Thermo

Xcalibur

Versions 2.1–2.3

XReport User Guide

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DOCUMENTATION
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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.

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DOCUMENTATION SURVEY

Related Documentation

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

- *Xcalibur Getting Started for Quantitative Analysis*
- *Xcalibur Data Acquisition and Processing User Guide*
- *Xcalibur Quantitative Analysis User Guide*
- *Xcalibur Qualitative Analysis User Guide*
- *Xcalibur Creating and Searching Libraries User Guide*
- *XReport User Guide*
- Help from within the software

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.

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Introduction to XReport

XReport 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 file), Microsoft™ Word™ document (.doc file), Microsoft Excel™ workbook (.xls file), rich text (.rtf file), portable display (.pdf file), or Web page (.htm or .html file) formats. Use these options to e-mail 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

- Overview of Report Templates

- Configuring XReport Objects

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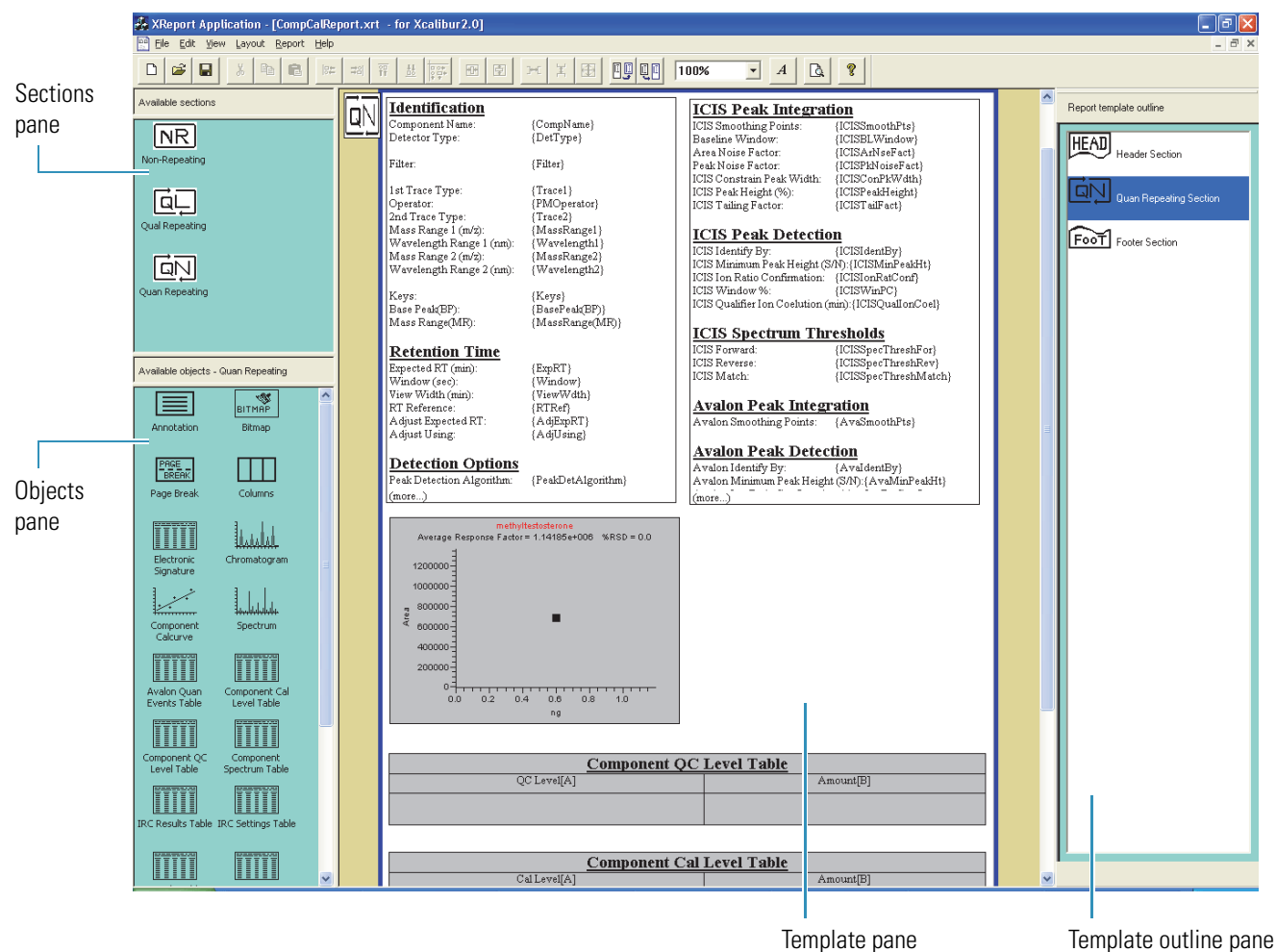
The Sections pane lists the available sections for the selected application (for example, Xcalibur). To add a section to a report, drag it from the Sections pane to the Template pane.

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 un-dock, reposition, or close it.

- To un-dock 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.

Overview of Report Templates

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

- Report Template

- Sections

- Report Objects (for more information, see Appendix B, "Types of Report Objects.")

- Data Source Files (.pmd, .raw, .rst, .sld, .xcal)

- 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 (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."

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" on page 170 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" on page 189 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" on page 170 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)

- Raw (.raw)

- Result (.rst)

- Sequence (.sld)

- Calibration (.xcal)

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 present 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

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

Use the Repeating Section Configuration dialog box to specify:

- The type of repeating section, Qual or Quan
- 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

Configuring a Table

Use the Table Configuration 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

Using the Chromatogram Wizard

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

Configuring a Component Calibration Curve

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.

Using the Data Source Browser

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

Sample XReport Templates

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 XReport, read these topics:

- Starting XReport

- Selecting a Report Template

- Creating and Generating Reports with XReport

- Exiting XReport

Starting XReport

❖ **To start XReport**

1. From your computer taskbar, double-click [icon] on the desktop, or choose
   Start > All Programs > Thermo Xcalibur > XReport.

   When more than one application is installed that uses XReport for reporting (for
   example, both Xcalibur 2.0 and LCquan™ 2.5), the Template Configuration dialog box
   opens (see Figure 2).

   Figure 2. Template Configuration dialog box
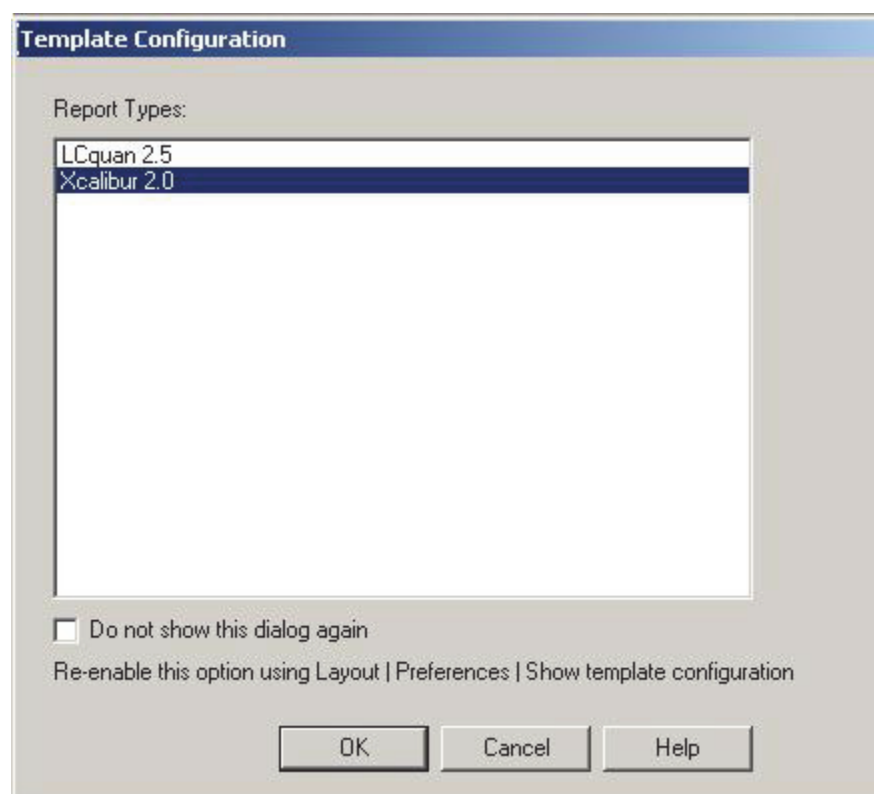
2. Select the application for the report template and click **OK**.

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

Figure 3. XReport window, showing a new template
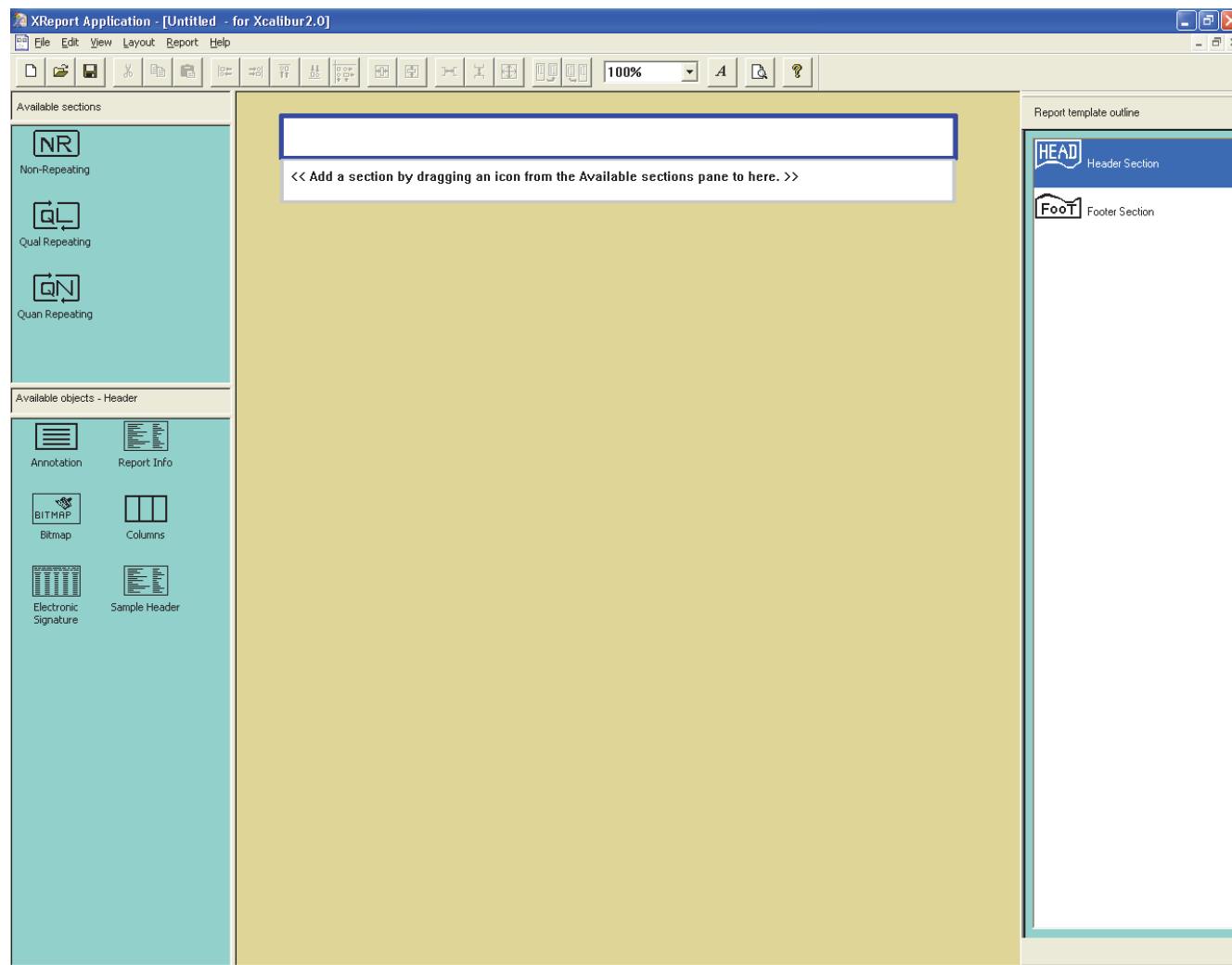
Selecting a Report Template

❖ **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" on page 15 and "Generating a Report" on page 29. 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 ![icon] to start XReport.

   A new XReport document appears in the report window (see Figure 3).

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, Xcalibur .pmd, .raw, .rst, .sld, and .xcal files).

For detailed information on how to generate a report from within the Xcalibur data system, see Chapter 3.

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 in .txt, .doc, .xls, .rtf, .pdf, or .htm format.

- From a data processing application (for example, Xcalibur): 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, Xcalibur): 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 personal report template. When you create a personal 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.

When you start XReport, XReport creates a new template that includes header and footer sections (see Figure 4). Either work with this new template, or choose **File > Open** to open an existing template and select an XReport template (.xrt) file. To create a template, do the procedures in this chapter in order.

Figure 4. XReport window, showing a new template
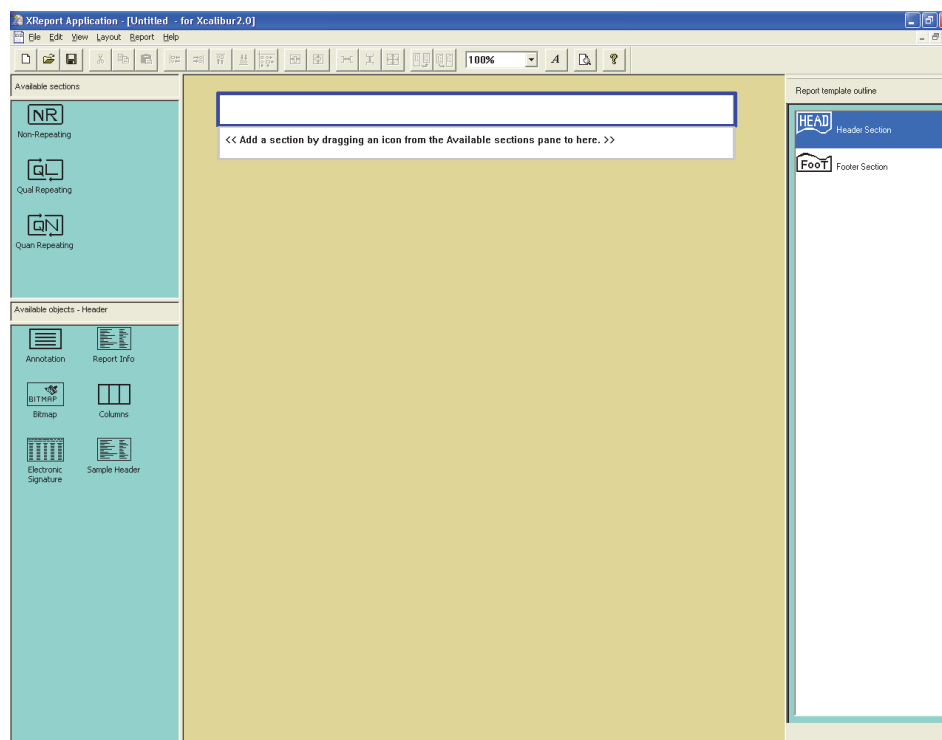
Contents

- Adding, Ordering, and Configuring Sections
- Adding and Configuring Report Objects
- Previewing and Saving the 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" on page 46.

Topics in this section:

- Adding, Deleting, or Reordering Sections

- Resizing Sections

- Configuring a Repeating Section

Adding, Deleting, or Reordering Sections

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

Resizing Sections

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 Repeating Section

❖ **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 (see Figure 5).

Figure 5. Repeating Section Properties dialog box
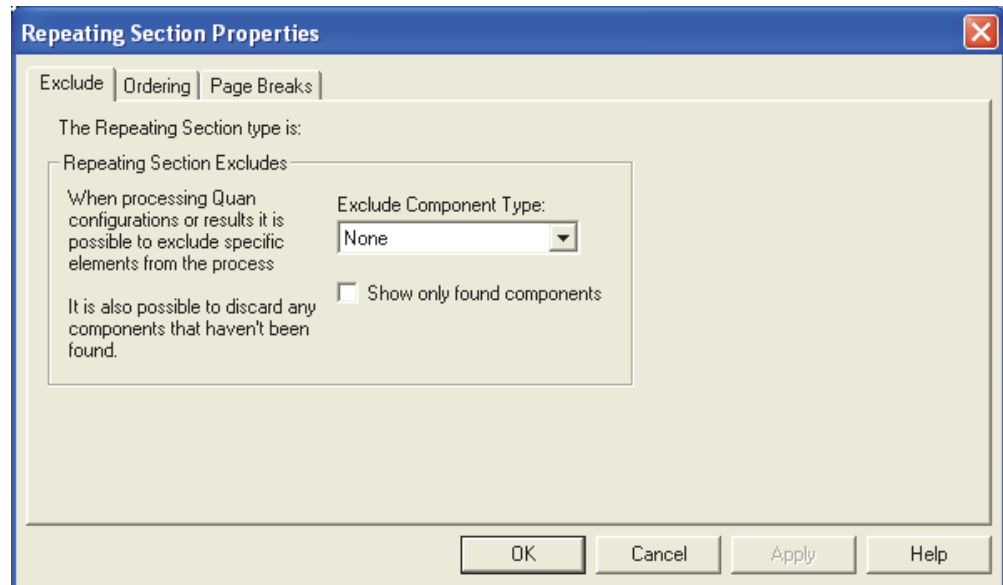
3. Set the parameters and click **OK**.

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 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 Page Layout

Adding, Deleting, Repositioning, and Resizing Objects

❖ **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 button on the toolbar that corresponds to the dimension you want to resize:

   Width, Height, or Both (⊨⊣ ⟂ ⊞).

   To **resize the columns** in a table object, double-click the table. Handles (small blue boxes) appear on the interior column borders. 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 button on the toolbar that corresponds to the edge to align: Left, Right, Top, Bottom.
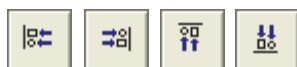
   Or click **Auto Align** to snap all objects to the nearest grid line.

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. Hold down the SHIFT key and select each object to center.

2. To center the objects on the page, click the **Center Horizontally** or **Center Vertically** button on the toolbar.

Using the Report Template Grid

The Template pane has a grid built in it. Choose **View > Report Template Grid** to view the grid lines.

To adjust the grid settings, choose **Layout > Preferences**. The Preferences dialog box opens (see Figure 6). Set the spacing between grid lines and whether to snap objects to the grid as they are added to the Template pane.

Figure 6. Preferences dialog box
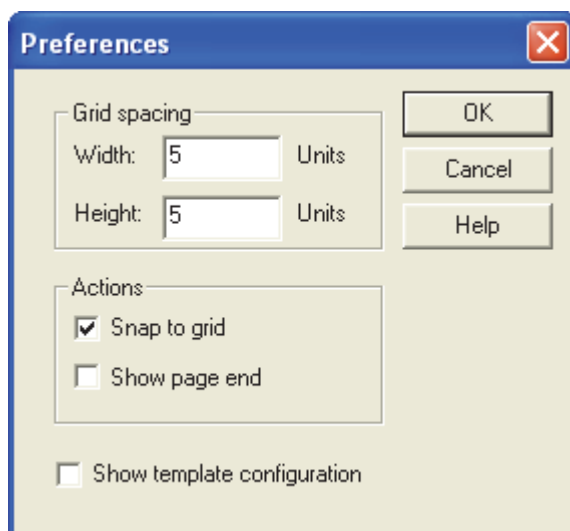
Using Columns

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 (see Figure 7). To learn how to configure columns and how columns work with different repeat types, see "Configuring Columns" on page 102.

Figure 7. Column Properties dialog box
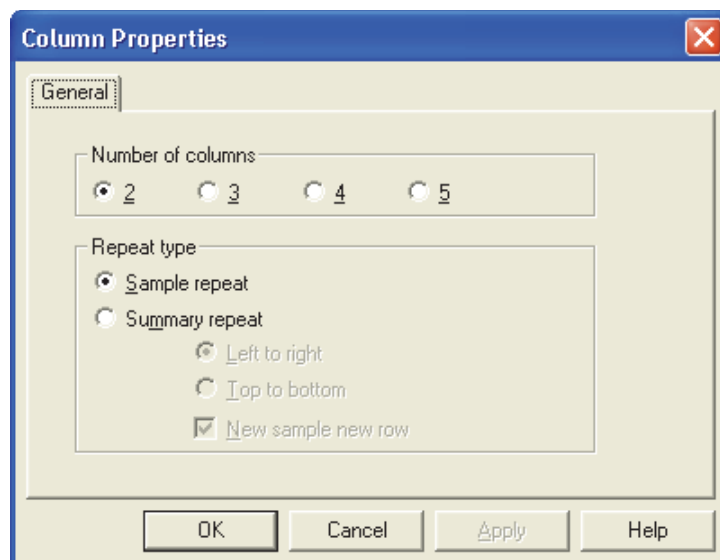
You can resize the entire column object (select it and drag the corner handles), but the columns within the column object remain equal in size.

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

Using Page Breaks

To add a page break to the template, drag the Page Break object from the Objects pane to the Template pane. After adding a page break to the template, drag the page break to reposition it.

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 where these automatic breaks occur, choose **Layout > Preferences**. The Preferences dialog box opens (Figure 6). Select the **Show Page End** check box.

Configuring 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.

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

1. Right-click the text object and choose **Properties** from the shortcut menu. The Data Page opens.

2. Select <User Text> in the Available Items list.

3. To add a text item to the Selected list, click **Add**.

4. To position the <User Text> item where you want your text displayed, click **Move Up** or **Move Down**.

5. Select the <User Text> item.

6. Type the text to display in the box below the Selected list and press **Apply**.

   The Xcalibur data system displays the text you entered in the Selected list.

❖ **To edit a <User Text> item**

1. Select the item to edit in the Selected list.

2. Edit your text in the User box.

3. Press **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.

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.

4. Type a title for this column in the User Column Title box.

5. Click **Edit Formula**. The Edit Formula For Dialog Box opens.

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

Use XReport to 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. Select the object and click A on the toolbar to open the Font dialog box, or right-click the object and choose **Properties** from the shortcut menu to open the Properties dialog box and display the Font page. Both of these pages provide the same settings.

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 A on 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 A on the toolbar. The Font dialog box opens.

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

Changing Page Layout

❖ **To change the page layout**

1. Choose **File > Page Setup**. The Page Setup dialog box opens (see Figure 8).

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.

Figure 8. Page Setup dialog box
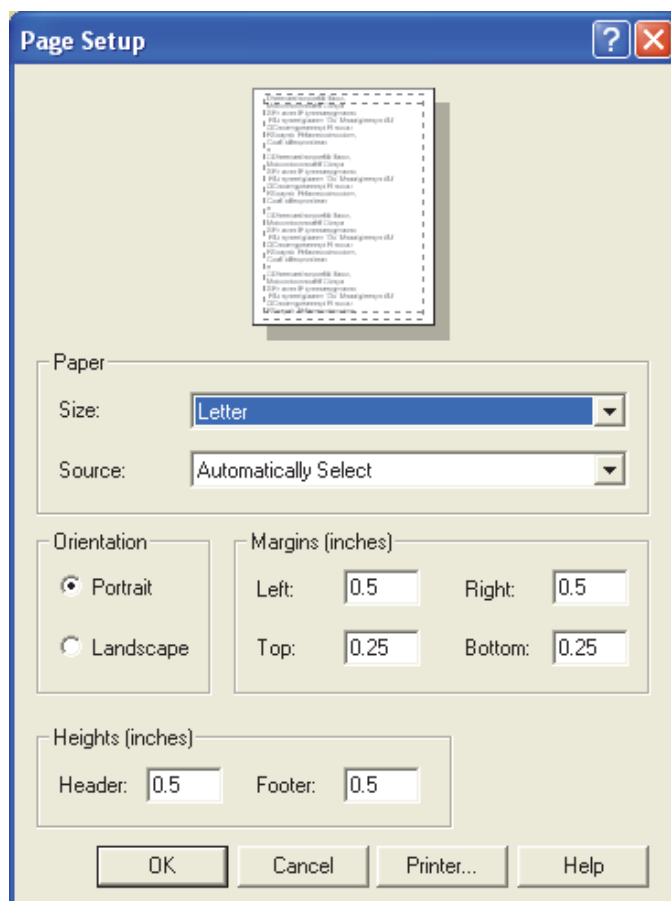
Previewing and Saving the Template

❖ **To preview the appearance of the template**

1. Choose **File > Simulate Report**. The Preview window opens (see Figure 9). The Preview window shows the report with the default data.

   Figure 9.   Preview window
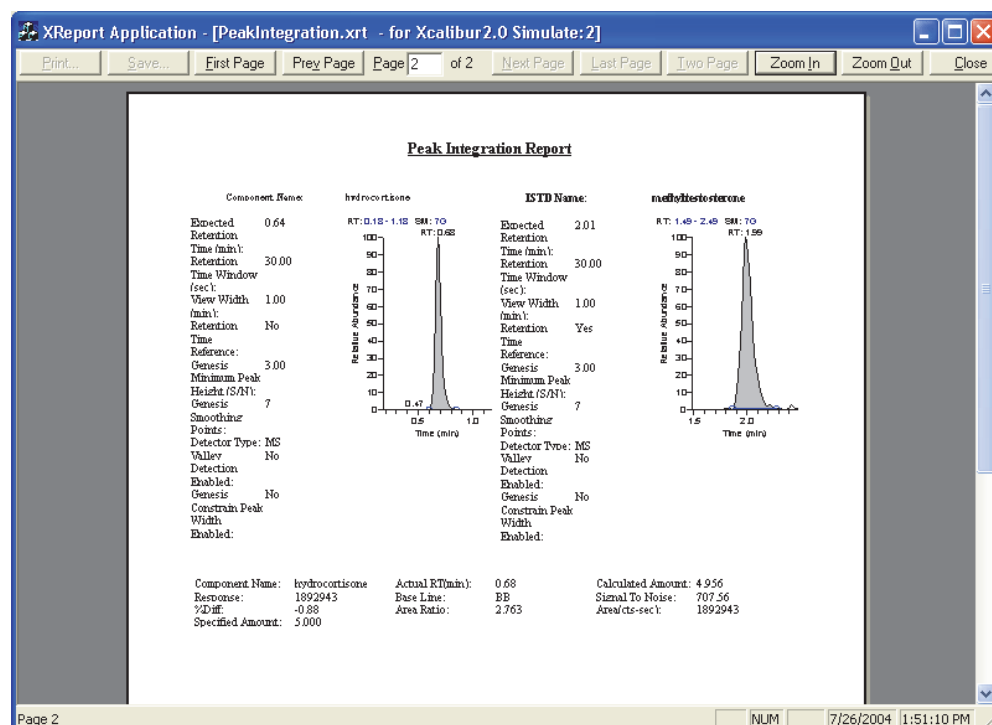
2. When the report is correct, click **Close** to close the preview window.

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 shipped with the Xcalibur software 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" on page 29.

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 (see Figure 10).

   Figure 10. Save As dialog box, showing XReport Templates
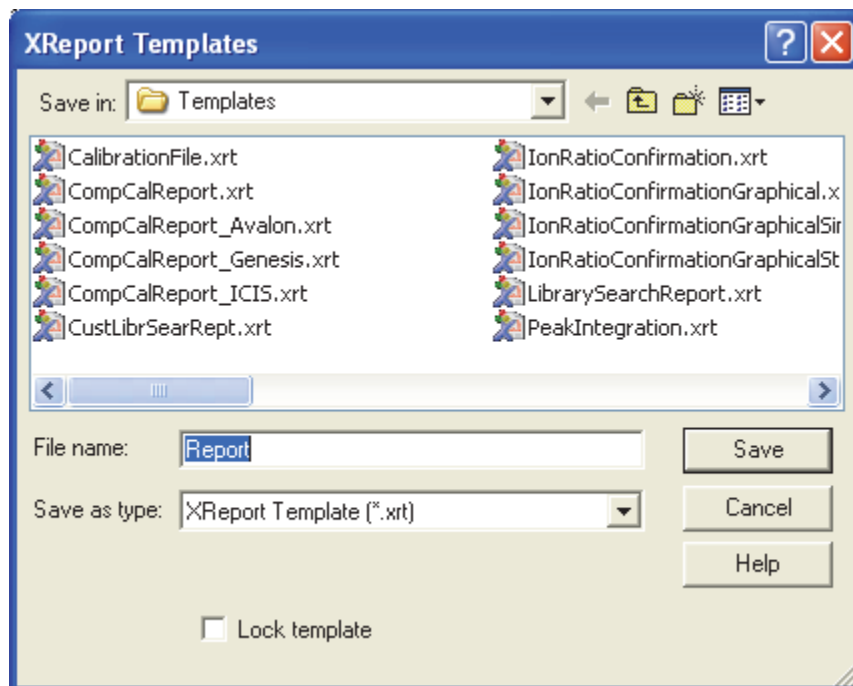
2. Give the report template an appropriate name and save it in the Xcalibur\templates folder with the templates that ship with the Xcalibur software.

3. Select the **Lock Template** check box and click **Save**.

Generating a Report

To generate an Xcalibur report (resolved document), combine a report template with one or more Xcalibur data source files (.pmd, .raw, .rst, .sld, .xcal files).

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.

2. Select the template and click **Open**.

3. Choose **Report > Data Sources**. The Data Sources dialog box opens (see Figure 11).

   Figure 11. Data Sources dialog box
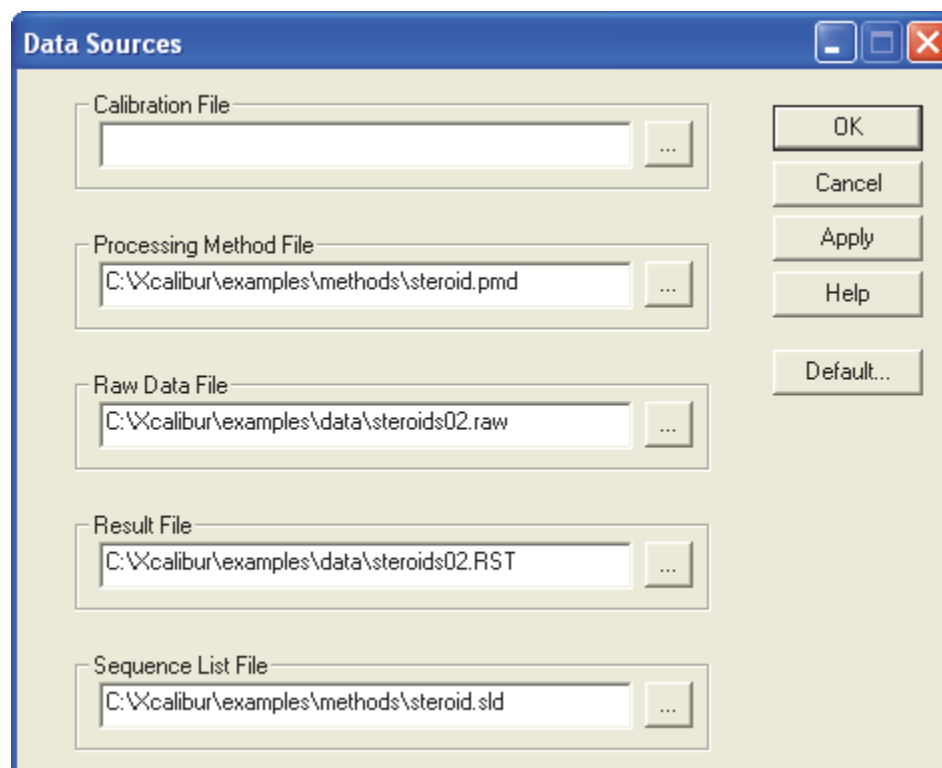
4. In each box, enter or search for a data file.

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

5. Click **OK**.

Generating, Saving, and Printing a Report

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

1. Choose **Report > Resolve Report** in XReport. The Preview window opens (see Figure 12). The Preview window shows a report combined with chosen data sources.

Figure 12. Preview window
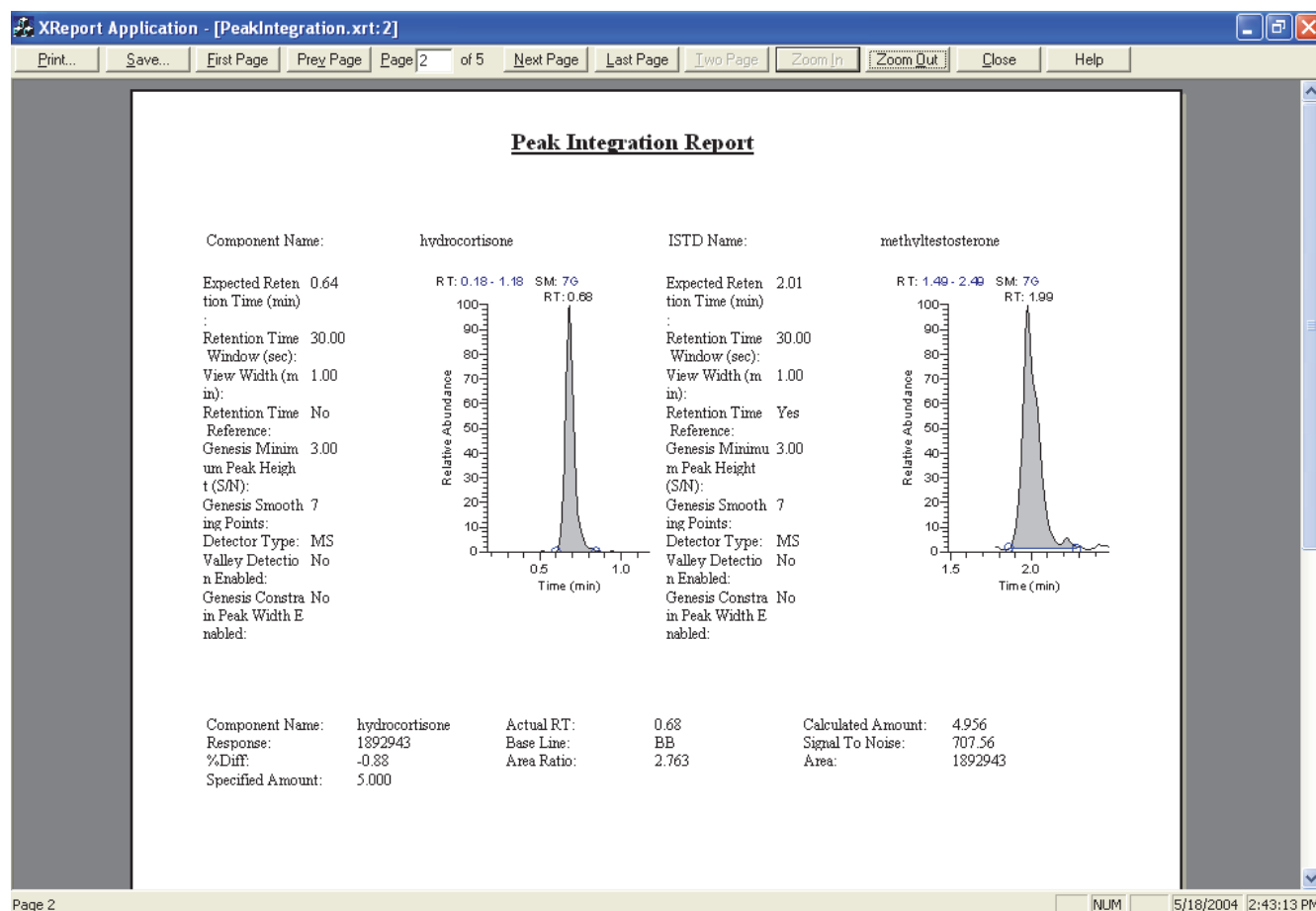
2. Click **Save** to save the report in the following file formats: Microsoft Word (.doc), Microsoft Excel (.xls), Web page (.htm or .html), rich text (.rtf), PDF (.pdf), or text (.txt).

3. To print the report, click **Print**.

4. 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" on page 107.

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 up Report Options in Processing Setup

- Generating Reports when Running a Sample or Sequence

- Generating Reports when Batch Processing a Sequence

Setting up Report Options in Processing Setup

❖ **To set up report settings in the Processing Setup window**

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:

   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), or **.txt**, **.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 Sample or Sequence

❖ **To generate reports when running a sample or a sequence**

1. Set report options in a processing method as described in Setting up Report Options in Processing Setup.

2. In the Xcalibur Sequence Setup window, open the sequence.

3. Specify the processing method that includes all of the report options in the Proc Meth column.
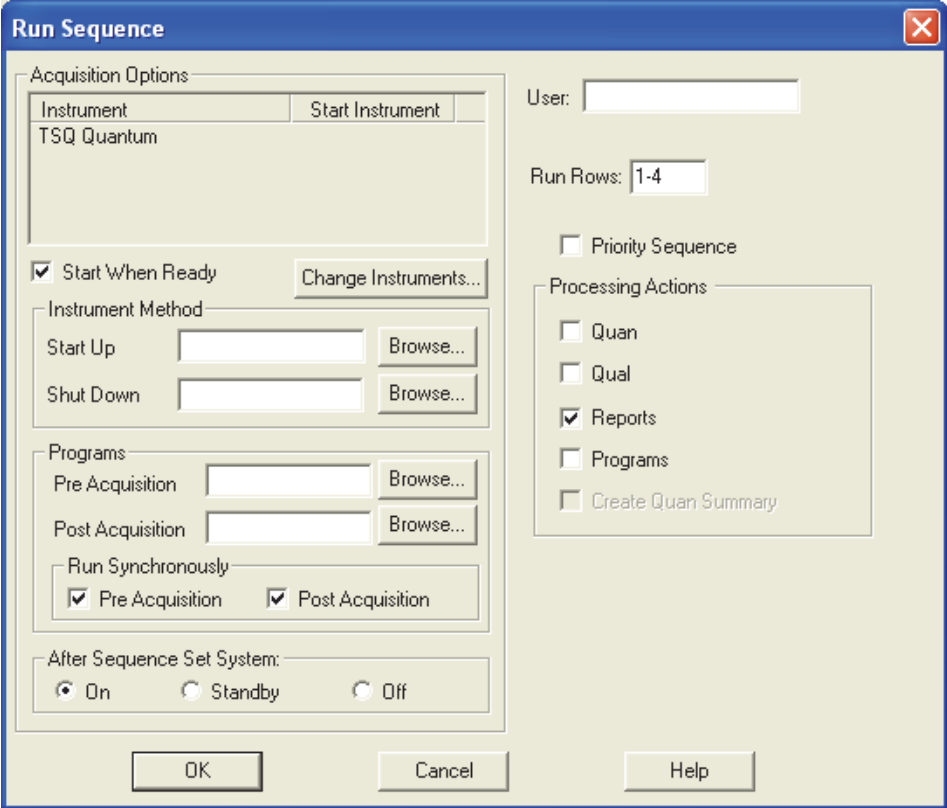
4. When running a sequence, drag the leftmost column to specify the rows to be processed from the current sequence. The application highlights the selected rows.

   When running a sample, select the leftmost column of the sample row.

5. Choose **Actions > Run This Sequence** or **Actions > Run This Sample**. The Run Sequence (see Figure 13) or Run Sample dialog box opens.

   Figure 13. Run Sequence dialog box

   The application displays the sequence rows or sample selected in step 4 in the Run Rows 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 starts processing the selected sample or samples.

Generating Reports when Batch Processing a Sequence

❖ **To generate reports when batch processing a sequence**

1. Set report parameters in the processing method as described in "Setting up Report Options in Processing Setup" on page 33.

2. In the Xcalibur Sequence Setup window, open the sequence.

3. Enter the processing method that includes all of the report options in the Proc Meth column.

4. Specify the rows to be processed from the current sequence by dragging the leftmost column. The data system highlights the selected rows.

5. Choose **Actions > Batch Reprocess**. The Batch Reprocess Setup dialog box opens (see Figure 14).

Figure 14. Batch Reprocess Setup dialog box
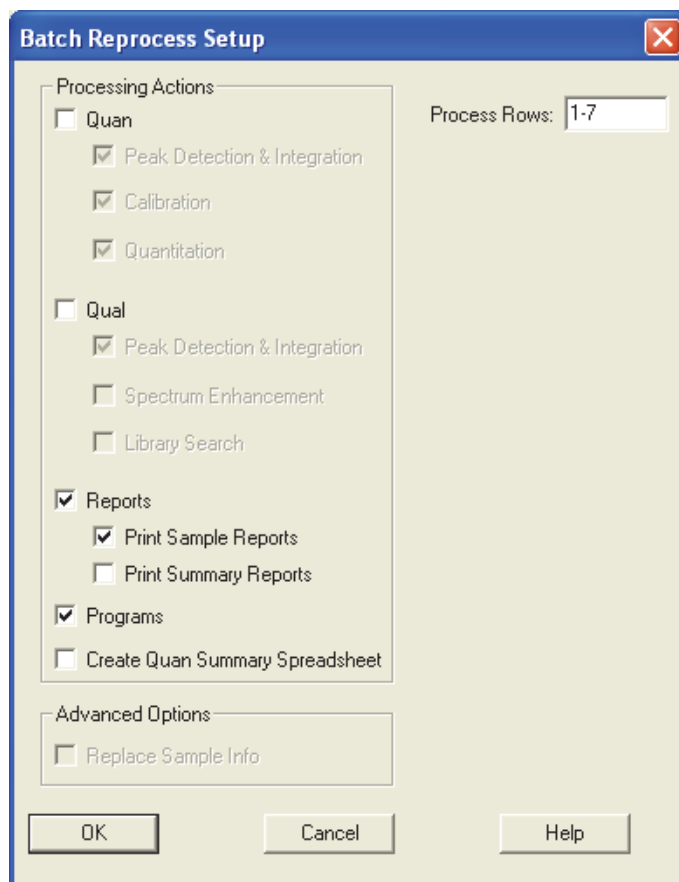
The Xcalibur data system displays the sequence rows selected in step 4 in the Process Rows box.

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

❖ **To generate a report from the Quan Browser window**

1. Open the Quan Browser window. The data system displays the Open dialog box.

2. To select a sequence, select an .sld file with samples to use in the reports.

3. Click **Open**.

4. Choose **View > Reports Dialog**. The Reports dialog box opens (see Figure 15).

Figure 15. Reports dialog box in the Quan Browser window

5. To make a row of the sample reports area active, click the **Enable** box in the first row and click the **Enable** box again. A check box appears in the box.

6. Click the check box. When you click the check box again, the application displays the word Yes in the Enable box to indicate that the entire row of options is selected.

7. To select the report type to print for the sample, click one of the following boxes: **Stds**, **QCs**, **Unks**, or **Other**. A check box control appears.

8. Click the check box. When you click the check box again, the application displays the word Yes in the Enable box to indicate that reports are to be printed for all selected samples of this sample type.

9. Repeat steps 6 and 7 to print reports for needed sample types.

10. 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 Xcalibur data system displays the full path and the file name of the report template .xrt document in the Report Template Name box.

11. To print reports for each report template document, repeat steps 5 through 10 for the next row.

12. 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.

13. To open the Select Report Samples dialog box, click **Select Samples**. The samples available from the .sld file opened in step 2 appear in the Sample Choices box (see Figure 16).

Figure 16. Select Report Samples dialog box
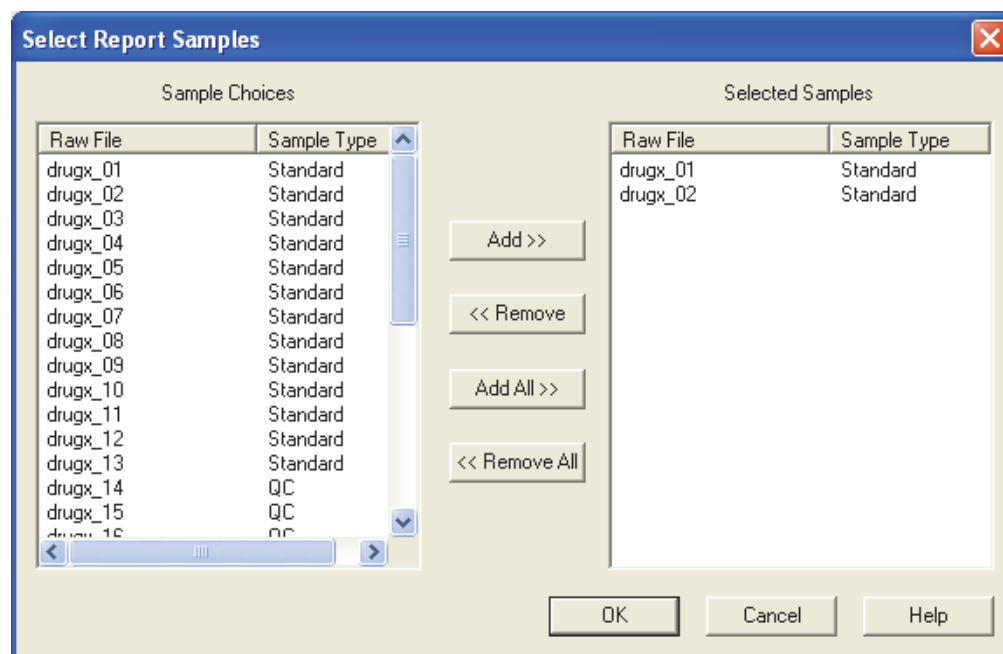
14. Select the samples:

   - 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 CTRL while you click each sample to select or clear it. The data system highlights the selected samples.

15. To copy the selected samples to the Selected Samples area, click **Add**.

16. To return to the Reports dialog box, click **OK**.

17. 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 application 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

In order 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 > All Programs > Thermo Foundation *x.x* > Authorization Manager**. The Authorization Manager window opens (see Figure 17).

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 logon names and passwords to electronically sign the report when it is generated.

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

6. To require signatures from additional groups, repeat step 5 to add them to the Signatures req'd list.

7. 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 17.

Figure 17. Sequence Setup settings for producing signed reports
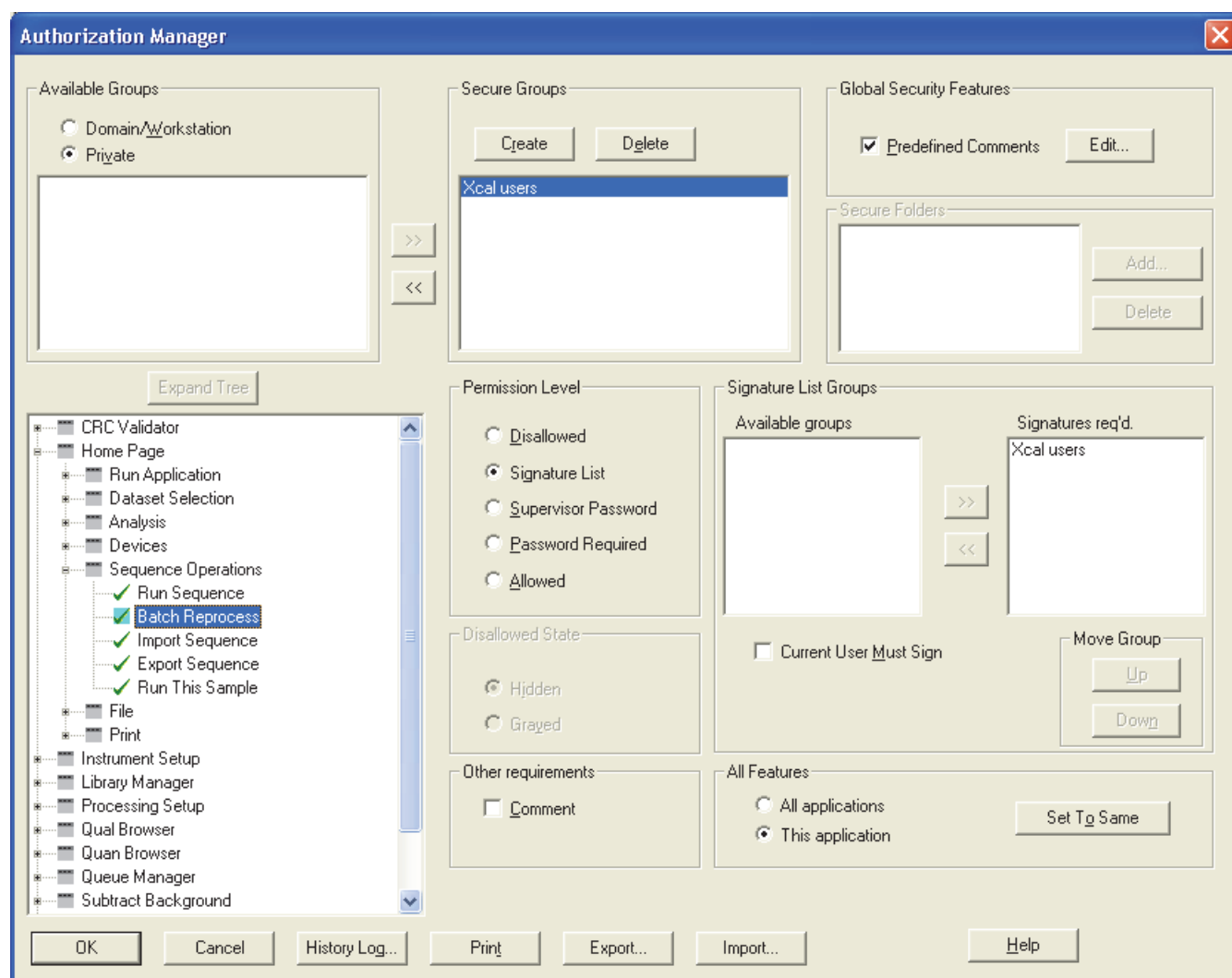
❖ **To set permissions for producing signed reports from Quan Browser**

1. Choose **Start > All Programs > Thermo Foundation *x.x* > Authorization Manager**. The Authorization Manager window opens (see Figure 18).

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**.

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 logon names and passwords to electronically sign the report when it is generated.

   > **Note** If you do not have any groups available or if the groups do not contain the correct members, refer to the *Xcalibur System and 21 CFR Part 11 Compliance Administrator Guide* for information on how to create and modify groups.

6. To require signatures from additional groups, repeat step 5 to add them to the Signatures Req'd list.

7. 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 18.

Figure 18. Quan Browser settings for producing signed reports
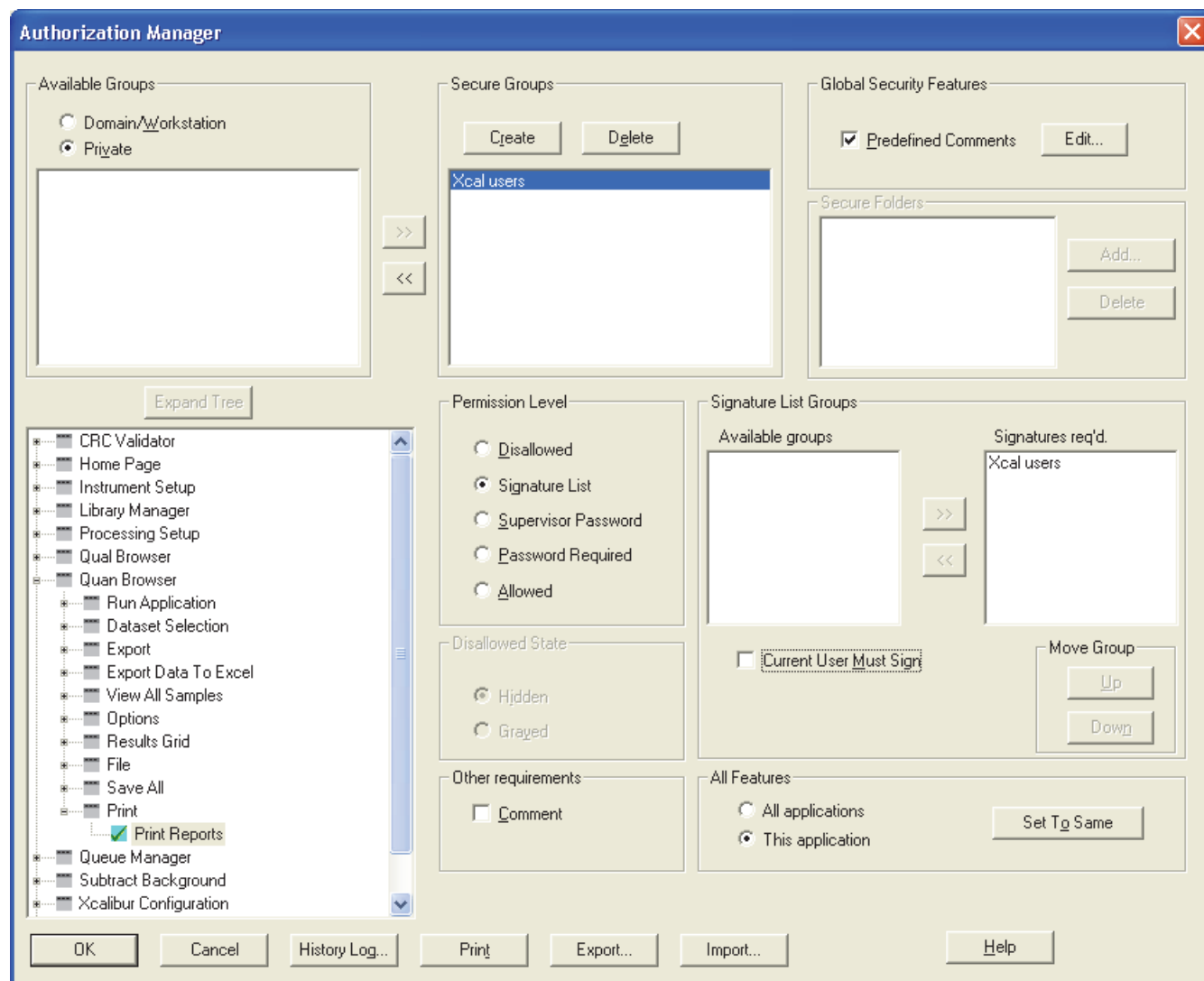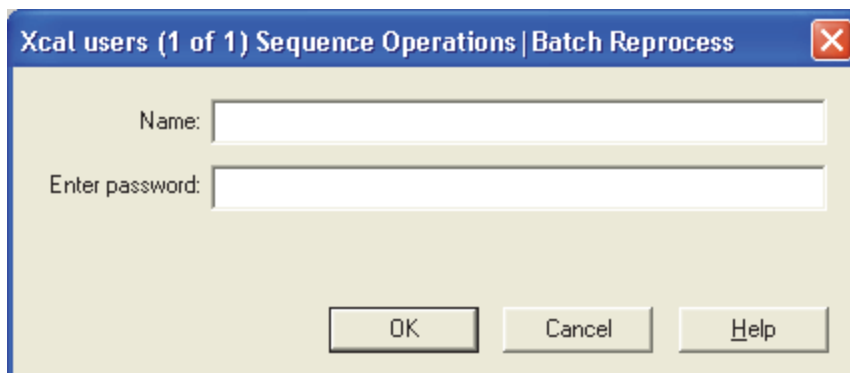
8. Click **OK** to save the settings and close the Authorization Manager dialog box.

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" on page 35 or in "Generating a Report From Quan Browser" on page 36. The Xcalibur data system prompts you to type signature information when the report is generated. Each user whose signature is required must type their logon name and password to sign the report. Figure 19 displays an example of a signature dialog box.

Figure 19. Example of a signature dialog box

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
- Configuring a Component Calibration Curve
- Configuring a Spectrum
- 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 (see Figure 20). This dialog box has three pages: Exclude (available for a Quan repeating section only), Ordering, and Page Breaks.

Figure 20. Exclude page in the Repeating Section Properties dialog box
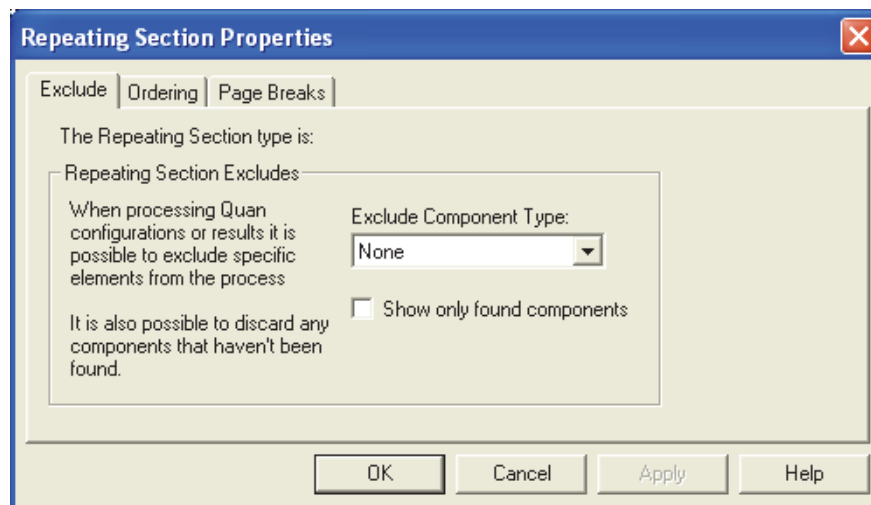
3. When configuring a Quan repeating section, use the Exclude page to exclude specific elements from the process and discard any components that have not been found.

   a. From the Exclude Component Type list, define the exclusions for the Quan repeating section by selecting one of the following options:

      • None (no exclusions) - the default

      • Internal Standards

      • Target Compounds

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

4. Click the **Ordering** tab to display the Ordering page. 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 (see Figure 21).

   Figure 21. Ordering page in the Repeating Section Properties dialog box
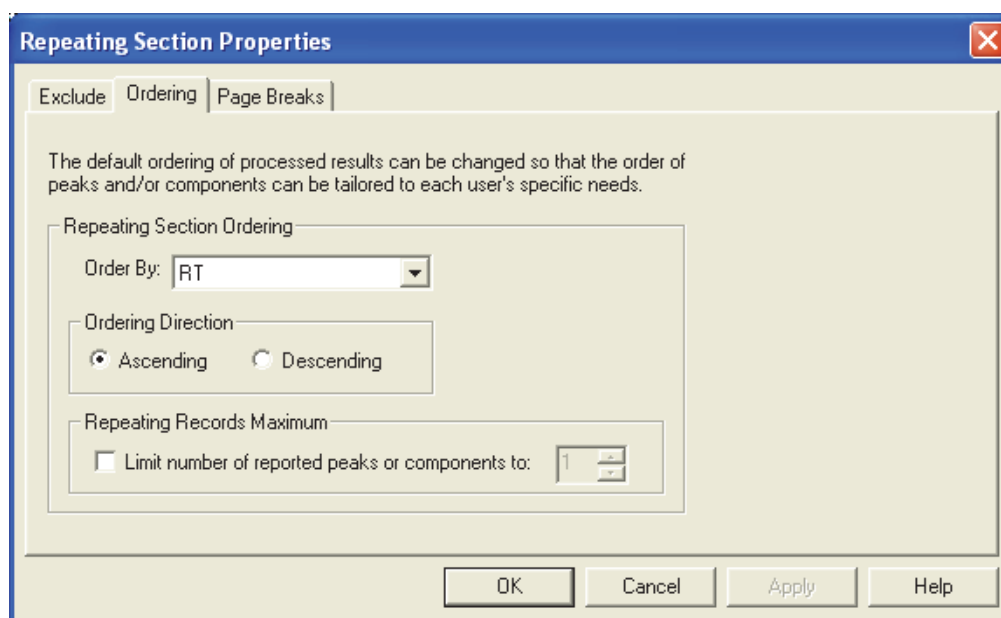
   a. To specify the order for the repeating section in the Repeating Section Ordering area, select one of the following options from the Order By list:

      • RT (Retention Time) - the default

      • Component Name (Quan only)

      • Peak Height Intensity

      • Peak Area Intensity

      • Peak Response Intensity (Quan only)

      • Component Concentration (Quan only)

b. To define the direction for the ordering in the Ordering Direction area, select one of the following options:

- Ascending: Sort data in ascending order

- Descending: Sort data in descending order

c. To set a maximum number of peaks or components to order (up to 999) in the Limit Repeating Records maximum area, select the **Limit number of reported peaks or components** check box and select a value from the active box.

5. 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 (see Figure 22).

Figure 22. Page Breaks page in the Repeating Section Properties dialog box
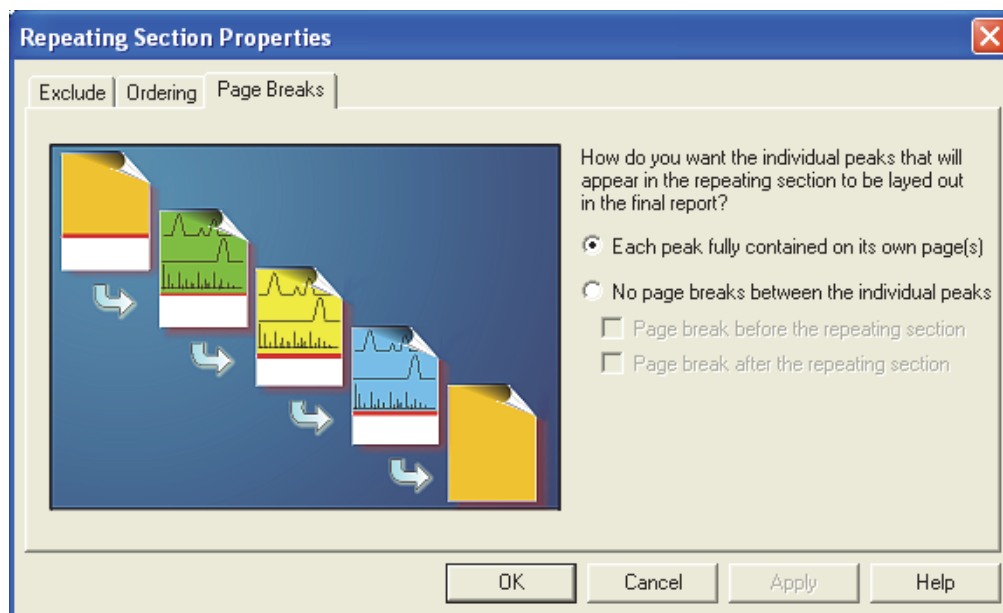
Select the option either to print each peak on its own pages or to avoid page breaks between the individual peaks.

6. When you have made selections in the Repeating Sections Properties dialog box, click **OK**.

7. Choose **File > Save** to save any changes.

Configuring a Text Object

To configure a text object, right-click the object and choose **Properties**. A dialog box opens (see Figure 23), 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 23. Data page in the Sample Header dialog box
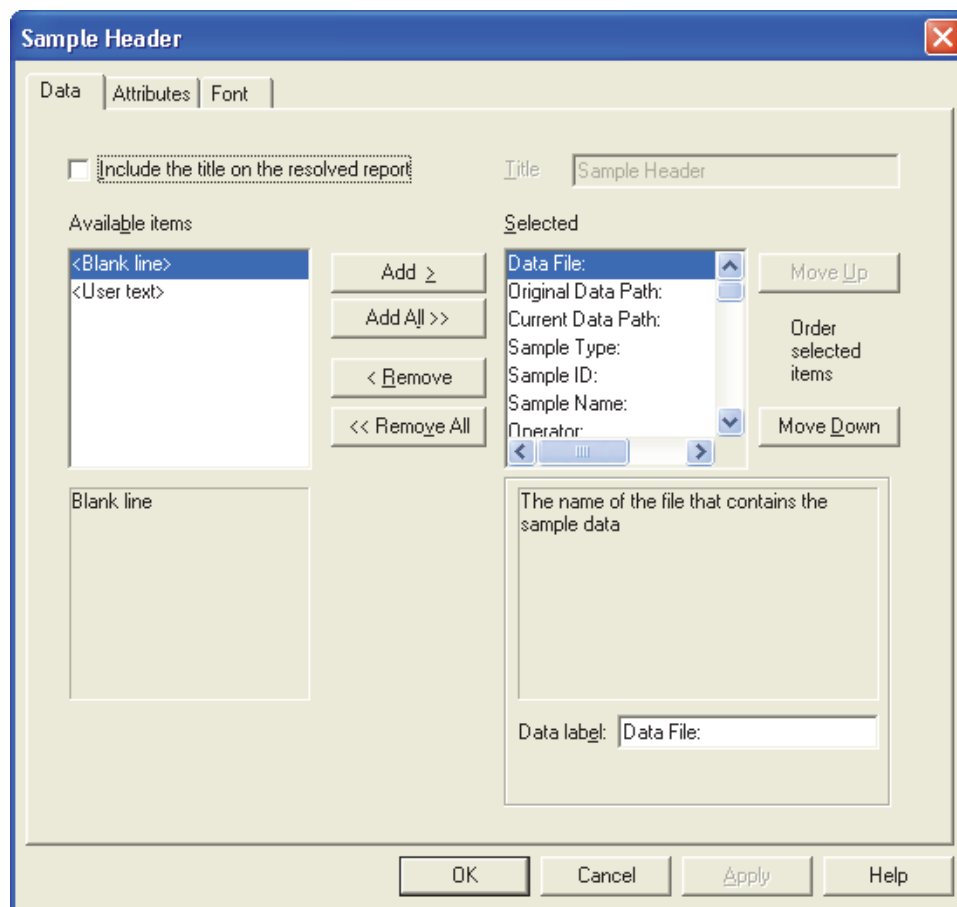
Use the dialog box to configure a text object within the report.

Use the Text Object Properties dialog box for these tasks:

- Configuring Text Fields

- Adding Custom Text Fields

- Configuring Text Attributes

- Setting Text Fonts

Configuring Text Fields

❖ **To configure the text object**

1. To include a custom title for the object, select the **Include the title on the resolved report** check box on the Data page of the Text Object Properties Dialog Box.

2. Click **Include** and type a name in the active 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 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.

❖ **To add a custom text field**

1. On the Data page, select **<User Text>** in the Available Items list and click **Add** (see Figure 24).

Figure 24. Adding a custom text field
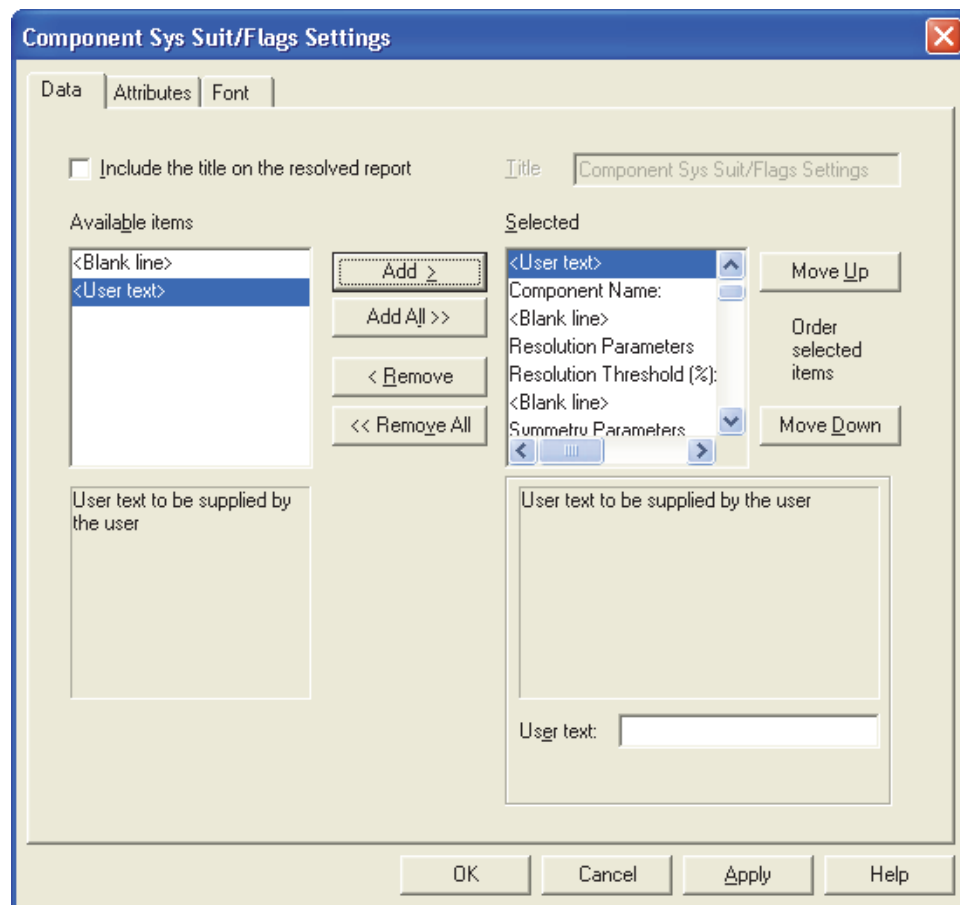
2. Select **<User Text>** in the Selected list.

3. Type the text in the text area and press ENTER (see Figure 25).

Figure 25. Customizing a text field
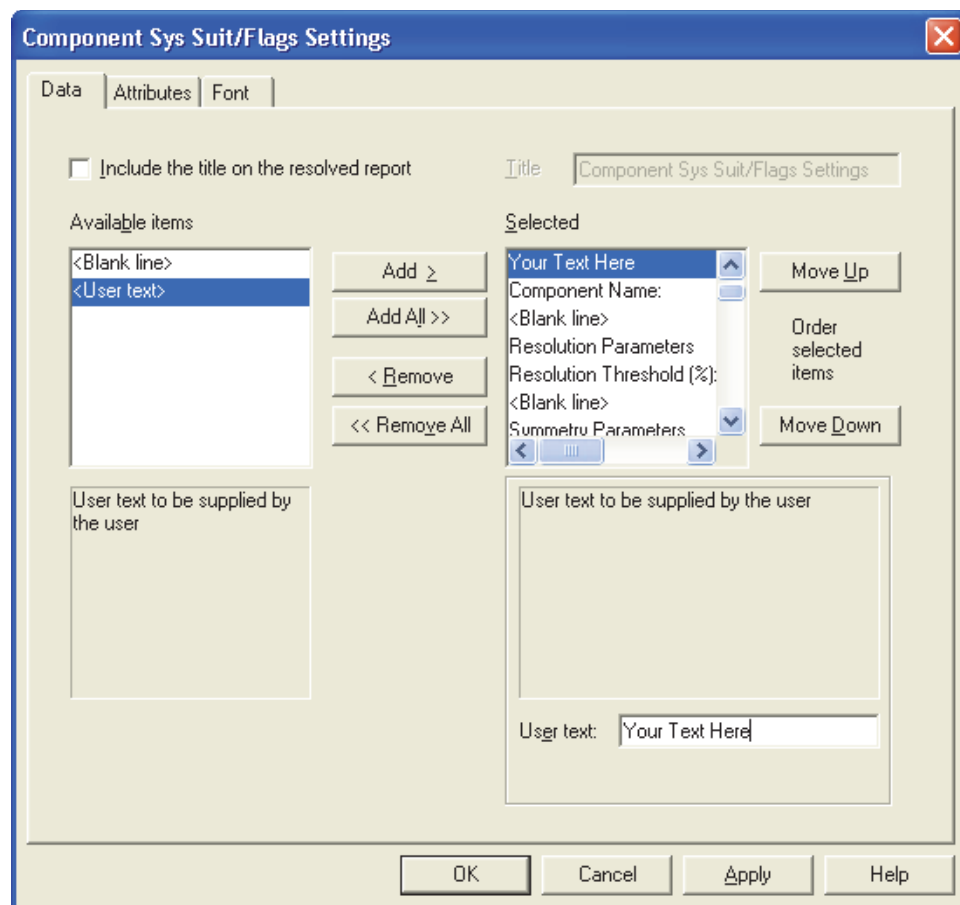
4. Click **OK** to save your changes.

Configuring Text Attributes

To configure text attributes, right-click a text object in the template and choose **Properties** from the shortcut menu. A dialog box opens. Click the **Attributes** tab (see Figure 26).

Figure 26. Attributes page in the Sample Header Properties dialog box
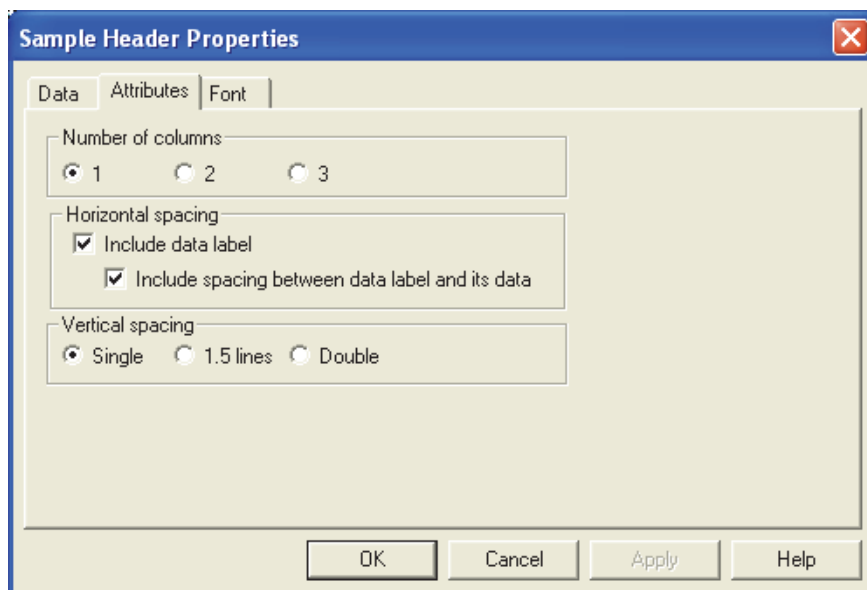
❖ **To configure attributes**

1. To format the text in columns, select the number of columns in the Number Of Columns area.

2. To include data labels in the object in the Horizontal Spacing area, select the **Include data label** check box.

3. To add extra space between data labels and data, select the **Include spacing between a label and its data** check box.

4. Select a line spacing option in the Vertical Spacing area.

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

Setting Text Fonts

To set text fonts, right-click a text object and choose **Properties** from the shortcut menu. A dialog box opens and you can select a font type for the title, heading, data label, and data. Click the **Font** tab (see Figure 27).

Figure 27. Setting fonts
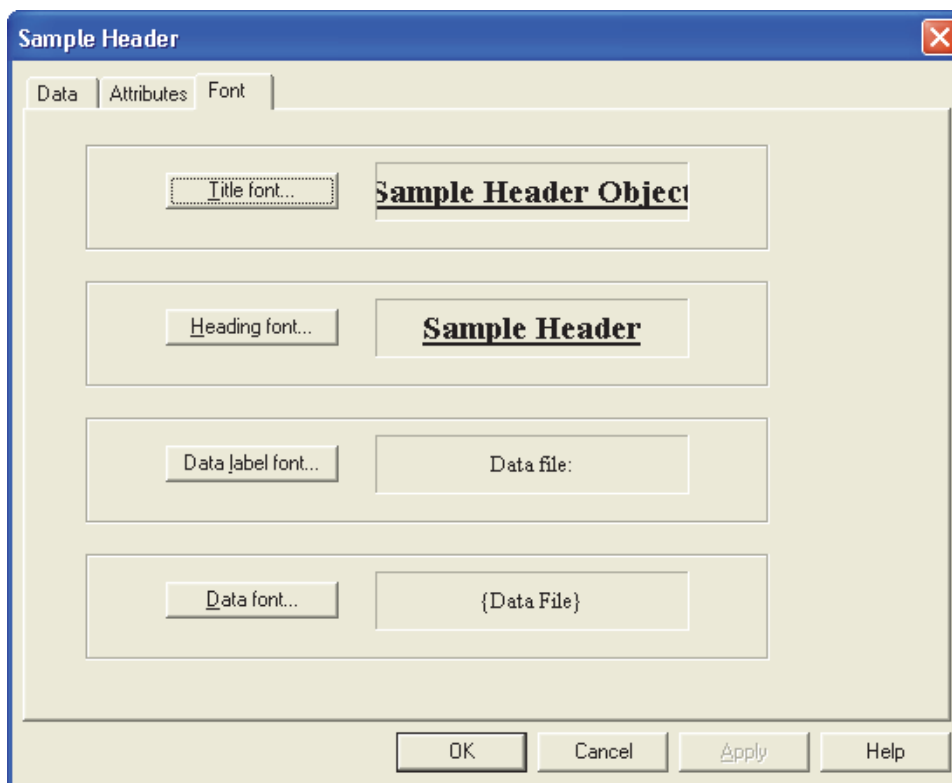
❖ **To set the font for a specific type of text for each button on the page**

1. Click a text type button. The Font dialog box opens (see Figure 28).

Figure 28. Font dialog box
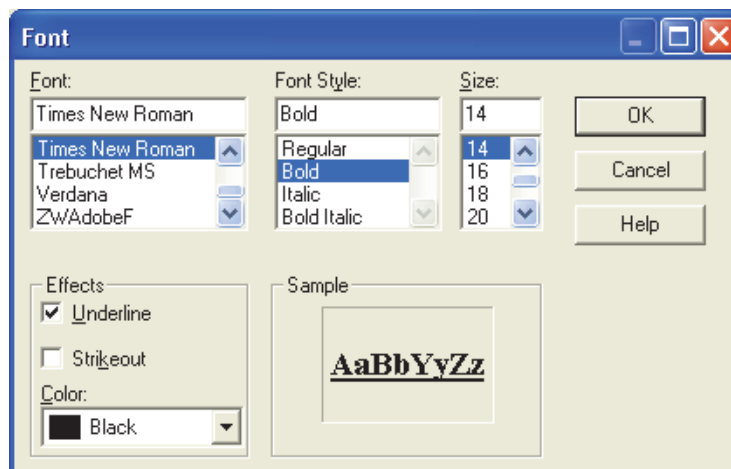
2. Make the font selections and click **OK**.

> **Note** The Heading Font selection is also used for User Text. See "Adding Custom Text Fields" on page 51.

Configuring an Annotation Object

You can include an annotation object in any section type.

❖ **To configure the Annotation object**

1. Right-click the annotation object in the template and choose **Properties** from the shortcut menu. The Annotation Properties dialog box opens (see Figure 29).

Figure 29. Data page in the Annotation Properties dialog box
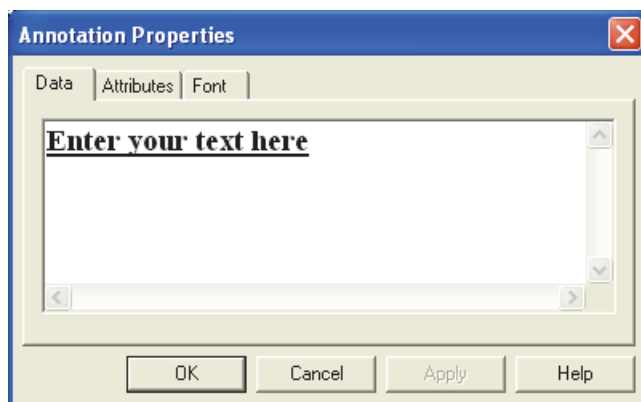
2. On the Data page, click the box on the Annotation Properties dialog box to get a cursor. Delete the words *Enter your text here* and type annotation text.

3. On the Attributes page, select the number of columns to display annotation text in the Number of columns area (see Figure 30).

Figure 30. Attributes page in the Annotation Properties dialog box
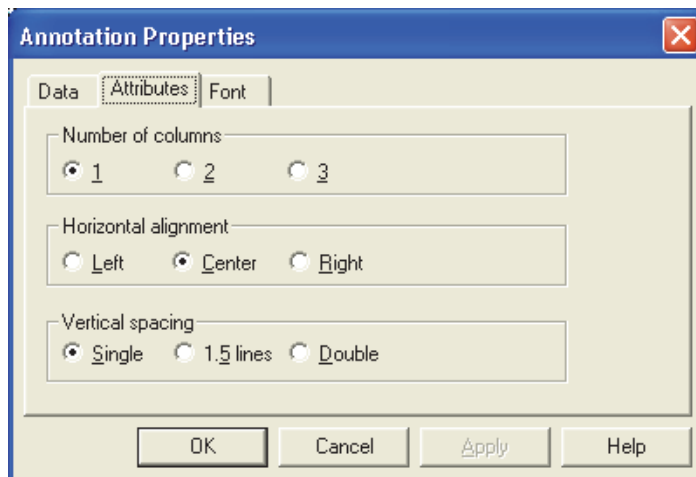
4. In the Horizontal alignment area, select an alignment option for the annotation text: **Left**, **Center**, or **Right**.

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 (see Figure 31).

Figure 31. Font page in the Annotation Properties dialog box
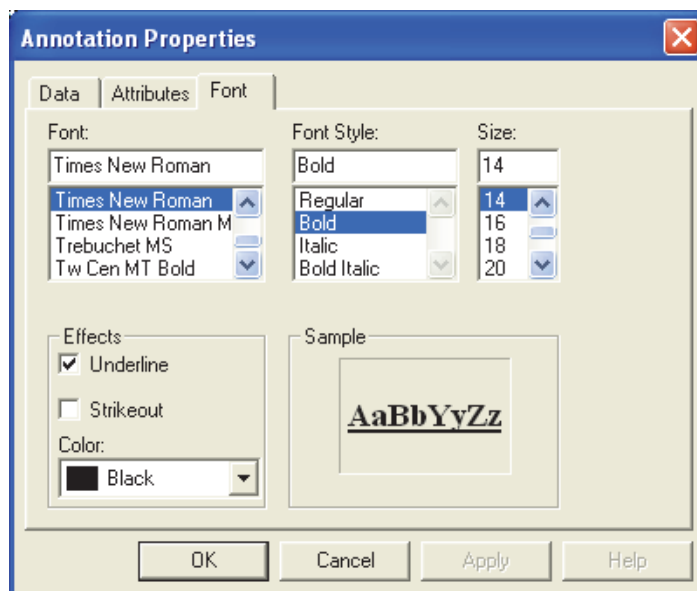
7. Click **OK** to save your changes.

Configuring a Table Object

❖ **To configure a table object**

1. Right-click the table object.

2. Choose **Properties** from the shortcut menu. The Table Properties wizard opens (see Figure 32), 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 32. Select Table Fields page
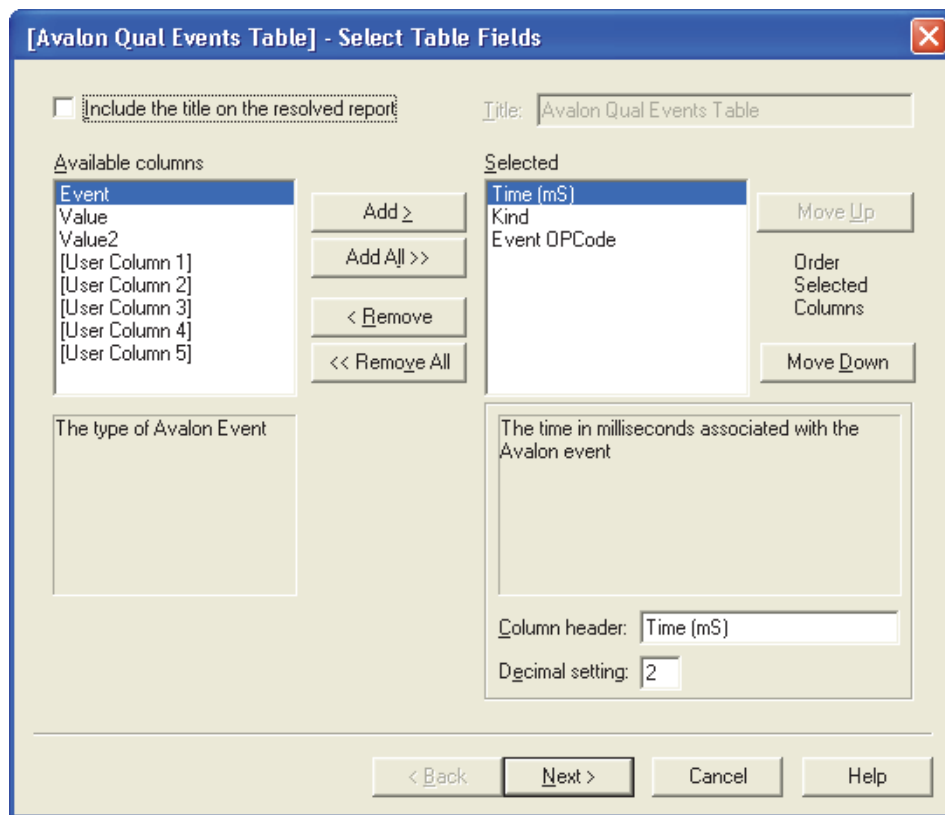
Using the Table Properties wizard, configure a table object included in the report template by changing its properties. Use the wizard for the following:

- 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 (see Figure 32), use the Select Table Fields page of the Table 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.

❖ **To select options for the Select Table Fields page of the Table wizard**

1. 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.

2. To select the columns to include in the table from the Available Columns list, choose one of these options.

   • 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.

3. Type the column heading text in the Column Header box.

4. To arrange the order of the selected columns in the Selected Columns list, click **Move Up** or **Move Down**.

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

Configuring Custom (User) Columns

The Configure User Column Parameters page of the Table wizard appears only if you chose to include custom User Columns in the table. Use this page to define parameters for each User Column in the table (see Figure 33).

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 33. Configure User Column Parameters page
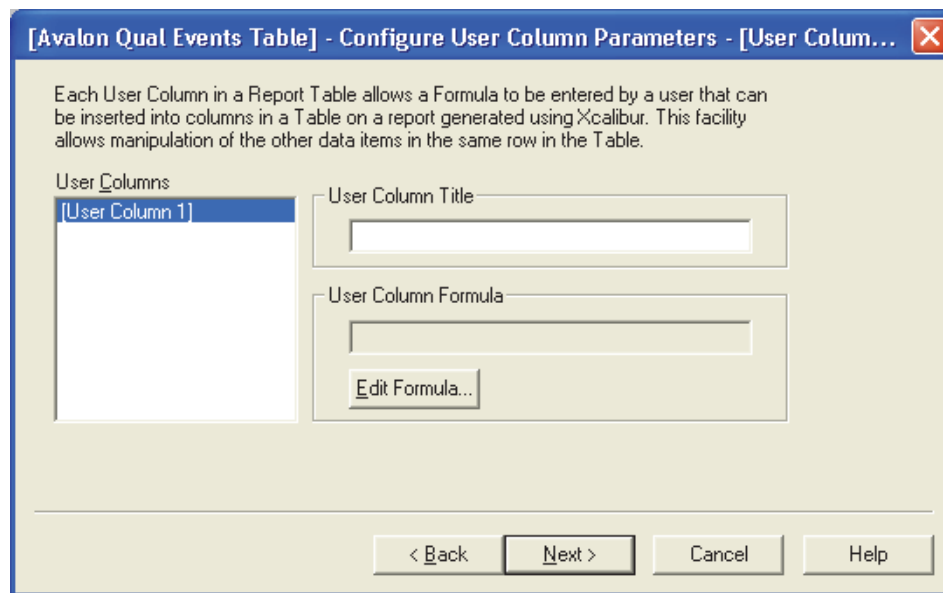
The data system displays the User Columns you have selected for the table in the User Columns list.

❖ **To define each user column**

1. Select a user column in the User Columns list.

2. Type a title for the user column in the User Column Title area.

3. Click **Edit Formula** in the User Column Formula area. The Edit Formula dialog box opens (see Figure 34).

Figure 34. Edit Formula For dialog box
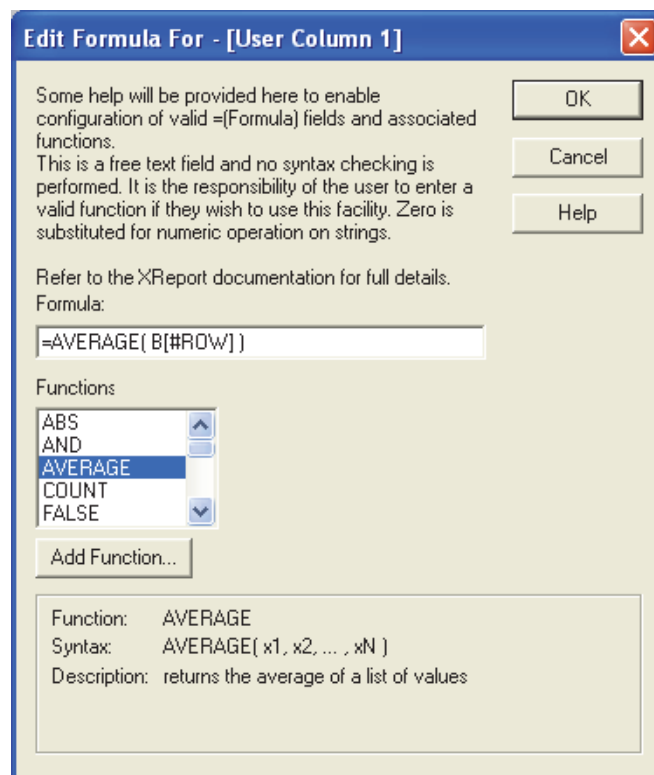
For the selected column, edit a formula for the user column and configure valid fields and associated functions. Below the functions list is a brief description of each function at the bottom of the dialog box.

4. 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.

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

6. To return to the Configure User Column Parameters page, click **OK**.

7. 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 wizard to define a method for sorting table data when you generate a report (see Figure 35).

Figure 35. Set Table Sort Filter page
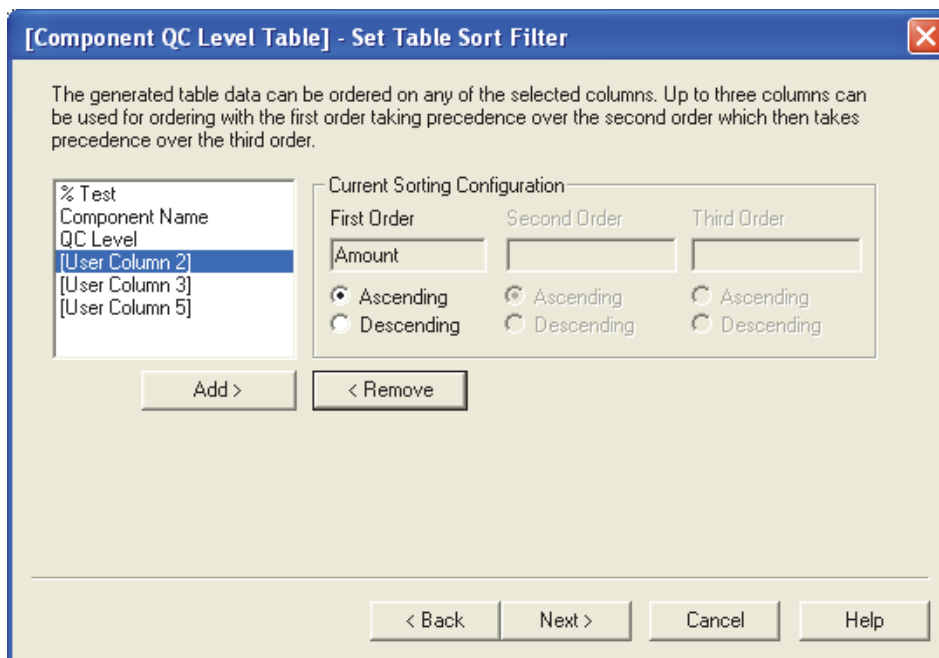
XReport displays the columns selected for the table in a list on the left side of the dialog box. Set the order for the table using any of the selected columns. Use up to three columns for ordering the table: The first order takes precedence over the second order, which takes precedence over the third order.

❖ **To define a method for ordering data in the table**

1. 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.

2. 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.

3. To define the second and the third variable used to order table columns, repeat the first two steps.

4. To move to the Font page, click **Next**.

Setting Table Fonts

Use the final page of the Table wizard, the Set Table Font page, to set the font type for elements in the table (see Figure 36).

Figure 36. Set Table Font page
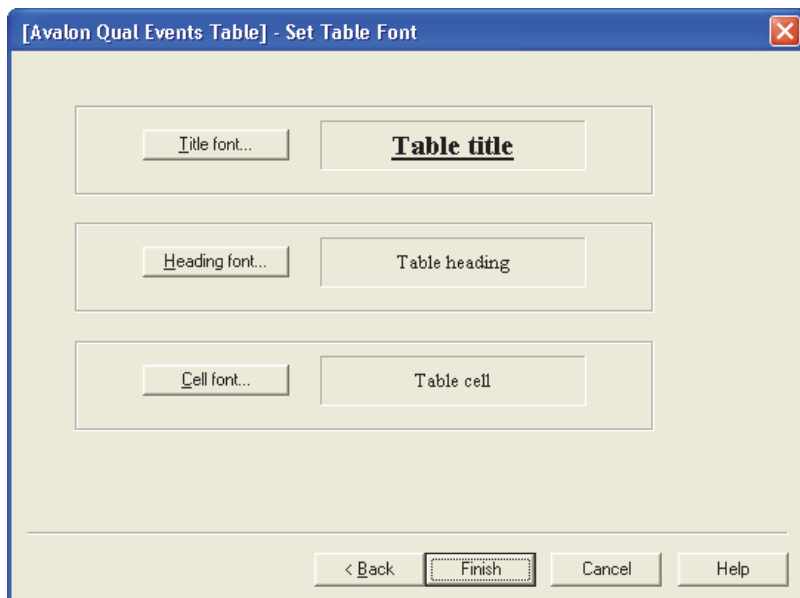
❖ **To define the font for a specific element**

1. Click the appropriate button. The Font dialog box opens (see Figure 37).

Figure 37. Font dialog box
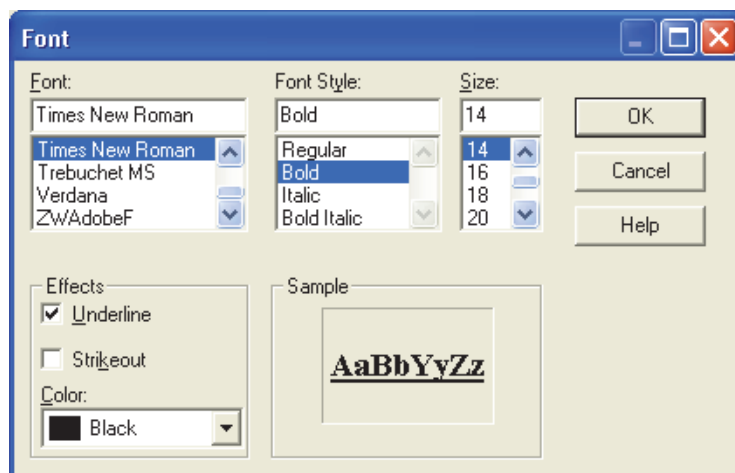
2. Select font options and click **OK**. Repeat the process as needed for other table elements.

Setting Additional Table Properties

After completing the Table 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

To set Library Search Graphics Table properties, right-click the table and choose **Properties** from the shortcut menu. The Table Properties wizard opens. When you complete the wizard and click Finish, the Library Search Graphics Table Properties dialog box opens (see Figure 38). Click **Cancel** to close the dialog box.

Figure 38. Library Search Graphics Table Properties dialog box
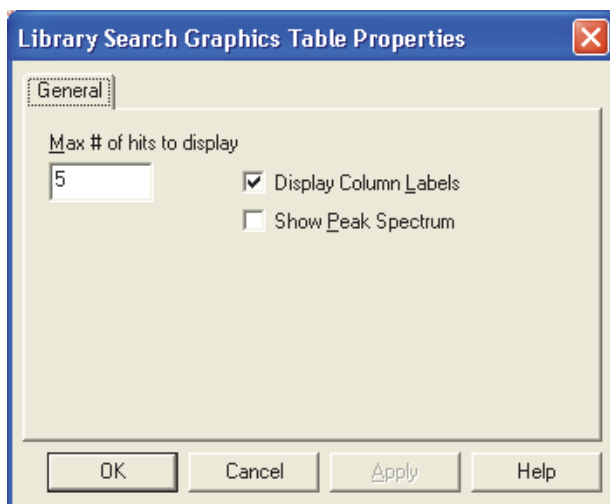
❖ **To set parameters in this dialog box**

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**. Choose **File > Save** to save any changes made.

Library Search Results Table Properties

To set Library Search Results Table properties, right-click the table and choose **Properties** from the shortcut menu. The Table Properties wizard opens. When you complete the wizard, the Library Search Results Table Properties dialog box opens (see Figure 39).

Figure 39. Library Search Results Table Properties dialog box
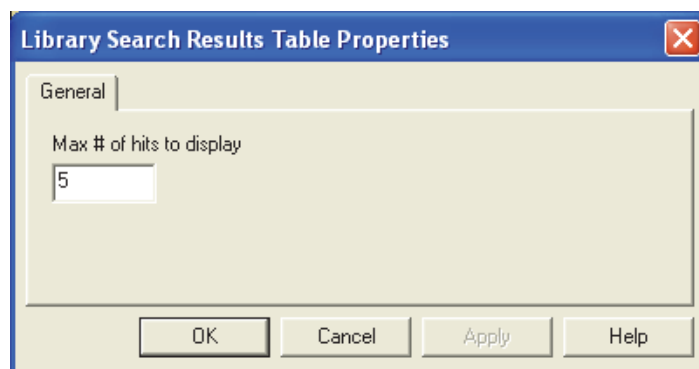
❖   **To set parameters in this dialog box**

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

To set Sample Table properties, right-click the table and choose **Properties** from the shortcut menu. The Table Properties wizard opens. After completing the wizard, the Sample Table Properties dialog box opens (see Figure 40).

Figure 40. Sample Table Properties dialog box
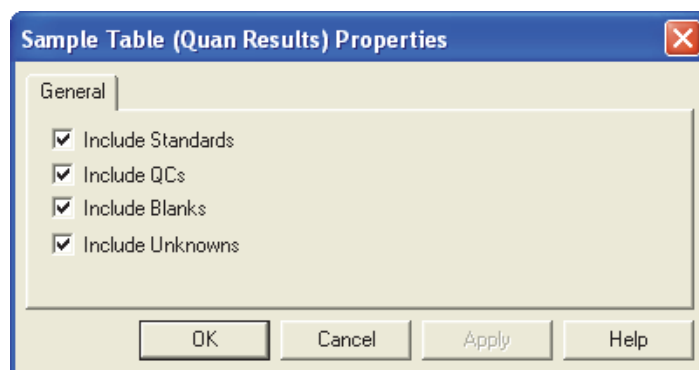
❖   **To set parameters in this dialog box**

1. To include standards, QCs, blanks, or unknowns in the Sample table, select the corresponding check boxes.

2. Click **OK**.

Spectrum List Table Properties

To set Spectrum List Table properties, right-click the table and choose **Properties** from the shortcut menu. The Table Properties wizard opens. After completing the wizard, the Spectrum List Table Properties dialog box opens (see Figure 41).

Figure 41. Options page in the Spectrum List Table Properties dialog box
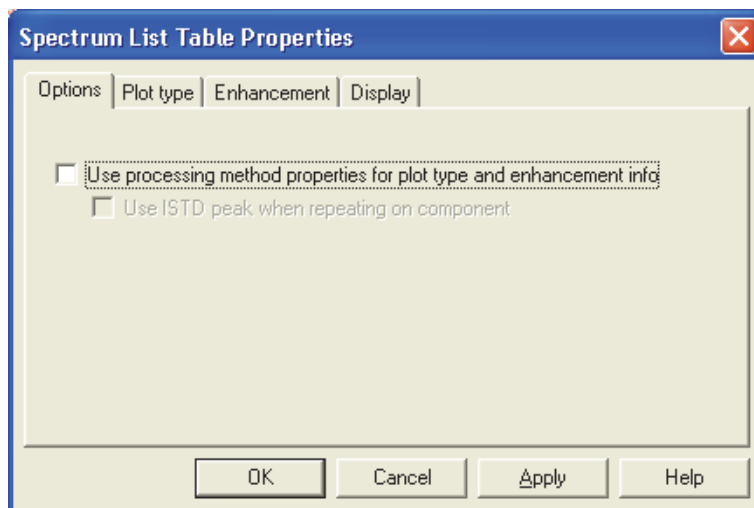
This dialog box has four pages:

- Options Page

- Plot Type Page

- Enhancement Page

- Display Page

Options Page

❖ **To set parameters on the Options page**

1. Select or clear the **Use processing method properties ...** check box (see Figure 41).

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

2. 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.)

3. Click **OK**.

Plot Type Page

Before viewing and selecting the parameters on the Plot Type page, clear the **Use processing method properties...** check box on the Options page and click the **Plot Type** tab.

❖ **To set parameters on the Plot Type page**

1. 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 (see Figure 42).

Figure 42. Plot Type page in the Spectrum List Table Properties dialog box
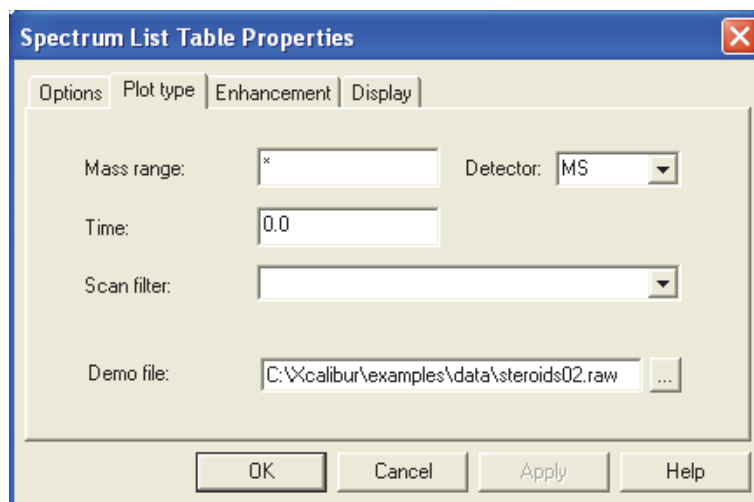
2. Select the type of detector that you are using from the Detector list: **MS** or **PDA**.

3. 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.

4. Enter the scan filter to use with the data in the Scan Filter list.

5. 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.

6. Click **OK**.

Enhancement Page

❖ **To set parameters on the Enhancement page**

1. To add smoothing to the data, select the **Enable** check box in the Smoothing area (see Figure 43).

Figure 43. Enhancement page in the Spectrum List Table Properties dialog box
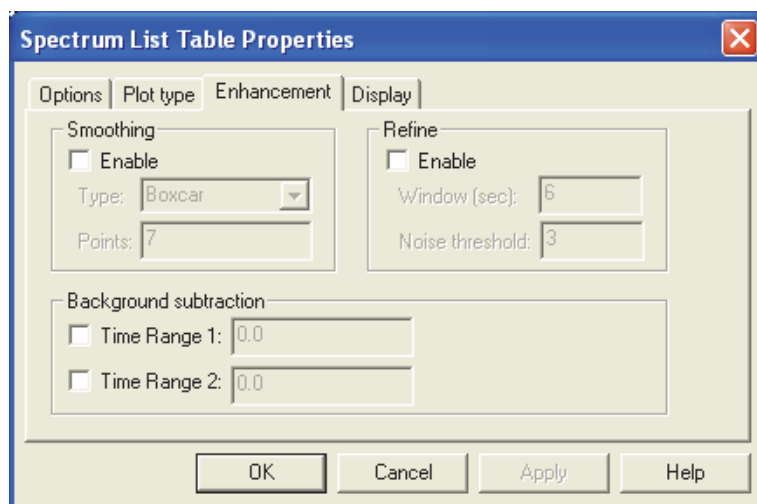
2. To select a type of smoothing, select **Boxcar** or **Gaussian** from the Type list.

3. Select the number of smoothing points (odd numbers from 3 to 15) to be used in the Points list.

4. To refine the data, select the **Enable** check box in the Refine area.

5. 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.

6. 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.

7. 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.

8. Click **OK**.

Display Page

❖ **To set parameters on the Display page**

1. 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 (see Figure 44).

   Figure 44. Display page in the Spectrum List Table Properties dialog box
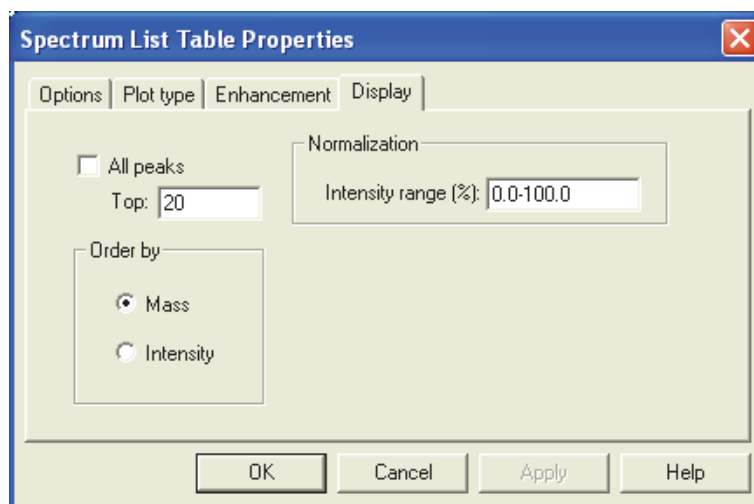
2. To order the data by mass or by intensity, select the appropriate option in the Order by area.

3. Type a value representing the relative abundance range of mass peaks to include in the table in the Normalization area.

4. 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.

❖ **To configure the Electronic Signature table object**

1. Right-click the **Electronic Signature** table object and choose Properties from the shortcut menu. The Electronic Signature Properties dialog box opens (see Figure 45).

   Figure 45. Electronic Signature Properties dialog box
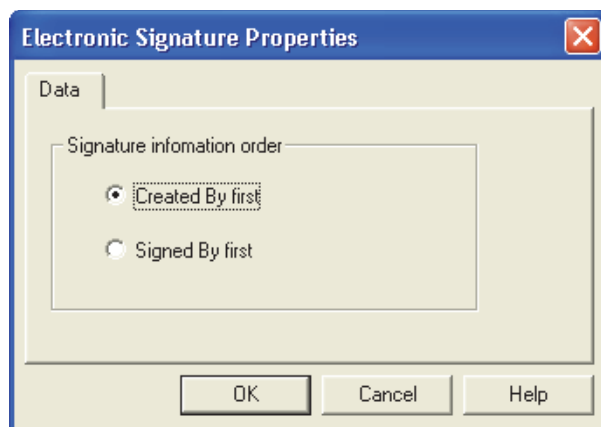
2. To display the Created By signature block before the Signed By signature block, select the **Created by first** option in the Signature Information Order area or, to display the Signed By block before the Created By block, select the **Signed by first** option.

3. Click **OK**.

Configuring a Bitmap Object

❖ **To configure the bitmap object**

1. Right-click the bitmap object and choose **Properties** from the shortcut menu. The Bitmap Properties dialog box opens (see Figure 46).

   Figure 46. Bitmap Properties dialog box
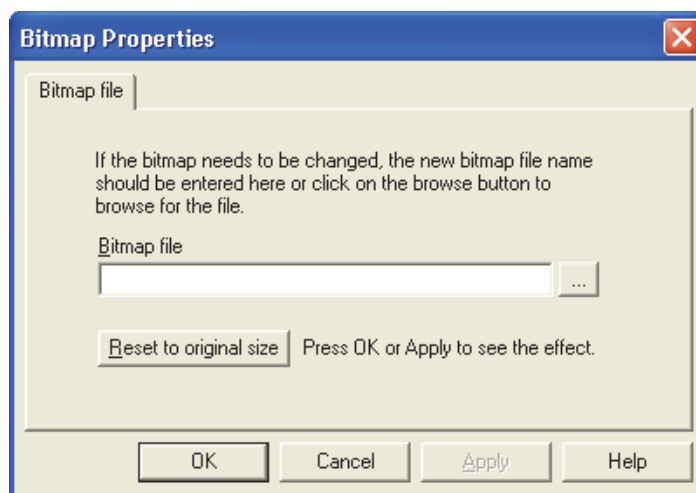
2. Enter the name of the image file. Choose one of the following file formats: .bmp, .dib, .gif, .jpg, or .ico.

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

❖ **To configure a chromatogram report object**

1. Right-click the object and choose **Properties** from the shortcut menu. The Chromatogram Properties dialog box opens (see Figure 47).

Figure 47. Chromatogram Properties dialog box
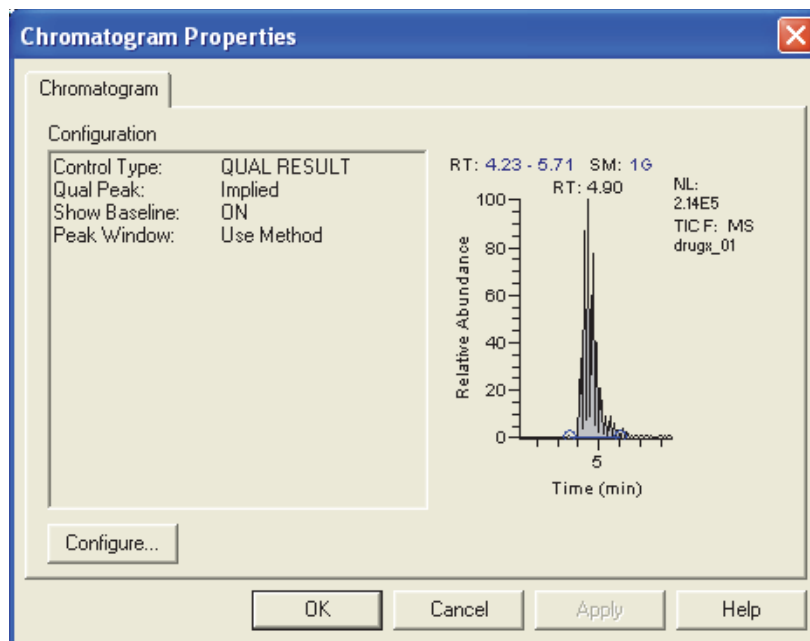
2. Click **Configure**. The Chromatogram Properties wizard opens.

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			Repeating section	
	Raw	**Quan**	**Qual**	**Quan**	**Qual**
Use Container Supplied Quan Peak				●	
Use Container Supplied Qual Peak					●
Select Chromatogram Type	●	●	●	●[*]	●
Select Demo File	●	●	●	●	●
Select the Quan Peak		●		●[**]	
Select Component				●	
Select the Qual Peak			●		●
Select Mass Spectrum Quan Traces to Display		●		●	
Configure How the Peak Window Will Look		●	●	●	●
Select Plot Details	●				
Select Enhance Details	●				
Select Chromatogram Style	●	●	●	●	●
Select the Peak Labeling	●	●	●	●	●
Select How the Chromatogram Axis Will Be Configured	●	●	●	●	●
Configure Normalization for the Chromatogram	●	●	●	●	●

[*] This page is not displayed if you selected Explicitly Specify the Chromatogram's Behavior on the Use Container Supplied Quan or Qual peak page.

[**] This page is only displayed if you selected Explicitly Specify the Chromatogram's Behavior on the Use Container Supplied Quan or Qual peak page.

> **Note** When you click 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 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.

❖ **To explicitly configure a Quan-based chromatogram type**

1. 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 (see Figure 48).

Figure 48. Use Container Supplied Quan Peak page
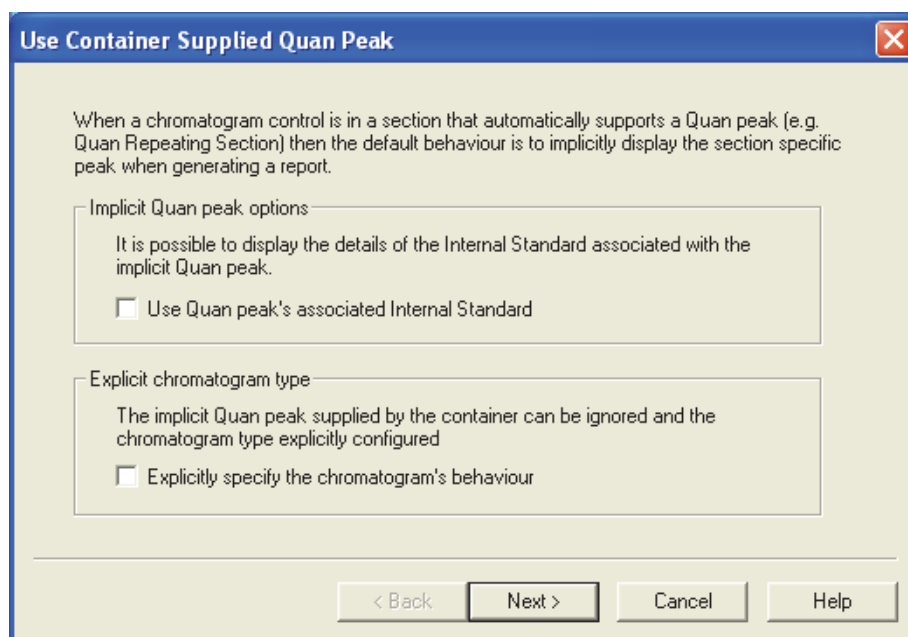
2. To ignore the implicit Quan peak supplied by the container and explicitly configure the chromatogram type, select the **Explicitly specify the chromatogram's behaviour** check box in the Explicit chromatogram type area.

3. 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 to ignore the implicit Quan peak and explicitly configure the chromatogram type.

❖ **To explicitly configure a Qual-based chromatogram type**

1. 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 (see Figure 49).

Figure 49. Use Container Supplied Qual Peak page
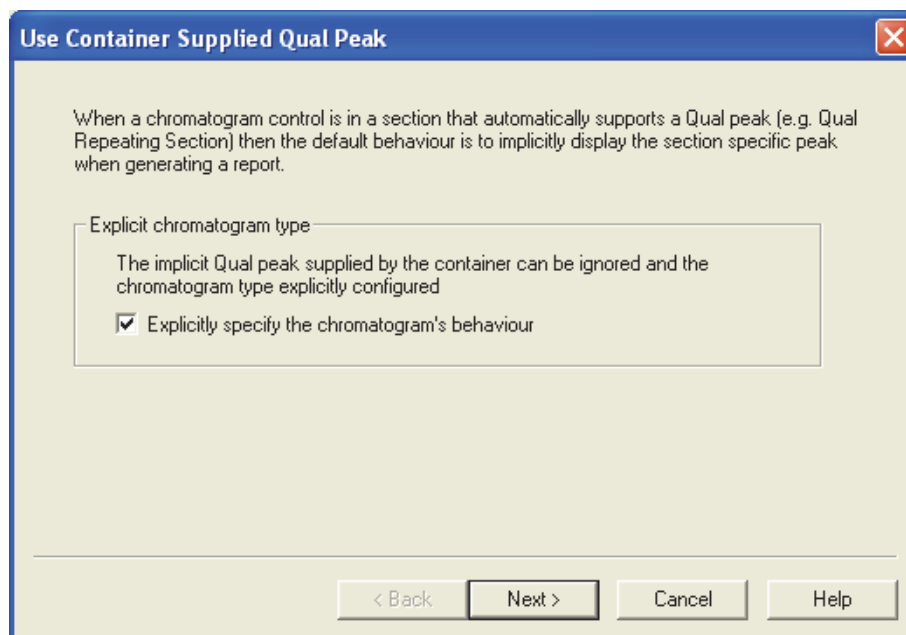
2. Click **Next** to go to the next page of the wizard.

Select Chromatogram Type Page

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

❖ **To select a chromatogram type**

1. Define the chromatogram type in the Chromatogram Type area (see Figure 50) by selecting one of the following options:

   • Raw file based chromatogram

   • Quan results based chromatogram

   • Qual results based chromatogram

Figure 50. Select Chromatogram Type page
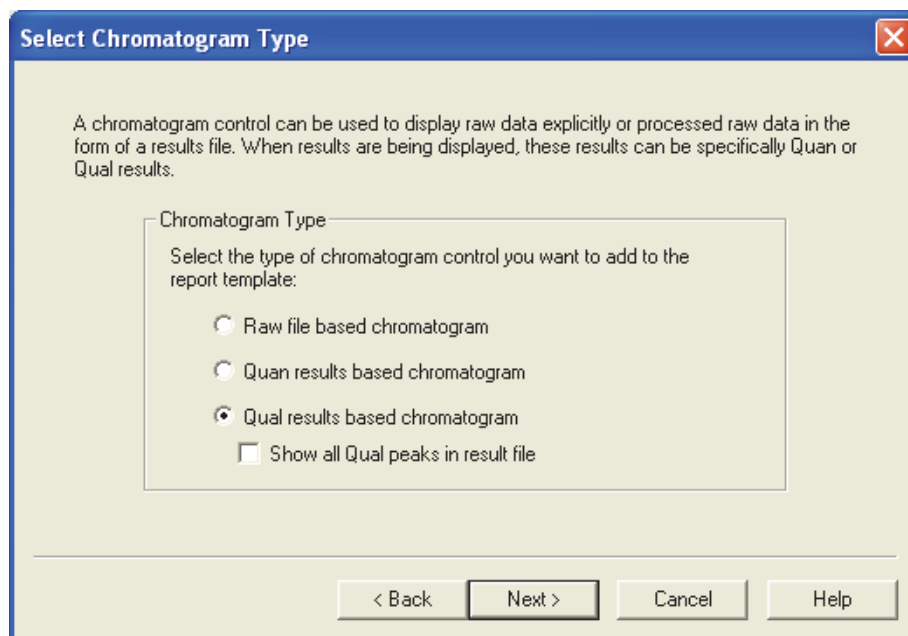
2. If you select a Qual results based chromatogram in step 1, select the **Show all Qual peaks in result file** check box to display all Qual peaks in a resolved Xcalibur report. This is a Peak Type setting.

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

Select Demo File Page

Use the Select Demo File page 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.

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 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 (see Figure 51).

   Figure 51. Select a raw file based chromatogram
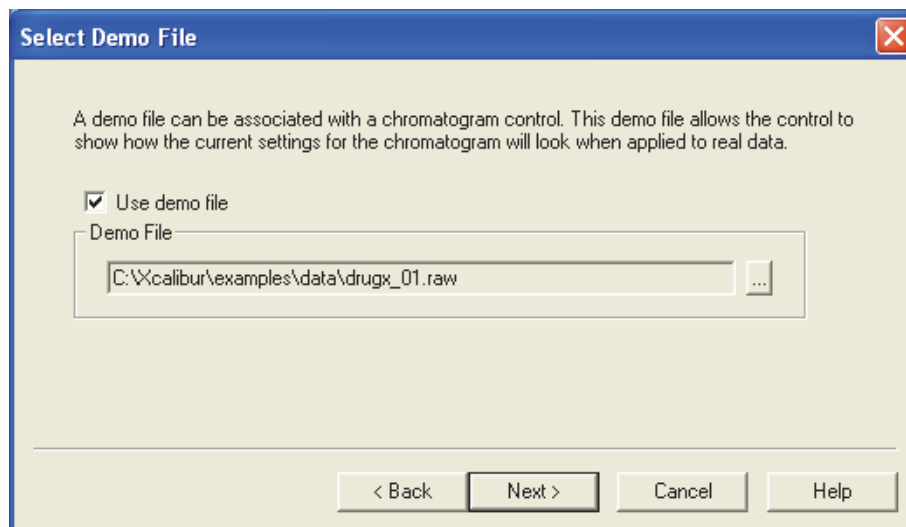
2. To search for the required demo file (.raw file), click the browse button in the Demo File area. The Select Raw Data File dialog box opens.

3. Select a demo file and click **Open**. 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.

❖ **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 (Figure 52).

   Figure 52. Selecting a Quan result based chromatogram
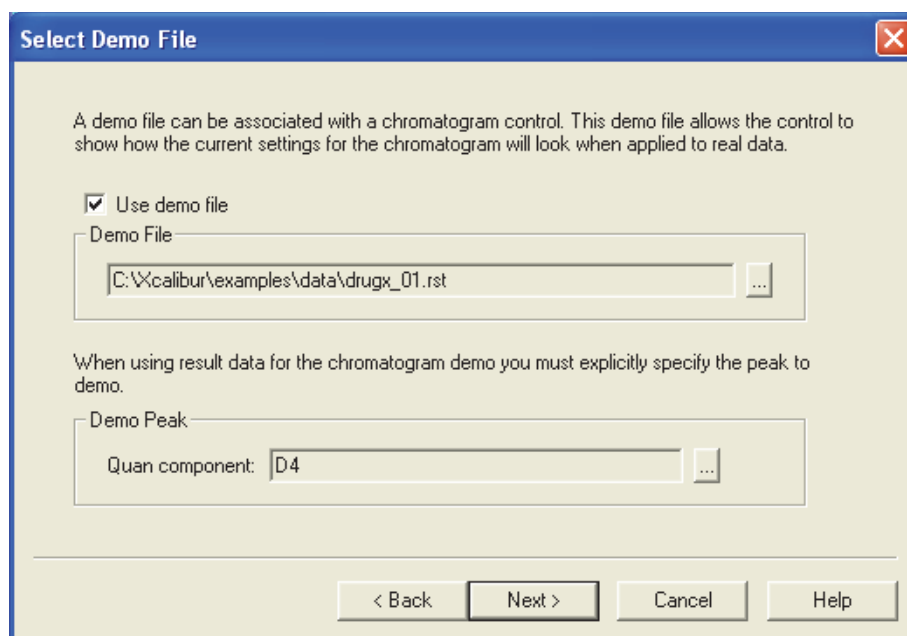
2. To search for the required demo file (.raw file), click the browse button in the Demo File area. The Select Raw Data File dialog box opens.

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.

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

1. Select the **Use demo file** check box to associate a demo file with the chromatogram report object (see Figure 50 on page 75).

   Figure 53. Selecting an explicit peak in a Qual result based chromatogram
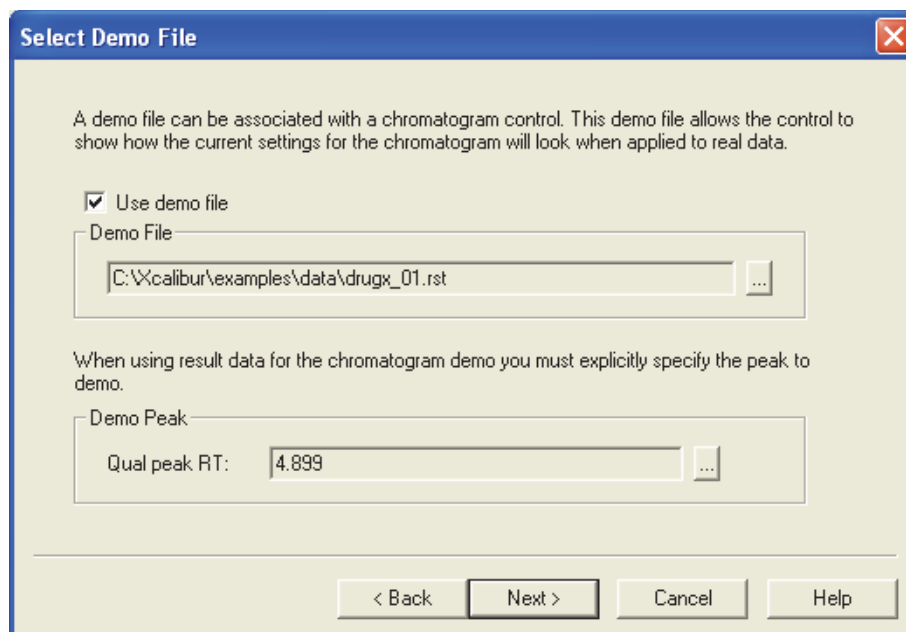
2. To search for the required demo file (.raw file), click the browse button in the Demo File area. The Select Raw Data File dialog box opens.

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.

❖ **To select a demo file for all available peaks**

1. To associate a demo file with the chromatogram report object (see Figure 51), select the **Use demo file** check box.

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

Select the Quan Peak Page

Use the Quan Peak page to explicitly specify the Quan peak (component) for a Quan results based chromatogram report object.

❖ **To specify a Quan peak**

1. To specify the Quan peak, type the text name of the component in the Quan Peak area (see Figure 54).

Figure 54. Select the Quan Peak page
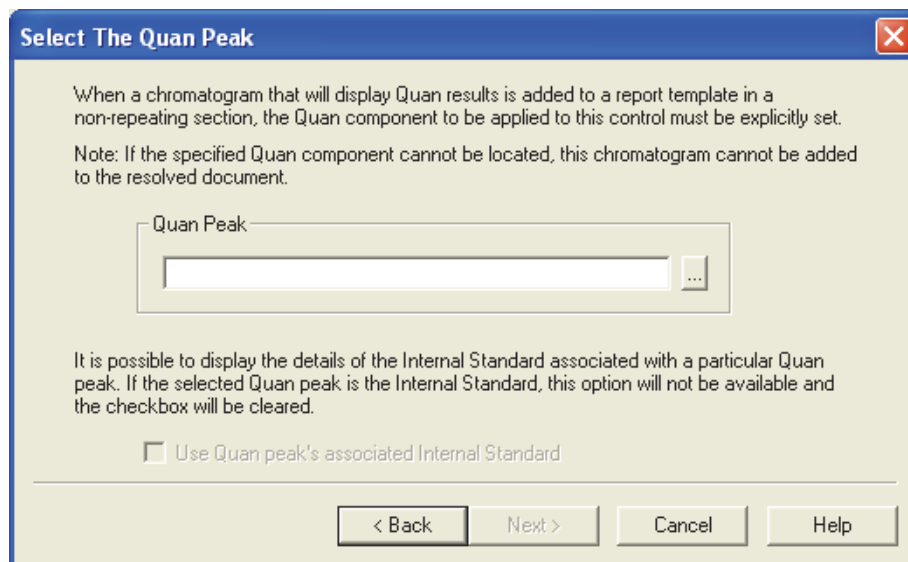
2. To search for the required processing method file (.pmd), click the browse button. The Select Component dialog box opens.

   a. Select a processing method file.

   b. Choose a component in the Use the Select Component dialog box. Click **OK** to return to the wizard. The Next button is active only after you have entered a component.

3. Select the **Use Quan peak's associated Internal Standard** check box of the Quan peak to use the selected the associated internal standard of the Quan peak instead of the Quan peak.

> **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.

Select the Qual Peak Page

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

❖ **To specify a Qual peak**

1. To specify the Qual peak in the Qual Peak to Display area, type the appropriate retention time in the Retention time box (see Figure 55).

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 55.   Select the Qual Peak page

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

Select Mass Spectrum Quan Traces to Display Page

Use the Select Mass Spectrum Quan Traces to Display page 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.

❖ **To specify a Quan trace**

1. Select the **Quan** trace in the Quan Traces area to be used from the Quan Traces list (see Figure 56).

   Figure 56. Select Mass Spectrum Quan Traces To Display page
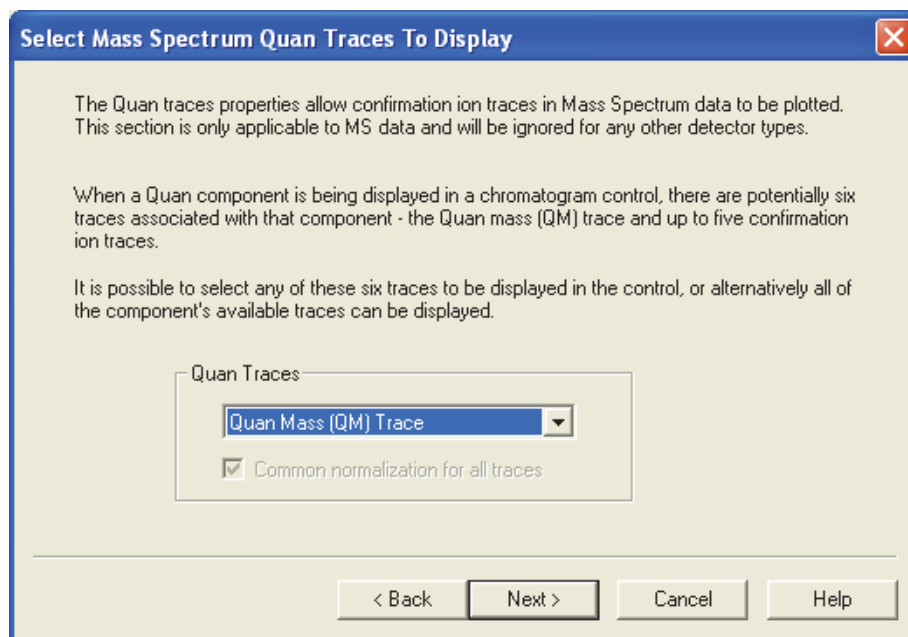
2. Select **All Quan Traces** from the list.

3. To normalize all the traces the same way, select the **Common normalization for all traces** check box.

4. 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 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 configure the Peak window**

1. Select the **Show Baselines** check box to display the baselines for a Chromatogram peak (Quan or Qual) (see Figure 57). When you clear this option, XReport does not display the baselines, peak tracing, or full peak annotation.

Figure 57. Configure How the Peak Window Will Look page
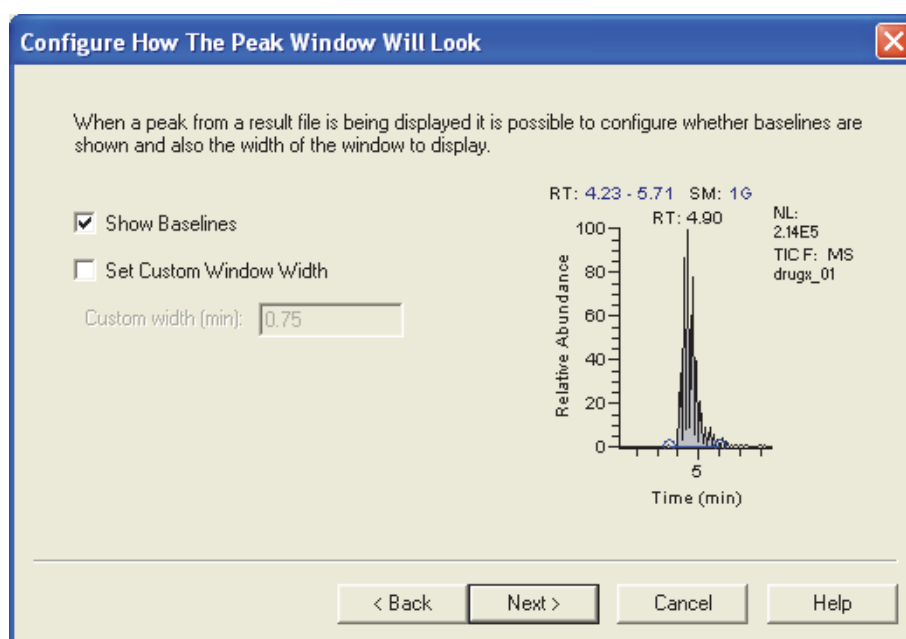
2. To manually override the default value of the peak window width (the default is peak width plus 1 min), select the **Set Custom Window Width** check box. Use the Custom width edit box to type a value for the window width (min). The default value for this field is 0.75 min.

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

Select Plot Details Page

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

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

1. Select the type of detector used to generate the raw file from the Detector list in the Plot Type area (see Figure 58). The type of detector determines the available traces.

   Figure 58. Select Plot Details page

2. 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.

3. From the Filter list, select the processing applied to a subset of the scans in a .raw 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.

4. 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

5. 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 ± Mass Range or Mass Range ± 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**.

6. 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.

7. 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.

8. 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

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

Select Enhance Details Page

Use the Select Enhance Details page to enhance a chromatogram plot by applying smoothing (see Figure 59).

Figure 59. Select Enhance Details page
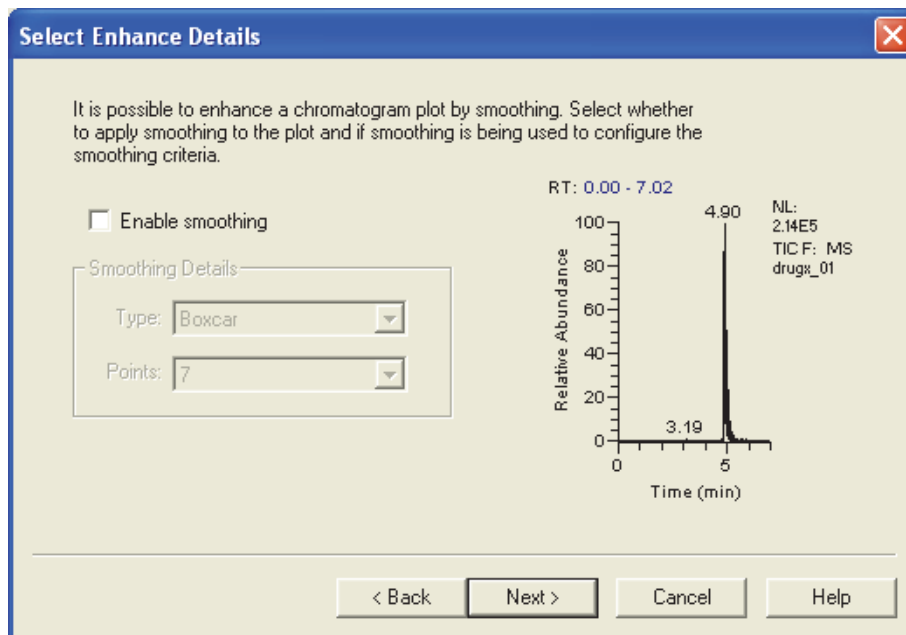
❖ **To enhance a chromatogram**

1. To apply smoothing to the chromatogram, select the **Enable Smoothing** check box.

2. To select a type of smoothing, select **Boxcar** or **Gaussian** from the Type list in the Smoothing Details area.

3. Select the number of smoothing points (odd numbers from 3 to 15) to use in the Points list.

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

Select Chromatogram Style Page

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

❖ **To define styles for a chromatogram**

1. To define the plotting style, select one of the following options in the Plotting area (see Figure 60):

   • **Point To Point**: Display point-to-point peak profiles.

   • **Stick**: Display the chromatogram as vertical lines.

Figure 60. Select Chromatogram Style page
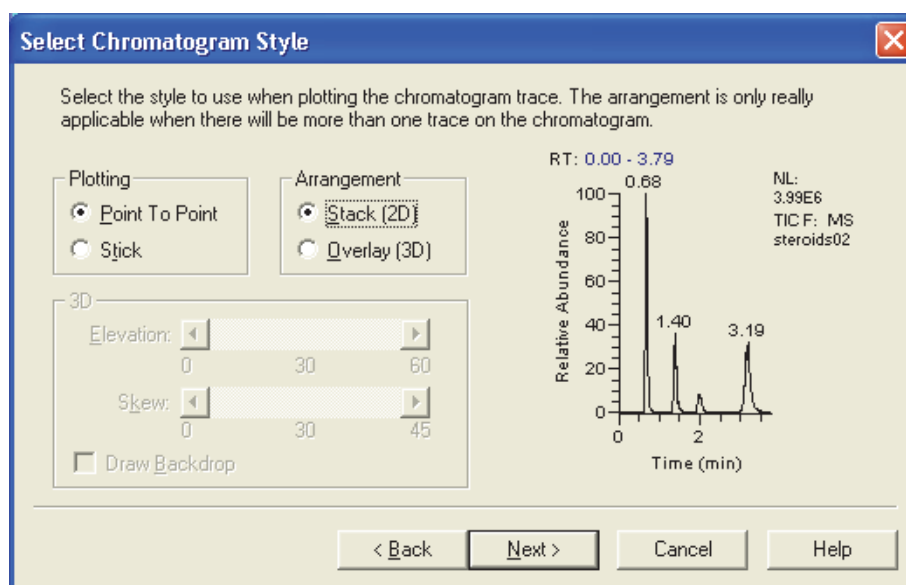
2. To define the plotting arrangement, select one of the following options in the Arrangement area:

   • **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 to choose the type and style of peak labels. From this page, click **Advanced** to open a dialog box to set advanced labeling options.

- Basic Options

- Advanced Options (Quan)

- Advanced Options (Qual)

Basic Options

❖ **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 (see Figure 61). The data system displays **RT** before the label.

Figure 61. Select the Peak Labeling page
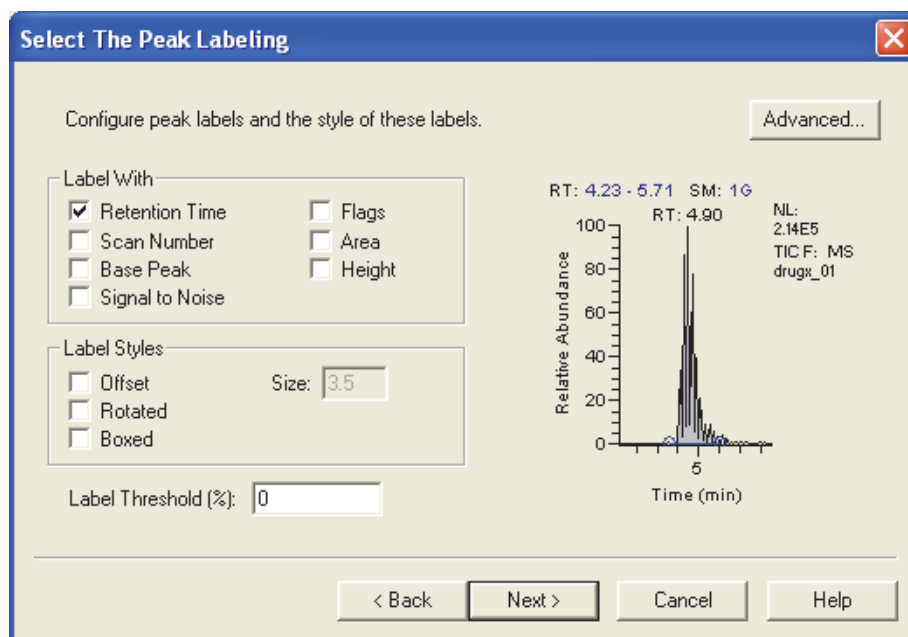
2. To label peaks with the number of mass scans at peak maximum, select the **Scan Number** check box. The data system displays **S#** before the label.

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

Advanced Options (Quan)

Click **Advanced** in the Select The Peak Labeling page. The Advanced Quan Peak Annotation Options dialog box opens. When you set Advanced Labeling options, the data system labels only the Quan peak.

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

1. To activate advanced Quan peak options, select the **Use advanced Quan peak annotation** check box (see Figure 62).

Figure 62. 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. When you turn on this check box, the Labels page shows the change when you return to it.

6. In the RT Labeling area, select the type of unit for the retention time from the Units list.

7. Select the number of decimal places to be displayed in the retention time label from the Decimals list.

8. Click **OK** to save the changes and close the dialog box.

Advanced Options (Qual)

Click **Advanced** in the Select the Peak Labeling page. The Advanced Qual Peak Annotation Options dialog box opens. When you set Advanced Labeling options, the Xcalibur data system labels only the Qual peak.

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

1. To activate the advanced Qual peak options, select the **Use advanced Qual peak annotation** check box (see Figure 63).

Figure 63. Advanced Qual Peak Annotation Options dialog box
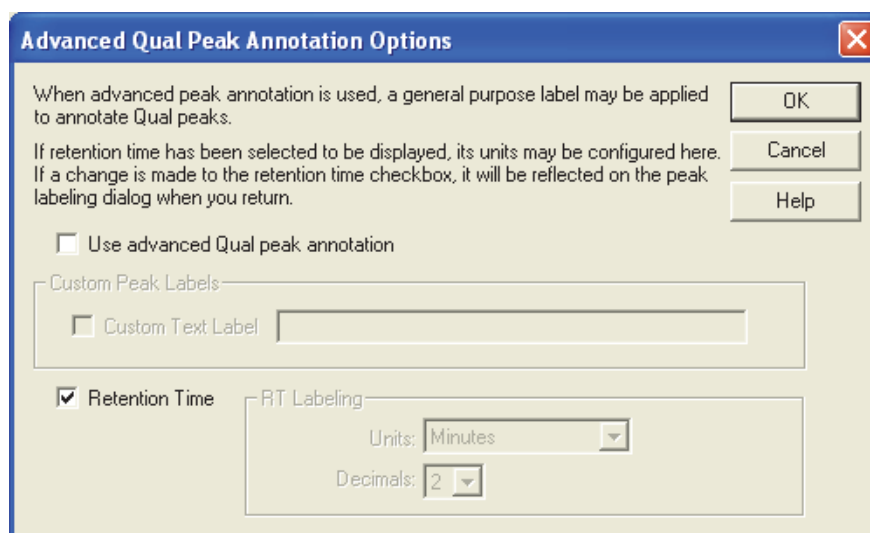
2. To specify a custom label, select the **Custom Text Label** check box in the active Custom Peak Labels area. Type a custom label for the Qual peak in the box.

3. To label the Qual peak with the retention time, select the **Retention Time** check box. When you turn on this check box, the Labels page shows the change when you return to it.

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.

Select How the Chromatogram Axes Will Be Configured Page

Use the Axes page to set chromatogram axes label and display options.

❖ **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 (see Figure 64).

Figure 64. Select How the Chromatogram Axes Will Be Configured page
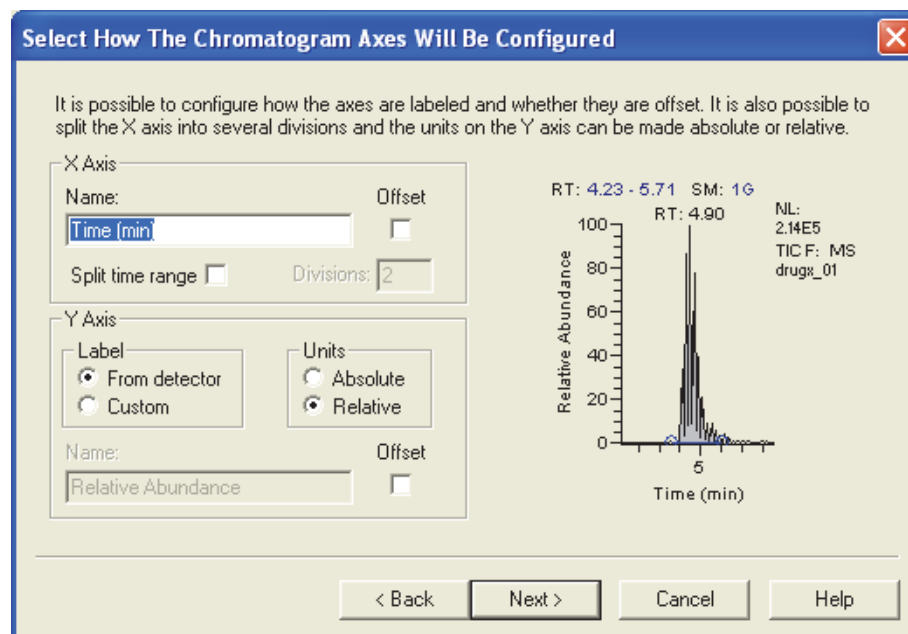
2. To offset the axis label from the chromatogram, select the **Offset** check box.

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 to select the normalization (*y*-axis scaling) method used for the chromatogram.

❖ **To specify normalization options**

1. Define the normalizing method in the Normalize method area (see Figure 65) 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 65. Configure Normalization for the Chromatogram page
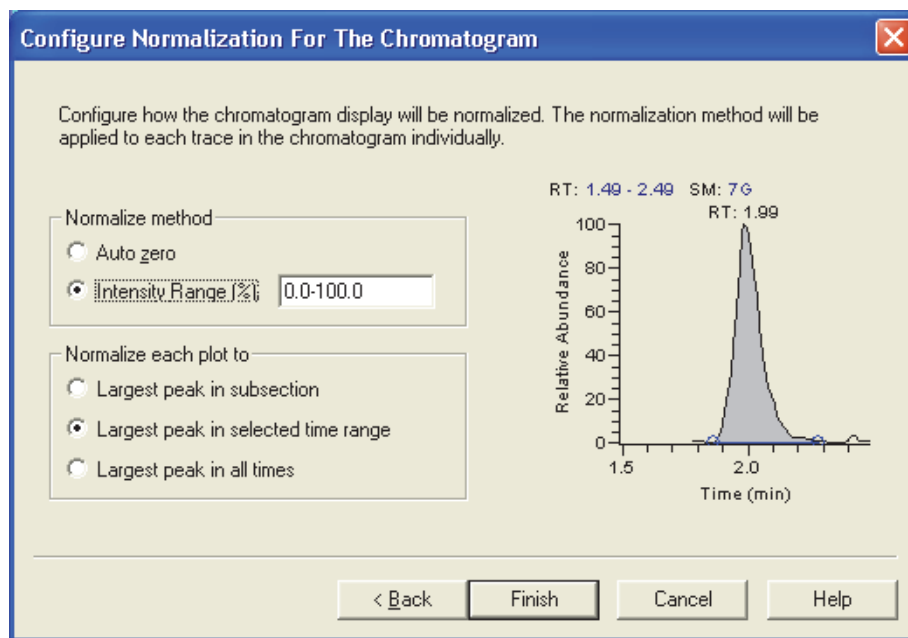
2. Define a peak to use for normalization in the Normalize each plot area by selecting one of the following options:

- **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-based chromatogram and you have selected the Fixed Scale check box on the Plot Type Page (see "Plot Type Page" on page 66).

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**.

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 (see Figure 66).

Figure 66. Component Calibration Curve Properties dialog box
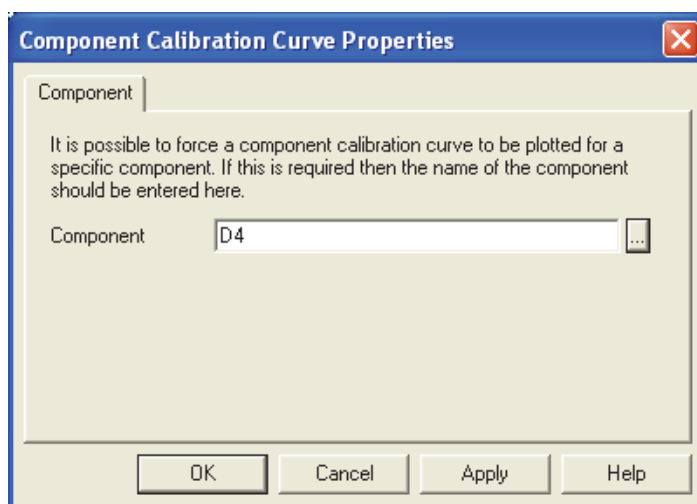
If your report has a nonrepeating Component Cal Curve report object, use the Component Calibration Curve wizard to specify the name of the component.

❖ **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 (see Figure 67).

   Figure 67. Select Component dialog box
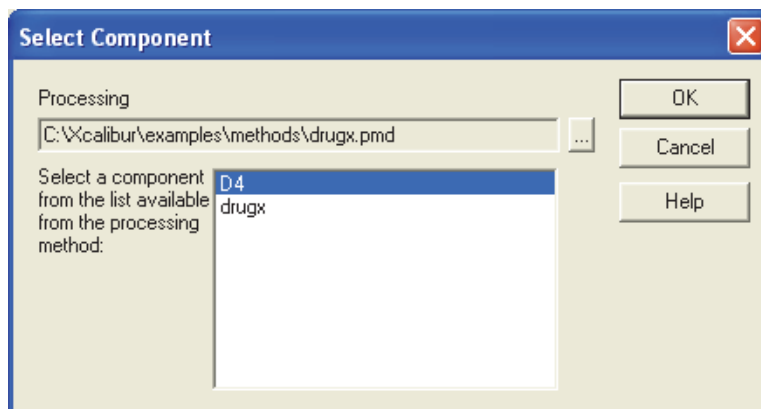
3. Select the required component from the list available for the chosen processing method and click **OK**. The Component Name page opens, displaying the specified name of the component in the box.

4. Click **OK**.

Configuring a Spectrum

To configure a Spectrum report object, right-click it and choose Properties from the shortcut menu. The Spectrum Properties Dialog Box opens to the Options page (see Figure 68).

Figure 68. Options page
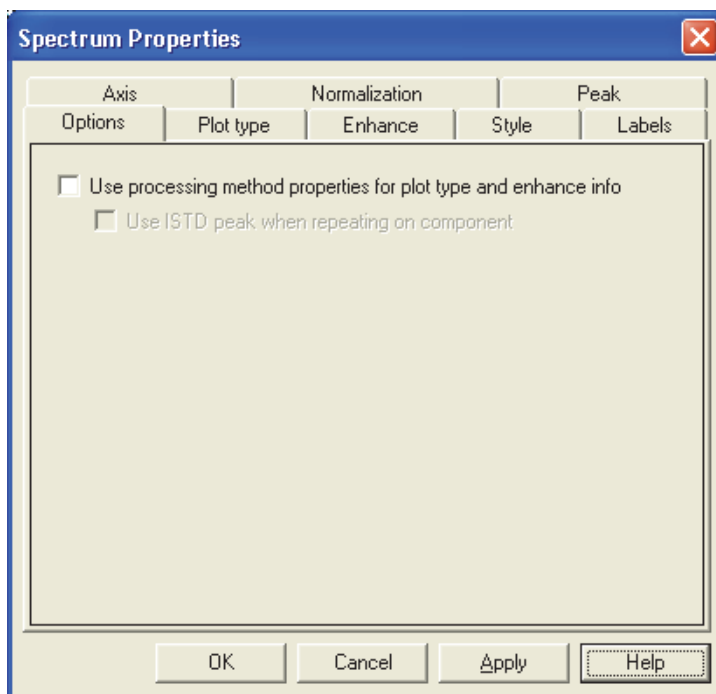
Use the XReport Spectrum Control Properties pages to do the following:

- Configure Options
- Configure Plot Types
- Enhance Spectra
- Configure Spectrum Style
- Configure 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.

Configure Options

To configure Spectrum options, use the Options Page.

❖ **To configure Spectrum options**

1. 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 (see Figure 68 on page 94).

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

2. 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
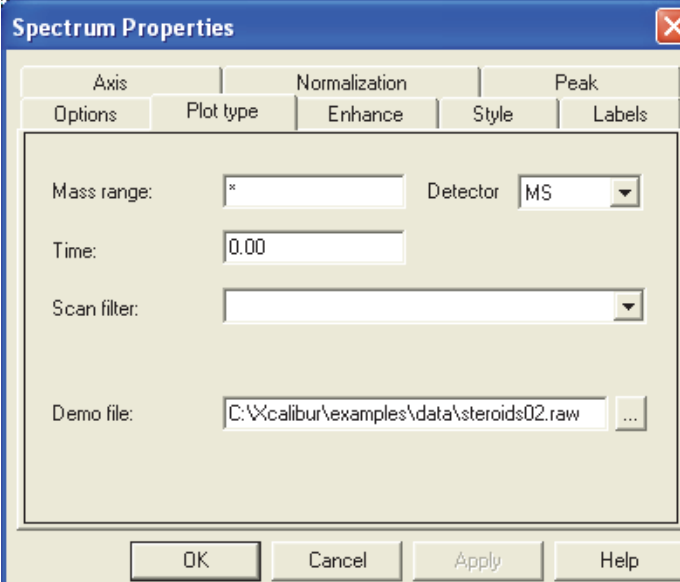
When raw data is being displayed in a Spectrum report object, use the Plot Type Page to configure how the plot is drawn.

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. Specify the mass or mass range for MS detector types in the Mass Range box (see Figure 69).

   Figure 69. 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:*.

2. Select the type of detector used to generate the raw file from the Detector list. Valid types are **MS** and **PDA**. The type of detector determines the available Plot types.

3. Select the time of the mass scan in the host chromatogram in the Time box. Type a new value or range as required.

4. From the Scan Filter list, select a filter or type a new one in the box using the scan filter format.

5. 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 to apply smoothing (the refine algorithm) to the spectrum and set background subtraction time ranges.

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 (see Figure 70).

Figure 70. Enhance page
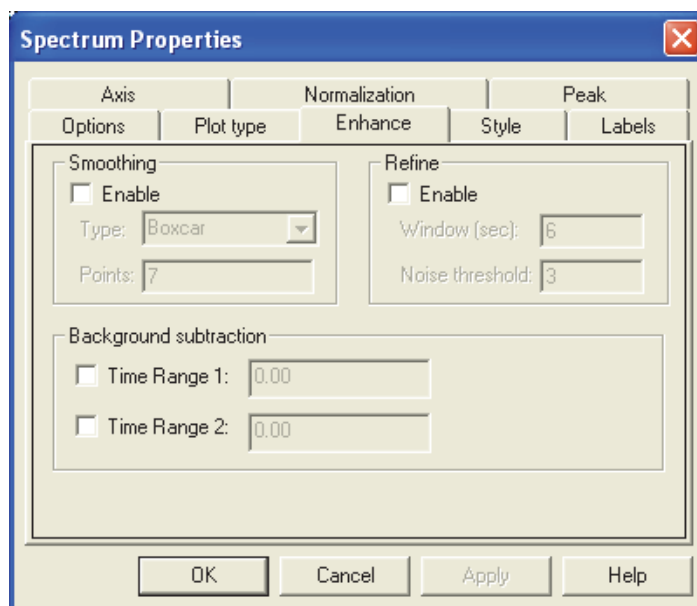
2. To select a type of smoothing, select **Boxcar** or **Gaussian** from the Type list.

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 a 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 a 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 (see Figure 71).

Figure 71. Style page
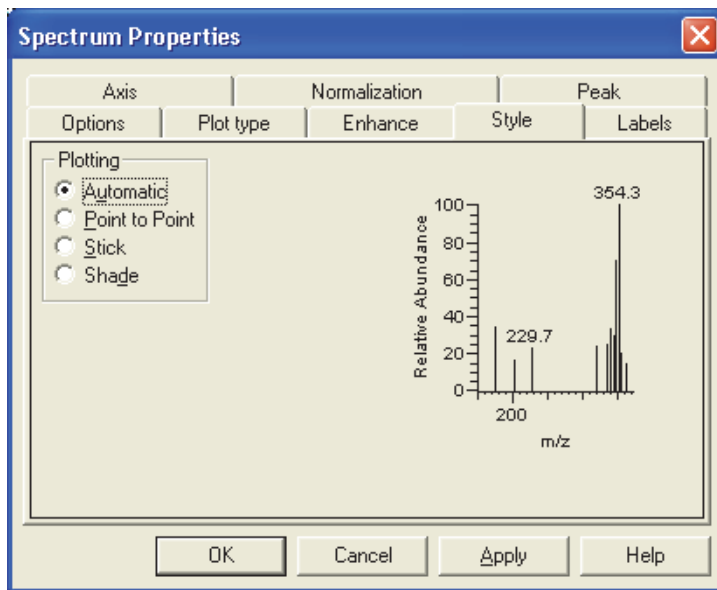
❖ **To set plotting options**

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 Peak Labels

To choose the type and style of peak labels, use the Labels Page.

❖ **To configure peak labels**

1. To label spectrum peaks with *m/z* value, select the **Mass** check box (see Figure 72) in the Label With area.

Figure 72. Labels page
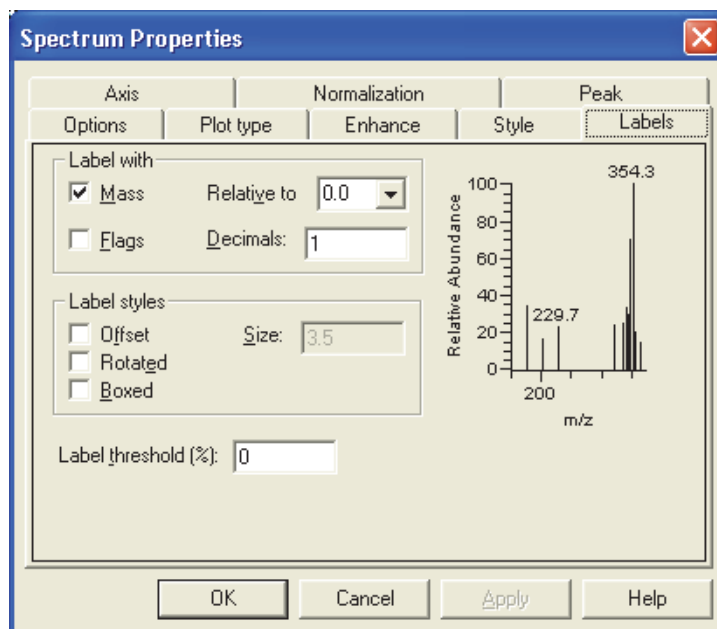
2. To label spectrum peaks with flags, select the **Flags** check box. Flags provide supplemental information about the peak data. For example, when a peak is saturated, the Xcalibur data system displays an **S** above the peak.

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.

❖ **To configure axis options**

1. Type the *x*-axis name in the Name box in the X Axis area (see Figure 73).

Figure 73. Axis page in the Spectrum Properties dialog box
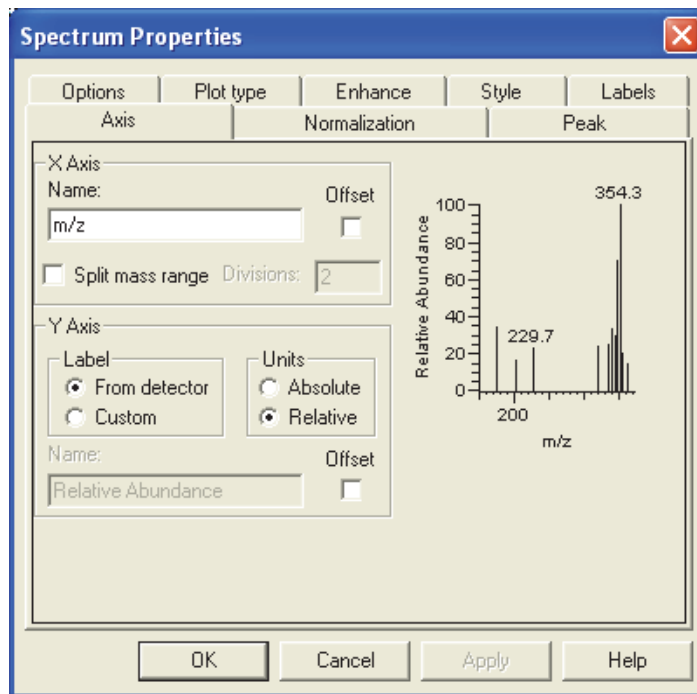
2. To offset the axis label from the spectrum, select the **Offset** check box.

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 to select normalization options for spectrum plots.

❖ **To select normalization options**

1. To define the normalization method, select one of the following options in the Normalize method area (see Figure 74).

   - **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 74. Normalization page
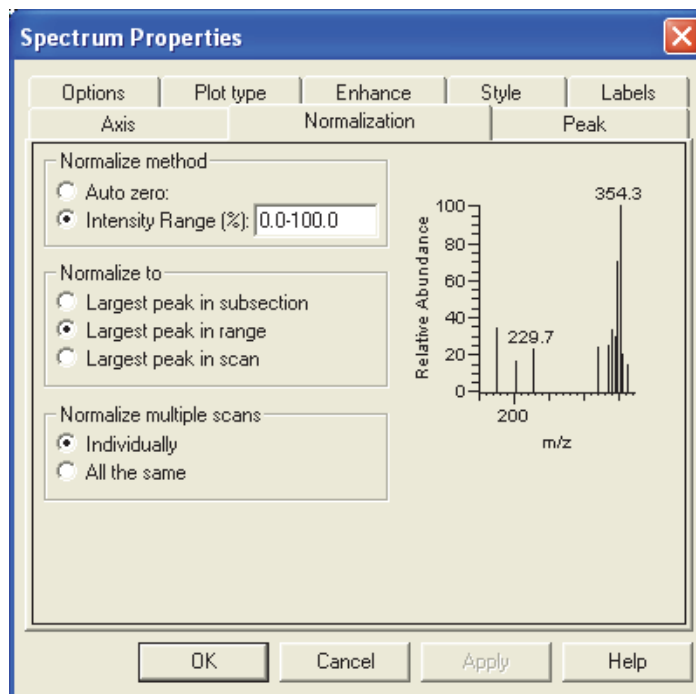
2. To define the peak that the spectrum is normalized to, select one of the following options in the Normalize To area:

- **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.

3. 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.

❖ **To specify a peak**

1. To specify a specific type of peak to appear in the spectrum, select the **Enable explicit peak type** check box (see Figure 75).

Figure 75. Peak page
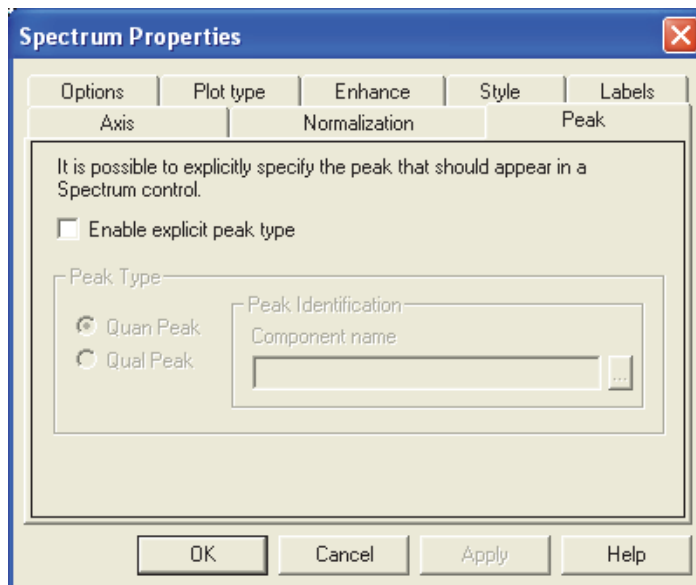
2. To specify the peak type to appear in the Spectrum, select the **Quan Peak** option to specify a Quan peak or select the **Qual Peak** option to specify a Qual peak.

3. 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

To configure a column object, right-click it and choose **Properties** from the shortcut menu. The Column Properties Dialog Box opens.

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

❖ **To configure a column object**

1. Select the number of columns to use in the Number of columns area (see Figure 76).

   Figure 76. Column Properties dialog box
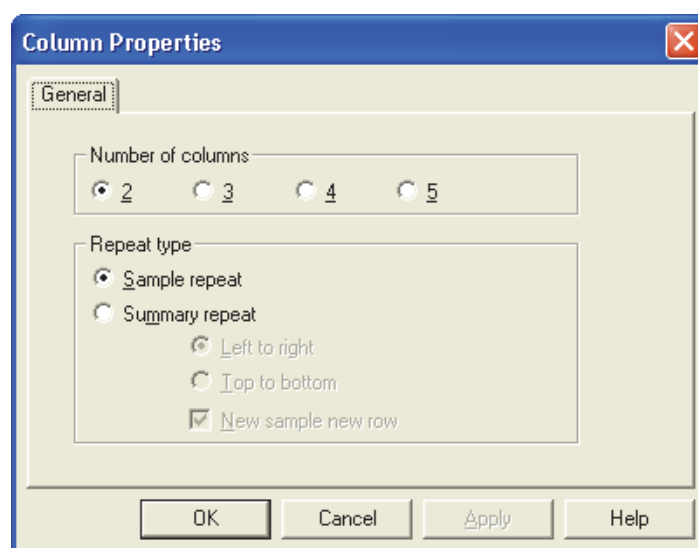
2. If the column object is in a nonrepeating section, configure the Repeat type. The Repeat type options are not available in Quan repeating or Qual repeating sections. In the Repeat type area, select **Sample repeat** or **Summary repeat** by clicking the appropriate option. For an example of using the two repeats, see Set Sample Repeat Options and Set Summary Repeat Options.

3. 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.

4. 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 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 77.

Figure 77. 2-column object behavior in a nonrepeating section, with a chromatogram object
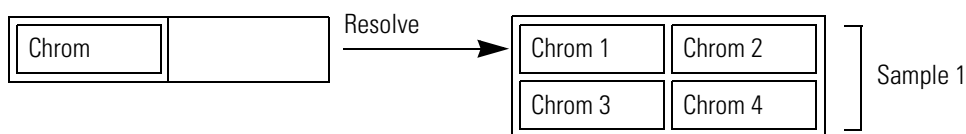
In another example, place a 2-column object in a nonrepeating section and add a chromatogram and a text object to the left column and a spectrum to the right column. Combine (resolve) the template using data of 1 sample with 4 components. All objects in the column are repeated for a single sample, and the report appears as in Figure 78.

Figure 78. 2-column object behavior in a nonrepeating section, with chromatogram and spectrum objects
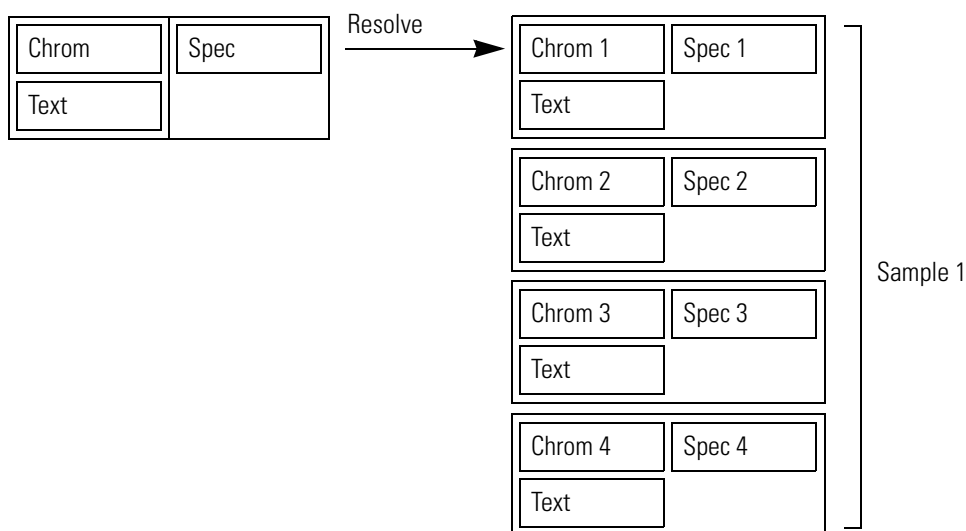
Set Summary Repeat Options

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 79.

Figure 79. 2-column object behavior in a nonrepeating section, with a chromatogram, Left to right option
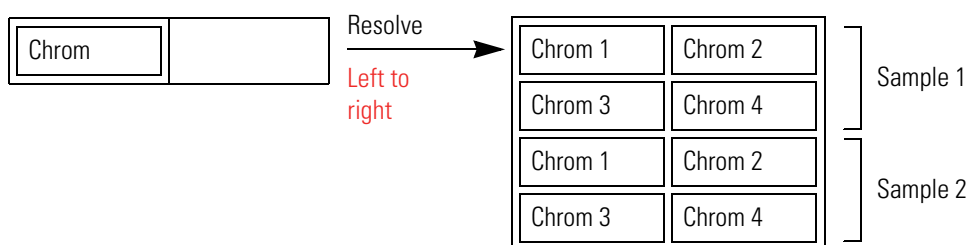
If you choose instead the Top To Bottom option, the report appears as in Figure 80.

Figure 80. 2-column object behavior in a nonrepeating section, with a chromatogram, Top to bottom option
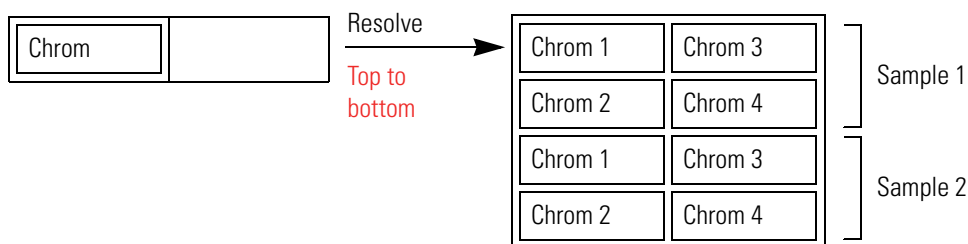
If you place an object in the right column and leave the left column empty, XReport combines the data as if the object is placed in the left column, as illustrated above.

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 81.

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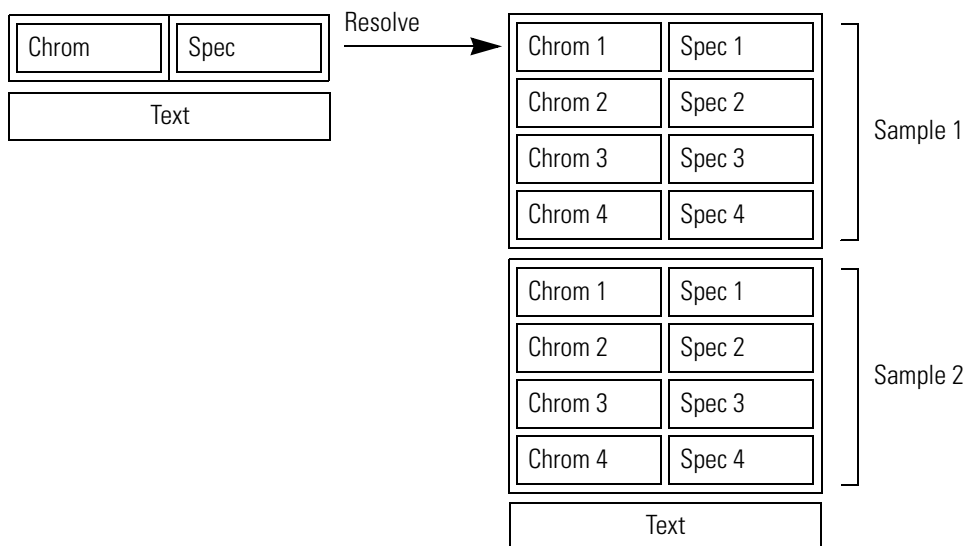
Sample XReport Template Files

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. Sample XReport template files (Sheet 1 of 2)

Report template file name	Data source files	Description/Use
CalibrationFile.xrt	.raw, .xcal	Generates sample reports with calibration data.
CompCalReport.xrt CompCalReport_Avalon.xrt CompCalReport_Genesis.xrt CompCalReport_ICIS.xrt	.rst, .raw, .pmd, .sld	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.
CustLibrSearRept.xrt LibrarySearchReport.xrt	.rst, .raw	Generates Qual sample reports that display Qual peaks and library search details. Use from Batch Processing in the Xcalibur data system.
IonRatioConfirmation.xrt	.rst, .raw, .pmd	Generates a Quan sample report containing non-graphical ion ratio confirmation results.
IonRatioConfirmationGraphical.xrt IonRatioConfirmationGraphical Simple.xrt IonRatioConfirmationGraphical Stacked.xrt	.rst, .raw, .pmd	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.
PeakIntegration.xrt	.rst, .raw, .pmd	Generates a Quan sample report containing peak integration data generated using Genesis.

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

Report template file name	Data source files	Description/Use
ProcessingMethod.xrt ProcessingMethod_Avalon.xrt ProcessingMethod_Genesis.xrt ProcessingMethod_ICIS.xrt	.pmd	Generates processing method sample reports. Use from Processing Method Setup in the Xcalibur data system.
QualPeakReport.xrt	.rst, .raw	Generates a simple Qual sample report. Use for data from Batch Processing in the Xcalibur data system.
QuanPeakResults_ESTD.xrt QuanPeakResults_ISTD.xrt QuanResults.xrt QuanSimple.xrt	.rst, .raw, .pmd	Generates Quan sample reports. Can be used from Batch Processing or Quan Browser in the Xcalibur data system.
QuantifySampleReport.xrt	.sld, .pmd, .rst, .raw	Generates a Quan summary report containing chromatograms and a Quan summary table.
SequenceReport.xrt	.sld	Generates a summary report showing the sequence being processed. Use from batch processing in the Xcalibur data system. Refer to the section "Processing a Batch of Samples" in Chapter 5 of the *Acquisition and Processing User Guide*.
SpectrumCandidates.xrt	.rst, .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 Objects

The table below lists 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, .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, .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, .sld	Displays general information about a sample, for example: • Sample Name • Operator • Sample Type • Run Time • Acquisition Date	Nonrepeating, header or footer

Table Objects

The table below lists 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 *m/z*, intensity, and relative intensity.	Qual or Quan repeating

Graphic Objects

The table below lists 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.	Quan repeating - repeats on component peak Nonrepeating - 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 (MS, PDA).	Qual or Quan repeating and nonrepeating sections

Formatting Objects

The table below lists 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

RT: 0.18 - 1.18 SM: 7G

RT: 0.68

NL: 5.01E5
m/z=
266.6-267.6+
308.6-309.6 F: + c Full
ms2 363.30 [
150.00-375.00] MS
Genesis steroids02

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

RT: 1.49 - 2.49 SM: 7G

1.99

NL: 9.60E4
m/z=
266.6-267.6+
284.7-285.7 F: + c Full
ms2 303.30 [
100.00-310.00] MS
Genesis steroids02
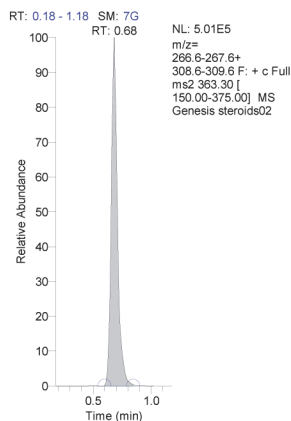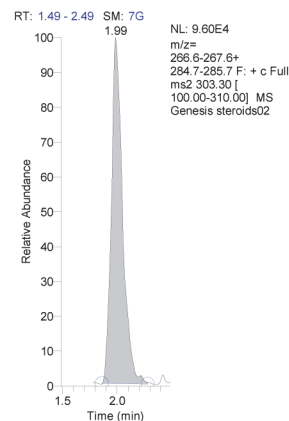
Component Name:	hydrocortisone	Actual RT(min):	0.67783	Calculated Amount:	4.95592
Response:	1892942.72621	Base Line:	BB	Signal To Noise:	707.56
%Diff:	-0.88	Area Ratio:	2.763	Area(cts-sec):	1892942.72621
Specified Amount:	5.00000				

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

RT: 0.90 - 1.90 SM: 7G
RT: 1.40

1.21   1.70

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

RT: 1.49 - 2.49 SM: 7G
1.99

NL: 9.60E4
m/z=
266.6-267.6+
284.7-285.7 F: + c Full
ms2 303.30 [
100.00-310.00] MS
Genesis steroids02
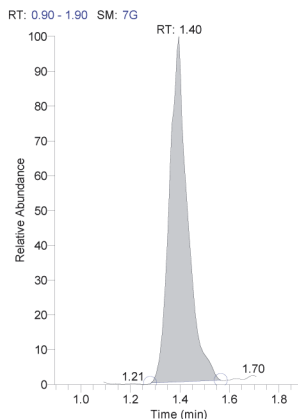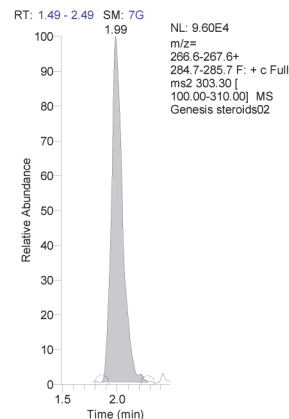
Component Name:	deoxycorticosterone	Actual RT(min):	1.39533	Calculated Amount:	5.10841
Response:	1040530.60245	Base Line:	BB	Signal To Noise:	148.23
%Diff:	2.17	Area Ratio:	1.519	Area(cts-sec):	1040530.60245
Specified Amount:	5.00000				

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
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

RT: 2.67 - 3.67 SM: 7G
RT: 3.17
2.89

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

RT: 1.49 - 2.49 SM: 7G
1.99
NL: 9.60E4
m/z= 266.6-267.6+ 284.7-285.7 F: + c Full ms2 303.30 [100.00-310.00] MS Genesis steroids02
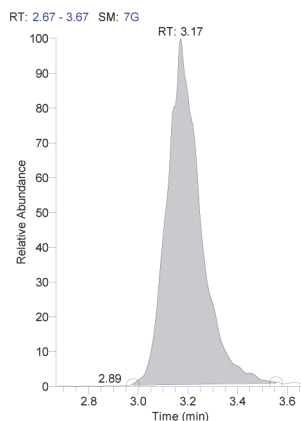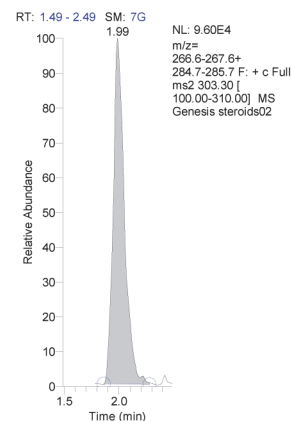
Component Name:	progesterone	Actual RT(min):	3.16867	Calculated Amount:	4.94898
Response:	2995893.97127	Base Line:	BB	Signal To Noise:	344.16
%Diff:	-1.02	Area Ratio:	4.373	Area(cts-sec):	2995893.97127
Specified Amount:	5.00000				

XReport Reference

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

Contents

- Reports View
- XReport Dialog Boxes
- Report Sections
- Report Objects
- Report Templates

Reports View

Use XReport 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 .xls and .html.

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

XReport Toolbar Buttons

Table 7. Toolbar buttons (Sheet 1 of 2)
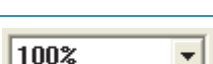
	Button	Description
	New	Create a new report template for the program you select.
	Open	Find and open .xrt files.
	Save	Save the current template as an .xrt file. This option is not available if you are using a locked template. In this case, choose **File > Save As** and save the template with a different 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.
	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 gridlines.

Table 7. Toolbar buttons (Sheet 2 of 2)

	Button	Description
	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:

- File Menu

- XReport Edit Menu

- XReport View Menu

- XReport Layout Menu

- XReport Report Menu

- XReport Help Menu

File Menu

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.
Recently Used Files	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. Edit menu commands (Sheet 1 of 2)

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.

Table 9. Edit menu commands (Sheet 2 of 2)

Command	Description
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. 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. 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.

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

Command	Description
Align > Auto	Snap all objects (selected or not) in the current section to the nearest upper and right gridlines.
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.
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. 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. 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

- Configure Repeating Section 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

- Configure 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

Configure Repeating Section Dialog Box

Use the Configure Repeating Section 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 Configure Repeating Section dialog box has these pages:

- Exclude Page

- Ordering Page

- Page Breaks Page

Exclude Page

Use the Exclude page to indicate components to exclude from a Quan repeating section, and whether or not to discard any components that have not been found.

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 to indicate the order for peaks or components in the repeating section.

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 hightest 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 to indicate where to apply page breaks in your report.

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 this 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 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. This 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. 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. 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. 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. Advanced Quan Peak Annotation Options page parameters

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.
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
	• 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 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. 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 to select the normalization (*y*-axis scaling) method used for the chromatogram.

Table 20. Configure Normalization for the Chromatogram page parameters

Parameter	Description
Normalize Method	
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 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. 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 to determine the appearance of the chromatogram.

Table 22. Select Chromatogram Style page parameters

Parameter	Description
Plotting	
Point-to-Point (see Figure 60)	Display point-to-point peak profiles.
Stick	Display the chromatogram as vertical lines.
Arrangement	
Stack (2D)	Stack plots vertically (same *x* axis) with no overlap (one *y* axis for each plot).
Overlay (3D)	Move plots vertically (same *x* axis) with an optional horizontal skew (*y*-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.

Table 23. Select Chromatogram Type page parameters

Parameter	Description
Chromatogram Type	
Raw File Based Chromatogram	Indicate the chromatogram is based on a raw file.
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 on the Select Component page to select a component to display when configuring a chromatogram.

Table 24. Select Component page parameters

Parameter	Description
Processing	View the name of the currently selected processing method (.pmd) file.
Component List	View a list of components found in the processing method file.

Select Demo File

Set parameters on the Select Demo File page 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 in the Chromatogram Type 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 to enhance a chromatogram plot by applying smoothing.

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.

Table 27. Select How the Chromatogram Axes Will Be Configured page parameters

Parameter	Description
X axis	
Name	View or change the name of the x axis.
Offset	Move the x-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 y axis (stored in the .raw file).
Custom	Use your own label for the y axis.
Units	
Absolute	Use absolute units for the y axis.
Relative	Use relative units for the y axis.
Name	Define the custom name of the y axis. This box is available only when you click the Custom option in the Label area.
Offset	Move the y 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 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. Select Mass Spectrum Quan Traces to Display page parameters

Parameter	Description
Quan Traces	
Quan Traces	Specify the Quan traces to display.
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 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. Select Plot Details page parameters (Sheet 1 of 2)

Parameter	Description
Plot Type	
Detector	View the type of detector used to generate the raw 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.

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

Parameter	Description
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
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 ± Mass Range or Mass Range ± 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 *Wavelength Range + Wavelength Range*, an additional Wavelength (nm) box opens.
	The valid range depends on the configured detector. The format is *low mass / wavelength–high mass / wavelength*. 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 to choose the type and style of peak labels.

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. Select the Qual Peak page parameters

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 to explicitly specify the Quan peak (component) for a Quan results-based chromatogram report object.

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 to ignore the implicit Qual peak and explicitly configure the chromatogram type.

Table 33. Use Container Supplied Qual Peak page parameters

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 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. 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
- Enhance Page
- Labels Page
- Normalization Page
- Options Page
- Peak Page
- Plot Type Page
- Style Page

Axis Page

Set spectrum axis labels and display options on the Axis page.

Table 35. Axis page parameters

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 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.
Units	
Absolute	Use absolute units on the *y* axis.
Relative	Use relative units on the *y* axis.

Enhance Page

Specify spectrum enhancement details on the Enhance page.

> **Note** Clear the Use Processing Method Properties For Plot Type And Enhancement Info check box on the Options Page to modify the Enhance page parameters.

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.

Table 36. Enhance page parameters (Sheet 2 of 2)

Parameter	Description
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	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

Choose the type and style of peak labels on the Labels page.

Table 37. Labels page parameters

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) or wavelength values (if PDA is selected as the detector on the Plot Type Page).
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.
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

Select normalization options for spectrum plots on the 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

Set spectrum parameters on the 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

Set parameters on the Peak page to explicitly specify the peak to display in the spectrum report object.

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

Configure how the spectrum is drawn on the Plot Type page.

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.

Table 41. Plot Type page parameters (Sheet 1 of 2)

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 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.

Table 41. Plot Type page parameters (Sheet 2 of 2)

Parameter	Description
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 file) that is used to generate a preview of the selected plot.

Style Page

Set parameters on the Style page that determine the appearance of the spectrum.

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 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. Complete the parameters on this page for each custom column that you selected.

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. 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. 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.
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.

Table 44. Select Table Fields page parameters (Sheet 2 of 2)

Parameter	Description
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 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. 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 - Ascending/Descending	Select the first column that the Xcalibur data system uses to sort the table. Select to sort in ascending or descending order.
Second Order - Ascending/Descending	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. Select to sort in ascending or descending order.
Third Order - Ascending/Descending	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. 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.

Table 46. Set Table Font page parameters

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 on the Edit Formula For dialog box. For more information on formula syntax, see "Adding a Formula to a Table" on page 23.

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(x)	Return the positive value of a number of a formula regardless of its actual positive or negative value.
AND	AND(x,y)	Return the value 1 if the logical expressions x and y are both true, or the value 0 if either expression is false.
AVERAGE	AVERAGE($x1$, $x2$, ...,xn)	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(x)	Return the number to the left of the decimal place in the value or formula x.
MAX	MAX($x1$, $x2$, ...,xn)	Return the largest value in a list.
MIN	MIN($x1$, $x2$, ...,xn)	Return the smallest value in a list.

Table 47. Edit Formula For dialog box parameters (Sheet 2 of 2)

Parameter	Description	
Function	**Syntax**	**Description**
MOD	MOD(*x,y*)	Return the remainder from dividing the value *x* by the value *y* a number of times in integers.
NOT	NOT(*x*)	Return the value 0 (zero, false) if the logical expression *x* is true, or the value 1 (true) of the expression *x* is false.
OR	OR(*x,y*)	Return the value 1 (true) if either or both logical expressions *x* and *y* are true, or the value 0 (zero, false) if both expressions are false.
PRODUCT	PRODUCT(*x1, x2, …,xn*)	Return the result of multiplying a list of values.
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, …,xn*)	Return the sum of a list of values or formulas.
TRUE	TRUE	Return 1.
Add Function	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

- Enhancement Page

- Options Page

- Plot Type Page

Display Page

Configure display parameters for the Spectrum List table on the 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

Configure spectrum enhancement parameters for the Spectrum List table on the Enhancement page.

> **Note** Clear the **Use Processing Method Properties For Plot Type And Enhancement Info** check box on the Options Page to modify parameters on the 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

Configure general parameters relating to the Spectrum List table on the 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

Configure plot information for the Spectrum List table on the Plot Type page.

> **Note** Clear the **Use Processing Method Properties For Plot Type And Enhancement Info** check box on the Options Page to modify the parameters in the Plot Type page.

Table 51. Plot Type page parameters (Sheet 1 of 2)

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 *First Mass–Last Mas*s. 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 *Short Wavelength–Long Wavelength*. 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**.

Table 51. Plot Type page parameters (Sheet 2 of 2)

Parameter	Description
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. 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. 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. Library Search Results Table Properties dialog box parameters

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. 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

- 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. 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 • 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	
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. 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.

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 58. 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 $\boxed{A}$. The Font Dialog Box opens.

Bitmap Properties Dialog Box

Specify the filename of the currently selected bitmap in the Bitmap Properties dialog box.

Table 59. 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.

Table 60. 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 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:

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:

Table 60. Column Properties dialog box parameters (Sheet 2 of 2)

Parameter	Description

Repeat Type - 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:
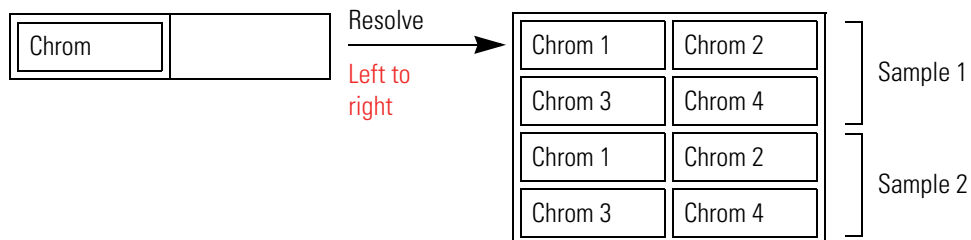
If you choose instead the Top To Bottom option, the report appears as follows:
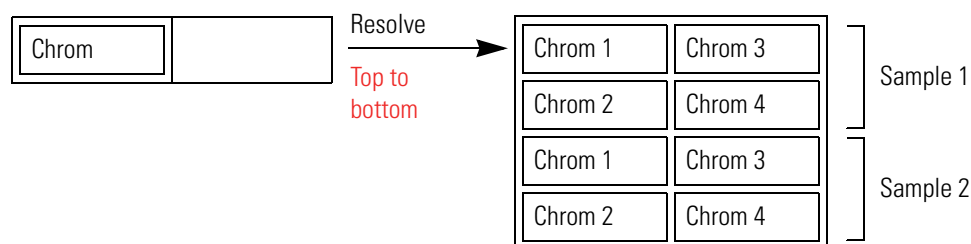
If you place an object in the right column, and leave the left column empty, the data is resolved as if the object is placed in the left column, as illustrated above.

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:
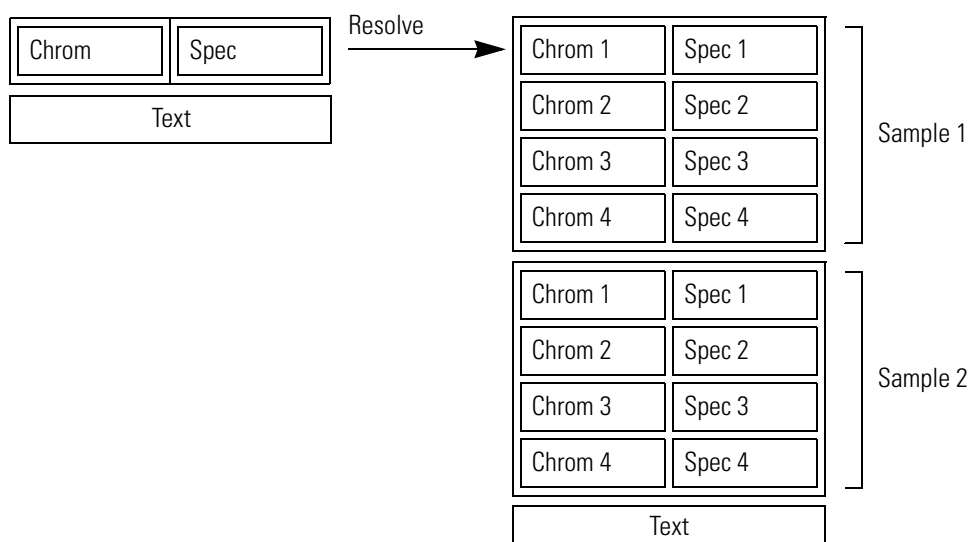
If you click the New Sample New Row option, data for a new sample always starts on a new row.

Configure Component Calibration Curve Dialog Box

Set parameters in the Configure 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 61. Configure 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 Configure 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 62. 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 in the Electronic Signature Properties dialog box.

Table 63. 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" on page 158)

- Text (see "Font Page" on page 158)

- Tables (see "Table Properties Wizard" on page 147)

Preferences Dialog Box

Set grid and configuration options for your report in the Preferences dialog box.

Table 64. Preferences dialog box parameters

Parameter	Description
Grid Spacing	
Width	Set the width between gridlines. (1 gridline unit = 0.1 inches)
Height	Set the height between gridlines. (1 gridline unit = 0.1 inches)
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, Xcalibur 2.0). This option is available only when two or more types of report templates are installed on the system (for example, both Xcalibur and LCQuan™.)

Preview Window

Preview and adjust the appearance of your report using the parameters in the Preview window. To open this window, choose **Report > Simulate Report**. XReport displays a preview of your template filled with sample data. In previewing the appearance of your report, adjust your template before you combine it with actual data. Choose **Report > Resolve Report** to see a preview of your report combined with your actual data.

Table 65. 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) • Microsoft Excel workbook (.xls) • Web page (.htm or .html) • Plain text (.txt) • Rich text format (.rtf) • Adobe™ PDF (.pdf)
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 X of Y	View X, the current page, and Y, the total number of pages in the report. Type in a new value for X 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 (for example, Xcalibur and LCquan).

Table 66. 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.

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" on page 170 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
- Columns

Graphic Objects

- Electronic Signature Table
- Bitmap
- Chromatogram
- Component Cal Curve
- Spectrum

Table Objects

- Avalon Qual Events Table
- Calibration File Table
- Component Cal Level Table
- Dilution Factor Table
- IRC Summary Table
- Processing Method Programs Table
- Processing Method Sample Reports Settings Table
- Processing Method Summary Reports Settings Table
- Qual Peak Table
- Quan Peak Table
- Sequence Table
- Spectrum Candidate Results Table

Text Objects

- Annotation

- Instrument Method

- Processing Method - General

- Processing Method - Qual

- Sample Table

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

Graphic Objects

- Bitmap

- Electronic Signature Table

- Table Objects

Text Objects

- Annotation

- Report Info

- Sample Header

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

- Columns

Graphic Objects

- Electronic Signature Table

- Bitmap

- Chromatogram

- Spectrum

Table Objects

- Library Search Graphics Table

- Library Search Results Table

- Spectrum List Table

Text Objects

- Annotation

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

- Columns

Graphic Objects

- Electronic Signature Table

- Bitmap

- Chromatogram

- Component Cal Curve

- Spectrum

Table Objects

- Avalon Quan Events Table

- Component Cal Level Table

- IRC Settings Table

- Component QC Level Table

- Component Spectrum Table

- IRC Settings Table

- Spectrum List Table

- Sample Table

Text Objects

- Annotation

- Component IdentDetectCal Settings

- Component ISTD Settings Summary

- Component Settings Summary

- Component Sys Suit/Flags Settings

- Quan ISTD Peak Summary

- Quan Peak Summary

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 (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	Bitmap
Spectrum	Columns
Component Cal Curve	Page Break

Chromatogram

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, .rst

Section placement: Qual, Quan, and nonrepeating sections

Spectrum

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, .rst

Section placement: Qual, Quan, and nonrepeating sections

Component Cal Curve

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, .rst

Section placement: Quan or nonrepeating sections. For the nonrepeating section, specify which component to display in the Configure Component Calibration Curve Dialog Box.

Bitmap

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

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

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	Library Search Results Table
Avalon Quan Events Table	Processing Method Programs Table
Calibration File Table	Processing Method Sample Reports Settings Table
Component Cal Level Table	Processing Method Summary Reports Settings Table
Component QC Level Table	Qual Peak Table
Component Spectrum Table	Quan Peak Table
Dilution Factor Table	Qual Summary Table
Electronic Signature Table	Quan Summary Table
Ion Ratio Confirmation Results Table	Sample Table
IRC Settings Table	Sequence Table
IRC Summary Table	Spectrum Candidate Results Table
Library Search Graphics Table	Spectrum List Table

Avalon Qual Events Table

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

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: .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

The Calibration File table displays calibration levels, raw file names, and acquisition dates of standards. This table provides information for each peak with each sample.

Required data file: .xcal, .sld, .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

The Component Cal Level table displays the calibration levels, amounts, and acceptance test values defined for a specific component.

Required data file: .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

The Component QC Level table displays the QC levels, amounts, and percent test values defined for a specific component.

Required data file: .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

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: .pmd

Section placement: Nonrepeating section

This table has the following possible fields:

- #
- *m/z*
- Intensity (%)
- User Columns 1 to 5

Dilution Factor Table

The Dilution Factor table displays the names of calibration levels and dilution factors for components other than internal standards.

Required data file: .rst

Section placement: Nonrepeating section

This table has the following possible fields:

- Calibration Level
- Dilution
- User Columns 1 to 5

Electronic Signature Table

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

The Ion Ratio Confirmation Results table displays data about each qualifier ion, based on search criteria specified in the processing method.

Required data 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

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: .pmd

Section placement: Nonrepeating section

This table has the following possible fields:

- Qualifier Ion #
- *m/z*
- Target Ratio (%)
- Window (±%)
- User Columns 1 to 5

IRC Summary Table

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: .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

The Library Search Graphics table displays the graphical results from a library search on a Qual peak.

Required data file: .rst, .raw

Section placement: Nonrepeating section

This table has the following possible fields:

- Hit Spectrum
- Delta
- Compound Structure

Library Search Results Table

The Library Search Results table displays the results of a library search on a Qual peak.

Required data file: .rst, .raw

Section placement: Nonrepeating 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

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: .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

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: .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

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: .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

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.

Required data 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

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.

Required data file: .pmd, .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

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.

Required data file: .sld, .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

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.

Required data file: .sld, .pmd, .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

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: .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

The Sequence table displays the contents of the sequence file. This table provides information for each peak with each sample.

Required data 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

The Spectrum Candidate Results table displays the results of spectrum candidate processing for GC/MS data on a per component basis.

Required data 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

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: .rst, .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	Processing Method - General
Component IdentDetectCal Settings	Processing Method - Qual
Component ISTD Settings Summary	Quan ISTD Peak Summary
Component Settings Summary	Quan Peak Summary
Component Sys Suit/Flags Settings	Report Info
Instrument Method	Sample Header

Annotation

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

The Component IdentDetectCal Settings object shows the peak detection, calibration, and integration parameters for a single component.

Required data file: .pmd

Section placement: Quan repeating section, repeats on component peak

For this object's possible fields and headings, see Table 67.

Component ISTD Settings Summary

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: .pmd

Section placement: Quan repeating section, repeats on component peak

For this object's possible fields, see Table 67.

Table 67. Component ISTD Settings object fields

- 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 Name
- 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

Component Settings Summary

The Component Settings Summary object displays a short list of peak detection and integration parameters for a specified component.

Required data file: .pmd

Section placement: Quan repeating section, repeats on component peak

For this object's possible fields and headings, see Table 68.

Table 68. 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

Component Sys Suit/Flags Settings

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: .pmd

Section placement: Quan nonrepeating, repeats on component peak

For this object's possible fields and headings, see Table 69.

Table 69. 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	**Detect Minimum Signal-to-Noise Ratio**	• Quantitation Limit
• Resolution Threshold	**Detect Column Overload**		• 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		**Calibration Flag**	• Area Threshold
Peak Classification Parameters		• R-Squared	• Height Threshold
Detect Peak Width			**Other**
• Width Peak Height			• <Blank Line > and <User Text> Data Items
• Min. Peak Width			
• Max. Peak Width			

Instrument Method

The Instrument Method object displays general instrument method parameters.

Required 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

The Processing Method - General object displays general processing method parameters.

Required data file: .pmd

Section placement: Nonrepeating section

For this object's possible fields and headings, see Table 70.

Table 70. 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

The Processing Method - Qual object displays Qual processing method parameters.

Required data file: .pmd

Section placement: Nonrepeating section

For this object's possible fields and headings, see Table 71.

Table 71. Processing Method – Qual object fields/headings

Identification	Avalon Peak Integration	ICIS Advanced Parameters	Options
• 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 Smoothing Points **Limit Peaks** • Select Top Peaks • Select By • Number To Select • Relative Peak Height Threshold • Percent of Highest Peak **Advanced Detection Options** **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	• 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	• 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

The Quan ISTD Peak Summary object displays summary parameters for a Quan component's associated ISTD peak.

Required data file: .pmd, .rst

Section placement: Quan nonrepeating, repeats on component peak

For this object's possible fields, see Table 72.

Table 72. Quan ISTD Peak Summary object fields

• Component Name	• Height	• Signal-to-Noise	• System Suitability
• ISTD Name	• Width	• Saturated	• Data Flags
• Actual RT	• Baseline Flags	• Expected RT	• <Blank Line > and <User Text> Data Items
• Response	• Area	• Peak Status	

Quan Peak Summary

The Quan Peak Summary object displays component peak summary parameters.

Required data file: .pmd, .rst

Section placement: Quan nonrepeating, repeats on component peak

For this object's possible fields, see Table 73.

Table 73. Quan Peak Summary object fields

• Component Name	• Area	• Peak Purity	• Component Type
• Actual RT	• Area Ratio	• Baseline Flags	• Peak Status
• Specified Amount	• Height	• Signal-to-Noise	• System Suitability
• Calculated Amount	• Height Ratio	• Saturated	• Data Flags
• %Diff	• Width	• Expected RT	• Calibration Flags
• Response	• Ion Ratio Status	• Sample Type	• <Blank Line > and <User Text> Data Items
• Response Ratio			

Report Info

The Report Info object displays general information about the report itself.

Required data file: None

Section placement: Report header and footer

For this object's possible fields, see Table 74.

Table 74. Report Info object fields

• Page [a] of [b]	• Layered App Version
• Date and Time	• <Blank Line > and <User Text> Data Items
• Template File	
• Layered App Name	

Sample Header

The Sample Header object displays general information about a sample.

Required data file: .raw, .sld

Section placement: Report header or footer or Nonrepeating section

For this object's possible fields, see Table 75.

Table 75. Sample Header object fields

• Data File	• Run Time	• Sample Weight	• Revision
• Original Data Path	• Comments	• ISTD Amount	• Barcode
• Current Data Path	• Vial	• Calibration Level	• Barcode Status
• Sample Type	• Injection Volume	• Dilution Factor	• User Labels 1 to 5
• Sample ID	• Scans	• Instrument Method	• <Blank Line > and <User Text> Data Items
• Sample Name	• Low Mass	• Processing Method	
• Operator	• High Mass	• Current Processing Method	
• Acquisition Date	• Sample Volume	• Calibration File	

System Suitability Flags

The Quan Summary Table, Quan ISTD Peak Summary, Sample Table, and Quan Peak Table 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.

These are the System Suitability flags.

Table 76. 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, Quan ISTD Peak Summary, Quan Peak Table, Qual Peak Table, Qual Summary Table, and Quan Summary Table 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.

These are the Baseline flags.

Table 77. 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, Quan ISTD Peak Summary, Quan Peak Table, and Quan Summary Table 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 78. 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, Quan Summary Table, and Quan Peak Table objects to indicate when certain peak characteristics exceed values specified in Quan Browser. These are the calibration flags that can appear.

Table 79. 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 data source files).

XReport comes with several example Xcalibur 2.0 report templates for you to use. These templates, described below, are located in the Xcalibur\Templates folder.

Table 80. XReport templates (Sheet 1 of 2)

Report names	Description	Files needed
CalibrationFile	For reporting calibration data.	.raw, .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, .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, .raw
IonRatio Confirmation	Generates a Quan sample report containing non-graphical ion ratio confirmation results.	.rst, .raw, .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, .pmd
Peak Integration	Generates a Quan sample report containing peak integration data generated using the Genesis peak integration algorithm.	.rst, .raw, .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, .raw
QuanPeakResults: _ISTD, _ESTD QuanResults QuanSimple	Generates Quan sample reports. Use this report with results from Xcalibur batch processing or Quan Browser.	.rst, .raw, .pmd
QuantifySampleReport	Generates Quan sample reports containing chromatograms and a Quan summary table.	.sld, .pmd, .rst, .raw

Table 80. 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, .raw

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