectrum Properties dialog box, set parameters that determine the appearance of the spectrum.

[Table 42](#) describes the parameters on the Spectrum Properties – Style page.

Table 42. Style page parameters

Parameter	Description
Plotting	
Automatic	Choose the graphic style based upon the data acquisition method that was used for the active spectrum.
Point To Point	Display point-to-point peak profiles.
Stick	Display the spectral mass peaks as vertical lines.
Shade	Display the spectrum as a shaded representation of intensity in each amu band for the active spectrum.

Table Properties Wizard

Use the table properties (*Table Name* Properties) wizard to customize the following settings for your table:

- Which columns to include in the table
- Custom table column settings
- Table sort order

The Table Properties wizard has these pages:

- [Configure User Column Parameters Page](#)
- [Select Table Fields Page](#)
- [Set Table Sort Filter Page](#)
- [Set Table Font Page](#)

Configure User Column Parameters Page

Configure any custom (User) columns that you selected to include in your table on the Configure User Column Parameters page of the table properties wizard. Complete the parameters on this page for each custom column that you selected.

For more information, see [Configuring Custom \(User\) Columns](#).

[Table 43](#) describes the parameters on the Configure User Column Parameters page of the table properties wizard.

Table 43. Configure User Column Parameters page parameters

Parameter	Description
User Columns	Define the custom columns to include in your table. Select the column to customize.
User Column Title	
User Column Title	Provide a descriptive title for the column.
User Column Formula	
User Column Formula	View the formula for the current column (read-only box). To edit the formula, click Edit Formula .
Edit Formula	Change your formula.

Select Table Fields Page

Choose the columns for the table on the Select Table Fields page of the table properties wizard. The columns available for a table are given in alphabetical order, but can be added to a report template in any order. The columns that you can select depend on the type of table object that you are configuring.

[Table 44](#) describes the parameters on the Select Table Fields page of the table properties wizard.

Table 44. Select Table Fields page parameters (Sheet 1 of 2)

Parameter	Description
Title	View the custom title of the selected object.
Include The Title In The Resolved Report	Include the custom title in the final report.
Available Columns	View columns that are available for the selected table. A user column is a column that you can configure to display what you want on a later page of the wizard.

Table 44. Select Table Fields page parameters (Sheet 2 of 2)

Parameter	Description
Add	Add one or more columns to the table. Select one or more columns from the Available Columns list and click Add to add them to the table.
Add All	Add all of the available columns to the table.
Remove	Remove one or more columns from the table. Select one or more columns from the Selected list and click Remove to remove them from the table.
Remove All	Remove all of the columns from the selected list.
Selected	View the columns that are currently selected to be included in the table. The columns are listed in the order that they appear in the table.
Column Header	View the heading for the currently selected column.
Decimal Setting	View or change the number of digits displayed after the decimal point for values displayed in this column. This parameter is only available for some table fields.
Move Up	Move a column up in the Selected list. Select a column in the Selected list and click Move Up to move the column up in the list. This action moves the column to the left in the finished table.
Move Down	Move a column down in the Selected list. Select a column in the Selected list and click Move Down to move the column down in the list. This action moves the column to the right in the finished table.

Set Table Sort Filter Page

Set parameters on the Set Table Sort Filter page of the table properties wizard to define the order for table data when you generate a report using the chosen table object in the report template.

Note This page is not available for the Library Search Graphics Results table.

Table 45 describes the parameters on the Select Table Sort Filter page of the table properties wizard.

Table 45. Set Table Sort Filter page parameters

Parameter	Description
Column List	View the list of columns that are currently selected for the table.
Current Sorting Configuration	
First Order column	Select the first column that the Xcalibur data system uses to sort the table.
Ascending or Descending option	Select to sort in ascending or descending order.
Second Order column	Select the second column that the data system uses to sort the table. For instance, use this option in columns that have identical entries in the First Order column.
Ascending or Descending option	Select to sort in ascending or descending order.
Third Order column	Select the third column that the data system uses to sort the table. For instance, use this option in columns that have identical entries in the First Order and Second Order columns.
Ascending or Descending option	Select to sort in ascending or descending order.
Buttons	
Add	Add the selected column to the next available sort order.
Remove	Remove the last selected sort order.

Set Table Font Page

Configure the formatting of the currently selected table object on the Font page of the table properties wizard.

Table 46 describes the parameter on the Select Table Font page of the table properties wizard.

Table 46. Set Table Font page parameter

Parameter	Description
Title Font, Heading Font, Cell Font	Set and view the font settings for all of the title, headings, and cells in the table object. To configure your font, click the button. The Font Dialog Box opens.

Edit Formula For Dialog Box

Edit a formula for use in a custom column of your table in the Edit Formula For dialog box. For more information on formula syntax, see [Adding a Formula to a Table](#).

[Table 47](#) describes the parameters in the Edit Formula For dialog box.

Table 47. Edit Formula For dialog box parameters (Sheet 1 of 2)

Parameter	Description	
Formula	View the current formula. Type in this box directly or add functions from the list.	
Functions		
A list of available functions. A brief description of each of the functions appears at the bottom of the dialog box when each function is selected.		
Function	Syntax	Description
ABS	ABS(<i>x</i>)	Return the positive value of a number of a formula regardless of its actual positive or negative value.
AND	AND(<i>x</i> , <i>y</i>)	Return the value 1 if the logical expressions <i>x</i> and <i>y</i> are both true, or the value 0 if either expression is false.
AVERAGE	AVERAGE(<i>x</i> 1, <i>x</i> 2,..., <i>x</i> <i>n</i>)	Return the average of the list of values.
COUNT	COUNT(list)	Return the count of the number of items in a list.
FALSE	=FALSE	Return 0 (zero).
INT	INT(<i>x</i>)	Return the number to the left of the decimal place in the value or formula <i>x</i> .
MAX	MAX(<i>x</i> 1, <i>x</i> 2,..., <i>x</i> <i>n</i>)	Return the largest value in a list.
MIN	MIN(<i>x</i> 1, <i>x</i> 2,..., <i>x</i> <i>n</i>)	Return the smallest value in a list.
MOD	MOD(<i>x</i> , <i>y</i>)	Return the remainder from dividing the value <i>x</i> by the value <i>y</i> a number of times in integers.
NOT	NOT(<i>x</i>)	Return the value 0 (zero, false) if the logical expression <i>x</i> is true, or the value 1 (true) of the expression <i>x</i> is false.
OR	OR(<i>x</i> , <i>y</i>)	Return the value 1 (true) if either or both logical expressions <i>x</i> and <i>y</i> are true, or the value 0 (zero, false) if both expressions are false.
PRODUCT	PRODUCT(<i>x</i> 1, <i>x</i> 2,..., <i>x</i> <i>n</i>)	Return the result of multiplying a list of values.

Table 47. Edit Formula For dialog box parameters (Sheet 2 of 2)

Parameter	Description	
ROUND	ROUND(x,y)	Return the value of x rounded to the specified number of decimal places y ; x can be either a number or a result of a formula.
SIGN	SIGN(x)	Return the value 1 if x is a positive value, or the value -1 if x is a negative value.
SUM	SUM($x1, x2, \dots, xn$)	Return the sum of a list of values or formulas.
TRUE	=TRUE	Return 1.
Add Function button	Configure the currently selected function and add it to the current formula.	

Configure Function Dialog Box

Configure the settings for a function in a formula for use in a custom column of your table in the Configure Function dialog box.

The Configure Function dialog box varies, depending on which function you are configuring.

FALSE and **TRUE**: No configuration options.

ABS, AVERAGE, INT, MAX, MIN, PRODUCT, ROUND, SIGN, SUM: Select one or more columns to perform the function on. These expressions all have the same options, but **ROUND** has the additional option to select the number of decimal places.

AND, NOT, and OR: enter one (NOT) or two (AND and OR) expressions to be evaluated. These expressions all have the same options.

COUNT: Enter a list.

MOD: Select either a column or a value for each of the first and second parameters.

Spectrum List Table Properties Dialog Box

Use the Spectrum List Table Properties dialog box to configure settings that apply to the Spectrum List table.

The Spectrum List Table Properties dialog box has the following pages:

- [Display Page for a Spectrum List Table](#)
- [Enhancement Page for a Spectrum List Table](#)
- [Options Page for a Spectrum List Table](#)
- [Plot Type Page for a Spectrum List Table](#)

Display Page for a Spectrum List Table

Configure display parameters for the Spectrum List table on the Display page of the Spectrum List Table Properties dialog box. For more information, see [Display Page](#).

[Table 48](#) describes the parameters in the Spectrum List Table Properties – Display page.

Table 48. Display page parameters

Parameter	Description
Display	
All Peaks	Display all peaks in the Spectrum List table.
Top	Limit the number of peaks in the table to a specified number.
Order By	
Mass/Intensity or Wavelength/Intensity	Toggle between ordering the data in the Spectrum List table by mass (or wavelength if the PDA Detector is selected) or intensity.
Normalization	
Intensity Range	Specify the relative abundance range of mass peaks that are included in the table. The valid range is –200.000 to 200.000%. To change the range of relative abundances, type the minimum and maximum relative abundance 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%, type 50.000–100.000 . XReport excludes spectrum peaks with relative abundances that range from 0.000 to 49.999% from the table.

Enhancement Page for a Spectrum List Table

Configure spectrum enhancement parameters for the Spectrum List table on the Enhancement page of the Spectrum List Table Properties dialog box. For more information, see [Enhancement Page](#).

Note Clear the **Use Processing Method Properties for Plot Type and Enhancement Info** check box on the [Options Page for a Spectrum List Table](#) to modify parameters on the Enhancement page.

[Table 49](#) describes the parameters in the Spectrum List Table Properties – Enhancement page.

Table 49. Enhancement page parameters

Parameter	Description
Smoothing	
Enable	Turn on spectrum smoothing.
Type	Specify the type of smoothing algorithm to apply to the spectrum. Choose from Boxcar or Gaussian.
Points	Specify the number of points for spectrum smoothing. This must be an odd number from 3 (minimum smoothing) to 15 (maximum smoothing).
Refine	
Enable	Turn on refine spectrum enhancement.
Window	Define an area for drawing a peak by specifying the number of seconds on either side of the specified point. A reasonable initial value is the peak width in seconds.
Noise Threshold	Specify the cutoff point for peaks. Type 0 to show all peaks in the spectrum and slowly increase the value until the noise peaks are eliminated. Use this setting to eliminate peaks generated from baseline noise.
Background Subtraction	
This area shows details of background subtraction if it was applied to the spectrum. The background contribution is determined by averaging the scans from one or two baseline regions.	
Time Range 1	Activate a first baseline region that is used for assessing the background. Clicking this option activates a box. Type the time range to use in the box.
Time Range 2	Activate a second baseline region that is used for assessing the background.

Options Page for a Spectrum List Table

Configure general parameters relating to the Spectrum List table on the Options page of the Spectrum List Table Properties dialog box. For more information, see [Options Page](#).

[Table 50](#) describes the parameters in the Spectrum List Table Properties – Options page.

Table 50. Options page parameters

Parameter	Description
Use Processing Method Properties For Plot Type And Enhancement Info	Use the information in the processing method when determining the plot type and other enhancement details.
Use ISTD Peak When Repeating On Component	Include internal standard peaks in the spectrum list. This parameter is only applicable to the Quan nonrepeating and is not available when this object is used in a Qual nonrepeating.

Plot Type Page for a Spectrum List Table

Configure plot information for the Spectrum List table on the Plot Type page of the Spectrum List Table Properties dialog box. For more information, see [Plot Type Page](#).

Note Clear the **Use Processing Method Properties for Plot Type and Enhancement Info** check box on the [Options Page for a Spectrum List Table](#) to modify the parameters in the Plot Type page.

[Table 51](#) describes the parameters in the Spectrum List Table Properties – Plot Type page.

Table 51. Plot Type page parameters

Parameter	Description
Mass/ Wavelength	For Detector = MS: View or change the current mass range of the active spectrum. To change the mass range, type 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. For 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.
Detector	View or change the currently selected detector data type: • MS • PDA
Time	View or change the time range (in minutes) for the active spectrum. 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: 0.10–9.10 .
Scan Filter	View or change the scan filter used for the active spectrum. Select a filter from the list or use the scan filter format to type a scan filter in the Filter box. This box is available only for MS detectors.
Demo File	View the filename of the demo file that is used in the template.

Average Scan Filter Selection Dialog Box

Configure the average scan filter that is used for the Spectrum List table in the Average Scan Filter Selection dialog box.

Display the Plot Type page, and type an asterisk (*) in the Time box.

Table 52 describes the parameter in the Average Scan Filter Selection dialog box.

Table 52. Average Scan Filter Selection dialog box parameters

Parameter	Description
Scan Filter	View a list of all scan filters in the time range. If there is more than one scan type in the selected time range, choose one scan type to average.

Library Search Graphics Table Properties Dialog Box

Configure additional parameters that apply to the Library Search Graphics Table in the Library Search Graphics Table Properties dialog box.

Table 53 describes the parameters in the Library Search Graphics Table Properties dialog box.

Table 53. Library Search Graphics Table Properties dialog box parameters

Parameter	Description
Max # Of Hits To Display	Specify the maximum number of matches from the library search to display in the Library Search Graphics table.
Display Column Labels	Display labels at the top of the columns in the table.
Show Peak Spectrum	Display the peak spectrum in the table. This check box is available only when you have selected to include the Hit Spectrum column in the Table Properties dialog box.

Library Search Results Table Properties Dialog Box

Configure an additional parameter that applies to the Library Search Results Table in the Library Search Results Table Properties dialog box.

Table 54 describes the parameter in the Library Search Results Table Properties dialog box.

Table 54. Library Search Results Table Properties dialog box parameter

Parameter	Description
General	
Max # Of Hits To Display	Specify the maximum number of matches from the library search to display in the Library Search Results table.

Sample Table Properties Dialog Box

Configure additional settings that apply to a Sample table in the Sample Table Properties dialog box.

[Table 55](#) describes the parameters in the Sample Table Properties dialog box.

Table 55. Sample Table Properties dialog box parameters

Parameter	Description
Include Standards	Include data from standards in the Sample table.
Include QCs	Include data from QCs in the Sample table.
Include Blanks	Include data from blank samples in the Sample table.
Include Unknowns	Include data from unknown samples in the Sample table.

Text Object Properties Dialog Box

Use the Text Object Properties dialog box to configure the settings of the currently selected text object.

This dialog box has the following pages:

- [Data Page](#)
- [Attributes Page](#)
- [Attributes Page for the Annotation Text Object](#)
- [Font Page](#)

Data Page

Indicate what text appears in the text object on the Data page.

The Data page of the Text Object Properties dialog box changes depending on the text object you select.

To create an Annotation object, you can type the annotation text to add to your report. You can either type the text directly in the box or copy and paste it in. Paste text in the box by either right-clicking in the box and choosing **Paste** from the shortcut menu, or by pressing CTRL+V. Add line breaks by pressing the ENTER key while the cursor is still in the box.

Table 56 describes the parameters on the Text Properties – Data page.

Table 56. Data page parameters (Sheet 1 of 2)

Parameter	Description
Title	The custom title of the selected object.
Include The Title In The Resolved Report	Include the custom title in the final report.
Available Items	
This box lists the items that are available to add to the text object. To add an item to the Selected list, select it to highlight it and click Add .	
The Available Items list varies, depending on which text object is selected:	
• Component ISTD Settings Summary Object • Component Settings Summary Object • Component Sys Suit/Flags Settings Object • Instrument Method Object • Processing Method – General Object • Processing Method – Qual Object • Quan ISTD Peak Summary Object • Quan Peak Summary Object • Report Info Object • Sample Header Object	
Add	Add the currently highlighted item in the Available Items list to the Selected list.
Add All	Add all of the items in the Available Items list to the Selected list.
Remove	Remove the currently highlighted item from the Selected list.
Remove All	Remove all of the items from the Selected list.
Selected	
This box lists the items that are already selected to be displayed in the text object.	
Move Up, Move Down	Rearrange the order of the items in the Selected list by moving the currently highlighted item up or down in the list.

Table 56. Data page parameters (Sheet 2 of 2)

Parameter	Description
Data Label	Show the data label or heading text for the currently highlighted data label or heading in the Selected list. Edit the data labels or headings by typing in this box.
Decimal Setting	Specify the number of digits displayed after the decimal point for values displayed with the selected data label. This parameter is only available for some data labels.

Attributes Page

Format the currently selected text object on the Attributes page.

Table 57 describes the parameters on the Text Properties – Attributes page.

Table 57. Attributes page parameters

Parameter	Description
Number of Columns	
1, 2, or 3	Display the data in 1, 2, or 3 columns.
Horizontal Spacing	
Include Data Label	Show or hide the data labels adjacent to the data.
Include Spacing Between Data Label and Its Data	Add space between data labels and the data so that all data values are aligned.
Vertical Spacing	
Single, 1.5 Lines, or Double	Set the amount of space between each line in the text object.

Attributes Page for the Annotation Text Object

Format the currently selected Annotation text object on the Attributes page (Figure 85).

Figure 85. Attributes page of the Annotation Properties dialog box

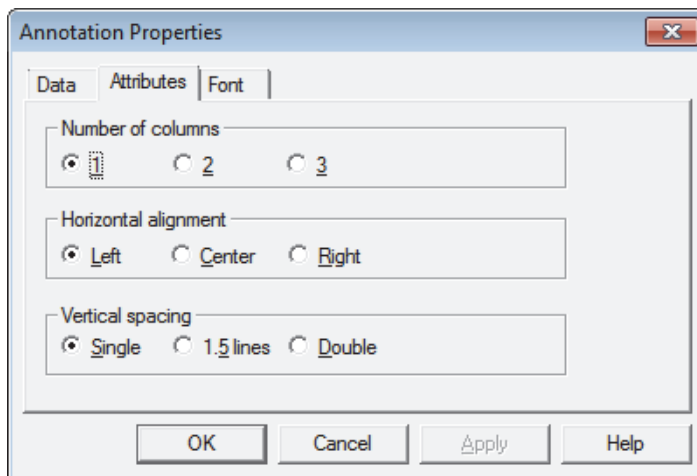


Table 58 describes the parameters on the Annotation Properties – Attributes page.

Table 58. Annotation Properties – Attributes page parameters

Parameter	Description
Number of Columns	
1, 2, or 3	Display the data in 1, 2, or 3 columns.
Horizontal Alignment	
Left, Center, or Right	Aligns the text to the left, center, or right.
Vertical Spacing	
Single, 1.5 Lines, or Double	Set the amount of space between each line in the text object.

Font Page

Format the currently selected text object on the Font page.

The parameters in the Font page depend on whether you are configuring an annotation or other text object.

The Annotation Font page has the standard Microsoft Windows font chooser. Here you can choose font, font size, color, emphasis, and so on.

[Table 59](#) describes the parameters for the Font page.

Table 59. Font page parameters

Parameter	Description
Title Font, Heading Font, Data Label Font, Data Font	Set and view the font settings for all of the title, headings, data labels, and data in the text object. To configure your font, click  . The Font Dialog Box opens.

Bitmap Properties Dialog Box

Specify the filename of the currently selected bitmap in the Bitmap Properties dialog box. For more information, see [Configuring a Bitmap Object](#).

[Table 60](#) describes the parameters for the Bitmap Properties dialog box.

Table 60. Bitmap Properties dialog box parameters

Parameter	Description
Bitmap File	Specify the filename for the currently selected bitmap. Type the full path or click the Browse button to browse for the file.
Reset to Original Size	Reset the size of the image in the template to the original size in the file.

Column Properties Dialog Box

Set parameters in the Column Properties dialog box to specify the number of columns for the column object and whether to repeat by sample or summary.

For more information about using the Columns object, see [Using Columns](#).

Table 61 describes the parameters for the Column Properties dialog box.

Table 61. Column Properties dialog box parameters (Sheet 1 of 2)

Parameter	Description
Number of Columns	
2, 3, 4, or 5	Specify the number of columns in the column object.
Repeat Type	
Sample repeat	View information relating to a particular raw data file of a sample and the results created when processing it. Use this repeat type as a layout tool to indicate where objects are placed on the page of the resolved report. Example 1: When you place a 2-column object in a Quan repeating section, add a chromatogram to the right column, and resolve the template given data of 1 sample with 4 components each, the report appears as follows: Chrom Resolve Chrom 1 Chrom 2 Chrom 3 Chrom 4 Sample 1 Example 2: Place a 2-column object in a Quan repeating section, add a chromatogram to the left column, a spectrum to the right column, and a text object below the column. Then, combine the data with the template given data of 1 sample with 4 components. All objects in the section are repeated by sample, and the report appears as follows: Chrom Spec Text Resolve Chrom 1 Spec 1 Text Chrom 2 Spec 2 Text Chrom 3 Spec 3 Text Chrom 4 Spec 4 Text Sample 1

Table 61. Column Properties dialog box parameters (Sheet 2 of 2)

Parameter	Description																																
Summary repeat	View information relating to all of the samples in an Xcalibur sequence and the results created when processing them. This setting is ignored when the column object is not located in a nonrepeating section. Example 3: If you place a 2-column object in a nonrepeating section, add a chromatogram (in either column), and resolve the template given data of 2 samples with 4 components each, the report appears as follows: Chrom Resolve Left to right <table><tr><td>Chrom 1</td><td>Chrom 2</td></tr><tr><td>Chrom 3</td><td>Chrom 4</td></tr><tr><td>Chrom 1</td><td>Chrom 2</td></tr><tr><td>Chrom 3</td><td>Chrom 4</td></tr></table> Sample 1 Sample 2 If you choose instead the Top To Bottom option, the report appears as follows: Chrom Resolve Top to bottom <table><tr><td>Chrom 1</td><td>Chrom 3</td></tr><tr><td>Chrom 2</td><td>Chrom 4</td></tr><tr><td>Chrom 1</td><td>Chrom 3</td></tr><tr><td>Chrom 2</td><td>Chrom 4</td></tr></table> Sample 1 Sample 2 If you place an object in the right column, and leave the left column empty, the data is resolved as if the object is placed in the left column, as illustrated above. If you place an object in each column, the Xcalibur data system ignores the Top To Bottom and Left To Right options. The report appears as follows: Chrom Spec Text Resolve <table><tr><td>Chrom 1</td><td>Spec 1</td></tr><tr><td>Chrom 2</td><td>Spec 2</td></tr><tr><td>Chrom 3</td><td>Spec 3</td></tr><tr><td>Chrom 4</td><td>Spec 4</td></tr><tr><td>Chrom 1</td><td>Spec 1</td></tr><tr><td>Chrom 2</td><td>Spec 2</td></tr><tr><td>Chrom 3</td><td>Spec 3</td></tr><tr><td>Chrom 4</td><td>Spec 4</td></tr></table> Sample 1 Sample 2 Text If you click the New Sample New Row option, data for a new sample always starts on a new row.	Chrom 1	Chrom 2	Chrom 3	Chrom 4	Chrom 1	Chrom 2	Chrom 3	Chrom 4	Chrom 1	Chrom 3	Chrom 2	Chrom 4	Chrom 1	Chrom 3	Chrom 2	Chrom 4	Chrom 1	Spec 1	Chrom 2	Spec 2	Chrom 3	Spec 3	Chrom 4	Spec 4	Chrom 1	Spec 1	Chrom 2	Spec 2	Chrom 3	Spec 3	Chrom 4	Spec 4
Chrom 1	Chrom 2																																
Chrom 3	Chrom 4																																
Chrom 1	Chrom 2																																
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Chrom 3	Spec 3																																
Chrom 4	Spec 4																																

Component Calibration Curve Dialog Box

Set parameters in the Component Calibration Curve dialog box to specify the component name that a nonrepeating Component Calibration Curve report object is plotted for in your report.

[Table 62](#) describes the parameters for the Component Calibration Curve dialog box.

Table 62. Component Calibration Curve dialog box parameters

Parameter	Description
Component Name	Specify the name of the component to display in your component calibration curve. Click the Browse button to open a dialog box and select a processing method file. After you select a processing method file, XReport provides a list of the components to choose from in that file. After you select a component, XReport returns to the Component Calibration Curve Dialog Box and adds the selected component to the Component Name box.

Data Sources Dialog Box

Select data files to apply to the current report in the Data Sources dialog box.

[Table 63](#) describes the parameters for the Data Sources dialog box.

Table 63. Data Sources dialog box parameters

Parameter	Description
Calibration File	Select the calibration (XCAL) file to apply to the current report.
Processing Method File	Select the processing method (PMD) file to apply to the current report.
Raw Data File	Select the raw (RAW) file to apply to the current report.
Result File	Select the result (RST) file to apply to the current report.
Sequence List File	Select the sequence list (SLD) file to apply to the current report.

Electronic Signature Properties Dialog Box

Configure the order of information displayed in the [Electronic Signature Table Object](#) object in the Electronic Signature Properties dialog box.

[Table 64](#) describes the parameters for the Electronic Signature Properties dialog box.

Table 64. Electronic Signature Properties dialog box parameters

Parameter	Description
Signature Information Order	
Created By First	Display the Created By signature block first. This block displays the electronic signature information for the person who created the report.
Signed By First	Display the Signed By signature block first. This block displays the electronic signature information for the people who signed the report.

Font Dialog Box

Use the Font dialog box to select the global fonts for all objects in your report or customized fonts for the selected objects in the report.

This dialog box has three pages that are the same as in the individual Font Properties pages that you access when you configure an individual object:

- Annotation (see [Font Page](#))
- Text (see [Font Page](#))
- Tables (see [Table Properties Wizard](#))

Preferences Dialog Box

Set grid and configuration options for your report in the Preferences dialog box.

[Table 65](#) describes the parameters for the Preferences dialog box.

Table 65. Preferences dialog box parameters (Sheet 1 of 2)

Parameter	Description
Grid Spacing	
Width	Set the width between grid lines. (1 grid line unit = 0.1 inches)
Height	Set the height between grid lines. (1 grid line unit = 0.1 inches)

Table 65. Preferences dialog box parameters (Sheet 2 of 2)

Parameter	Description
Actions	
Snap To Grid	Snap objects to the grid. For Snap To Grid to work, the grid must be displayed (choose View > Report Template Grid).
Show Page End	Display a dashed blue line that indicates the location for page breaks.
Show Template Configuration	Show the Template Configuration Dialog Box when you open XReport or choose File > New . Use the Template Configuration dialog box to select a type of report to create (for example, the Xcalibur data system). This option is available only when two or more types of report templates are installed on the system.

Preview Window

Preview and adjust the appearance of your report using the parameters in the Preview window. In previewing the appearance of your report, adjust your template before you combine it with actual data.

❖ To open the preview window

Choose **Report > Simulate Report**.

XReport displays a preview of your template filled with sample data.

❖ To view the report's appearance with actual data

Choose **Report > Resolve Report**

The application shows a preview of the report combined with your actual data.

Table 66 describes the parameters for the Preview window.

Table 66. Preview window parameters

Parameter	Description
Print	Print your report preview. This option is available only for resolved reports, not for simulated reports.
Save	Save your report in the following formats (available only for resolved reports, not simulated reports): • Microsoft word document (DOC file) • Microsoft Excel workbook (XLS file) • Web page (HTM or HTML file) • Plain text (TXT file) • Rich text format (RTF file) • Adobe™ PDF (PDF file)
Next Page/Prev Page	Scroll the preview to the next or previous page in the report.
First Page/Last Page	Scroll the preview to the first or last page in the report.
Page <i>X</i> of <i>Y</i>	View <i>X</i> , the current page, and <i>Y</i> , the total number of pages in the report. Type in a new value for <i>X</i> to scroll to that page.
Two Page	View the preview two pages at a time.
Zoom In/Zoom Out	Increase or decrease the size of the report in the preview window.
Close	Close the preview window and go to XReport.
Help	View XReport Help.

Save As Dialog Box

Use the Save As dialog box to save your report template.

The Save As dialog box is the standard Microsoft Save dialog box, with the addition of a Lock Template check box. If you select this check box, the template cannot be saved with the same name again. It can, however, be opened, edited, and resolved with data. To save an edited version, save it as a different filename.

The title bar of XReport indicates whether the displayed template is locked or unlocked. For a locked template, *Locked* appears in the title bar. For an unlocked template, nothing appears in the title bar.

There is no audit trail when a new template is created or when an existing template is changed.

Template Configuration Dialog Box

Select the type of report to create in the Template Configuration dialog box. This dialog box is only displayed if you have more than one type of report installed.

Table 67 describes the parameters for the Template Configuration dialog box.

Table 67. Template Configuration dialog box parameters

Parameter	Description
Report Types	View a list of available report types. Select the program for which you would like to create a report.
Do Not Show This Dialog Again	Hide this dialog box when you open XReport or choose File > New again. To redisplay this dialog box, choose Layout > Preferences and select the Show Template Configuration check box.

Page Setup Dialog Box

Use the Page Setup dialog box to set up the page layout for reports printed from the Qual Browser window, Sequence Setup view, or the XReport application.

The page setup settings for the Qual Browser window, Sequence Setup view, and XReport application are independent of each other.

❖ To set up the page layout for a report template

- Do one of the following:
 - From the menu bar of the Qual Browser window, Sequence Setup view, or XReport application, choose **File > Page Setup**.—or—
 - In the XReport application, set up the page breaks for the report template as follows:
 - Drag the **Page Break** object to the template pane.
 - Right-click the **Page Break** object and choose **Properties** from the shortcut menu.

The Page Setup dialog box opens.

- Set up the following properties:
 - In the Paper area, do the following:
 - Select the paper size.
 - Select the paper source.
 - In the Orientation area, select the **Portrait** or **Landscape** option.

- c. In the Margins area, type the appropriate margins in the Left, Right, Top, and Bottom boxes.

The range of valid values depends on the paper size and page orientation.

- d. (XReport only) In the Heights area, do the following:
- Type the appropriate value for the placement of the header in the Header box.
 - Type the appropriate value for the placement of the footer in the Footer box.

As you change the properties, the graphic at the top of the dialog box displays the effect of the changes.

3. Click **OK** to accept the changes and return to the template pane.

Table 68 describes the parameters in the Page Setup dialog box.

Table 68. Page Setup dialog box parameters

Parameter	Description
Paper	
Size	Specifies the paper size for printing. Default selection: Letter
Source	Specifies the paper source. Some printers have multiple paper trays. Default selection: Automatically Select
Orientation	
Portrait	Selecting this option prints pages vertically.
Landscape	Selecting this option prints pages horizontally.
Margins (inches)	
Left, Right, Top, and Bottom	Adjusts the space between the edge of the document and the corresponding edge of the page.
Heights (inches) XReport application only	
Header	Specifies the distance of the header from the top of the page.
Footer	Specifies the distance of the footer from the bottom of the page.
Buttons	
OK	Accepts the new settings and closes the dialog box.
Cancel	Cancels the new settings and closes the dialog box.

Report Sections

You can divide your report template into sections and add report objects to those sections. To add sections into a report template, drag them from the Sections pane.

The types of sections used in XReport are as follows:

- [Nonrepeating Section](#)
- [Report Header and Footer](#)
- [Qual Repeating Section](#)
- [Quan Repeating Section](#)

A report object that is placed in a repeating section can behave differently from the same report object placed in a nonrepeating section. See [Report Objects](#) for information on how a report object functions when it is placed inside or outside a repeating section.

Nonrepeating Section

A nonrepeating section is any portion of a report template that is not classified as a repeating section. A nonrepeating section usually displays static details associated with either data or methods that apply once and globally within the system.

A nonrepeating section can have these objects:

- Formatting Objects
 - [Page Break Object](#)
 - [Columns Object](#)
- Graphic Objects
 - [Electronic Signature Table Object](#)
 - [Bitmap Object](#)
 - [Chromatogram Object](#)
 - [Component Cal Curve Object](#)
 - [Spectrum Object](#)

- Table Objects
 - Avalon Qual Events Table Object
 - Calibration File Table Object
 - Component Cal Level Table Object
 - Dilution Factor Table Object
 - IRC Summary Table Object
 - Processing Method Programs Table Object
 - Processing Method Sample Reports Settings Table Object
 - Processing Method Summary Reports Settings Table Object
 - Qual Peak Table Object
 - Quan Peak Table Object
 - Sequence Table Object
 - Spectrum Candidate Results Table Object
- Text Objects
 - Annotation Object
 - Instrument Method Object
 - Processing Method – General Object
 - Processing Method – Qual Object
 - Sample Table Object

Report Header and Footer

The report header and footer sections contain data to be repeated at the top and bottom of each page in your report, for example, the report date, page number, and a company logo.

A Report Header or Footer section can have these objects:

- Formatting Objects
 - Columns Object
- Graphic Objects
 - Bitmap Object
 - Electronic Signature Table Object
 - Table Objects

- Text Objects
 - [Annotation Object](#)
 - [Report Info Object](#)
 - [Sample Header Object](#)

Repeating Sections

A repeating section is a section of a report template that is automatically repeated for every component or peak in a resolved document. You can change the properties of a repeating section to customize its behavior. XReport can have two types of repeating sections:

- [Qual Repeating Section](#)
- [Quan Repeating Section](#)

Qual Repeating Section

A Qual Repeating section displays details relating to a single Qual peak within some data. This section is then repeated for all Qual peaks found.

A Qual Repeating section can have these objects:

- Formatting Objects
 - [Page Break Object](#)
 - [Columns Object](#)
- Graphic Objects
 - [Electronic Signature Table Object](#)
 - [Bitmap Object](#)
 - [Chromatogram Object](#)
 - [Spectrum Object](#)
- Table Objects
 - [Library Search Graphics Table Object](#)
 - [Library Search Results Table Object](#)
 - [Spectrum List Table Object](#)
- Text Objects
 - [Annotation Object](#)

Quan Repeating Section

A Quan repeating section is also called a Component section. Its purpose is to display details relating to a single Quan peak in some data or a component configured in a processing method. This section is then repeated for all Quan peaks or components.

A Quan repeating section can have the following objects:

- Formatting Objects
 - [Page Break Object](#)
 - [Columns Object](#)
- Graphic Objects
 - [Electronic Signature Table Object](#)
 - [Bitmap Object](#)
 - [Chromatogram Object](#)
 - [Component Cal Curve Object](#)
 - [Spectrum Object](#)
- Table Objects
 - [Avalon Quan Events Table Object](#)
 - [Component Cal Level Table Object](#)
 - [IRC Settings Table Object](#)
 - [Component QC Level Table Object](#)
 - [Component Spectrum Table Object](#)
 - [IRC Settings Table Object](#)
 - [Spectrum List Table Object](#)
 - [Sample Table Object](#)
- Text Objects
 - [Annotation Object](#)
 - [Component IdentDetectCal Settings Object](#)
 - [Component ISTD Settings Summary Object](#)
 - [Component Settings Summary Object](#)
 - [Component Sys Suit/Flags Settings Object](#)
 - [Quan ISTD Peak Summary Object](#)
 - [Quan Peak Summary Object](#)

Report Objects

Report objects are predefined chunks of data that you can drag to the XReport template from the Objects pane. When you combine a report template with Xcalibur data source files, XReport replaces the report objects in the template with data to generate an Xcalibur report.

Report objects include the following:

- [Graphic and Formatting Objects](#)
- [Table Objects](#)
- [Text Objects](#)

Graphic and Formatting Objects

Graphic objects display graphics. Graphic objects can be configured and customized. The graphic object is replaced with a graphic when a report template is resolved with Xcalibur data. Formatting objects help to configure the layout of the report.

The following graphic and formatting objects are available in XReport:

- [Chromatogram Object](#)
- [Spectrum Object](#)
- [Component Cal Curve Object](#)
- [Bitmap Object](#)
- [Columns Object](#)
- [Page Break Object](#)

Chromatogram Object

The Chromatogram object displays a graphical trace that can show either raw data or processed data for any acquisition device that is supported by the Xcalibur data system (MS, Analog, A/D card, PDA, UV).

Required data file: RAW or RST

Section placement: Qual, Quan, and nonrepeating sections

Spectrum Object

The Spectrum object displays a graphical spectrum that can show either raw data or processed data for any acquisition device supported by the Xcalibur data system (MS, PDA).

Required data file: RAW or RST

Section placement: Qual, Quan, and nonrepeating sections

Component Cal Curve Object

The Component Calibration Curve object displays the calibration curve that is used to quantify a specified component. The curve is specified in the processing method as the response versus the amount of standard.

Required data file: PMD or RST

Section placement: Quan or nonrepeating sections. For the nonrepeating section, specify which component to display in the [Component Calibration Curve Dialog Box](#).

Bitmap Object

The Bitmap object displays a graphical image, for example, a company logo.

Required data file: BMP, DIB, GIF, JPG, or ICO

Section placement: possible in all sections

Columns Object

Use the Columns object to manipulate the layout and repeating properties of graphic and text objects. Format the columns in the [Column Properties Dialog Box](#).

Required data file: none

Section placement: possible in all sections.

Page Break Object

Use the Page Break object to insert a manual page break in your report.

Required data file: None

Section placement: Possible in Qual repeating, Quan repeating, and nonrepeating sections.

Table Objects

Table objects contain tabular information. The columns of table objects can be added, deleted, and ordered. You can also create custom columns. The columns in the table fill with data when a report template is resolved with Xcalibur data.

These table objects are available in XReport:

- [Avalon Qual Events Table Object](#)
- [Avalon Quan Events Table Object](#)
- [Calibration File Table Object](#)
- [Component Cal Level Table Object](#)
- [Component QC Level Table Object](#)
- [Component Spectrum Table Object](#)
- [Dilution Factor Table Object](#)
- [Electronic Signature Table Object](#)
- [Ion Ratio Confirmation Results Table Object](#)
- [IRC Settings Table Object](#)
- [IRC Summary Table Object](#)
- [Library Search Graphics Table Object](#)
- [Library Search Results Table Object](#)
- [Processing Method Programs Table Object](#)
- [Processing Method Sample Reports Settings Table Object](#)
- [Processing Method Summary Reports Settings Table Object](#)
- [Qual Peak Table Object](#)
- [Quan Peak Table Object](#)
- [Qual Summary Table Object](#)
- [Quan Summary Table Object](#)
- [Sample Table Object](#)
- [Sequence Table Object](#)
- [Spectrum Candidate Results Table Object](#)
- [Spectrum List Table Object](#)

Avalon Qual Events Table Object

The Avalon Qual Events table displays details of the Avalon peak detection algorithm events configured in the Qual section of a processing method. This table provides information for each peak with each sample. There is a separate row for each sample peak combination. The rows are grouped so that all peaks in a sample are shown together.

Required data file: PMD

Section placement: Nonrepeating section

This table has the following possible fields:

- Time (ms)
- Kind
- Event OPCode
- Event
- Value
- Value 2
- User Columns 1 to 5

Avalon Quan Events Table Object

The Avalon Quan Events table displays details of the Avalon peak detection algorithm events configured for a component in the Quan section of a processing method. This table provides information for each peak with each sample. There is a separate row for each sample peak combination. The rows are grouped so that all peaks in a sample are shown together.

Required data file: processing method (PMD)

Section placement: Nonrepeating section

This table has the following possible fields:

- Time
- Kind
- Event OPCode
- Event
- Value
- Value2
- User Columns 1 to 5

Calibration File Table Object

The Calibration File table displays calibration levels, raw data file names, and acquisition dates of standards. This table provides information for each peak with each sample.

Required data file: calibration file (XCAL), sequence file (SLD), or raw data file (RAW)

Section placement: Nonrepeating section

This table has the following possible fields:

- Level
- Response Factor
- Component Name
- Average Response Factor
- %RSD
- User Columns 1 to 5

Component Cal Level Table Object

The Component Cal Level table displays the calibration levels, amounts, and acceptance test values defined for a specific component.

Required data file: processing method (PMD)

Section placement: Nonrepeating section

This table has the following possible fields:

- Component Name
- Cal Level
- Amount
- User Columns 1 to 5

Component QC Level Table Object

The Component QC Level table displays the QC levels, amounts, and percent test values defined for a specific component.

Required data file: processing method (PMD)

Section placement: Nonrepeating section

This table has the following possible fields:

- QC Level
- Amount
- Test (%)
- Component Name
- User Columns 1 to 5

Component Spectrum Table Object

The Component Spectrum table displays m/z and intensity data for up to fifty spectrum peaks. The Xcalibur data system uses this data to identify components when the Spectrum Peak Identification Method is specified in the processing method. This table provides information for each peak with each sample. There is a separate row for each sample peak combination. The rows are grouped so that all peaks in a sample are shown together.

Note This method is only used for GC chromatography.

Required data file: processing method (PMD)

Section placement: Nonrepeating section

This table has the following possible fields:

- #
- m/z
- Intensity (%)
- User Columns 1 to 5

Dilution Factor Table Object

The Dilution Factor table displays the names of calibration levels and dilution factors for components other than internal standards.

Required data file: result file (RST)

Section placement: Nonrepeating section

This table has the following possible fields:

- Calibration Level
- Dilution
- User Columns 1 to 5

Electronic Signature Table Object

The Electronic Signature table object displays up to six electronic signatures in table format.

Required data file: none

Section placement: possible in all sections.

Note The data system generates Electronic Signature information at the time the report is created, and the signature information can only be included in reports generated from either the Xcalibur Sequence Setup or Quan Browser. Reports generated from within XReport do not display signature information.

The Electronic Signature table object displays two blocks of signatures. The Created By block displays the signature of the person who created the report. The Signed By block displays the signatures of the people who entered electronic signature information at the time the report was created. This object displays the electronic signature data in the following columns:

- Logon Name
- Full Name
- Date and Time
- Comment

Ion Ratio Confirmation Results Table Object

The Ion Ratio Confirmation Results table displays data about each qualifier ion, based on search criteria specified in the processing method.

Required data file: result file (RST)

Section placement: Nonrepeating section

This table has the following possible fields:

- Qualifier Ion #
- Mass
- Qualifier Ion Found
- Coelution Passed
- Ion Ratio Passed
- Absolute Window (%)
- Actual Ion Ratio (%)
- Target (%)
- Target Range (%)
- User Columns 1 to 5

IRC Settings Table Object

The IRC Settings Table displays up to five qualifier ions within tolerance limits to confirm the detection of a target analyte. The ions are specified in the processing method.

Required data file: processing method (PMD)

Section placement: Nonrepeating section

This table has the following possible fields:

- Qualifier Ion #
- m/z
- Target Ratio (%)
- Window ($\pm$ %)
- User Columns 1 to 5

IRC Summary Table Object

The IRC Summary table displays all of the information for the qualifier ion for each component. Most useful when the Name column is the first column.

Required data file: result file (RST)

Section placement: Nonrepeating section

This table has the following possible fields:

- Component Name
- RT
- Mass
- Response
- Calculated Amount
- Actual Ion Ratio (%)
- Ion Ratio Passed
- Target Range (%)
- Qualifier Ion #
- User Columns 1 to 5

Library Search Graphics Table Object

The Library Search Graphics table displays the graphical results from a library search on a Qual peak.

Required data file: result file (RST) and raw data file (RAW)

Section placement: Nonrepeating section

This table has the following possible fields:

- Hit Spectrum
- Delta
- Compound Structure

Library Search Results Table Object

The Library Search Results table displays the results of a library search on a Qual peak.

Required data file: result file (RST) or raw data file (RAW)

Section placement: Non-repeating section

This table has the following possible fields:

- SI
- RSI
- Compound Name
- Cas #
- Probability
- Area
- Area (%)
- Library
- Molecular Formula
- Molecular Weight
- RT
- Scan #
- User Columns 1 to 5

Processing Method Programs Table Object

The Processing Method Programs table displays a list of programs to be run by the data system after the sample has been analyzed and the data has been processed. The application runs programs in the order listed.

Required data file: processing method (PMD)

Section placement: Nonrepeating section

This table has the following possible fields:

- Num
- Enable
- Std
- QC
- Unk
- Action
- Other
- Parameters
- Program or Macro Name
- Sync
- User Columns 1 to 5

Processing Method Sample Reports Settings Table Object

The Processing Method Sample Reports Settings table displays sample report information for each sample in a sequence, including the template name and the report file name. Specify the sample type in the processing method.

Required data file: processing method (PMD)

Section placement: Nonrepeating section

This table has the following possible fields:

- Num
- Enable
- Std
- QC
- Unk
- Other
- Report Template Name
- Save As
- User Columns 1 to 5

Processing Method Summary Reports Settings Table Object

The Processing Method Summary Reports Settings table displays summary reports to be issued after processing the samples in a bracketed or non-bracketed sequence.

Required data file: processing method (PMD)

Section placement: Nonrepeating section

This table has the following possible fields:

- Num
- Enable
- Save As
- Report Template Name
- User Column 1 to 5

Qual Peak Table Object

The Qual Peak table displays information specific to chromatogram peaks detected by qualitative analysis for a single sample.

Note To display information on chromatogram peaks for an entire sequence, use the [Qual Summary Table Object](#).

Required data file: result file (RST)

Section placement: Nonrepeating section

This table has the following possible fields:

- RT
- Peak Area
- Peak Height
- BL
- S/N
- Area (%)
- Peak Width
- Saturated
- User Column 1 to 5

Quan Peak Table Object

The Quan Peak table displays information specific to component peaks detected by quantitative analysis for a single sample.

Note To display component peak information for all samples in a sequence, use the [Quan Summary Table Object](#) object.

Required data file: processing method (PMD), result file (RST)

Section placement: Nonrepeating section

The Quan Peak table has the following possible fields:

- Component Name
- RT
- Calculated Amount
- Response
- BL
- %Diff
- Area
- Area (%)
- Area Ratio
- [Calibration Flags](#)
- Component Found
- Component Type
- [Data Flags](#)
- Expected RT
- Height
- Height Ratio
- Ion Ratio Status
- ISTD Area
- ISTD Height
- ISTD Name
- ISTD Response
- Keys
- Peak Purity
- Peak Status
- Response Ratio
- S/N
- Sample Type
- Saturated
- Specified Amount
- System Suitability
- Units
- Width
- User Columns 1 to 5

Qual Summary Table Object

The Qual Summary table displays information specific to chromatogram peaks detected by qualitative analysis for all samples in a sequence.

Note To display peak information for a single sample only, use the [Qual Peak Table Object](#) object.

Required data file: sequence file (SLD) or result file (RST)

Section placement: Nonrepeating section

The Qual Summary table has the following possible fields:

- RT
- Peak Area
- Peak Height
- BL
- Data File Name
- Sample ID
- S/N
- Area (%)
- Peak Width
- Saturated
- User Column 1 to 5

Quan Summary Table Object

The Quan Summary table displays information specific to component peaks detected by quantitative analysis for all samples in a sequence.

Note To display component peak information for a single sample only, use the [Quan Peak Table Object](#) object.

Required data file: sequence file (SLD), processing method (PMD), result file (RST)

Section placement: Nonrepeating section

The Quan Summary table has the following possible fields:

- Component Name
- RT
- Calculated Amount
- Response
- BL
- %Diff
- Area
- Area (%)
- Area Ratio
- [Calibration Flags](#)
- Component Found
- Component Type
- Data File Name
- [Data Flags](#)
- Expected RT
- Height
- Height Ratio
- Ion Ratio Status
- ISTD Area
- ISTD Height
- ISTD Name
- ISTD Response
- Keys
- Peak Purity
- Peak Status
- Response Ratio
- S/N
- Sample ID
- Sample Type
- Saturated
- Specified Amount
- System Suitability
- Units
- Width
- User Columns 1 to 5

Sample Table Object

The Sample table displays system suitability and flag processing results for each component in a sample, and repeats this information for every sample in a sequence. This table provides information for each peak with each sample. There is a separate row for each sample peak combination. The rows are grouped so that all peaks in a sample are shown together.

Required data file: sequence file (SLD)

Section placement: Nonrepeating section

The Sample table has the following possible fields:

- Sample ID
- Data File Name
- Area
- Area Ratio
- ISTD Area
- Specified Amount
- %Diff
- %RSD
- Actual RT
- Calculated Amount
- [Calibration Flags](#)
- [Data Flags](#)
- Excluded
- Height
- ISTD Height
- Height Ratio
- QC Failed
- System Suitability
- User Columns 1 to 5

Sequence Table Object

The Sequence table displays the contents of the sequence file. This table provides information for each peak with each sample.

- Required data file: sequence file (SLD)
- Section placement: Nonrepeating section

The Sequence table has the following possible fields:

- Sample Type
- File Name
- Sample ID
- Path
- Inst Method
- Cal File
- Dil Factor
- Inj Vol
- ISTD Corr Amt
- Level
- Proc Method
- Sample Vol
- Sample Wt
- Position
- User Labels 1 to 5
- User Columns 1 to 5

Spectrum Candidate Results Table Object

The Spectrum Candidate Results table displays the results of spectrum candidate processing for GC/MS data on a per component basis.

Required data file: result file (RST)

Section placement: Nonrepeating section

The Spectrum Candidate Results table has the following possible fields:

- Component Name
- Cand. #
- Forward Fit
- Reverse Fit
- Match
- Area
- End RT
- Found RT
- Height
- Start RT
- User Columns 1 to 5

Spectrum List Table Object

The Spectrum List table displays the text equivalent of the spectrum graphic object. This table provides information for each peak with each sample. There is a separate row for each sample peak combination. The rows are grouped so that all peaks in a sample are shown together.

Required data file: result file (RST) or raw data file (RAW)

Section placement: Nonrepeating section

The Spectrum List table has the following possible fields:

- *m/z*
- Intensity
- Relative
- Wavelength
- User Columns 1 to 5

Text Objects

Text objects contain text labels and associated text fields. These fields can be deleted, cut/copied, and pasted anywhere in the report template (for example, a header). The text object fields are replaced with textual information when a report template is resolved with Xcalibur data.

These text objects are available in XReport:

- [Annotation Object](#)
- [Component IdentDetectCal Settings Object](#)
- [Component ISTD Settings Summary Object](#)
- [Component Settings Summary Object](#)
- [Component Sys Suit/Flags Settings Object](#)
- [Instrument Method Object](#)
- [Processing Method – General Object](#)
- [Processing Method – Qual Object](#)
- [Quan ISTD Peak Summary Object](#)
- [Quan Peak Summary Object](#)
- [Report Info Object](#)
- [Sample Header Object](#)

Annotation Object

Use the Annotation object to insert static text into your report. To enter the text, right-click the object and choose **Properties** from the shortcut menu. The Annotation Properties dialog box opens. Type your text in the box.

Required data file: None

Section placement: Possible in all sections.

Component IdentDetectCal Settings Object

The Component IdentDetectCal Settings object shows the peak detection, calibration, and integration parameters for a single component.

Required data file: processing method (PMD)

Section placement: Quan repeating section, repeats on component peak

For this object's possible fields and headings, see [Table 69](#).

Component ISTD Settings Summary Object

The Component ISTD Settings object displays a summary of the configuration details for each component's ISTD configuration in the Quantitation section of a processing method.

Required data file: processing method (PMD)

Section placement: Quan repeating section, repeats on component peak

Table 69 lists the this object's possible fields.

Table 69. Component ISTD Settings object fields

• Component Name	• Expected Retention Time	Genesis Peak Integration/Detection	ICIS Peak Integration/Detection
• Detector Type	• Retention Time Window	• Genesis Smoothing Points	• ICIS Smoothing Points
• Filter	• View Width	• Valley Detection Enabled	• ICIS Constrain Peak Width
• Trace	• Retention Time Reference	• Genesis Constrain Peak Width	• ICIS Identify By
• Mass Range	• Component Type	• Genesis Identify By	• ICIC Minimum Peak Height
• Wavelength Range 1	• ISTD Name	• Genesis Minimum Peak Height	Avalon Peak Integration/Detection
• Wavelength Range 2	• Peak Detection Algorithm		• Avalon Smoothing Points
			Other
			• <Blank Line > and <User Text> Data Items

Component Settings Summary Object

The Component Settings Summary object displays a short list of peak detection and integration parameters for a specified component.

Required data file: processing method (PMD)

Section placement: Quan repeating section, repeats on component peak

Table 70 lists this object's possible fields and headings.

Table 70. Component Settings Summary object fields/headings

• Component Name • Detector Type • Filter • Trace • Mass Range • Wavelength Range 1 • Wavelength Range 2	• Expected Retention Time • Retention Time Window • View Width • Retention Time Reference • Component Type • ISTD • Standard Dilution – Base Amount • Peak Detection Algorithm	Genesis Peak Integration/Detection • Genesis Smoothing Points • Valley Detection Enabled • Genesis Constrain Peak Width • Genesis Identify By • Genesis Minimum Peak Height	ICIS Peak Integration/Detection • ICIS Smoothing Points • ICIS Constrain Peak Width • ICIS Identify By • ICIC Minimum Peak Height Avalon Peak Integration/Detection • Avalon Smoothing Points Other • <Blank Line > and <User Text> Data Items
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Component Sys Suit/Flags Settings Object

The Component Sys Suit/Flags Settings object displays calibration, quantitation, and detection flags along with system suitability parameters, which allow automatic chromatographic checks that assign a pass/fail qualification to a target peak.

- Required data file: processing method (PMD)
- Section placement: Quan nonrepeating, repeats on component peak

Table 71 lists this object's possible fields and headings.

Table 71. Component Sys Suit/Flags Settings object fields/headings

System Suitability	Detect Tailing	Detect Baseline Clipping	Quantitation Flags
• Component Name	• Tail Peak Height	• Num. of Peak Widths for Noise Detection	• Detection Limit
Resolution Parameters	• Tail Failure Threshold		• Quantitation Limit
• Resolution Threshold	Detect Column Overload	Detect Minimum Signal-to-Noise Ratio	• Linearity Limit
Symmetry Parameters	• Over Peak Height	• Signal-to-Noise Ratio	• Carry Over Limit
• Symmetry Peak Height	• Over Failure Threshold	Calibration and Quantitation Flags	Detection Flags
• Symmetry Threshold			• Area Threshold
Peak Classification Parameters		Calibration Flag	• Height Threshold
		• R-Squared	Other
Detect Peak Width			• <Blank Line > and <User Text> Data Items
• Width Peak Height			
• Min. Peak Width			
• Max. Peak Width			

Instrument Method Object

The Instrument Method object displays general instrument method parameters.

Required data file: raw data file (RAW)

Section placement: Nonrepeating section

This object displays instrument method information for all the instruments associated with a RAW file. This object uses the default data, attribute, and font settings from Qual Browser, and has no configurable properties.

Processing Method – General Object

The Processing Method – General object displays general processing method parameters.

Required data file: processing method (PMD)

Section placement: Nonrepeating section

Table 72 lists this object's possible fields and headings.

Table 72. Processing Method – General object fields/headings

Identification	Baseline	Options	Other
- Created By - When Created - Last Modification - Modified By - Summary - Void Time	- Baseline and Noise Window - Baseline Noise Tolerance - Min. Number of Scans in Baseline	- Chromatography By - Calibration By	<Blank Line > and <User Text> Data Items

Processing Method – Qual Object

The Processing Method – Qual object displays Qual processing method parameters.

Required data file: processing method (PMD)

Section placement: Nonrepeating section

Table 73 lists this object's possible fields and headings.

Table 73. Processing Method – Qual object fields/headings (Sheet 1 of 2)

Identification • Detector Type • Detector Delay • Filter • 1st Trace Type • Operator • 2nd Trace Type • Mass Range 1 • Wavelength Range 1 • Mass Range 2 • Wavelength Range 2 • Range	Detection Options • Peak Detection Algorithm Genesis Peak Integration • Genesis Smoothing Points • S/N Threshold • Valley Detection • Expected Peak Width • Genesis Constrain Peak Width • Genesis Peak Height • Genesis Tailing Factor	Avalon Peak Integration • Avalon Smoothing Points Limit Peaks • Select Top Peaks • Select By • Number To Select • Relative Peak Height Threshold • Percent of Highest Peak	Genesis Peak Detection • Genesis Identify By • Minimum Masses Required • Minimum Percent of Masses Found • Minimum Peak Height Genesis Peak Edge Detection • Peak S/N Cutoff • Report Noise As
ICIS Advanced Parameters • Noise Method • Minimum Peak Width • Multiplet Resolution • Area Tail Extension • Area Scan Window	Spectrum Enhancement Spectrum Enhancement Usage	Refine • Window Size • Noise Threshold	Combine Background Subtraction Left Region • Left Region Width • Region End Peak Top Region • Width

Table 73. Processing Method – Qual object fields/headings (Sheet 2 of 2)

Options • Maximum Number of Hits • Reverse Search • Search with MW	Append to User Library • Availability • User Library • Match Factor • Reverse Match Factor • Probability Search Libraries		Library Search Constraints • Molecular Weight Range • Other Databases • Name Fragment • Element Constraints Enabled • Elements in Compound • Element Infiltration • Mass Spectral Peak Constraints Enabled • Mass Spectral Peak Measurement
ICIS Peak Integration • ICIS Smoothing Points • Baseline Window • Area Noise Factor • Peak Noise Factor • ICIS Constrain Peak Width • ICIS Peak Height • ICIS Tailing Factor	Genesis Apex Detection • Window Size • Filter Width Genesis Valley Detection • Rise % • Valley S/N Genesis Background Subtraction • Recomputation Interval • Number of Scans in Background	Background Subtraction Right Region • Right Region Width • Region Start Threshold • Cutoff Threshold Library Search Options Search Type • Identity • Similarity	Peak Purity Options • Scan Threshold • Peak Coverage • Limit Scan Wavelength Range Other • <Blank Line > and <User Text> Data Items

Quan ISTD Peak Summary Object

The Quan ISTD Peak Summary object displays summary parameters for a Quan component's associated ISTD peak.

Required data file: processing method (PMD) or result file (RST)

Section placement: Quan nonrepeating, repeats on component peak

[Table 74](#) lists this object's possible fields.

Table 74. Quan ISTD Peak Summary object fields

• Component Name • ISTD Name • Actual RT • Response	• Height • Width • Baseline Flags • Area	• Signal-to-Noise • Saturated • Expected RT • Peak Status	• System Suitability • Data Flags • <Blank Line > and <User Text> Data Items
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Quan Peak Summary Object

The Quan Peak Summary object displays component peak summary parameters.

Required data file: processing method (PMD) or result file (RST)

Section placement: Quan nonrepeating, repeats on component peak

[Table 75](#) lists this object's possible fields.

Table 75. Quan Peak Summary object fields

• Component Name • Actual RT • Specified Amount • Calculated Amount • %Diff • Response • Response Ratio	• Area • Area Ratio • Height • Height Ratio • Width • Ion Ratio Status	• Peak Purity • Baseline Flags • Signal-to-Noise • Saturated • Expected RT • Sample Type	• Component Type • Peak Status • System Suitability • Data Flags • Calibration Flags • <Blank Line > and <User Text> Data Items
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Report Info Object

The Report Info object displays general information about the report itself.

Required data file: None

Section placement: Report header and footer

Table 76 lists this object's possible fields.

Table 76. Report Info object fields

• Page [a] of [b] • Date and Time • Template File • Layered App Name	• Layered App Version • <Blank Line > and <User Text> Data Items
---	---

Sample Header Object

The Sample Header object displays general information about a sample.

Required data file: raw data file (RAW) or sequence file (SLD)

Section placement: Report header or footer or Non-repeating section

Table 77 lists this object's possible field.

Table 77. Sample Header object fields

• Data File • Original Data Path • Current Data Path • Sample Type • Sample ID • Sample Name • Operator • Acquisition Date	• Run Time • Comments • Vial • Injection Volume • Scans • Low Mass • High Mass • Sample Volume	• Sample Weight • ISTD Amount • Calibration Level • Dilution Factor • Instrument Method • Processing Method • Current Processing Method • Calibration File	• Revision • Barcode • Barcode Status • User Labels 1 to 5 • <Blank Line > and <User Text> Data Items
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System Suitability Flags

The [Quan Summary Table Object](#), [Quan ISTD Peak Summary Object](#), [Sample Table Object](#), and [Quan Peak Table Object](#) objects have an available System Suitability field, which displays the results of any system suitability tests carried out on the specified peak. Each test is represented by a flag letter. XReport displays the flags in categories according to whether the peak passed, failed, or was not tested.

[Table 78](#) describes the System Suitability flags.

Table 78. System Suitability flags

Flag	Description
S	Symmetry: A peak passes this test if its calculated symmetry is greater than the symmetry threshold specified in the System Suitability page of Quan View in Processing Setup.
R	Resolution: A peak passes this test if its calculated resolution is greater than the resolution threshold specified in the System Suitability page of Quan View in Processing Setup.
W	Peak Width: A peak passes this test if its width falls between the minimum and maximum values specified in the System Suitability page of Quan View in Processing Setup.
T	Tailing: A peak passes this test if its calculated tailing falls below the threshold specified in the System Suitability page of Quan View in Processing Setup.
O	Column Overload: A peak passes this test if its calculated overloading falls below the threshold specified in the System Suitability page of Quan View in Processing Setup.
B	Baseline Clipping: A peak passes this test if baseline clipping is not detected.
N	Signal to Noise Ratio: A peak passes this test if its signal-to-noise ratio falls above the threshold specified in the System Suitability page of Quan View in Processing Setup.
C	Concave: A peak passes this test if it does not exhibit a concave depression due to noise.
D	Saturation: A peak passes this test if the detector did not saturate during data acquisition.

<Blank Line > and <User Text> Data Items

All text objects except for the Annotation object and Instrument Method object have two special data items, <Blank Line> and <Text>. These data items appear in the Available Items list of the [Data Page](#).

When you insert the <Blank Line> data item in the Selected list, XReport inserts a blank line at that spot. You can use this to control the spacing between items in a text object. Unlike ordinary data items, a <Blank Line> can appear in the Selected list more than once.

The <User Text> item allows you to insert additional custom text into the text object. The <User Text> item can be added to the Selected list more than once, and each instance can be configured to display different custom text. Custom text is displayed using the font settings for Headings.

Baseline Flags

The [Quan Peak Summary Object](#), [Quan ISTD Peak Summary Object](#), [Quan Peak Table Object](#), [Qual Peak Table Object](#), [Qual Summary Table Object](#), and [Quan Summary Table Object](#) objects have an available Baseline flags field that displays how the data system detected the left and right peak edges of the current peak. The flags are displayed in pairs, with the first letter of the pair indicating the detection method for the left edge of the peak, and the second letter indicating the detection method for the right edge of the peak.

[Table 79](#) describes the baseline flags.

Table 79. Baseline flags

Flag	Description
B	Baseline: The edge of the peak is at baseline level.
V	Valley: The edge of the peak is in a peak valley.
M	Manual: The edge of the peak has been adjusted manually.
S	Stripe: The edge of the peak reached the Constrain Peak Height Percent specified in the method.
T	Tail: The edge of the peak reached the Constrain Peak Height Tailing Factor limit before the Height Percent.
–	Tilt: An error occurred before the edge of the peak could be determined.
?	Unknown: An unknown error occurred.

Data Flags

XReport can display Data Flag letters in the [Quan Summary Table Object](#), [Quan ISTD Peak Summary Object](#), [Quan Peak Table Object](#), and [Quan Summary Table Object](#) objects to indicate when a peak has exceeded threshold area or height values specified in Quan Browser. These are the data flags that can appear.

[Table 80](#) describes the data flags.

Table 80. Data flags

Flag	Description
A	Indicates that the peak area is outside the specified tolerance.
H	Indicates that the height is outside the specified tolerance.

Calibration Flags

XReport can display Calibration Flag letters in the [Quan Peak Summary Object](#), [Quan Summary Table Object](#), and [Quan Peak Table Object](#) objects to indicate when certain peak characteristics exceed values specified in Quan Browser. These are the calibration flags that can appear.

[Table 81](#) describes the calibration flags.

Table 81. Calibration flags

Flag	Description
E	Detection limit: Indicates that the detection threshold for the concentration of the quantified peak is outside the specified tolerance.
L	Carry Over limit: Indicates that the carryover threshold for the concentration of the quantified peak is outside the specified tolerance.
Q	R-squared: Indicates that the coefficient of determination is outside the specified tolerance.
U	Quantitation limit: Indicates that the quantitation threshold for the concentration of the quantified peak is outside the specified tolerance.
Y	Linearity limit: Indicates that the linearity threshold for the concentration of the quantified peak is outside the specified tolerance.

Report Templates

An XReport template is an XReport document (XRT file) that defines the content, layout, and style of an Xcalibur report. You can include sections and report objects in the report template. An Xcalibur report is generated when a report template is resolved (combined) with Xcalibur data source files).

XReport comes with several example Xcalibur report templates for you to use. These templates, described below, are located in the Xcalibur\Templates folder.

Table 82 describes the standard XReport templates.

Table 82. XReport templates (Sheet 1 of 2)

Report names	Description	Files needed
CalibrationFile	For reporting calibration data.	RAW and XCAL
CompCalReport: _Avalon,_Genesis,_ICIS	Generates summary reports showing processing method details, calibration curve, and sample table (Quan results). Use this report with results from Xcalibur batch processing and Quan Browser.	RST, RAW, PMD, and SLD
CustLibrSearRept LibrarySearchReport	Generates Qual sample reports that display Qual peaks and library search details. Use this report with results from Xcalibur batch processing.	RST and RAW
IonRatio Confirmation	Generates a Quan sample report containing non-graphical ion ratio confirmation results.	RST, RAW, and PMD
IonRatio Confirmation: Graphical, GraphicalSimple, GraphicalStacked	Generates Quan sample reports containing graphical ion ratio confirmation results. These report templates take advantage of the explicit qualifier ion settings available when using the Chromatogram Properties Dialog Box and Wizard .	RST, RAW, and PMD
Peak Integration	Generates a Quan sample report containing peak integration data generated using the Genesis peak integration algorithm.	RST, RAW, and PMD
ProcessingMethod: _Avalon, _Genesis, _ICIS	Generates processing method reports. Use this report with results from Xcalibur Processing Method Setup.	PMD
QualPeak Report	Generates a simple Qual sample report. Use this report with results from Xcalibur batch processing.	RST and RAW
QuanPeakResults: _ISTD, _ESTD QuanResults QuanSimple	Generates Quan sample reports. Use this report with results from Xcalibur batch processing or Quan Browser.	RST, RAW, and PMD
QuantifySampleReport	Generates Quan sample reports containing chromatograms and a Quan summary table.	SLD, PMD, RST, and RAW

Table 82. XReport templates (Sheet 2 of 2)

Report names	Description	Files needed
Sequence Report	Generates a summary report showing the sequence being processed. Use this report with results from Xcalibur batch processing.	SLD
Spectrum Candidates	Generates a Quan sample report (only applicable to GC/MS). Use this report with results from Xcalibur batch processing or Quan Browser.	RST and RAW

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