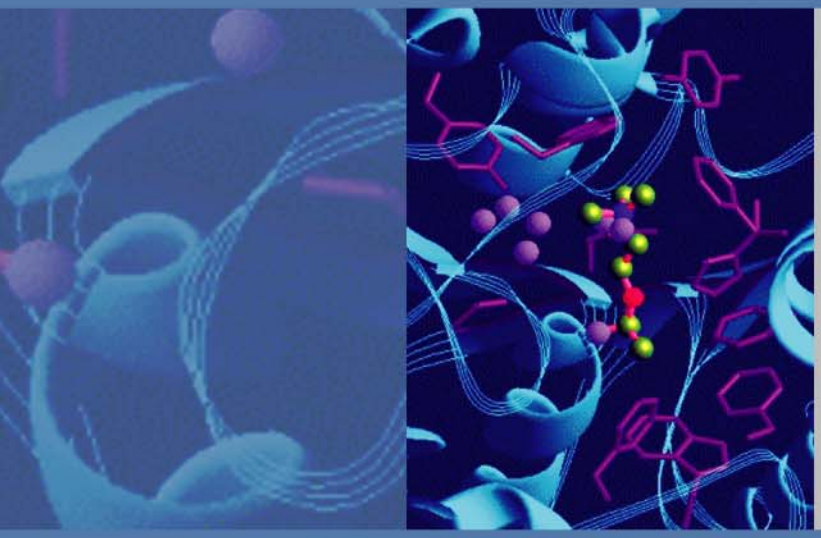

Thermo Xcalibur

Acquisition and Processing

Version 2.2

User Guide

XCALI-97209 Revision D May 2011

DOCUMENTATION SURVEY

Part of Thermo Fisher Scientific

Thermo SCIENTIFIC

Release history: Revision A, January 2009; Revision B, September 2010; Revision C, January 2011 (to reflect Microsoft Windows 7 compatibility); Revision D, May 2011

Software version: Thermo Xcalibur version 2.2

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

Contents

Preface

The Thermo Xcalibur™ mass spectrometry data system uses a sequence to specify samples of various types and a processing method to automatically detect and analyze the sample. This manual describes how to create and work with processing methods and sequences.

To provide us with comments about this document, please click the link below. Thank you in advance for your help.

Related Documentation

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

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

Special Notices

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

Special notices include the following:

IMPORTANT Highlights information necessary to prevent damage to software, loss of data, or invalid test results; or may contain information that is critical for optimal performance of the system.

Note Highlights information of general interest.

Tip Highlights helpful information that can make a task easier.

Contacting Us

There are several ways to contact Thermo Scientific for the information you need.

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Phone	800-532-4752
Fax	561-688-8736
E-mail	us.techsupport.analyze@thermofisher.com
Knowledge base	www.thermokb.com

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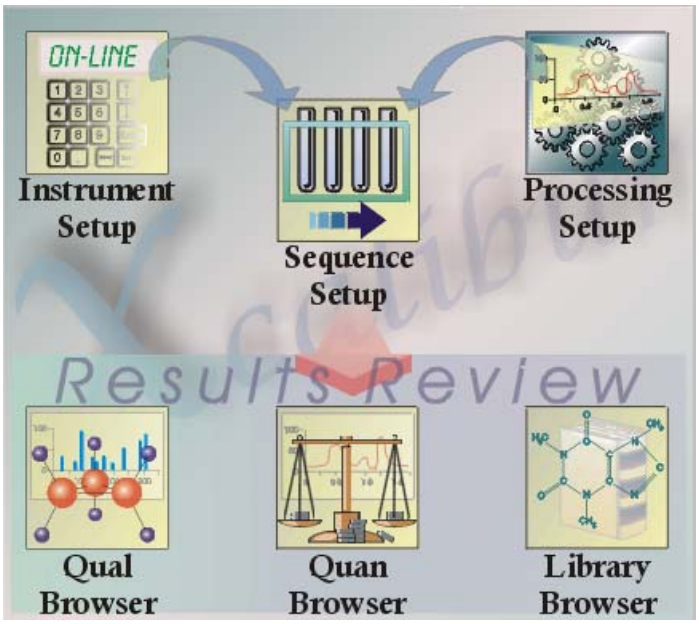
Introduction

Within the Xcalibur application, use the Thermo Xcalibur Sequence Setup module to acquire information and use the Thermo Xcalibur Processing Setup module to set up procedures for analyzing data (see Figure 1). Unlike an instrument method, which is required for data acquisition, you can create a processing method before or after you acquire raw data files. If you create a processing method before you inject your samples, you can add it to your acquisition sequence and analyze the data as it is acquired. If you create a processing method after you have acquired your raw data, you can add the processing method to the acquisition sequence, and then batch process the data files.

Figure 1. Xcalibur Roadmap view



Contents

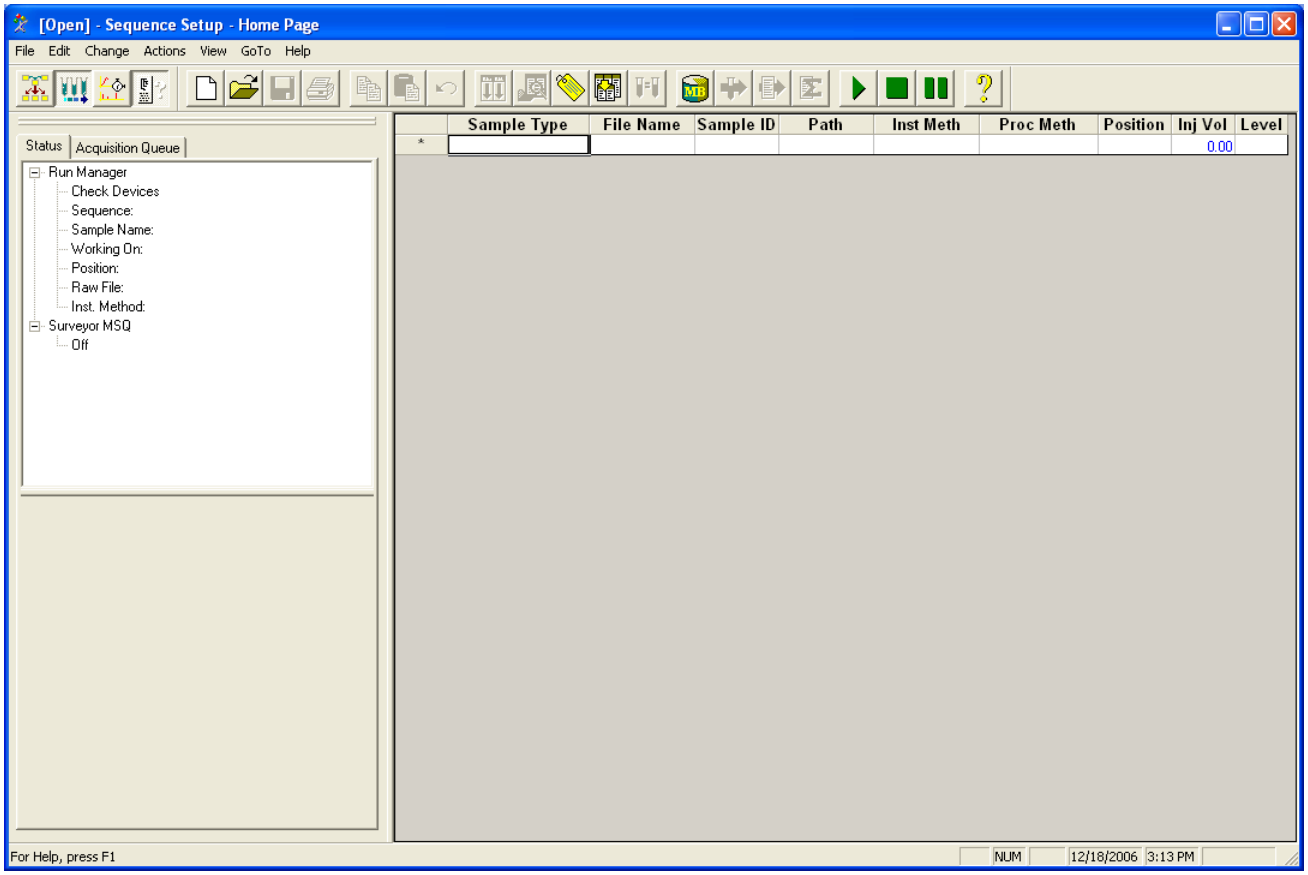
About the Sequence Setup View

Use the Sequence Setup view to set up a sequence containing unknown samples, calibration standard samples, quality control samples, and blank samples. You can also use this view to

- Control your autosampler or syringe pump and run a sample
- Run a sequence of samples
- Process a batch of previously acquired raw data files

Sequence Setup uses the processing method to initiate processing for qualitative and quantitative data, create reports, and run additional programs or macros (such as shutdown procedures).

Figure 2. Sequence Setup view



One row of the sequence corresponds to one sample injection. Each sample is defined by the settings in its sequence row. You can also manually inject samples from the front panel injector, as predefined in the sequence.

For quantitative analysis, you can generate a sequence semi-automatically based on a processing method. For example, Sequence Setup can divide a large number of samples into smaller groups that are bracketed by calibration sets. When you create a processing method, you can define the number of calibration levels in each calibration set in the processing method. Calibration sets can be shared between brackets to make overlapping brackets, if required. the Xcalibur data system supports sequences with no bracket, open bracket(s), overlapped bracket(s), and non-overlapped brackets. See "Creating a New Sequence" on page 10 for more information about creating a sequence or using brackets.

About the Processing Setup Window

Use the Processing Setup Window to

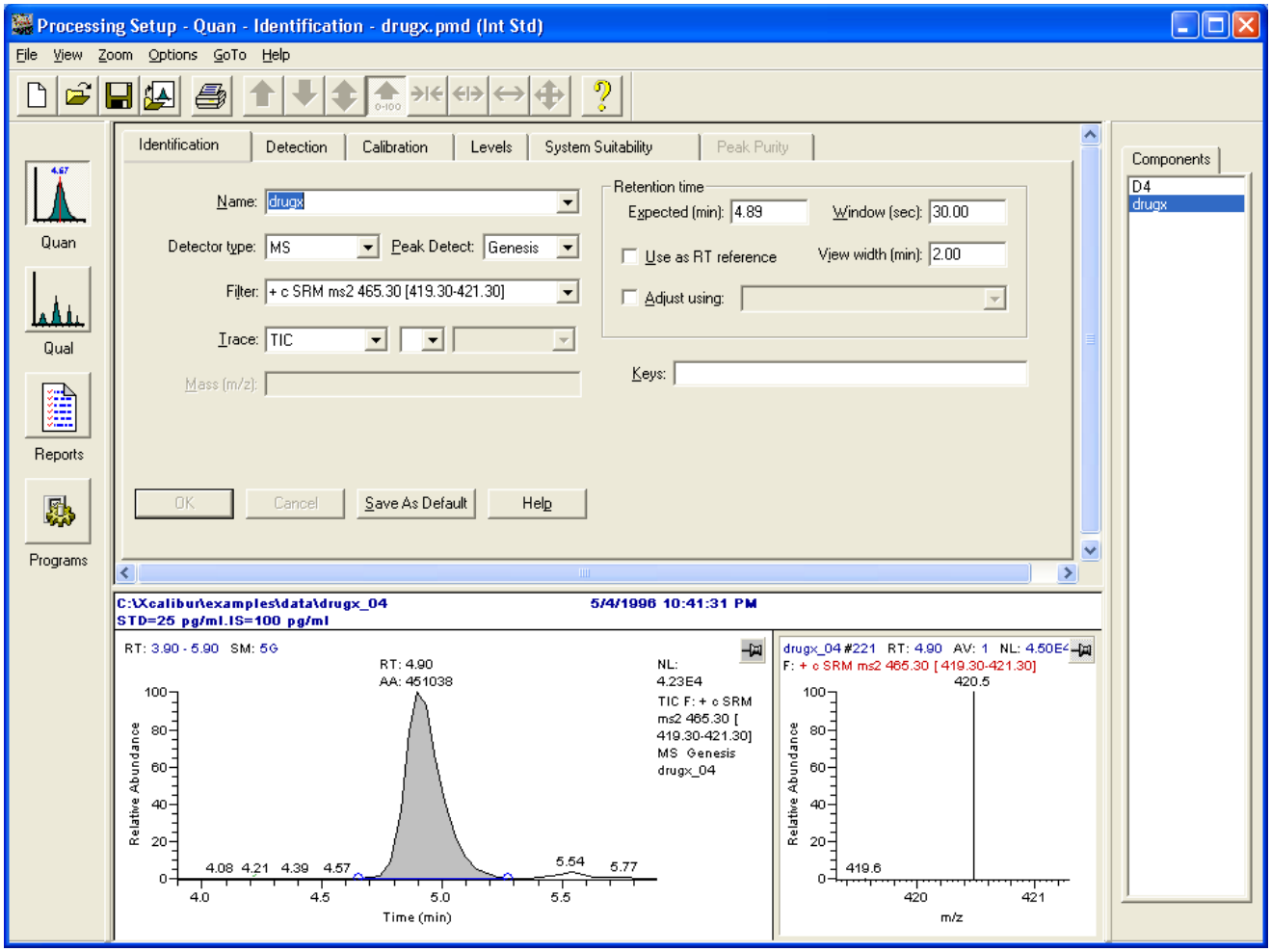
- Create a processing method for automated batch analysis.
- Modify existing methods.

Save method files or use Processing Setup to build a processing method for the qualitative or quantitative analysis of data. After you create a processing method, you can perform post-acquisition processing of your raw data files and print reports. This manual describes how to

- Create a processing method for the quantitative analysis of data. Processing methods are saved as a .pmd file type.
- Restore existing method files.

The Processing Setup window consists of the view bar, title bar, menu bar, toolbar, workspace, and status bar with access to the Help. To process the raw data properly, the processing method must contain the appropriate information. The Processing Setup view changes depending on which view option you select. The Quan view contains six tabbed pages (see Figure 3).

Figure 3. Processing Setup Identification page (Quan view)



Use the Processing Setup window to set values for the following procedures:

- "Setting Quan Browser Process Parameters" on page 45
- "Setting Qual Browser Process Parameters" on page 65
- "Working with Reports" on page 72

For information about searching libraries, refer to the *Creating and Searching Libraries User Guide*.

Preparing for Acquisition

A sequence is a list containing sample acquisition and batch processing information. Sequence files in the Xcalibur data system have an .sld file extension. Sequences in the application use two types of methods: an instrument method and a processing method. Use the instrument method to acquire the data file and use the processing method to process the information contained in the data files after they are acquired. Initially, the sequence file contains only a list of potential injections. After you acquire data files using the information in the sequence list, the data system links the sequence file to the acquired data files.

Contents

Configuring Instruments

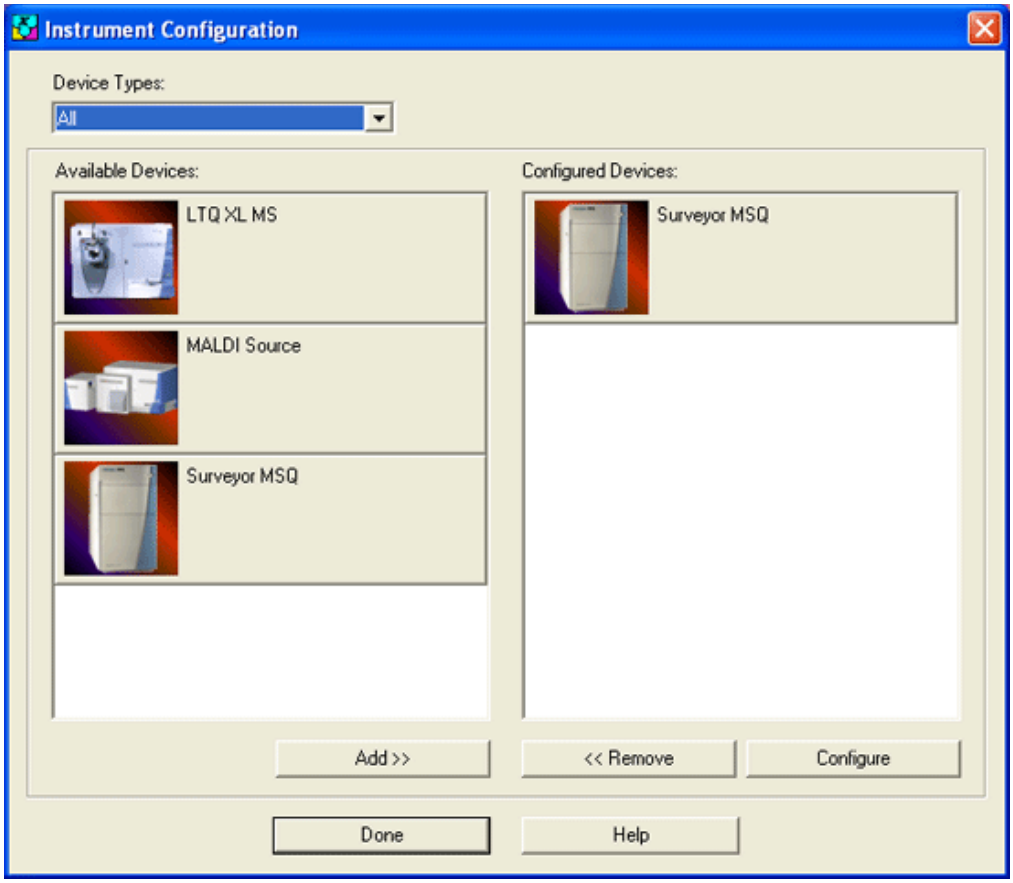
Choose from one of the following procedures to configure instruments:

Adding Hardware Devices to the Xcalibur Configuration

❖ **To add hardware devices to your Xcalibur hardware configuration**

1. Choose **Start > Programs > Thermo Foundation 2.0 > Instrument Configuration.** The Instrument Configuration dialog box opens (see Figure 4).

   Figure 4. Instrument Configuration window



2. To select the type of hardware device to add to your Xcalibur configuration, click the device icon in the Device Types list. The application displays all configurable devices as buttons in the Available Devices area. The Device button depresses to indicate that it is selected.

   If you do not see the device you want to configure, you might need to install the device driver.

3. To add the device to the Configured Devices area, click **Add**. The application copies the selected Available Devices button to the Configured Devices area, displayed as a Configured Devices button.

4. To select a device to configure, click the device icon in the Configured Devices area. The Configured Devices button depresses to indicate that it is selected.

5. To configure the selected device, click the **Configure** button. The *DeviceName* Configuration dialog box opens (the device name corresponds to the selected device).
6. Enter all required configuration information for the device. Complete entries and options for all pages.
7. To save settings and close the *DeviceName* Configuration dialog box, click **OK**. The application returns you to the Xcalibur Hardware Configuration dialog box.
8. Repeat steps 2 through 8 for all devices to be configured. To configure a device quickly, double-click the device button.
9. To save settings and close the dialog box, click **Done**.

Removing Hardware Devices from the Xcalibur Configuration

❖ **To remove hardware devices from your Xcalibur hardware configuration**

1. Choose **Start > Programs > Thermo Foundation 2.0 > Instrument Configuration.** The Instrument Configuration dialog box opens (see Figure 4 on page 6).
2. To select a device to remove from the configuration, click the device icon in the Configured Devices area. The Configured Devices button depresses to indicate that it is selected.
3. To remove the selected device, click **Remove**. The Xcalibur application removes the selected Configured Device button from the Configured Devices area.
4. To save settings and close the *DeviceName* Configuration dialog box, click **OK**. The application returns you to the Xcalibur Hardware Configuration dialog box.
5. Repeat steps 2 through 5 for all devices to be removed.
6. To save settings and close the dialog box, click **Done**.

Setting Up Instruments

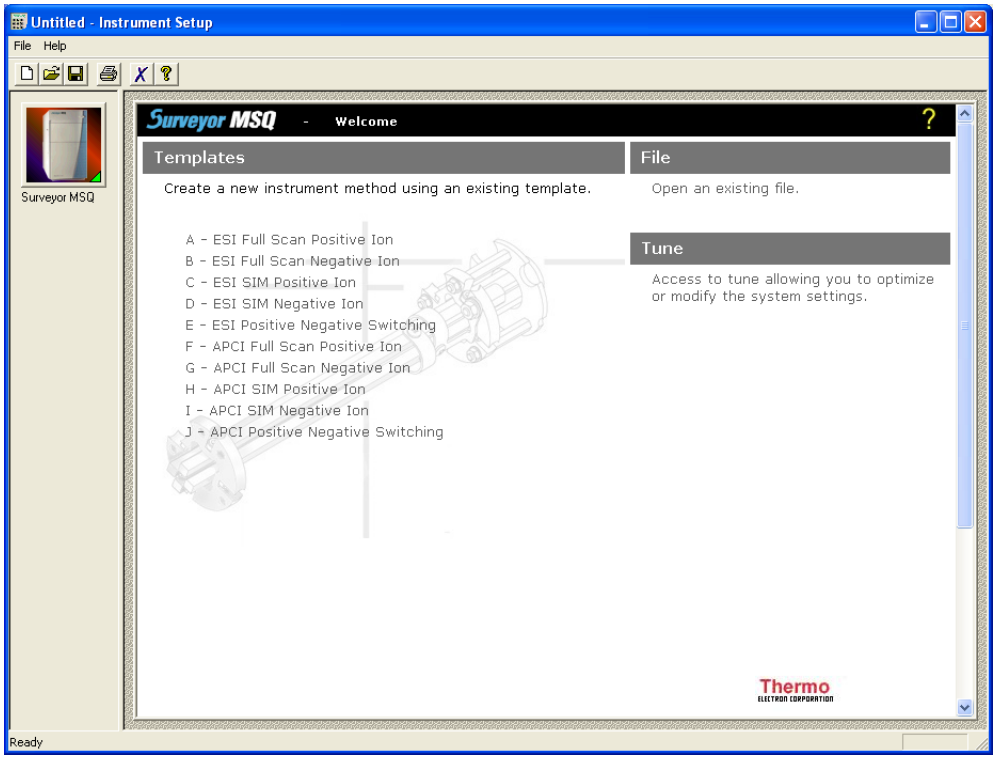
This procedure provides a general outline for setting up an instrument. For specific information about setting up a particular instrument, see Help for that instrument.

Note You must configure an instrument before you can set it up. To configure an instrument, close both the Home Page window and the Instrument Setup view and choose **Start > Programs > Thermo Foundation 1.0 > Instrument Configuration**. The Instrument Configuration dialog box opens. See "Configuring Instruments" on page 5 for more information.

❖ To set up an instrument

1. From any Xcalibur window, choose **GoTo > Instrument Setup**. The Instrument Setup window opens (see Figure 5).

Figure 5. Instrument Setup view



The application displays the Instrument Setup view with icons for all of the currently configured instrument components displayed down the left side of the view. Instrument Setup pages and dialog boxes for the selected instrument component are displayed on the right side of the view.

2. To select an instrument component to set up, click the picture icon of the instrument. If you have several instruments configured, you might need to scroll down to view and select the instrument icon.

   The application displays the Instrument Setup view for the instrument you selected. This can consist of one or more pages or dialog boxes.

3. To select Instrument Setup options, enter the instrument settings that are appropriate for the experiment that you want to perform.

   - For more information about the instrument, choose **Help > *Instrument* Help**.
   - For more information about how to perform an instrument setup, choose **Help > Instrument Setup Help**.
   - For more information about the current instrument setup page or dialog box, choose **Help > Help On Current Item**.
   - To display the main Xcalibur Help, choose **Help > Xcalibur Help**.
   - To display the Glossary, choose **Help > Glossary**.

4. Repeat step 3 for each Instrument Setup view page or dialog box.

   When you are done with the Instrument Setup for the current instrument, go to step 5.

5. Repeat steps 2 through 4 for each instrument to set up.

   When you have completed the Instrument Setup for all configured instruments, go to step 6.

6. To save the Instrument Setup method, choose **File > Save As**. The Save As dialog box opens. Browse to the folder to hold the method.

7. Enter the Instrument Setup method name and click **OK**. The application creates a new Instrument Setup method with a .meth extension.

8. To close the Instrument Setup view, choose **File > Exit**.

Creating a New Sequence

You can create a new sequence manually or semi-automatically.

To create a sequence manually, enter the appropriate information for each sample: File Name, Sample ID, Path, Experiment Method, Processing Method, Position, Injection Volume, Level, Sample Weight, Sample Volume, ISTD Amount, and Dil Factor.

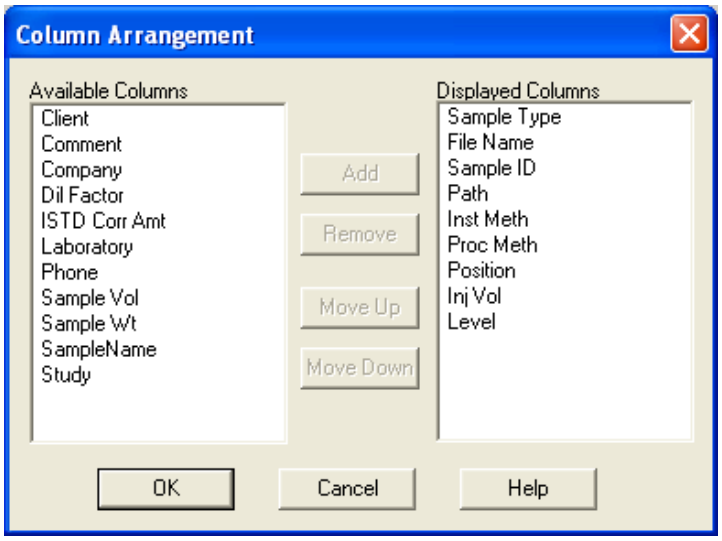
To create a sequence semi-automatically, use the New Sequence Template Dialog Box to assist in the preparation of the sequence. This time-saving method is especially useful when you are running large numbers of similar samples or when you are running bracketed, calibration, or QC samples.

Creating a Sequence Manually

❖ To create a sequence manually

1. Click  from the Roadmap view of the Home Page window. The Sequence Setup view opens.
2. To specify the sequence columns that you want to include, choose **Change > Column Arrangement.** The Column Arrangement Dialog Box opens (see Figure 6).

Figure 6. Column Arrangement dialog box



3. Select columns from the Available Columns list and click **Add** to move them to the Displayed Columns list.
4. Click **OK** to close the dialog box.

5. In the Sequence Setup view, right-click in a Sample box and select one of the following sample types: Unknown, Blank, QC, Std Bracket, Std Update, Std Clear, Start Bracket, or End Bracket.

   The sample types that appear in the Sample Type list are dependent upon the bracket type selected for the sequence.

6. To specify the sample data file name, type a name in the File Name box.

7. To specify a sample identification number, type a sample identification number in the Sample ID box.

   This entry is optional. If you do not enter a Base Sample ID, the Xcalibur application automatically uses the vial position as the Base Sample ID. If you enter a Base Sample ID, The application automatically appends the vial position to your entry.

8. To specify the sample data file drive and folder, type a file location in the Path box or double-click in the Path box to open a Select Directory dialog box and select the path and file name for the sample data file.

9. To specify the path and file name for the instrument method, enter the path and file name of the instrument method file in the Exp Method box or double-click in the Inst Method box to open a Select Instrument Method dialog box and select the path and file name for the instrument method.

   Instrument methods have a .meth file extension.

10. To specify a drive and directory for the processing method file, type the path and file name for the .pmd file.

    The application requires a processing method if the sample type is QC, Std Bracket, Std Clear, or Std Update or if you want to process the raw data obtained for the sample automatically.

11. To specify a position number, type the position number in the Position box.

    If you are using an autosampler, the position number must correspond to the autosampler's position number.

12. To specify the injection volume, type a value in the Inj Vol box. The application sends this volume to the syringe pump or autosampler.

    The injection volume displayed in the Inj Vol column matches the injection volume in your instrument setup method. You can override this injection volume value. If you do not enter an injection volume, the data system uses the default injection volume set in the instrument method that you selected in step 9.

13. To specify a level, if the sample type is QC, Std Bracket, Std clear, or Std Update, enter a level in the Level box. Double-click in the Level box. The Select Level dialog box opens. Select a level and click **OK**. The application displays the level in the Level box.

14. If the sample type is QC, Std Bracket, Std Clear, or Std Update, specify a sample weight (amount) in the Samp Wt box. Type the sample weight (amount) of the target compound in the QC or Standard sample. The units are defined in the processing method.

15. Specify or do not specify an internal standard bulk correction factor.

    The units are defined in the processing method selected in step 10, but are not to be included in this box.

    - If the internal standard amount in the sample is the same as the internal standard amount specified in the active processing method, confirm that the value in the Sequence Setup ISTD Corr Amt box is 0.000. No correction is applied.
    - If the internal standard amount in the sample is not the same as the internal standard amount specified in the active processing method (due to preparation error), type the actual total amount or concentration of the internal standard in the sample in the ISTD Corr Amt box. The Xcalibur application applies a bulk adjustment to the internal standard response factor.

16. To specify the component dilution factor, type a value in the component Dil Factor box.

17. To alter the current column arrangement, click the Column Arrangement toolbar button. The Column Arrangement Dialog Box opens (see Figure 7).

    - To add a column to the sequence, select the column from the Available Columns list and click **Add**.
    - To remove a column from the sequence, select the column from the Displayed Columns list and click **Remove**.
    - To alter the position of the columns in the sequence, select the column from the Displayed Columns list and click either **Move Up** or **Move Down** as appropriate.

18. Repeat steps 3 through 16 for all samples.

    To save time in duplicating column entries for sample rows below the row of the setting to be duplicated, use the Fill Down command by choosing Edit > Fill Down or by clicking the Fill Down button.

19. To save the sequence, choose **File > Save As**. The File Summary Information dialog box opens. Enter a description of the sequence and click **OK**. The Save As dialog box opens.

20. Enter the file name, select the location for the sequence, and click **Save**.

Changing the Sequence Display

To change the sequence display, use these procedures:

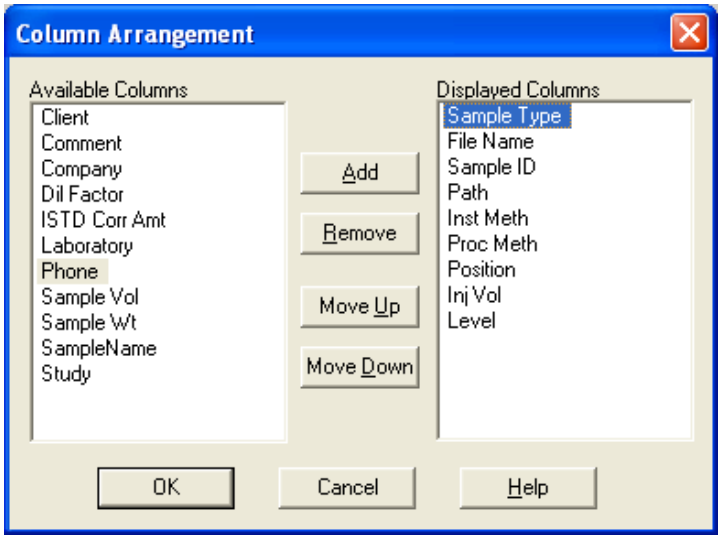
- Arranging Sequence Columns
- Changing User Labels
- Going to a Sequence Row
- Filling Down Sequence Parameters
- Transferring Row Information
- Changing the List Separator Character
- Printing a Vial or Sequence List

Arranging Sequence Columns

❖ **To select columns to display and a column display order in a sequence**

1. In the Sequence Setup view, click  in the toolbar or choose **Change > Column Arrangement**. The Column Arrangement Dialog Box opens (see Figure 7).

Figure 7. Column Arrangement dialog box



2. To add sequence columns, select a column name to add to the current sequence display in the **Available Columns** list and click **Add**. The Xcalibur data system moves the column name from the Available Columns list to the Displayed Columns list and displays the new column in the sequence.

3. To delete sequence columns, select a column name to delete from the current sequence display in the **Displayed Columns** list and click **Remove**. The application moves the column name from the Displayed Columns list to the Available Columns list and removes the selected column from the current sequence.

4. To select the sequence column position, select the column name in the **Displayed Columns** list and change the position.

   - Click **Move Up** to move the column name up the Displayed Columns list. This action corresponds to moving the column to the left in the sequence.
   - Click **Move Down** to move the column name down the Displayed Columns list. This action corresponds to moving the column to the right in the sequence.

   Note The Xcalibur data system displays the columns that are listed in the Displayed Columns list. The displayed left-to-right sequence column order corresponds to the top-to-bottom order in the Displayed Columns list.

5. Repeat step 4 until all columns are positioned correctly in the sequence.

6. To select sequence column widths, move the cursor to the column headings row at the top of the sequence and place the cursor at the right or left boundary of the column that is the incorrect width. The application changes the cursor to ⇤|⇥. Drag the column boundary to obtain the desired column width.

   Repeat step 6 until all columns are the correct widths.

7. Click **OK**.

Changing User Labels

You can define the heading names of the five columns that are located under the toolbar on the right side of the Sequence Setup view. These column heading names and the information entered in their respective boxes are stored with the active row of the sequence. The default names for the headings are as follows:

Heading 1: *Study*

Heading 2: *Client*

Heading 3: *Laboratory*

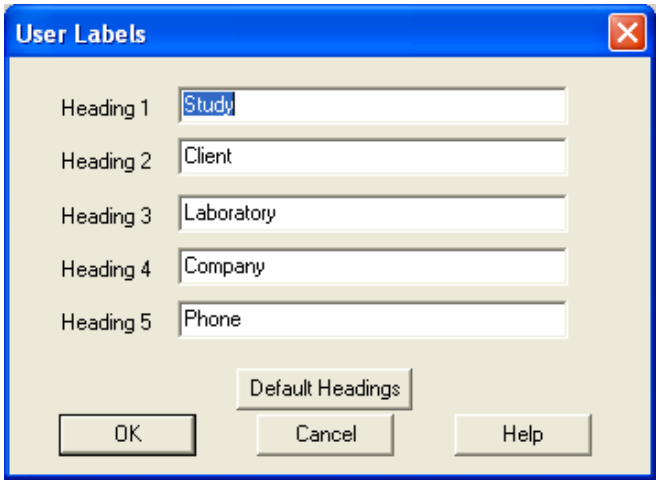
Heading 4: *Company*

Heading 5: *Phone*

❖ To change a heading name for the active sequence row

1. In the Sequence Setup view, click  in the Sequence Editor toolbar or choose **Change > User Labels**. The User Labels Dialog Box opens (see Figure 8).

   Figure 8. User Labels dialog box

2. To specify the new heading name, select a current heading name and type the new heading in the appropriate heading box.

   If you do not want to use a heading, select and delete the text and leave the box blank.

3. Repeat step 2 for each of the five heading names that you want to change.

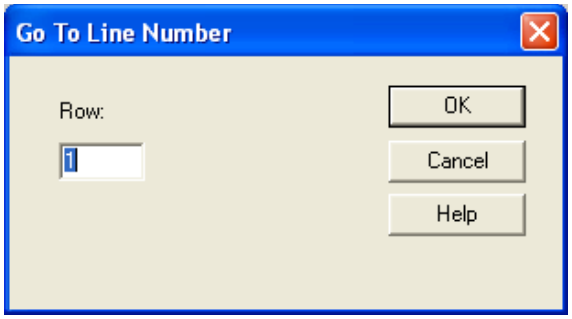
4. To save your new column heading names in the active row and close the dialog box, click **OK**. If you want other rows to have the same headings, see "Filling Down Sequence Parameters" on page 16.

Going to a Sequence Row

❖ **To go to a specified row in the current sequence**

1. In the Sequence Setup view, choose **Edit > Go To Row**. The Go To Line Number Dialog Box opens (see Figure 9).

   Figure 9. Go to Line Number dialog box

2. To specify a sequence row number, enter a valid sequence row number in the Row box. The Xcalibur application displays this number in the leftmost column of the sequence.
3. To go to the line number, click **OK**. The application closes the Go To Line Number dialog box and selects the Sample Type cell of the selected row in the current sequence.

Filling Down Sequence Parameters

❖ **To fill selected rows of selected columns with duplicate text entries or sequenced number entries**

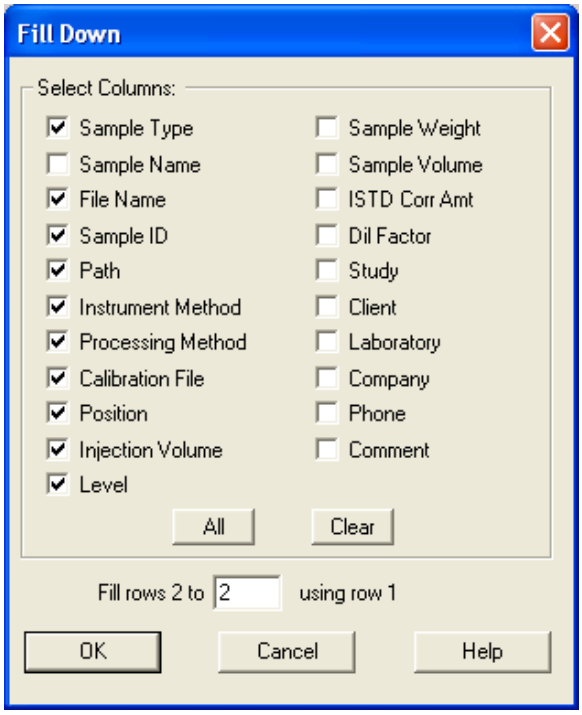
1. To activate the Fill Down command, select the cells in the sequence row that you want to copy data from and the cells in row(s) that you want to copy data to. The rows must be contiguous (grouped together).

   The data system activates the Fill Down command in the Edit menu and the Fill Down button on the toolbar.

   The top row that you select provides the information that is duplicated in the selected rows below it.

2. In the Sequence Setup window, click  in the toolbar or choose **Edit > Fill Down**. The Fill Down Dialog Box opens (see Figure 10).

Figure 10. Fill Down dialog box



The application displays check boxes for each of the sequence columns and selects the columns that you selected in step 1.

The application also displays the following message at the bottom of the dialog box based upon your selection:

Fill rows [B] to [C] using row [A]

where

A is the row number of the first row selected,

B is the row number of the second row selected, and

C is the row number of the last row selected.

The cells you select define A and B, which you cannot change; however, you can edit C to change the row number of the last row to be filled.

3. To specify the columns to be duplicated, select the columns that you want duplicated with the settings from row A.

Note The columns do not need to be next to each other.

- To select all the column check boxes, click **All**.
- To clear all the column check boxes, click **Clear**.

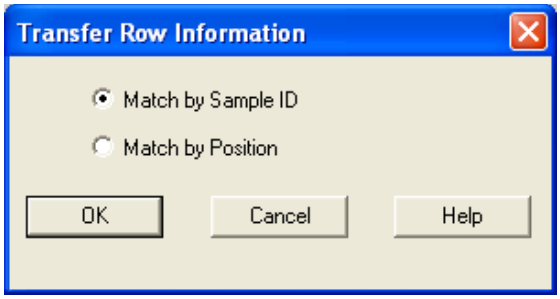
4. To fill the rows and close the dialog box, click **OK**.

Transferring Row Information

❖ **To copy information from one sample row to other rows in the sequence**

1. Click  in the toolbar or choose **Change > Transfer Row Info**. The Transfer Row Information Dialog Box opens (see Figure 11).

   Figure 11. Transfer Row Information dialog box

2. Specify whether to use Sample ID or Position.
3. To copy the row information from the first occurrence of a Sample ID to all sample rows that have the same Sample ID, select the **Match by Sample ID** option.

   To copy the row information from the first occurrence of a Position number to all sample rows that have the same position, select the **Match by Position** option.
4. To copy the information and close the dialog box, click **OK**. The data system performs the selected copy operation.

   Note The File Name and Sample Type columns are not affected.

   If you must undo the copy operation, immediately choose **Edit > Undo** or click  in the Sequence Editor toolbar.

Changing the List Separator Character

When you export a sequence, the Xcalibur data system creates an exported comma-separated-value text file with a .csv file extension by inserting a list separator character between each field of each column of the sequence. This file format can be read by a text editor or spreadsheet program.

When you import a sequence, the list separator character used in the sequence file to be imported must be the same as the current list separator character set for your computer operating system. The application generates an invalid file message if you try to import a file where the list separator character is different than the list separator currently set in the International dialog box. For example, an invalid file message is generated if the list to be imported uses a comma (,) for a separator character and the separator character setting for your operating system is a semicolon (;).

❖ To change the list separator character

1. Choose **Start > Settings > Control Panel**. The Control Panel window opens.
2. Double-click **Regional and Language Options.** The Regional and Language Options dialog box opens.
3. On the Regional Options page, click **Customize**. Click the **Numbers** tab.
4. Type a comma in the List Separator box.

   Note Each country has a default list separator. If you have not changed the list separator character before, the default character appears in the List Separator box. For example, the default list separator for the United States is the comma. In this case, the Xcalibur data system places a comma between each sequence field in the exported file. The list separator can be changed to any alphanumeric character. However, characters that cannot be distinguished from the characters used in the sequence text fields, such as alphabetic characters, should be avoided because they result in unreadable (invalid) files. The most common list separators are the comma (,) and the semicolon (;).

   If the list separator character has been changed and you want to return it to the default value for your country, do the following: In the Regional Options page of the Regional and Language Options dialog box, select a different country from the list box and click **OK**. Then, immediately open the Regional and Language Options dialog box again and select your country from the list. Click **OK** to save the default settings.

5. To store the new list separator setting and close the dialog box, click **OK**. Click **OK** again to close the Customize Regional Options dialog box.

Printing a Vial or Sequence List

To preview your autosampler position list or sequence before printing, go to step 1. To print your list without a preview, go to step 3.

❖ To print a vial position list or sequence

1. To preview your vial list or sequence, choose **File > Print Preview** in the Sequence Setup view. The Print Selection dialog box opens.

   - To preview your vial position list, select the **Vial Position List** option and choose **OK**.
   - To preview your sequence, select the **Full Sequence** option and choose **OK**.

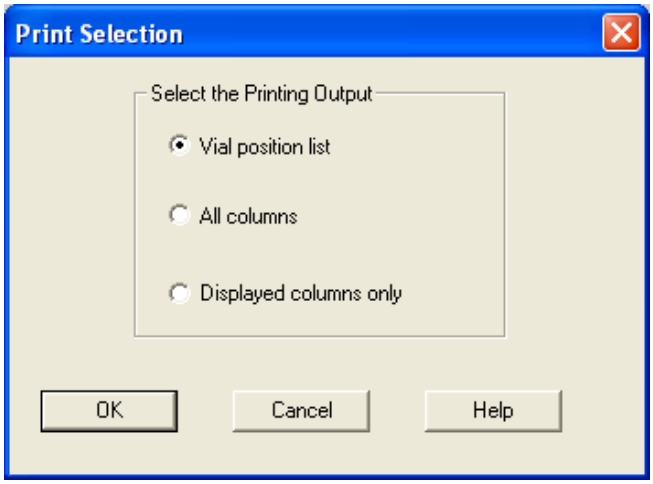
   The application displays the first page of the selected list in the Print Preview view with the cursor active.

   - Click to increase the size of the list to make it easier to read.
   - Click again to further increase the size of the list. The application displays the default icon.
   - Click again to return to the original (full page) size.

2. To review the displayed list, use the **Next Page**, **Prev Page**, **Two Page**, **Zoom In**, and **Zoom Out** buttons.

3. To print the selected list, click **Print**. The Print Selection dialog box opens (see Figure 12).

   Figure 12. Print Selection dialog box

4. To print your vial position list or sequence, choose **File > Print** in the Sequence Setup view. The Print Selection dialog box opens.

5. Select what you want to print.
   - To print your vial position list, select the **Vial Position List** option and choose **OK**.
   - To print your sequence, select the **All Columns** option and choose **OK**.
   - To print only displayed columns, select the **Displayed Columns Only** option and choose **OK**.

   The Print dialog box opens.
6. Select print options under Print range and Copies, and choose **OK**.

   The application prints the selected list.

Acquiring Data

This chapter provides procedures used in acquiring data.

Contents

Creating a Sequence Semi-Automatically

To create a sequence semi-automatically, do these procedures:

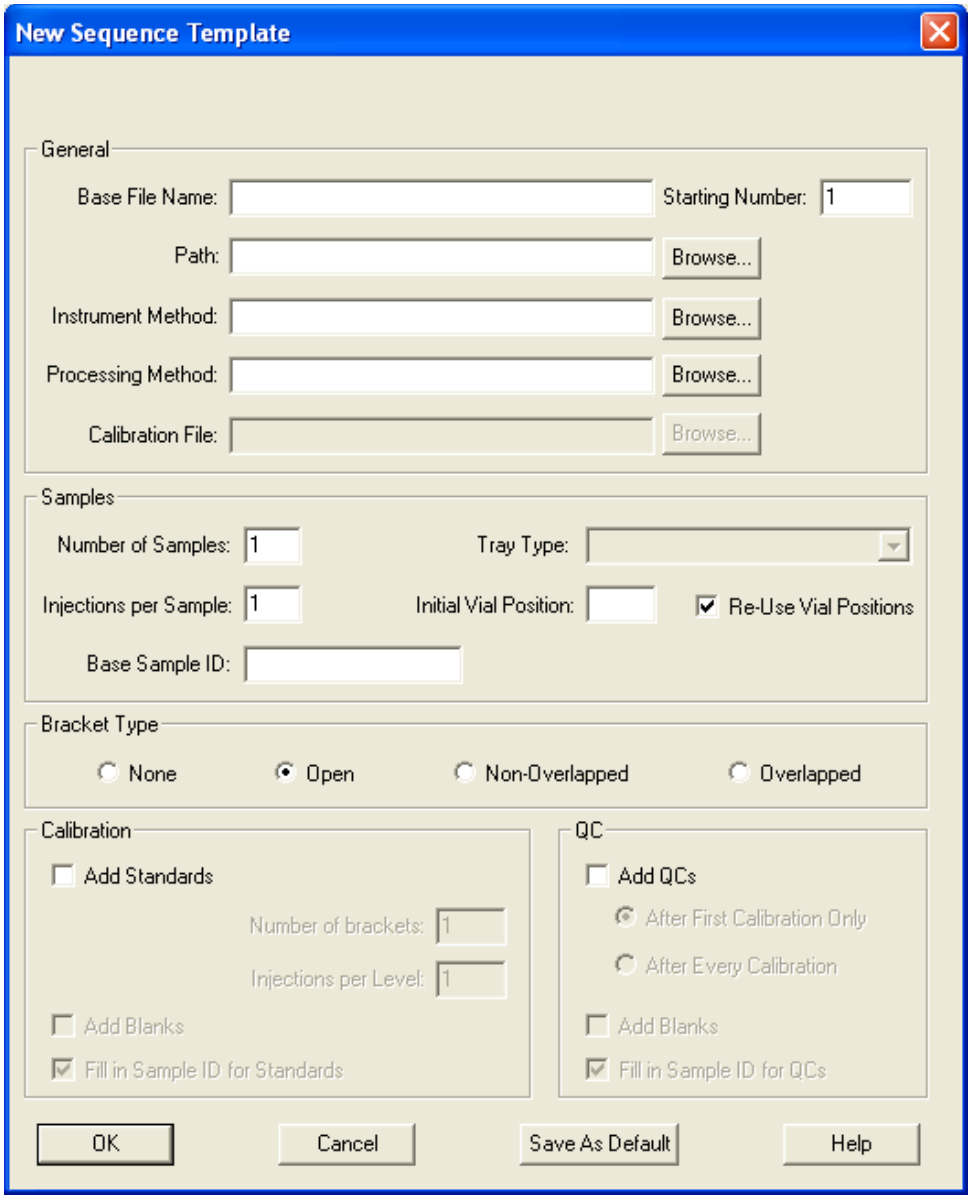
1. Opening the New Sequence Template Dialog Box
2. Entering Base File Name, Path, and Methods
3. Entering Sample Settings
4. Selecting the Bracket Type.
5. Entering Calibration Settings
6. Entering Quality Control Settings
7. Saving the Changes and Closing the Dialog Box

Opening the New Sequence Template Dialog Box

❖ **To open the New Sequence Template dialog box**

In the Sequence Setup view, choose **File > New** or click  in the toolbar. The New Sequence Template Dialog Box opens (see Figure 13).

Figure 13. New Sequence Template dialog box



Entering Base File Name, Path, and Methods

❖ To specify the names of the methods and base and calibration files

1. In the New Sequence Template dialog box, define base file parameters in the General area (see Figure 14).

   Figure 14. General area

2. Type the base file name of the raw file in the Base File Name box. The Xcalibur data system applies this name to all of the raw files that it creates using the new sequence.

   If you do not specify a base file name, the application assigns a default file name of 001 to the first sample.

   The application starts file name numbering at 001. To have it start numbering at another file name number, enter the number in the Starting Number box.

3. To indicate a location for the sample raw files, type a path location in the Path box or click **Browse** to select the drive and directory where the files are to be stored.

4. To specify an existing instrument method, type the path and file name of an existing instrument method in the Instrument Method box or click **Browse** to select the drive, directory, and file name.

5. To select an existing processing method (optional), type the path and file name of an existing processing method in the Processing Method box or click **Browse** to select the drive, directory, and file name.

6. Enter a calibration file (active only for Bracket Type None).

7. To use a previously created calibration file, click **Browse** to select the file. The application enters the path and file name in the Calibration File box.

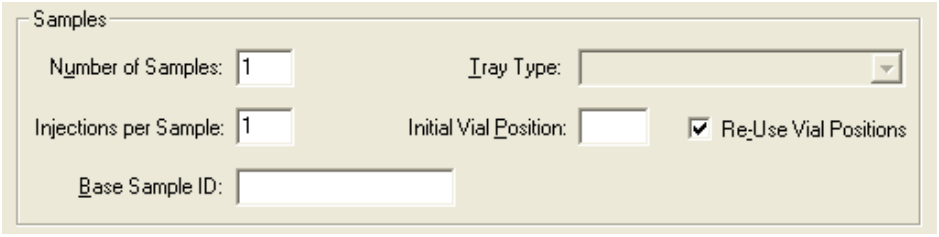
   To have the application create a new calibration file, type a folder and file name in the Calibration File box. Do not include the .XCAL file extension.

Entering Sample Settings

❖ To enter sample and auto-sampler settings

1. To specify the number of samples in the Samples area (see Figure 15) of the New Sequence Template dialog box, type the number of samples in the Number of Samples box.

   Figure 15. Samples area

2. To specify the number of injections per sample, type the number of injections for each sample (number of replicates) in the Injections Per Sample box.
3. To specify the base sample ID, type the base sample ID in the Base Sample ID box.
4. To specify the autosampler tray type, select the autosampler tray type from the Tray Type list.
5. To specify the initial vial position, type the first vial number in the Initial Vial Position box.
6. To re-use vial positions, select the **Re-Use Vial Positions** check box. Clear this check box if you have separate vials for each sample.

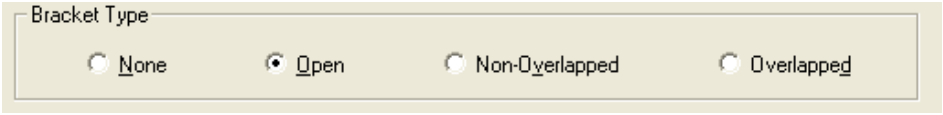
Selecting the Bracket Type

❖ To enter the bracket type to be used for the current sequence

In the New Sequence Template dialog box, select a bracket type in the **Bracket Type** area (see Figure 16) by choosing one of the following options. See the "New Sequence Template Dialog Box" on page 109 for more information about bracket types.

- None
- Open
- Non-Overlapped
- Overlapped

Figure 16. Bracket Type area



Entering Calibration Settings

❖ To enter calibration settings

1. To add calibration standard samples in the Calibration area (see Figure 17) of the New Sequence Template dialog box, select the **Add Standards** check box. This process is optional.

   Figure 17. Calibration area

   The Xcalibur data system activates the Number of Brackets box and the Injections Per Level box (not active for Bracket type Open).

   a. Type a value for the number of calibration sets in the Number of Brackets box.

   b. Type a value for the number of injections (replicates) for each calibration level in the Injections Per Level box.

2. To add blank samples, select the **Add Blanks** check box. This process is optional.

3. To have the data system enter the sample ID for each calibration sample, select the **Fill In Sample ID For Standards** check box. This process is optional.

Entering Quality Control Settings

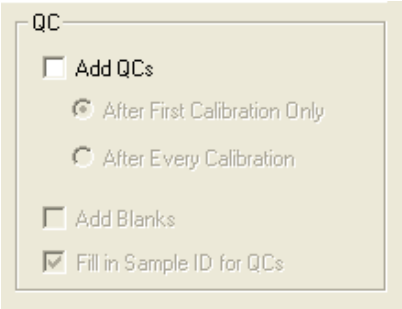
You need to create and select a processing method with Calibration or QC levels before you can select one of the levels for a quality control sample type [QC] or standard update sample type [Std Update] to use in a sequence.

In the Sequence Setup view, the Level box displays the current calibration or QC level for the Sequence row. This level is defined in the processing method displayed in the Processing Method box.

❖ To enter quality control settings in the QC area

- To add quality control samples (see Figure 17), select the **Add QCs** check box. This process is optional.

  Figure 18. QC area

  The Xcalibur data system activates the After First Calibration Only option and the After Every Calibration option.

  – To add QC samples after only the first calibration, select the **After First Calibration Only** option.

  – To add QC samples after every calibration, select the **After Every Calibration** option.

- To add quality control blank samples, select the **Add Blanks** check box. This process is optional.
- To have the data system enter the Sample ID for each QC sample, select the **Fill In Sample ID for QCs** check box. This process is optional.

Saving the Changes and Closing the Dialog Box

❖ To save settings and close the dialog box

Click **OK**. The settings are saved and the New Sequence Template dialog box closes.

The Xcalibur data system uses the information in the New Sequence template to create a new sequence. The application displays the rows and columns that have been selected using the Column Arrangement Dialog Box in the Sequence Setup view.

Preparing to Run Xcalibur Samples

Before you run an Xcalibur sample, select or set up a tune method, instrument setup method, processing method (optional), and a sample sequence.

❖ To prepare to run Xcalibur samples

1. To open the Home Page window, choose **Start > Programs > Thermo Xcalibur > Xcalibur**.
2. To select or create a tune method, choose **GoTo > Instrument Setup**. The Instrument Setup window opens. Choose **MS Detector or Mass Spectrometer > Tune Plus**. The Tune window opens. Select tune options and save the Tune Method. The Tune Method file type can vary with the instrument.
3. To select or create an instrument method, select instrument setup options and save the instrument method from the Instrument Setup window. The instrument method file type has a .meth extension.
4. To select or create a processing method (optional), choose **GoTo > Processing Setup** from the Home Page window. The Processing Setup window opens. Select Processing Setup options and save the processing method. The Processing Setup file type has a .pmd extension.
5. To select or create a sequence, choose **View > Sequence Setup View** to open the Sequence Setup view from the Home Page window. Select Sequence Setup options and save the sequence method. The sequence method file type has an .sld extension.

   Note To acquire data, the sequence must specify an instrument method for each sample. An instrument method specifies the control parameters to run your LC/MS instrument, including the tune method for the mass spectrometer. If you select an invalid tune method, the Xcalibur data system displays an error message when you try to run the sequence.

   Processing methods specify parameters for the post-processing of data and are not required to acquire raw data files. To batch process a sequence, it must contain a processing method.

6. From the Sequence Setup window, select a single sample or a list of samples.
   - To run a single sample, select the sample from the sequence by clicking in the leftmost column to select the entire sample row. Choose **Actions > Run This Sample**. The Run Sequence Dialog Box opens. Select sequence options and click **OK** to save options and close the dialog box.
   - To run multiple samples, select sequential samples from the sequence by clicking and dragging in the leftmost column to select multiple sample rows. If the samples you want to run are not sequential in the sequence, choose **Edit > Insert Row** or use cut and paste commands to place the samples in consecutive order before selecting them.

The data system runs samples in the sequence in the relative order they appear in the sequence (top to bottom). From the Sequence Setup window, choose **Actions > Run Sequence.** The Run Sequence Dialog Box opens.

7. Select sample run options and then select sequence options. Click **OK** to save the options and close the dialog box.

❖ To select or change a calibration or QC level for a sample

1. From the Sequence Setup view, for a sample of type Std Update or QC, select a processing method file that defines one or more levels.
2. Double-click the Level box to open a list of levels from the processing method.
3. To select the QC or calibration level, click the correct level for the sample.
4. To enter the settings into the Sequence Setup table, click away from the list store the level. The application displays the new level in the Level box for the sample.

Running a Sample

❖ To run a sample selected from the current sequence

1. To select a sample from the current sequence to run or process, on the far left click a row number with the current sequence. The application highlights the entire row.
2. Choose **Actions > Run This Sample** in the Sequence Setup view or click  in the toolbar.

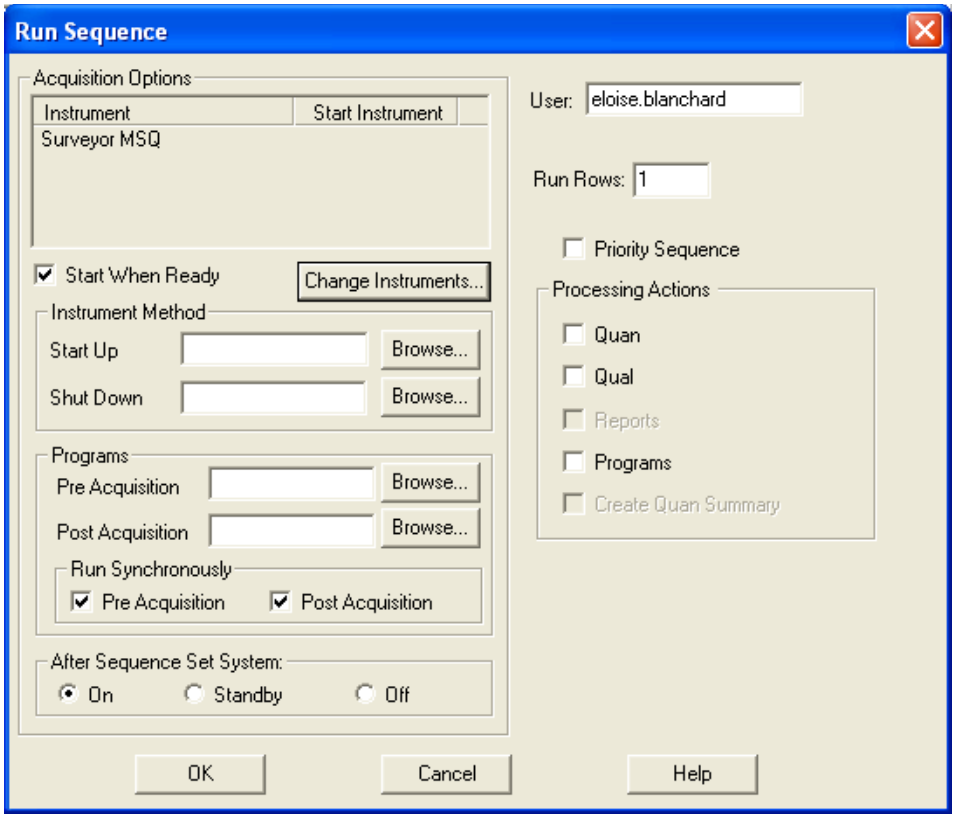
   The Run Sequence Dialog Box (covered) and the Change Instruments In Use Dialog Box (on top) open.
3. To select the start instrument for the current sequence and the instruments that you want to use to run the selected sample, use the Change Instruments In Use Dialog Box.

   Click the Instrument or Start Instrument fields to turn the Yes display on and off. Yes indicates that the instrument is active. Click **OK** to save changes and close the dialog box.

   The selections you have made are displayed in the Acquisition Options area of the Run Sequence Dialog Box.

> **Note** You can make instrument changes at any time using the Change Instruments button.

Figure 19. Run Sequence dialog box



4. To indicate the operator who started the sample, type up to 10 characters in the User box.
5. To confirm the run rows, check the sample row displayed in the Run Rows box to see that it is correct.

> **Note** If you did not select a sequence row in step 1, the Xcalibur data system defaults to using sample row 1.

6. Specify the priority of the sample.
   - To have the application begin acquisition of the sample immediately after the current sequence is completed, select the **Priority Sequence** check box.
   - To enter this sample at the end of the current processing queue, clear the **Priority Sequence** check box.
7. Specify when to run the sample.
   - To have the application begin the acquisition as soon as all devices are ready, select the **Start When Ready** check box.
   - To have the application wait so that you can perform a manual check or any other needed action before starting, clear the **Start When Ready** check box. In this case, when you have completed all actions and all the devices are ready, click **Start** in the toolbar.

8. Specify an instrument method.
    - In the Start Up box, specify the (optional) instrument method to be run when the sequence starts.
    - In the Shut Down box, specify the (optional) instrument method to be run when the sequence is completed.
9. Specify programs to be run.
    - In the Pre Acquisition box, specify the program to be run prior to running the sequence.
    - In the Post Acquisition box, specify the program to be run when the sequence is completed.
10. Specify whether the programs are to be run asynchronously or synchronously.
    - To run programs synchronously (in series) with data collection, select the **Pre Acquisition** check box or **Post Acquisition** check box.
    - To run programs asynchronously (in parallel) with data collection, clear the **Pre Acquisition** and **Post Acquisition** check boxes.
11. In the After Sequence Set System area, select a status for the system after the data system completes the sequence.
    - On option
    - Standby option
    - Off option
12. Select one or more of the following processing actions:
    - To access check boxes for peak detection and integration, calibration, and quantitation processing, select the **Quan** check box.
    - To access check boxes for peak detection and integration, spectrum enhancement, and library search processing, select the **Qual** check box.
    - To print Sample Reports and Summary Reports, select the **Reports** check box.
    - To run programs, select the **Programs** check box.
    - To print a summary of the quantitation data, select the **Create Quan Summary** check box.
13. To save the settings and close the dialog box, click **OK**. The Xcalibur data system either places the sample in the run queue or starts processing when the current sample is completed.

Running a Sequence

❖ To run a series of samples selected from the current sequence

1. To select the samples you want to run or process, click the row numbers on the far left in the current sequence. The data system highlights the selected rows.
2. In the Sequence Setup view, click  in the toolbar or choose **Actions > Run Sequence**. The Run Sequence Dialog Box (covered) and the Change Instruments In Use Dialog Box (on top) appear.
3. Select the instruments to run the selected samples and the start instrument for the current sequence.
   a. In the Change Instruments In Use dialog box, select the instrument under the Instrument column and click **Yes**. Clicking in the In Use column turns Yes on and off.
   b. Repeat step a for multiple instruments.
   c. Click **OK** to save changes and close the dialog box.

   The selections you have made appear in the Acquisition Options area of the Run Sequence dialog box.

   Note You can make instrument changes at any time using the Change Instruments button.
4. To enter a user ID and indicate the operator who started the sequence, type up to 10 characters in the User box.
5. Confirm that the sample rows displayed in the Run Rows box are correct. Change entries that are not correct.

   If you did not select sequence rows in step 1, the data system starts the sequence with Sample 1 by default.
6. Specify the priority of the sequence.
   - To have the application begin acquisition of the sequence immediately after the current sequence is completed, select the **Priority Sequence** check box.
   - To enter this sequence at the end of the current processing queue, clear the **Priority Sequence** check box.
7. Specify when to run the sequence in the Acquisition Options area.
   - To have the application begin the acquisition as soon as all devices are already, select the **Start When Ready** check box.
   - To have the application wait so that you can perform a manual check or any other needed action before starting, clear the **Start When Ready** check box. When you have completed all actions and all the devices are ready, click **Start** in the toolbar.

8. To specify an instrument method to run when the sequence starts, use the Start Up box. Specify the instrument method to be run when the sequence is completed in the Shut Down box.
9. To specify programs to be run:
    - Type a program name in the **Pre Acquisition** box. This program runs before the sequence starts.
    - Type a program name in the **Post Acquisition** box. This program runs after the sequence is completed.
10. To specify whether programs are to be run asynchronously or synchronously:
    - To run programs synchronously (in series) with data collection, select the Pre acquisition or Post Acquisition check box.
    - To run programs asynchronously with (at the same time as) data collection, clear the Pre Acquisition and Post Acquisition check boxes.
11. In the After Sequence Set System area, select a status option for post-processing (after the sequence is completed).
    - On
    - Standby
    - Off
12. Select one or more of the following in the Processing Actions area:
    - To select peak detection and integration, calibration, and quantitative analysis processing, select the **Quan** check box.
    - To select peak detection and integration, spectrum enhancement, and library search processing, select the **Qual** check box.
    - To print sample reports and summary reports, select the **Reports** check box.
    - To run programs, select the **Programs** check box.
    - To print a summary of the quantitation data, select the **Create Quan Summary** check box.
13. To save the settings and close the dialog box, click **OK**. The data system either places the sample at the end of the run queue or starts processing when the current sample is completed.

IMPORTANT If you add a processing method to your acquisition sequence, do not close Home Page during the sequence run. If you close Home Page during the sequence run, batch process your raw data files to perform the appropriate post-acquisition processing.

Viewing the Data As It Is Acquired

❖ **To view data as it is acquired using the Real Time Plot facilities**

1. Click the **Real Time Plot View** button  on the Home Page toolbar.
2. If the display is not already locked, click the **Lock Display** button to lock the display so you can monitor the real-time progress of your run.

   In the unlocked position, you cannot monitor the real-time progress of your run, but you can review your data. For example, you can display the spectrum for a particular peak that has already eluted. Data collection continues offscreen as you review your data.

Reviewing Real-Time Data

❖ **To review data as it is being collected**

1. Unlock the display by clicking the **Lock Display** button.

   After you unlock the display, data collection continues offscreen.
2. Pin the **Mass Spectrum** cell by clicking  in the upper-right corner of the cell.

   The pin in the upper-right corner of the Mass Spectrum cell turns green. Cursor actions in other cells such as the chromatogram cell now affect the view displayed in the Spectrum cell.
3. Click the peak of interest in the **Chromatogram** cell.

   In the Mass Spectrum cell, a mass spectrum appears for the time-point that you clicked on.
4. Click the **Lock Display** button to resume monitoring real-time data acquisition.
5. Pin the **Chromatogram** cell by clicking the pin in the upper-right corner of the cell.

   The pin in the upper-right corner of the Chromatogram cell turns green. Cursor actions in other cells such as the Spectrum cell now affect the view displayed in the Chromatogram cell.
6. Click the *m/z* value of interest in the Mass Spectrum cell.

   In the Chromatogram cell that contained the total ion chromatogram (TIC), a chromatogram appears for the *m/z* value you clicked.
7. Click the **Lock Display** button to resume monitoring real-time data acquisition.

Monitoring a Chromatogram in Real Time

The Real Time Plot view of the Home Page window provides a real-time display of the chromatogram of the current sample. The display settings are defined in the instrument method used for the sample run. The horizontal X-axis displays the time in minutes and the vertical Y-axis displays the relative abundance of the mass range, TIC (total ion current), base peak, UV1, UV2, UV3, or UV4.

Note If the Relative Abundance caption displays horizontally in your computer task bar, choose **Start > Settings > Control Panel**. The Control Panel dialog box opens. Double-click the Fonts icon to open the Fonts dialog box and automatically re-initialize the fonts. Close the Fonts dialog box. The software should now display the Relative Abundance caption vertically.

❖ To view a chromatogram in locked and unlocked modes

1. To unlock the display, choose **View > Lock Display**, click , or click the display to unlock the data from the instrument. You can then review the data obtained up to that point in time. The Xcalibur data system continues to store all real-time sample data.

   In locked mode, the Lock Display menu command has a check by it and the toolbar appears to be depressed.

2. To select the chromatogram, click to indicate that the chromatogram display is the active display ( ). The chromatogram display is contained in a grid cell and can be controlled by toolbar and menu commands.

3. Select an X-axis range:

   - To display all data on the X-axis, click or choose **View > Zoom > Display All**.
   - To show more data, click to zoom out the X-axis or choose **View > Zoom > Zoom Out X**.
   - To show more detail, click to zoom in the X-axis at the center or choose **View > Zoom > Zoom In X**.

4. Select a Y-axis range:

   - To normalize the intensity scale, click or choose **View > Zoom > Normalize**. The tallest peak has relative abundance = 100.
   - To show more data, click to zoom out the Y-axis or choose **View > Zoom > Zoom Out Y**.
   - To show more detail, click to zoom in the Y-axis from the current baseline or choose **View > Zoom > Zoom In Y**.

5. To lock the data display to the instrument so that you can resume monitoring real-time data collection, click or choose **View > Lock Display**. The data system displays the most recent update of the chromatogram.

Monitoring a Spectrum in Real Time

The Real Time Plot view of the Home Page window provides a real-time display of the spectrum of the current sample. The horizontal X-axis displays the mass-to-charge ratio and the vertical Y-axis displays the relative abundance of the ions.

❖ To view a spectrum in locked and unlocked modes

1. To unlock the display, click , choose **View > Lock Display** or click the display at any time. Unlocking the data from the instrument lets you review the data obtained up to that point in time. The data system continues to store all real-time sample data.

   In locked mode, the Lock Display menu command has a check by it and the toolbar appears to be depressed.

2. To select the spectrum, click in the upper right corner of the spectrum. The application changes the cell target to to indicate that the spectrum display is the current display. The spectrum display is contained in a grid cell and can be controlled by toolbar and menu commands.

3. Select the scan you want to view:

   - To display the previous mass scan, click or choose **View > Pan > Previous Scan**.
   - To display the next mass scan, click or choose **View > Pan > Next Scan**.

4. Select X-axis range:

   - To display all data on the X-axis, click or choose **View > Zoom > Display All**.
   - To zoom out the X-axis to show more data, click or choose **View > Zoom > Zoom Out X**.
   - To zoom in the X-axis at the center to show more detail, click or choose **View > Zoom > Zoom In X**.

5. Select Y-axis range:

   - To normalize the intensity scale, click or choose **View > Zoom > Normalize**. The tallest peak has relative abundance = 100.
   - To zoom out the Y-axis to show more data, click or choose **View > Zoom > Zoom Out Y**.
   - To zoom in the Y-axis from the current baseline to show more detail, click or choose **View > Zoom > Zoom In Y**.

6. To lock the display, click or choose **View > Lock Display**. This locks the data display to the instrument so that you can resume monitoring real-time data collection. The application displays the most recent update of the spectra.

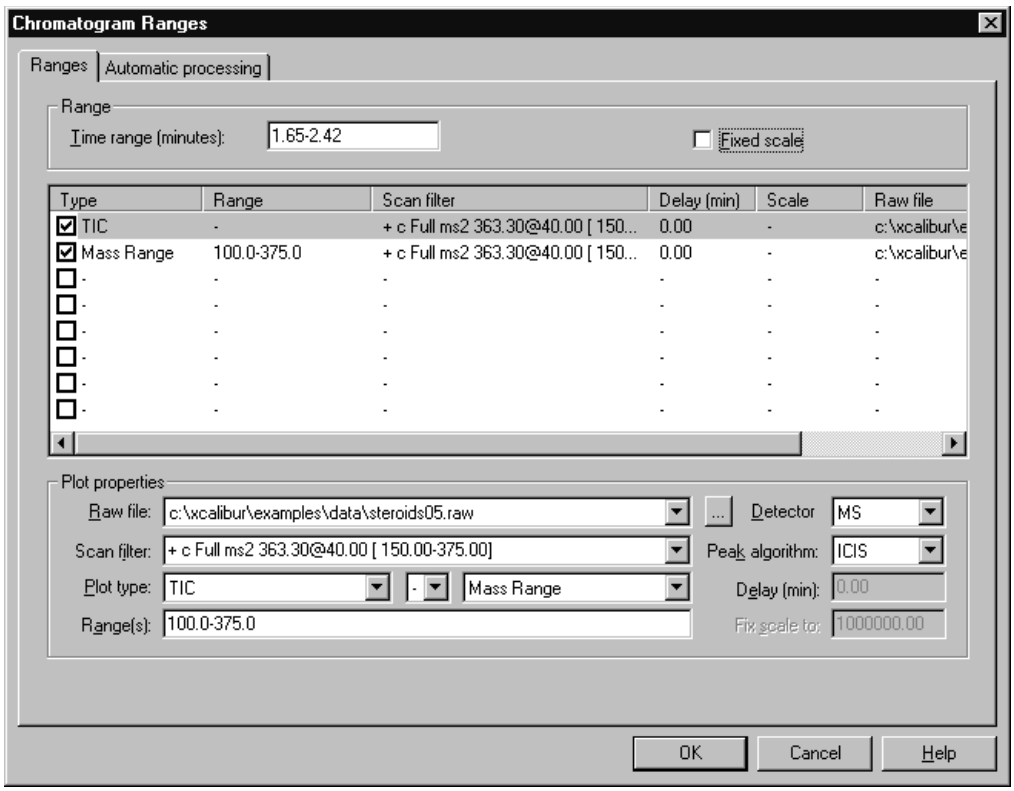
Adding Cells to the Display

You can display multiple cells in the Real Time display view.

❖ To display multiple chromatogram cells

1. Click the **Chromatogram** cell to make it the active cell with a gray border.
2. Choose **View > Ranges**. The Chromatogram Ranges dialog box opens.

   Figure 20. Chromatogram Ranges dialog box



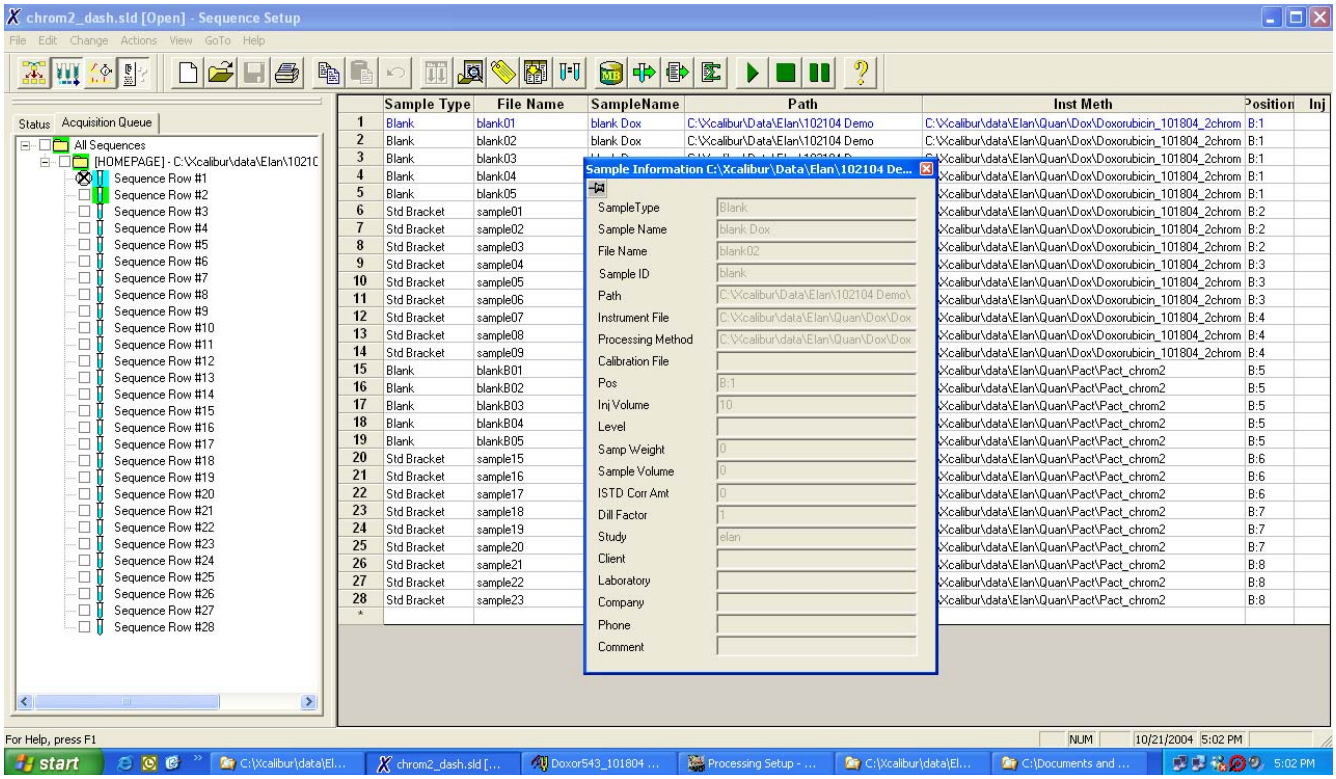
3. For each cell that you want to add, do the following:
   a. Select a Type check box.
   b. From the Detector list, select a detector.
   c. From the Plot Type list, select a plot type.
4. Click **OK** to close the Chromatogram Ranges dialog box.
5. Choose **View > Lock Display** to resume monitoring real-time data acquisition.

Using the Acquisition Queue

The Acquisition Queue (see Figure 21) shows all the sequences and samples submitted for analysis. The file tree view shows two levels of detail: the sequence names and, within each branch, the raw sample file names. Use the Acquisition Queue to do the following:

- Delete sequences unless they are currently being run.
- Delete samples within a sequence unless they have already been acquired, are currently undergoing acquisition, or are part of the quantitation bracket currently being acquired.

Figure 21. Acquisition Queue with the Sample Information window displayed



Manipulate entries in the acquisition queue:

- Right-click the name of the sequence or sample to open a shortcut menu. Choose **Properties** to display the Sample Information dialog box.
- Double-click a sequence to load it into Sequence Setup.
- Double-click a sample. The Sample Information dialog box opens.

A check box appears alongside each sequence and sample. Select one or more items for deletion. To delete a sample or sequence from the queue, select the check box and then press the DELETE key.

Deleted samples are identified by a large cross in the check box (⊠). The Xcalibur data system also adds the word DELETED after the sample or sequence identifier.

Sample Information Dialog Box

The Sample Information dialog box shows the parameters for all sequence fields. See "Acquiring Data" on page 23 for field descriptions.

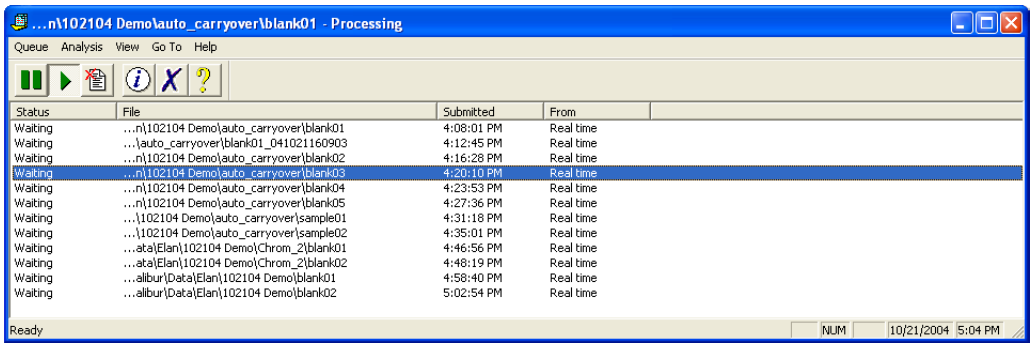
The Sample Information dialog box closes if you click anywhere outside it. Click the pin icon to keep it open. Click the close icon to close the dialog box or unpin the dialog box (by clicking the pin icon again) and click anywhere outside the dialog box before continuing.

The data system updates a pinned dialog box with the details of any selected sequence.

Managing Tasks

The Queue Manager, shown in Figure 22, provides additional functions for managing queued tasks. The Queue Manager is active whenever samples or sequences are queued for batch processing. If this window is not visible, it might be minimized on your computer toolbar.

Figure 22. Queue Manager window



Use the following procedures to manage the Xcalibur Processing Queue.

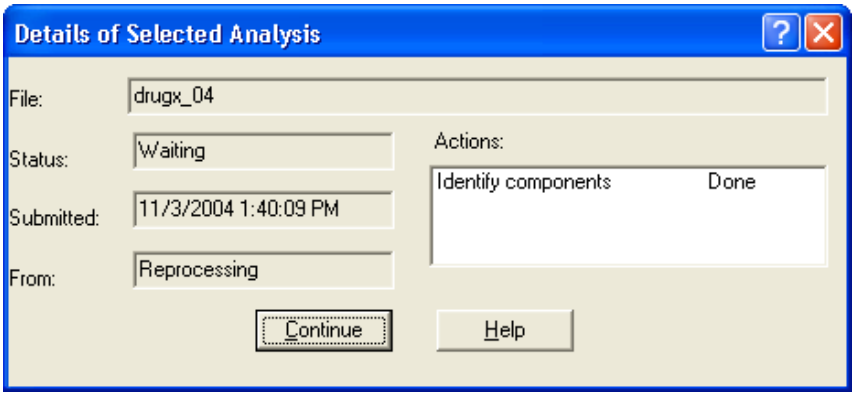
Pausing the Processing Queue	To temporarily pause the processing queue, click the **Pause** button or choose **Queue > Pause**.
Resuming the Processing Queue	To resume the processing queue when it is in the Pause mode, click the **Resume** button or choose **Queue > Resume**.
Updating the Display	To update the display with the latest information, choose **View > Refresh**.
Removing Tasks	To remove a task from the queue, select the task to be removed. Click the **Remove Job** button or choose **Analysis > Remove From Queue** from Queue. To remove all tasks from the queue, choose **Queue > Purge Queue**.

Viewing the Details of a Selected Analysis

To view the details of a selected analysis, select the required analysis in Queue Manager. Click the **Details** button in the toolbar or choose **Analysis > Details**.

The Details of Selected Analysis Dialog Box opens (see Figure 23).

Figure 23. Details of Selected Analysis dialog box



This dialog box contains the following readouts:

- The File readout displays the name of the data file.
- The Status readout displays the status of the queue.
- The Submitted readout displays the time and date that the processed job was submitted.
- The From readout displays the source of the processing job.
- The Actions display lists the tasks required to complete the selected processing job and their current status.

Preparing for Processing

Design a process to analyze your data using either Qual Browser or Quan Browser.

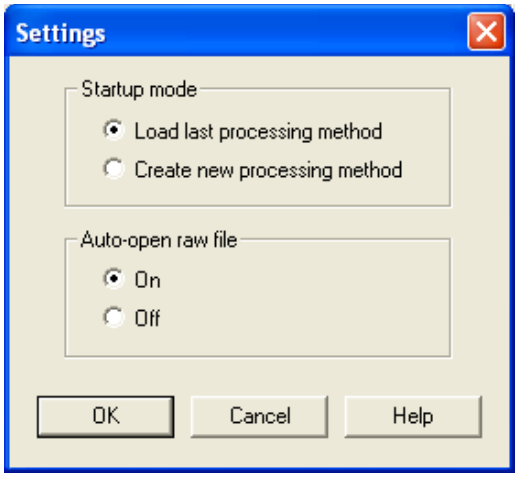
Contents

Setting Default Process Parameters

❖ **To select the default startup and autofile options in the Processing Setup view**

1. Choose **Options > Settings.** The Settings Dialog Box opens (see Figure 24)**.**

   Figure 24. Settings dialog box



2. Choose the Startup mode for Processing Setup.
   - To load the last used processing method at startup, select the **Load Last Processing Method** option.
   - To start each new session with a new processing method, select the **Create New Processing Method** option.
3. Choose from the Auto-Open Raw File options.
   - To open methods with the chromatogram and spectrum cells populated with their associated raw files, select the **On** option.
   - To open methods with the chromatogram and spectrum cells empty, select the **Off** option.
4. To save the new settings and close the dialog box, click **OK**.

Setting Quan Browser Process Parameters

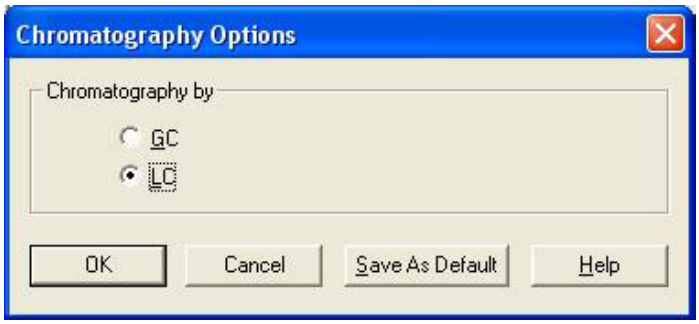
Select one of these procedures to view:

Changing Chromatography Detection Mode

❖ **To change the chromatography detection mode**

1. In the Quan view of Processing Setup, choose **Options > Chromatography By**. The Chromatography Options Dialog Box opens (see Figure 25).

   Figure 25. Chromatography Options dialog box

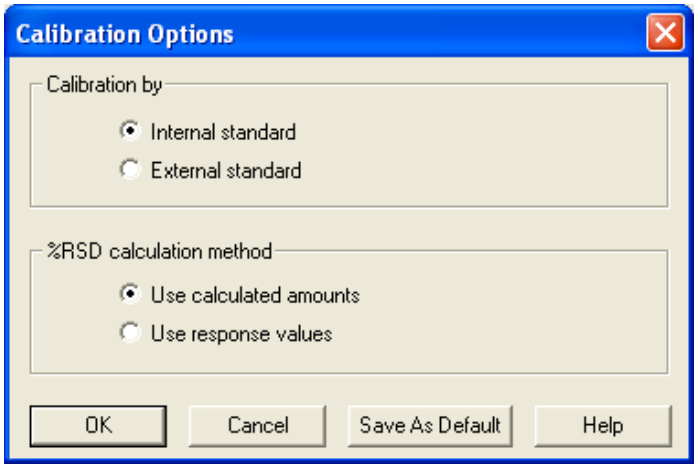
2. Select a detection mode:
   - To choose GC detection modes, including the Spectrum detection option, select the **GC** option.
   - To choose LC detection modes, select the **LC** option.
3. To save the new setting and close the dialog box, click **OK**.
4. To save the detection mode as the default option for new processing methods, click **Save As Default**.

Changing Calibration Mode

❖ To change the calibration mode

1. In the Quan view of Processing Setup, choose **Options > Calibration Options.** The Calibration Options Dialog Box opens (see Figure 26).

   Figure 26. Calibration Options dialog box

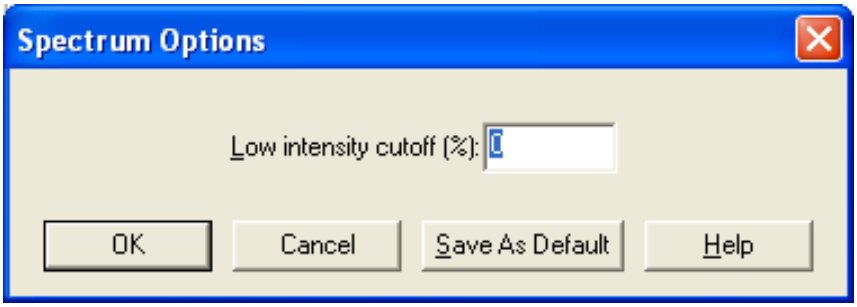
2. Select a calibration mode:
   - To choose internal standard calibration, select the **Internal Standard** option.
   - To choose external standard calibration, select the **External Standard** option.
3. To save the new setting and close the dialog box, click **OK**.
4. To save the calibration mode as the default option for new processing methods, click **Save As Default**.

Selecting Spectrum Detection Options

❖ To change the low intensity cutoff threshold for spectrum detection

1. In the Quan view of Processing Setup, choose **Options > Chromatography By**. The Calibration Options Dialog Box opens. Select the **GC** option and click **OK**.
2. Click the **Detection** tab within Quan view. In the Genesis Peak Detection area, select the **Spectrum** option, and then choose **Options > Spectrum**. The Spectrum Options Dialog Box opens (see Figure 27).

Figure 27. Spectrum Options dialog box



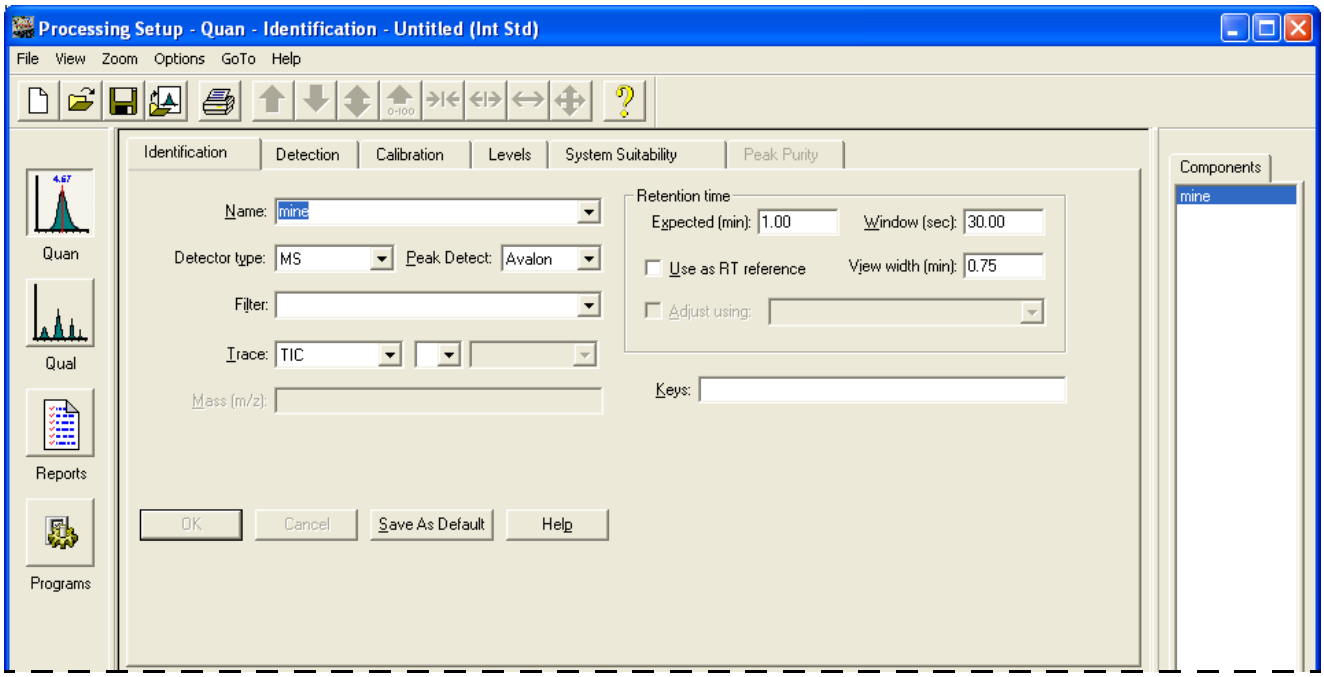
3. To enter a spectrum detection threshold, type a value in the Low Intensity Cutoff (%) box.
4. To save the new setting and close the dialog box, click **OK**.

Setting Quan View Identification Parameters

❖ To set identification parameters

1. From the Quan view of the Processing Setup window, select the **Identification** tab (see Figure 28).

Figure 28. Identification page for Quan view



2. In the Name box, type or select a component name for the new processing method. For example, type **sample01**.
3. From the Detector Type list, select the detector type: **MS**, **Analog**, **A/D card**, **PDA**, or **UV**.
4. From the Peak Detect list, select a peak detection algorithm: **Genesis**, **ICIS**, or **Avalon**.
5. If you selected MS as a detector type, select or type the name of a scan filter for the selected component in the Filter box.
6. Select a Trace type or Trace combination in the three Trace lists.
   a. Select a Trace type from the first Trace list.
   b. To use a Trace type combination, select an operator (+ or –) in the second Trace list.
   c. Select the second Trace type in the third list.
7. If needed, type the mass range or wavelength range of the selected component in the Mass or Wavelength box.
8. Type a text comment in the Keys box.
9. In the Retention Time area, type the expected retention time of the selected component in the Expected (min) box.
10. Type the allowable time deviation for the expected retention time (the window for the retention time) in the Window (sec) box.
11. Specify whether the retention time of the selected component is to be used as a reference time for other components:
    - To use the selected component for a retention time reference, select the **Use As RT Reference** check box.
    - To adjust the expected retention time of the selected component by using a retention time reference, use the Adjust Using box to select a reference.
12. To apply the changes you made to the Identification Page for Quan View, click **OK**. The window remains open and the other tabs become available.

Selecting Advanced Detection Options

❖ **To select advanced detection options**

1. From the Quan view of the Processing Setup window, select the **Identification** tab.
2. From the Peak Detect list, select a peak detection algorithm, either **Genesis**, **ICIS**, or **Avalon**. Then click **OK**.
3. Click the **Detection** tab.

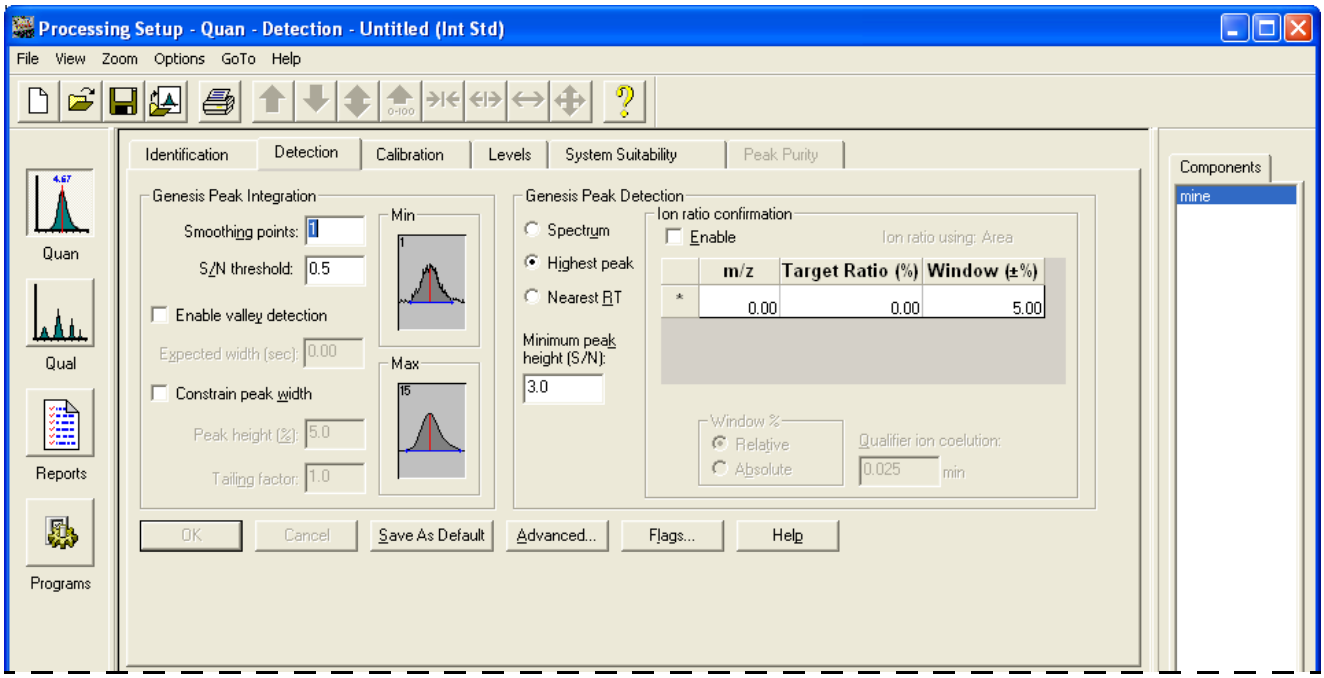
4. To specify the advanced parameters for the selected algorithm, on the Detection page click **Advanced**. One of these dialog boxes appears:
   - Genesis Advanced Chromatogram Options Dialog Box
   - ICIS Advanced Parameters Dialog Box
   - Avalon Event List Dialog Box
5. Specify the parameters for the currently selected algorithm.
6. To save the new settings and close the dialog box, click **OK**.

Setting Genesis Detection Parameters

❖ **To set Genesis detection parameters for a component**

1. On the Identification Page for Quan View in the Processing Setup window, make sure the Peak Detect type is **Genesis**. Click **OK**.
2. Select the **Detection** tab. The Genesis Detection Page for Quan View appears (see Figure 29).

Figure 29. Genesis Detection page for Quan view



3. To enter the smoothing level that the Xcalibur data system applies to the chromatogram prior to peak integration, type a value in the Smoothing Points box in the Genesis Peak Integration area.
4. To enter a signal-to-noise ratio threshold value, type a value in the S/N Threshold box. The application does not integrate peaks with a signal-to-noise ratio less than this value, but it integrates peaks with a signal-to-noise ratio greater than this value.

5. To approximate the start and end points of unresolved peaks, select the **Enable Valley Detection** check box and type a value for the minimum width of the peak in the Expected Width (sec) box.
6. To apply peak height and tailing factor integration criteria, select the **Constrain Peak Width** check box. Type the start integration threshold in the Peak Height (%) box and type the stop integration criteria in the Tailing Factor box.
7. To specify peak detection criteria, select one of the following component identification options:
   - To use a reference spectrum in GC mode only, select the **Spectrum** option.
   - To choose the highest peak in the chromatogram, select the **Highest Peak** option.

     For GC mode only, to use Ion ratio confirmation, select the **Enable** check box in the Ion Ratio Confirmation area.
   - To use the peak with the nearest retention time, select the **Nearest RT** option.

     For GC mode only, to choose Ion ratio confirmation, select the **Enable** check box in the Ion Ratio Confirmation area.
8. To enter a signal-to-noise ratio threshold, type a value in the Minimum Peak Height (S/N) box. The application ignores all chromatogram peaks that have a signal-to-noise value less than this parameter value.
9. To save the new settings and close the dialog box, click **OK**.

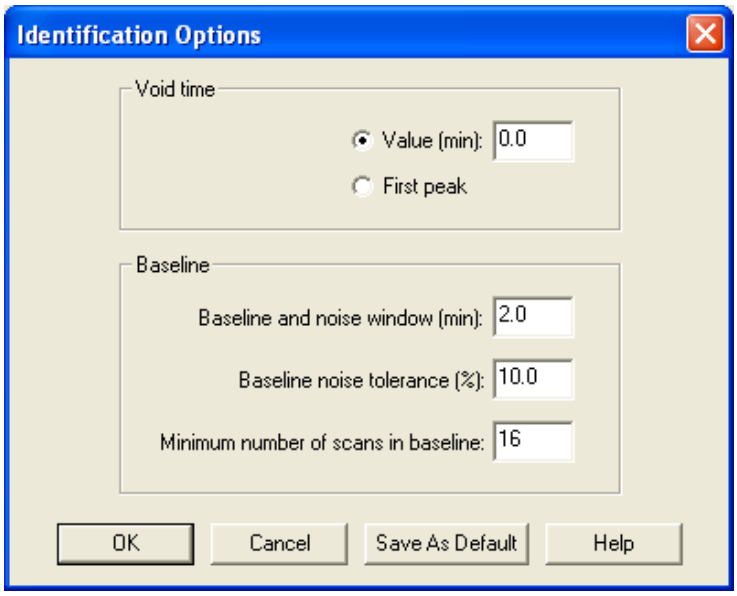
Setting Identification Option Parameters

Use the Identification Options dialog box to set options for Genesis detection.

❖ To select Identification options

1. To display the Identification Options Dialog Box, choose **Options > Identification** (see Figure 30) from either the Quan view or the Qual view of the Processing Setup window.

   Figure 30. Identification Options dialog box



2. To set a void time, select the **Value (min)** option to set an absolute value. Type the void time in the associated box.

   Select the **First Peak** option if you want the data system to use the retention time of the first peak as the void time.

3. To adjust the Baseline parameters, use the Baseline and Noise Window box to enter a new value for the baseline and noise window parameter.

   - Use the Baseline Noise Tolerance % box to enter a new value for the baseline and noise tolerance.
   - Use the Minimum Number of Scans in Baseline box to enter a new value for the minimum number of scans in baseline parameter.

4. To save your settings, click **OK**.

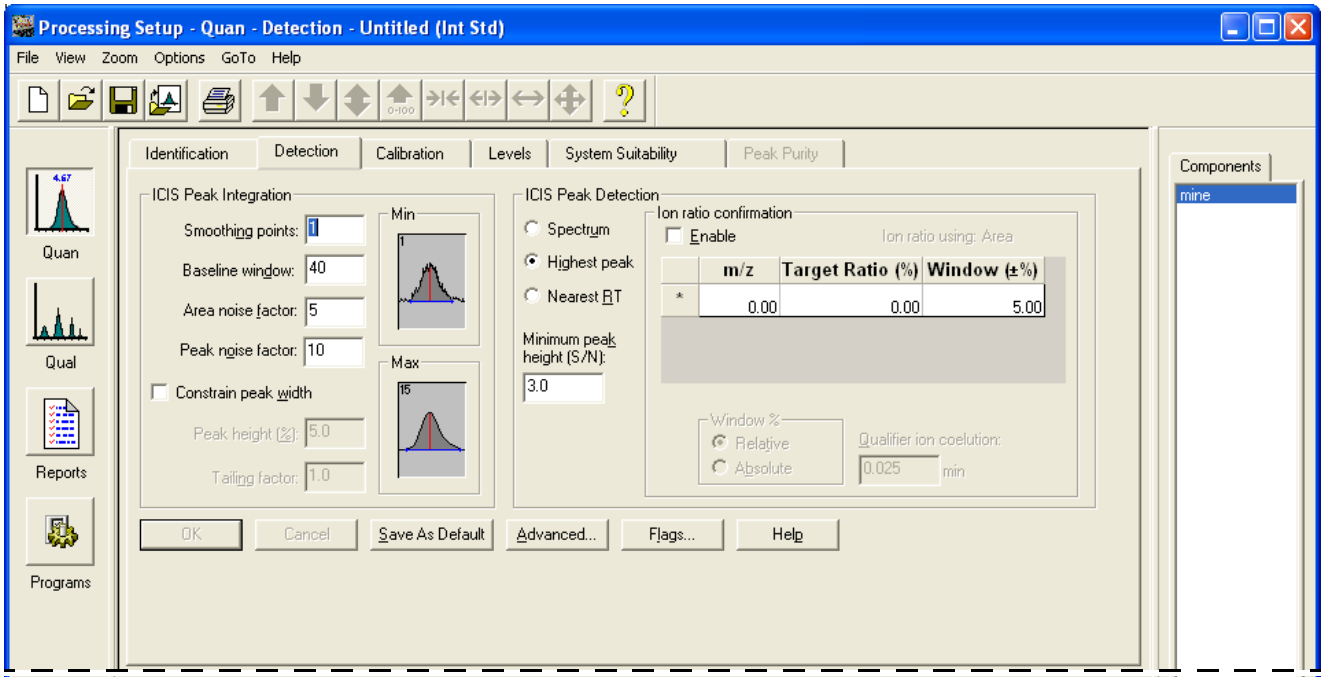
5. To save the new values as the default identification parameters, click **Save As Default**.

Setting ICIS Detection Parameters

❖ To set ICIS detection parameters for a component

1. On the Identification Page for Quan View in the Processing Setup window, make sure the Peak Detect type is **ICIS**. Click **OK**.
2. Select the **Detection** tab. The ICIS Detection Page for Quan View appears.

Figure 31. ICIS Detection page for Quan view



3. To set the smoothing level that the application applies to the chromatogram prior to peak integration, type a value in the Smoothing Points box in the ICIS Peak Integration area.
4. To set the baseline window parameter, type a value in the Baseline Window box.
5. To set the area noise factor, type a value in the Area Noise Factor box.
6. To set the peak noise factor, type a value in the Peak Noise Factor box.
7. To apply peak height and tailing factor integration criteria, select the **Constrain Peak Width** check box.
   - To enter the start integration threshold, type a value in the Peak Height (%) box.
   - To enter the stop integration criteria, type a value in the Tailing Factor box.

8. To specify peak detection criteria, select one of the following component identification options:
   - To choose a reference spectrum in GC mode only, select the **Spectrum** option.
   - To use the highest peak in the chromatogram, select the **Highest Peak** option.

     For GC mode only, to use Ion Ratio Confirmation, select the **Enable** check box in the Ion Ratio Confirmation area.
   - To use the peak with the nearest retention time, select the **Nearest RT** option.

     For GC mode only, to use Ion Ratio Confirmation, select the **Enable** check box in the Ion Ratio Confirmation area.
9. To save the new settings and close the dialog box, click **OK**.

Setting Avalon Detection Parameters

❖ To set the Avalon detection parameters for a component

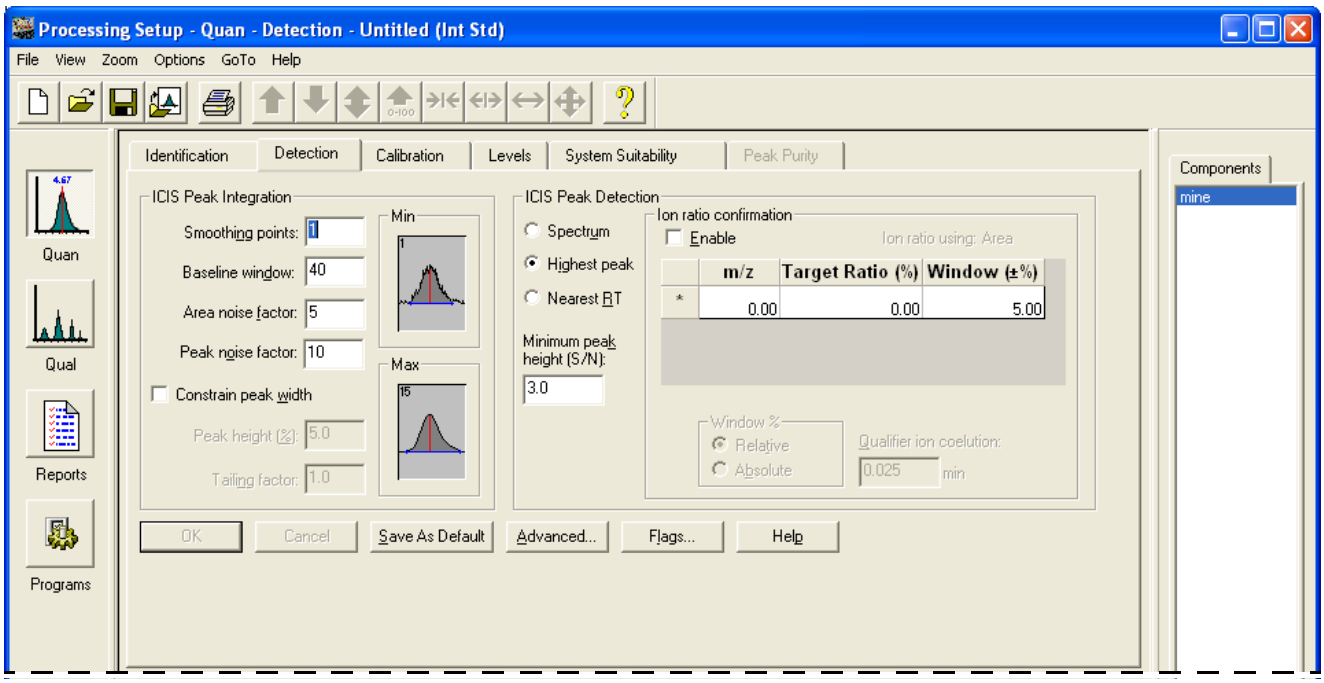
1. On the Identification Page for Quan View in the Processing Setup window, make sure the Peak Detect type is **Avalon**. Click **OK**.
2. Select the **Detection** tab. The Avalon Detection Page for Quan View appears.
3. To enter the smoothing level that the application applies to the chromatogram prior to peak integration, type a value in the Smoothing Points box in the Avalon Peak Integration area.
4. Click the **Advanced** button. The Avalon Event List dialog box opens.
5. To edit the Event list, highlight the row you want to change, one row at a time, and enter the revised settings in the boxes. Click **Change**.
6. To save the new settings and close the dialog box, click **Exit**.

Setting Data Flags

❖ To select data flag settings

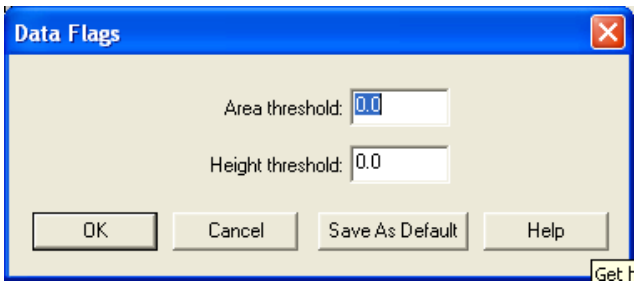
1. To open the Detection Page for Quan View, select the **Detection** tab (see Figure 32) from the Quan view of the Processing Setup window.

Figure 32. Detection page for Quan view



2. To open the Data Flags dialog box, click **Flags** in the Processing Setup window (see Figure 33).

Figure 33. Data Flags dialog box



3. To set the threshold value for the Area Threshold flag, type a value in the Area Threshold box.

4. To set the threshold value for the Height Threshold flag, type a value in the Height Threshold box.

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

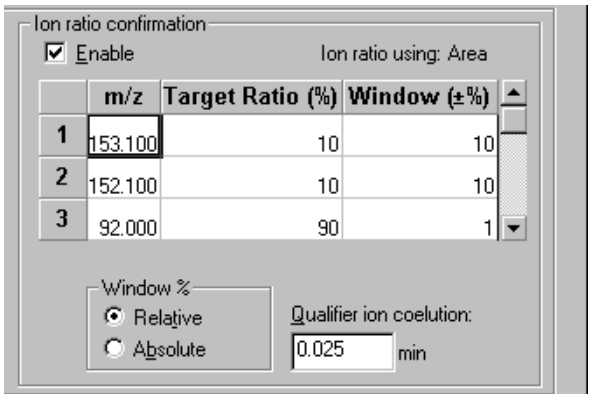
Setting Ion Ratio Confirmation

This supplementary procedure for setting detection parameters applies only to the Xcalibur GC detection mode.

❖ To set up ion ratio confirmation for a component

1. In the Quan view of the Processing Setup window, select the **Detection** tab.
2. Select the **Highest Peak** option or the **Nearest RT** option in the Peak Detection area.
3. To turn on Ion Ratio Confirmation, select the **Enable** check box in the Ion Ratio Confirmation area (see Figure 34).

   Figure 34. Ion ratio confirmation area

4. To enter details of the qualifier ions for the current component,

   - Select an *m/z* box and type the value for an ion characteristic of the component.
   - Select the Target Ratio (%) box and type a value for the target ratio.
   - Select the Window (± %) box and type a value for the relative intensity of the ion.

     Repeat this procedure for all the ions (up to a maximum of 5). A context menu is available for you to insert, delete, clear, or move rows in the table.

   To insert a row, click the row number above the position. Right-click and select **Insert Row** from the shortcut menu.

   To delete a row, click the row number of the row to delete. Right-click and select **Delete Rows** from the shortcut menu, or press DELETE. You can delete a range of rows by dragging the cursor from the first to the final row in the selected range. Then right-click and select **Delete Rows**.

5. Set the Window% mode:

   - To use the target ratio tolerances in the Window ± % column as absolute percentages of the target ratio, select the **Absolute** option.
   - To use the target ratio tolerances in the Window ± % column as relative percentages of the target ratio, select the **Relative** option.

6. To set a value in minutes for the qualifier ion coelution window, type a value in the Qualifier Ion Coelution box.
7. To save your settings, click **OK**.

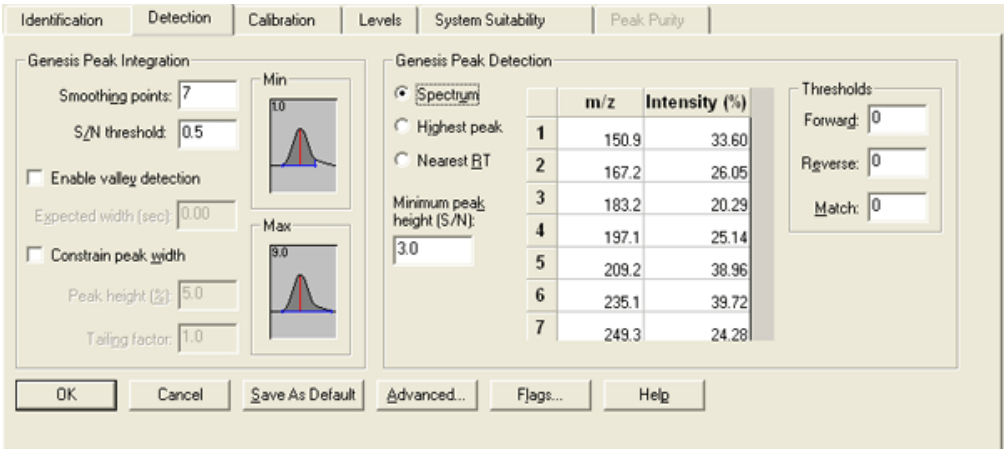
Setting Spectrum Detection Parameters

This supplementary procedure for setting detection parameters applies only to the Xcalibur GC detection mode.

❖ To select spectrum detection options for a component

1. From the Quan view of the Processing Setup window, select **Options > Chromatography By**.
2. Click **GC**.
3. Select the **Detection** tab (see Figure 29).
4. To display spectrum options in the Peak Detection area, select the **Spectrum** option.
5. To enter mass/charge [*m/z*] and intensity data for up to 50 spectrum peaks, type data in the Spectrum peak identification table.

Figure 35. Spectrum peak identification table



You can do this manually or use a raw file containing good quality spectral data for the component.

To enter data manually:

- Select an *m/z* Table cell and type the value for an ion characteristic of the component.
- Select the Intensity (%) Table cell and type a value for the relative intensity of the ion.

  Repeat this procedure for all the ions in the reference spectrum (up to a maximum of 50). Right-click a row to display a menu where you can insert, delete, clear, or move rows in the table.

To insert a row, click the row number above the position. Right-click and select **Insert Row** from the shortcut menu.

To delete a row, click the row number of the row to delete. Right-click and select **Delete Rows** from the shortcut menu, or press DELETE. You can delete a range of rows by dragging the cursor from the first to the final row in the selected range. Then right-click and select **Delete Rows**.

To enter data using an open raw file:

- Pin the Spectrum preview.
- Drag the cursor across the appropriate component peak in the Chromatogram preview. The data system displays the spectrum from the scan closest to the peak apex in the Spectrum cell.
- Drag the cursor across the required Spectrum range. The application copies the ion *m/z* and intensity values to the peak identification table. It discards any ions with intensities below the Low Intensity Cutoff % parameter in the Spectrum Options Dialog Box. To adjust this parameter, select **Options > Spectrum**.

6. To select threshold values for spectrum matching in the Thresholds area, choose one of these options.
   - Type a forward search threshold in the Forward box.
   - Type a reverse search threshold in the Reverse box.
   - Type a match search threshold in the Match box.
7. To save your settings, click **OK**.

Setting Standard Dilution Parameters

❖ To create calibration levels for target components

1. From the Quan view of the Processing Setup window, select the **Levels** tab. The Levels Page for Quan View opens.
2. Choose **Options > Standard Dilution**. The Standard Dilution Dialog Box opens.
3. Enter the base amount for each component in the Amount boxes in the Base Amounts table.
4. Enter information in the Dilution Factors table:
   - Enter calibration levels in the Cal Level boxes.
   - Enter the amount of dilution factor at each calibration level in the Dilution boxes.
5. To save the new settings and close the dialog box, click **OK**. The Xcalibur data system uses the parameters to calculate calibration levels for all the target components defined in the method.

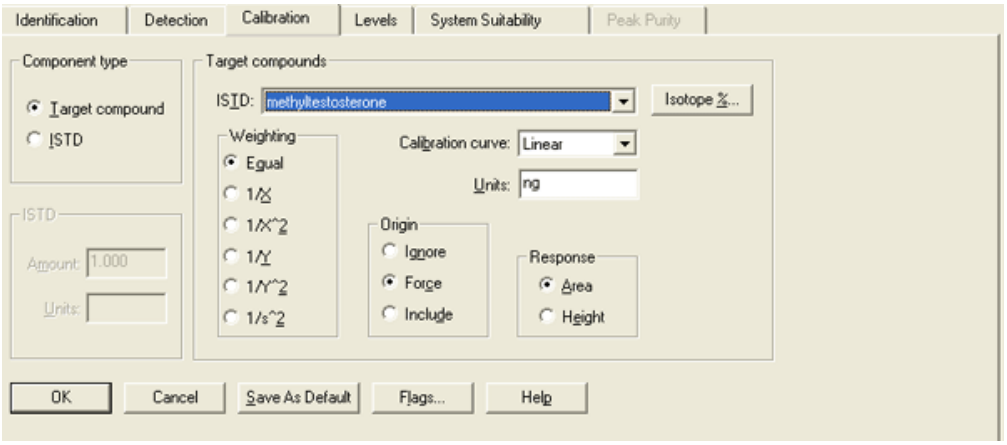
Setting Calibration Parameters

❖ To set calibration parameters

1. From the Quan view of the Processing Setup window, select the **Calibration** tab. The Calibration Page for Quan View opens.
2. To select a component, click a component name from the Component list on the right side of the Processing Setup window.
3. To define the type of the selected component, select the **Target Compound** option or the **ISTD** option.
   - If you select the Target Compound option, the Target Compounds area becomes active. Go to Step 4.
   - If you select the ISTD option, the ISTD area becomes active. Go to Step 10.

   Note When creating an internal standard method, you must assign an internal standard to at least one component before you can assign target compounds to any other components.
4. To select an internal standard (ISTD) for the calibration, select from the ISTD list.

   Figure 36. Target compounds area



   To correct for isotope contributions, click **Isotope %**. The Correction for Isotope Contribution dialog box opens. See "Correcting for Calibration Impurities" on page 61 for information about entering values into this box.
5. To select a locally weighted calibration curve type, select from the Calibration Curve list. If you select **Linear** or **Quadratic**, the Weighting area becomes active. Go to Step 6.

   If you select any of the other curve types, the Weighting area is not active. Go to Step 7.
6. To apply the correct regression weighting method when the data system calculates the least-squares regression calibration curve, select the **Equal**, **1/X**, **1/X^2**, **1/Y**, **1/Y^2**, or **1/s^2** option.

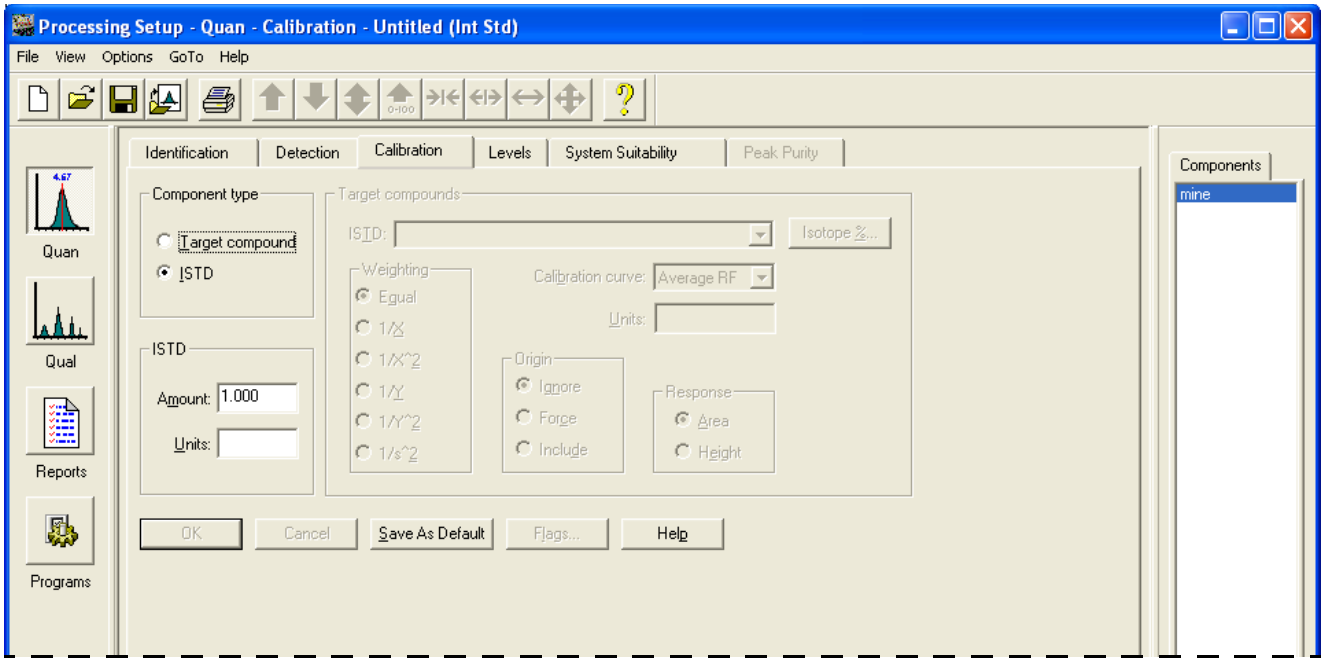
7. To select how to treat the origin in the calibration curve calculation:
   - Select the **Ignore** option to exclude the origin from the calibration curve calculation.
   - Select the **Force** option to require that the calibration curve passes through the origin.
   - Select the **Include** option to include the origin as one data point.
8. To select the units to be displayed on graphs and reports, type the required units in the Units box.
9. In the Response area, define the basis for the quantitation:
   - To quantitate based on the integrated area of component peaks, select the **Area** option. Go to step 10.
   - To quantitate based on the calculated height of component peaks, select the **Height** option. Go to step 10.
10. Select internal standard settings:
    - To specify the amount of the internal standard injected into each sample, type a value in the Amount box.
    - To specify the units of the internal standard injected into each sample, type a value in the Units box.
11. Repeat this procedure for all components.

Setting Calibration and Quantitation Flags

❖ To set calibration and quantitation flags

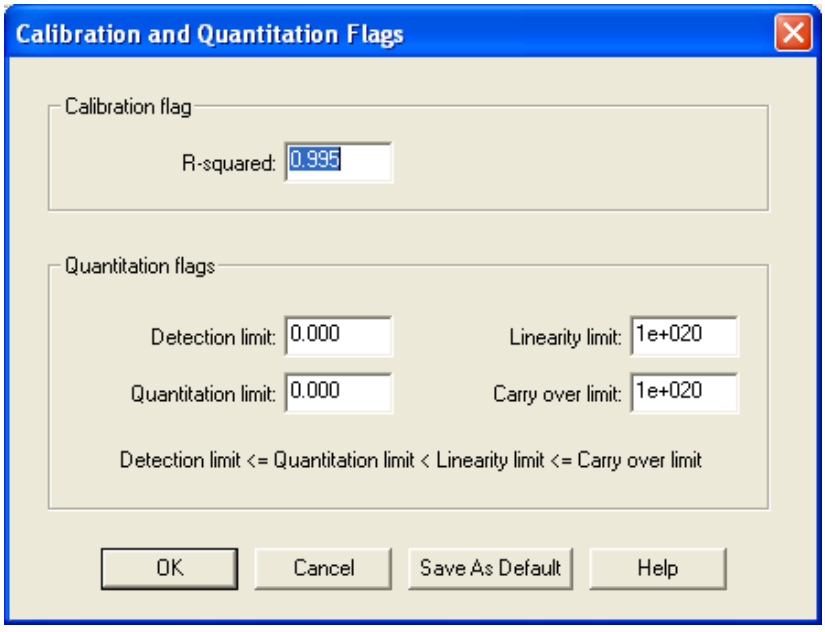
1. From the Quan view of the Processing Setup window, select the **Calibration** tab (see Figure 37). The Calibration Page for Quan View opens.

Figure 37. Calibration page for Quan view



2. Click **Flags**. The Calibration and Quantitation Flags Dialog Box opens (see Figure 38).

Figure 38. Calibration and Quantitation Flags dialog box



3. To specify a calibration flag threshold, adjusting the R-squared flag threshold value, type a value in the R-squared box.
4. Specify quantitation flag threshold values:
   - To adjust the detection limit flag threshold value, type a value in the Detection Limit box.
   - To adjust the linearity limit flag threshold value, type a value in the Linearity Limit box.
   - To adjust the quantitation limit flag threshold value, type a value in the Quantitation Limit box.
   - To adjust the carry over limit flag threshold value, type a value in the Carry Over Limit box.
5. To save the new settings and close the dialog box, click **OK**.

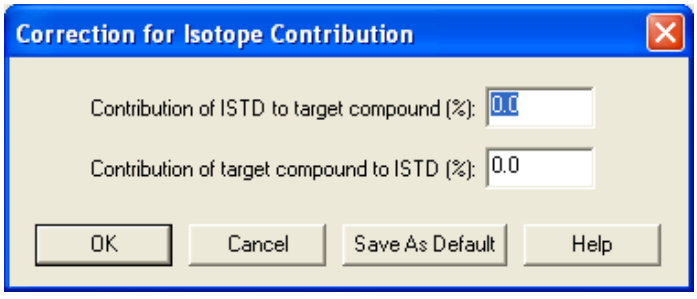
Correcting for Calibration Impurities

Use the Correction for Isotope Contribution dialog box to correct for an impurity in the internal standard reagent ISTD [impurity] that elutes at the same time as the target molecule [TM] or correct for an impurity in the target molecule reagent TM [impurity] that elutes at the same time as the internal standard [ISTD].

❖ To correct for calibration impurities

1. From the Quan view of the Processing Setup window, select the **Calibration** tab (see Figure 37). The Calibration Page for Quan View opens.
2. Click **Isotope %**. The Correction for Isotope Contribution Dialog Box opens (see Figure 39).

Figure 39. Correction for Isotope Contribution dialog box



- If you have an impurity in your internal standard that elutes at the same time as the target molecule, type the ISTD [impurity] / ISTD [pure] ratio in the Contribution of ISTD to Target Compound (%) box.

  To determine this ratio experimentally, analyze the ISTD reagent using the method for quantitation of the target compound. Use the respective peak areas or heights to determine the ratio of impurity [peak at retention time of TM] to pure compound [peak at retention time of ISTD]: ISTD [impurity] / ISTD [pure].

- If you have an impurity in your target molecule reagent that elutes at the same time as the ISTD molecule, type the TM [impurity] / TM [pure] ratio in the Contribution of Target Compound to ISTD (%) box.

  To determine this ratio experimentally, analyze the TM reagent using the method for quantitation of the target compound. Use the respective peak areas or heights to determine the ratio of impurity [peak at the retention time of ISTD] to pure compound [peak at retention time of TM]: TM [impurity] / TM [pure].

  Using the data you provide in Steps 1 and 2, The data system corrects for the ISTD [impurity] or TM [impurity] and reports the corrected amounts of ISTD and TM.

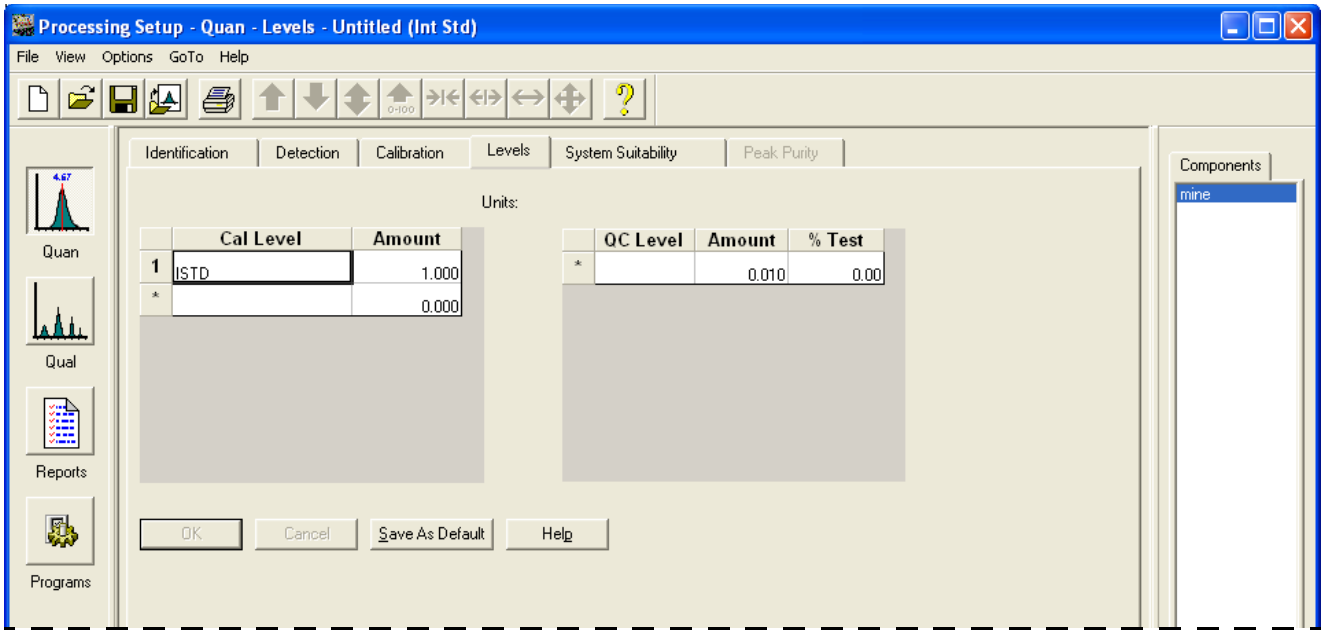
3. To save the new settings and close the dialog box, click **OK**.

Setting Levels Parameters

❖ To set calibration and QC level parameters for a component

1. From the Quan view of the Processing Setup window, select the **Levels** tab (see Figure 40) The Levels Page for Quan View opens.

Figure 40. Levels page for Quan view



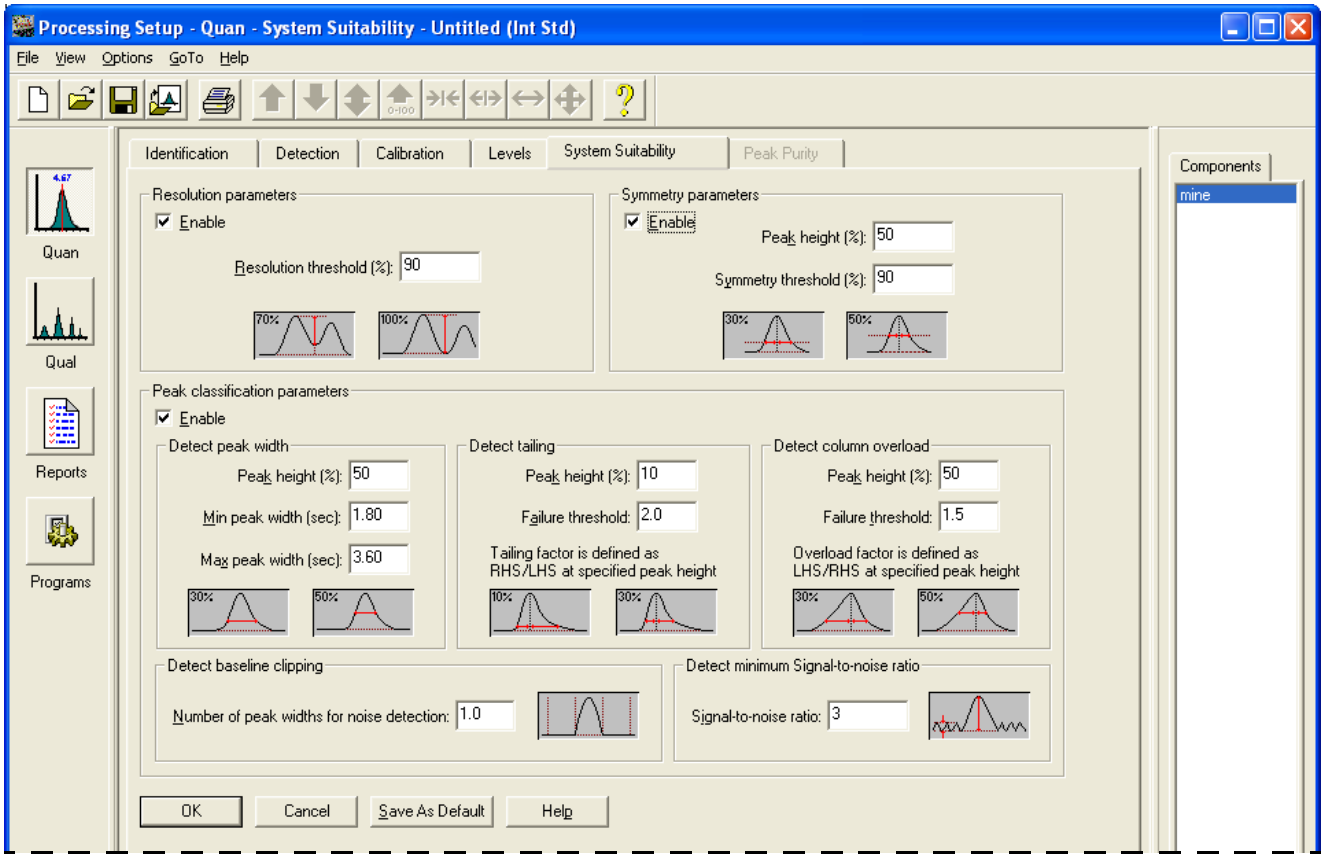
2. To select a component, click a target component in the Component list on the right side of the Processing Setup window. The Levels page is not available for ISTD components.
3. To set calibration levels for all components, use the Standard Dilution Dialog Box. The data system uses the values to calculate the Calibration Levels table for each component or you can type the parameters manually in the Calibration Levels table:
   - To enter calibration levels, type values in the Cal Level boxes.
   - To enter the amount of internal standard added at each level, type values in the Amount boxes.
4. If the component is a target, enter quality control level data in the QC Levels table:
   - To enter quality control levels, type values in the QC Level boxes.
   - To enter the amount of internal standard added at each level, type values in the Amount boxes.
   - To enter the percent tested at each quality control level, type values in the % Test boxes.
5. Repeat the procedure for each target component.
6. To save your settings, click **OK**.

Setting System Suitability Parameters

❖ **To set system suitability parameters**

1. From the Quan view of the Processing Setup window, select the **System Suitability** tab (see Figure 41). The System Suitability Page for Quan View opens.

Figure 41. System Suitability page for Quan view



2. To perform resolution testing, select the **Enable** check box in the Resolution Parameters area and type a threshold for peak resolution in the Resolution Threshold (%) box.

3. To perform symmetry testing, select the **Enable** check box in the Symmetry Parameters area. Type a peak height for symmetry testing in the Peak Height (%) box and type a threshold for symmetry testing in the Symmetry Threshold (%) box.

4. To carry out classification tests, select the **Enable** check box in the Peak Classification Parameters area. Then set the following parameters:

   a. To adjust Xcalibur peak width testing thresholds, type parameters in the Detect Peak Width area.

      - To enter a peak height for the test, type a value in the Peak Height box.
      - To enter a minimum peak width threshold, type a value in the Min Peak Width (sec) box.

- To enter a maximum peak width threshold, type a value in the Max Peak Width (sec) box.

b. To adjust the Xcalibur peak tailing test, type parameters in the Detect Tailing area.

- To enter a peak height for the test, type a value in the Peak Height (%) box.
- To enter a threshold limit for peak tailing, type a value in the Failure Threshold box.

c. To adjust the Xcalibur column overload test, type parameters in the Detect Column Overload area.

- To enter a peak height for the test, type a value in the Peak Height (%) box.
- To enter a threshold limit for peak tailing, type a value in the Failure Threshold box.

d. To adjust the Xcalibur baseline clipping test, type parameters in the Detect Baseline Clipping area and the Detect Minimum Signal-to-Noise Ratio area.

- To define the test window, type a value in the Number of Peak Widths for Noise Detection box.
- To define the Signal-to-Noise Threshold, type a value in the Signal-to-Noise Ratio box.

5. To save your settings, click **OK**.

Setting Qual Browser Process Parameters

Set parameters using these procedures:

- Setting Qual View Identification Parameters
- Selecting Advanced Chromatogram Options
- Setting Combine Option Parameters for Spectrum Enhancement
- Setting Refine Option Parameters for Spectrum Enhancement
- Setting Threshold Option Parameters for Spectrum Enhancement
- Changing Chromatography Detection Mode
- Changing Calibration Mode
- Selecting Spectrum Detection Options

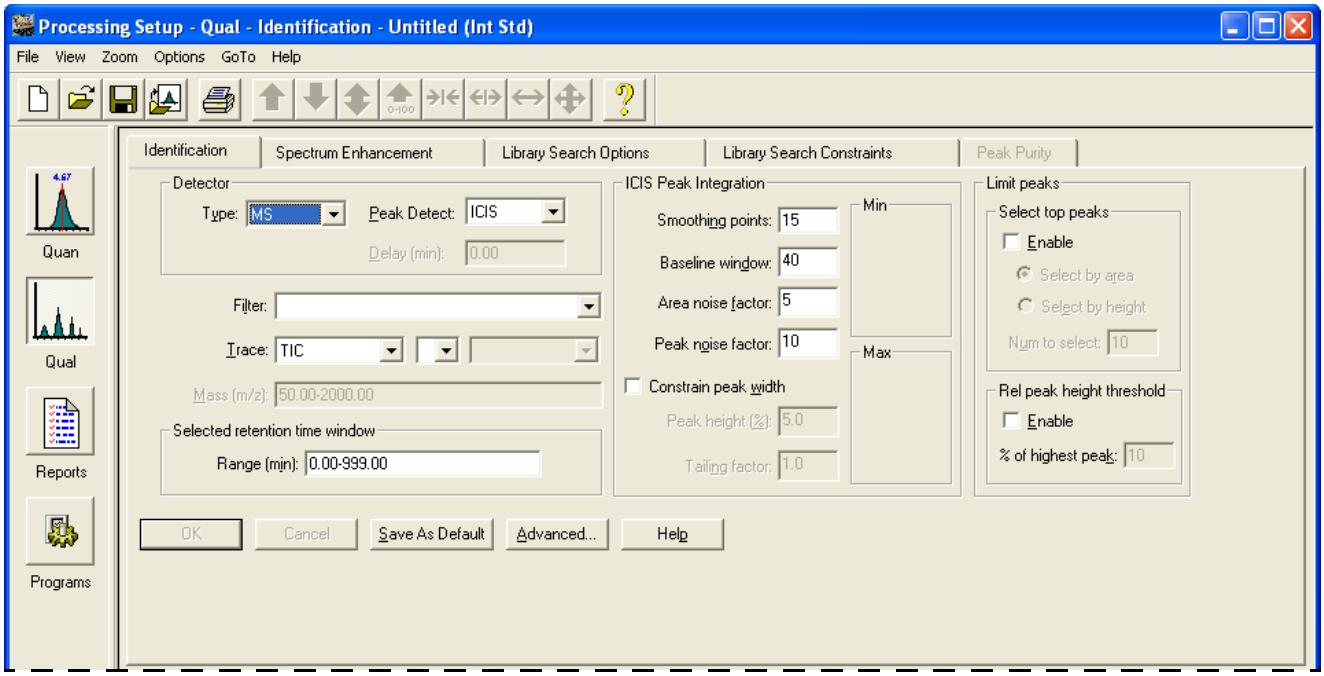
Refer to the *Creating and Searching Libraries User Guide* for more information about using libraries to search for spectra.

Setting Qual View Identification Parameters

❖ To set Qual view identification parameters

1. From the Qual view of the Processing Setup window, select the **Identification** tab to display the Identification page for Qual view (see Figure 42) and open a raw data file.

Figure 42. Identification page for Qual view



2. Choose **File > Open Raw File** from the menu bar. The Open Raw File dialog box opens.
3. Select a raw file to analyze.
4. In the Detector area, select a detector from the Type list. Valid detector types are MS, Analog, A/D Card, PDA, or UV.

   If you select a non-MS trace type, type the time difference in minutes between MS and non-MS detection in the Delay box to synchronize the data with the MS detector.
5. To select an algorithm that the data system can use to identify and integrate peaks, use the Peak Detect list. Choose from among the Avalon peak detection algorithms.
6. Select a Trace type or Trace combination in the three Trace lists:
   - Select a Trace type from the first Trace list box.
   - To use a Trace type combination, select an operator (+ or –) in the second Trace list box and then select the second Trace type in the third list box.
7. To select or enter a scan filter for an MS trace type, type or select the name of the filter to be used for the selected component in the Filter box.

8. To enter the mass range (or wavelength range for non-MS detectors) for the chromatogram, type the mass or mass ranges or wavelength or wavelength ranges in the Mass or Wavelength boxes.
9. Specify a selected retention time window or time range to limit qualitative processing of the chromatogram:
   - Type the time range in the Range box (for example, 0.30–1.55).
   - Use a representative raw file and have the data system calculate an effective window from the relevant peak. To do this:
     i. Select a representative raw file in the Open Raw File dialog box (choose **File > Open Raw File**).
     ii. To bring up the spectrum preview, click  .
     iii. Drag the cursor horizontally across the peak in the chromatogram preview. The application updates the Range (min) box with a time span centered on the apex of the dragged peak.
10. Select from among these peak integration options:

Peak detect	Peak integration options
Genesis	In the Smoothing Points box, type the number for the amount of smoothing that the data system applies before integration. The value must be odd and between 3 (minimum smoothing) and 15 (maximum smoothing).
	Type the signal-to-noise threshold value in the S/N Threshold box.
	Select or clear the **Enable Valley Detection** check box and, if selected, enter the value in seconds in the Expected Width box.
	To constrain the peak width, select the **Constrain Peak Width** check box and type a value in the Tailing Factor box.
	To change the advanced detection parameters if required, click **Advanced**. The Genesis Advanced Chromatogram Options Dialog Box opens.

Peak detect	Peak integration options
ICIS	In the Smoothing Points box, type the number of points used for a moving average.
	In the Baseline Window box, type the number of scans to scan for a local minima.
	In the Area Noise Factor box, type the noise level multiplier used to determine the peak edge after the location of a possible peak.
	In the Peak Noise Factor box, type the noise level multiplier used to determine the potential peak signal threshold.
	To change the advanced detection parameters, click **Advanced** in the ICIS Advanced Parameters Dialog Box.
Avalon	In the Smoothing Points box, type the number for the amount of smoothing that the data system applies before integration. The value must be odd and between 3 (minimum smoothing) and 15 (maximum smoothing). To display initial peak detection settings in the Avalon Peak Integration area, click **Auto Calc Initial Events**.
	To edit the peak detection settings in the Event list, click **Advanced**. The Avalon Event List Dialog Box opens.
	Make changes to the Event list and click **Change** to apply them automatically to the chromatogram plot and to the Event list on the Identification page.
	After editing the peak detection settings, click **Exit** to close the dialog box and return to the Identification page.

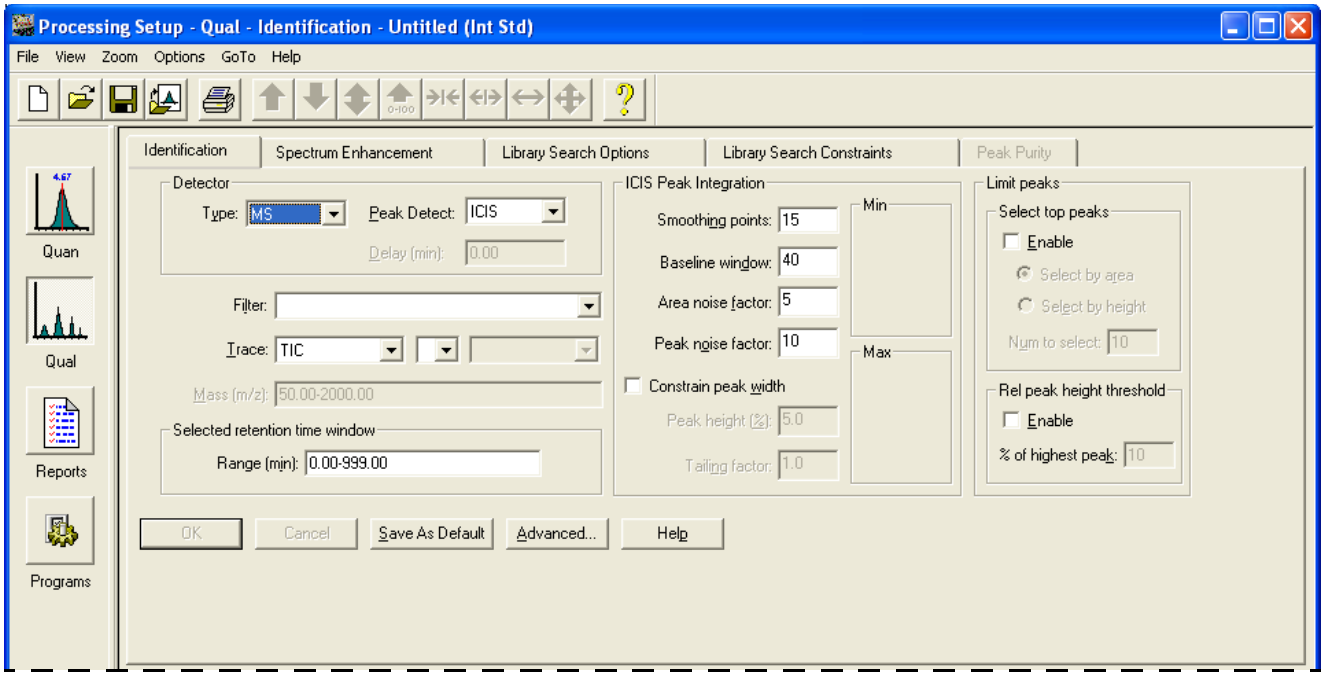
11. To reduce the number of chromatogram peaks submitted for further processing, select from the options under Limit Peaks:
    a. In the Select Top Peaks area, select the **Enable** check box.
        - To restrict processing to the most significant peaks based on area, select the **By Area** option.
        - To restrict processing to the most significant peaks based on height, select the **By Height** option.
        - Type the maximum number of peaks to be processed in the Num to Select box.
    b. In the Rel Peak Height Threshold area, select the **Enable** check box and enter the peak height threshold in the Percent of Highest Peak box.
12. To save your settings, click **OK**.

Selecting Advanced Chromatogram Options

❖ **To select advanced chromatogram options**

1. From the Qual view of the Processing Setup window, select the **Identification** tab (see Figure 43).

Figure 43. Identification page for Qual view



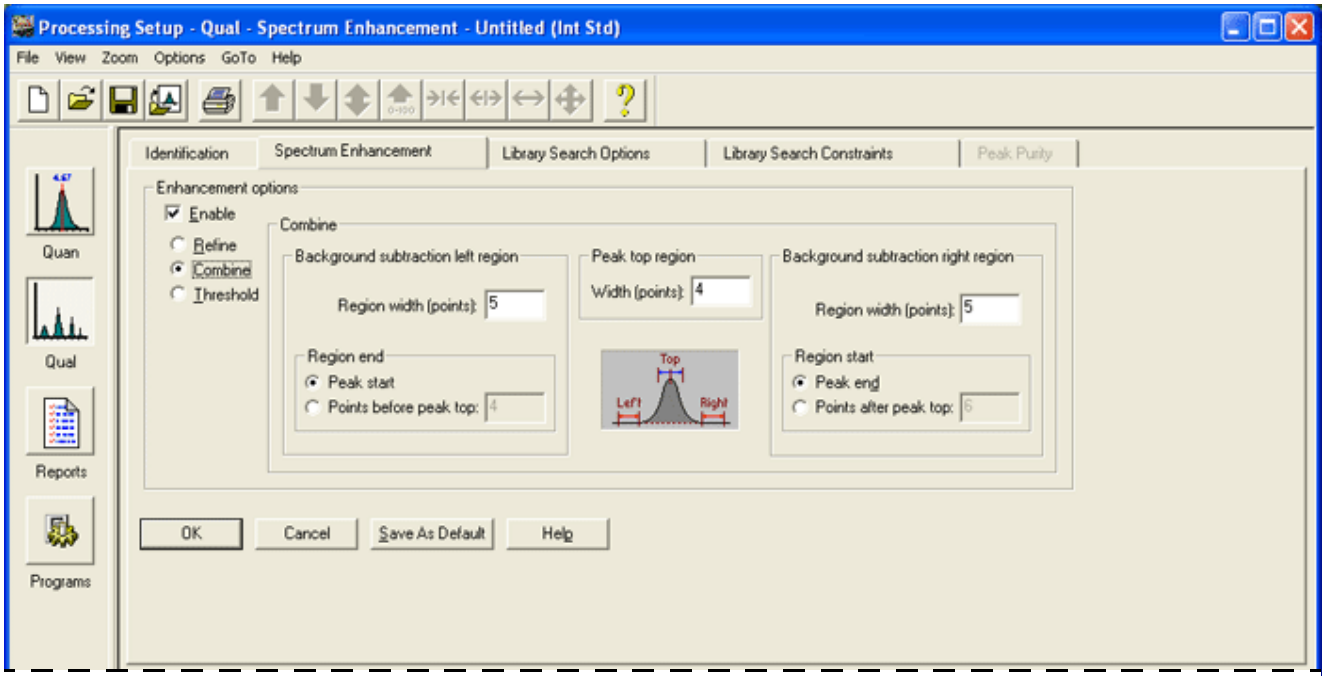
2. In the Detector area, select a peak detection algorithm from the Peak Detect list: Genesis, ICIS, or Avalon.
3. To specify advanced parameters for the selected algorithm, click **Advanced** in the Processing Setup window. One of the following dialog boxes appears:
   - Genesis Advanced Chromatogram Options Dialog Box
   - ICIS Advanced Parameters Dialog Box
   - Avalon Event List Dialog Box
4. Specify parameters for the selected algorithm.
5. To save the new settings and close the dialog box, click **OK**.

Setting Combine Option Parameters for Spectrum Enhancement

❖ To set combine option parameters

1. From the Qual view of the Processing Setup window, select the **Spectrum Enhancement** tab (see Figure 44). The Spectrum Enhancement Page for Qual View opens.

Figure 44. Spectrum Enhancement page for Qual view



2. To display Spectrum Enhancement options, select the **Enable** check box.
3. To select the Combine method and average multiple scans, select the **Combine** option.
4. To define the Peak Top Region, type the number of scans you want to average across the apex of the peak in the Width (points) box. Examine the chromatogram peak and estimate the number of good scans across the peak apex.
5. In the Background Subtraction Left Region area, define the baseline region used for background analysis before a peak:
   a. In the Region Width (points) box, type the number of scans to average in the analysis of the background spectrum.
   b. In the Region End area, select one of the two starting options to define the end time of the Left region:
      - Select the **Peak Start** option to use the detected peak start time.
      - Select the **Points Before Peak Top** option to specify the Left region end point as a specific number of scans before the peak top.

        Type the number of scans in the Points Before Peak Top box.

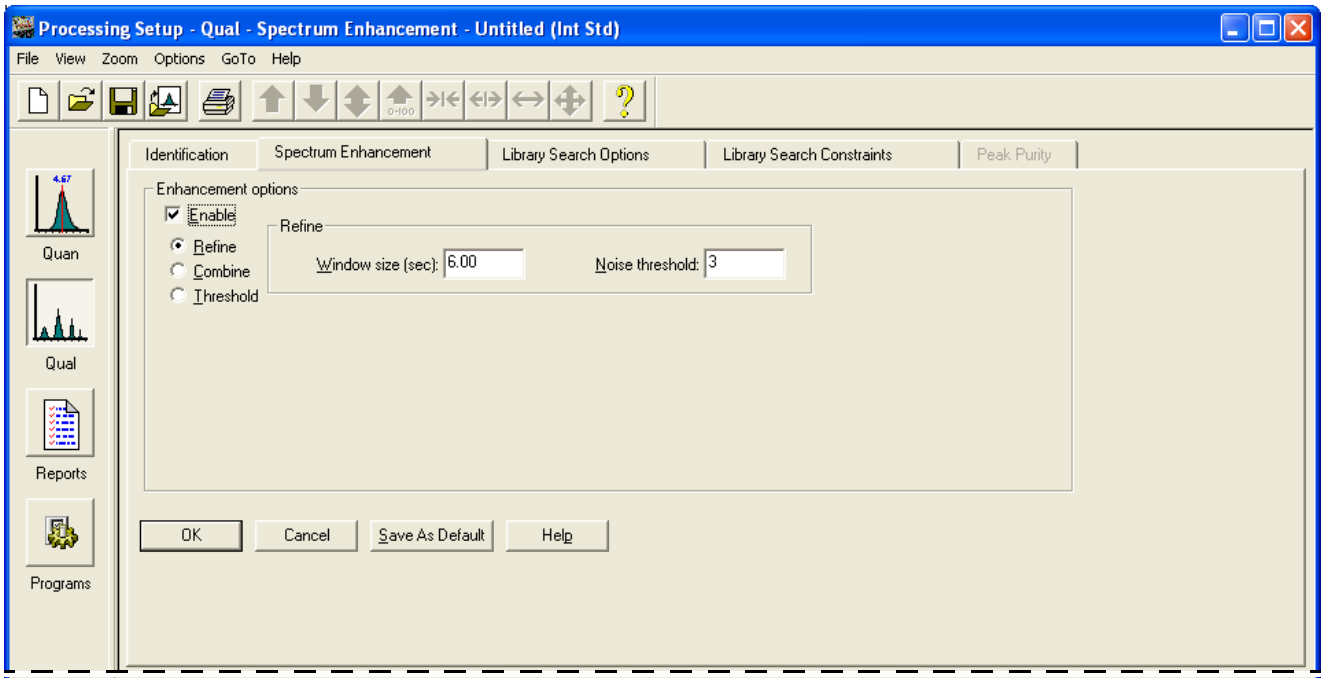
6. In the Background Subtraction Right Region area, define the baseline region used for background analysis after a peak:
   a. In the Region Width (points) box, type the number of scans to average in the analysis of the background spectrum.
   b. In the Region Start area, select one of the two ending options to define the end time of the Right region:
      - Select the **Peak End** option to use the detected peak end time.
      - Select the **Points After Peak Top** option to specify the Right region end point as a specific number of scans after the peak top.
      - Type the number of scans in the associated Points After Peak Top box.
7. To save your settings, click **OK**.

Setting Refine Option Parameters for Spectrum Enhancement

❖ To set refine option parameters

1. From the Qual view of the Processing Setup window, select the **Spectrum Enhancement** tab (see Figure 45). The Spectrum Enhancement Page for Qual View opens.

Figure 45. Spectrum Enhancement page for Qual view



2. To view spectrum enhancement options, select the **Enable** check box in the Enhancement Options area.
3. To select the refine enhancement method, select the **Refine** option.
4. To enter a time range for Refine, type a window size in the Window Size (sec) box. Set this parameter to the expected peak width.
5. To enter a noise threshold, type a limit for low intensity ions in the Noise Threshold box. Start with a value of zero, increasing the setting until the procedure eliminates spurious masses generated by background noise.
6. To save your settings, click **OK**.

Setting Threshold Option Parameters for Spectrum Enhancement

❖ **To set threshold option parameters for spectrum enhancement**

1. From the Qual view of the Processing Setup window, select the **Spectrum Enhancement** tab. The Spectrum Enhancement Page for Qual View opens.
2. To view spectrum enhancement options, select the **Enable** check box in the Enhancement Options area.
3. Select the **Threshold** option.
4. To enter an intensity threshold, type a value as a percentage of the most intense ion in the Cutoff Threshold (%) box.
5. To save your settings, click **OK**.

Working with Reports

Use reports to display your data so that you can access it easily.

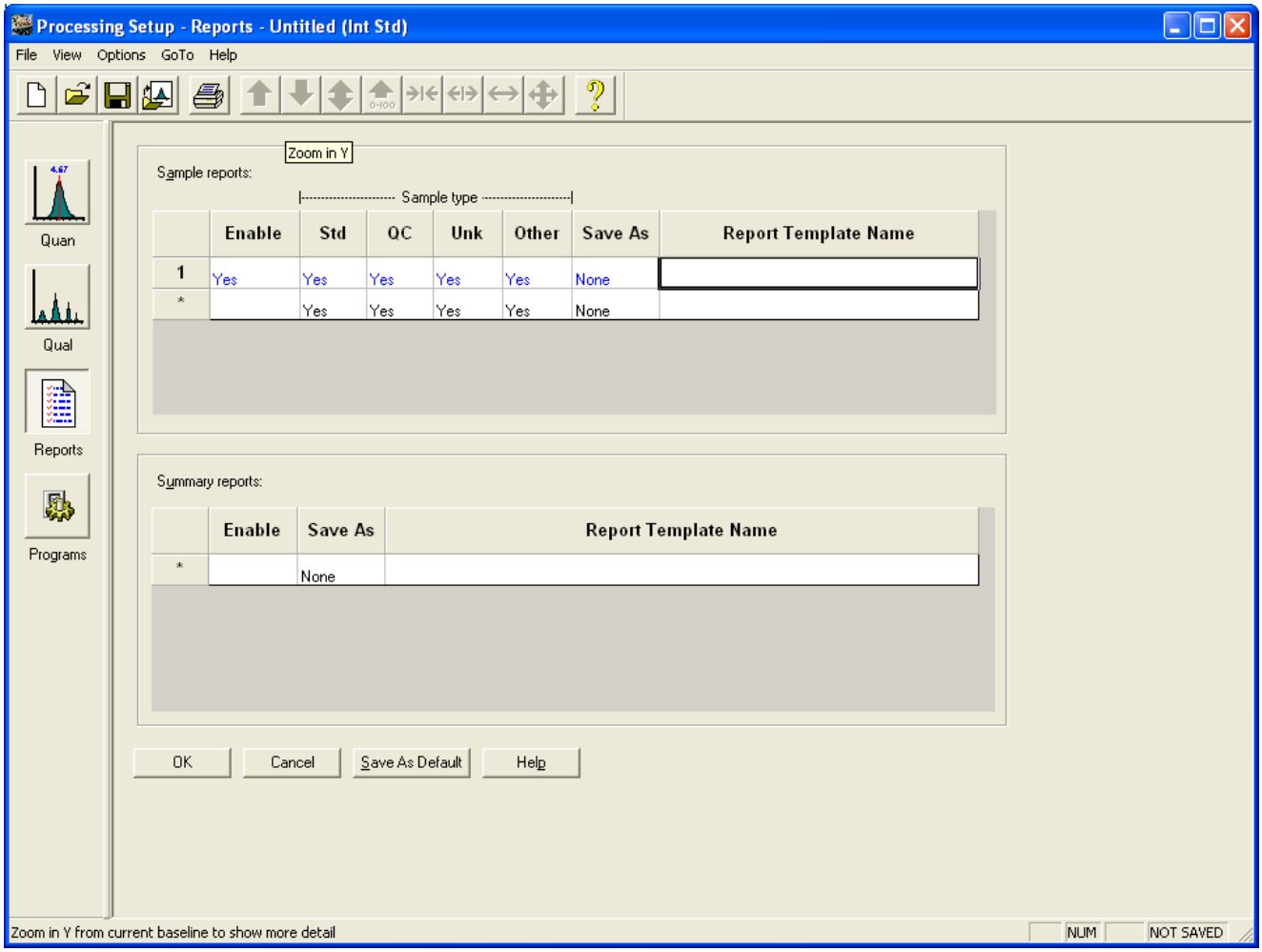
- Setting Report Parameters
- Selecting a Sample Report Template
- Selecting a Summary Report Template

Setting Report Parameters

❖ To set report parameters

1. Choose **View > Reports** or click  in the View bar to display the Reports View (see Figure 46).

Figure 46. Reports view



2. To add a report to either the Sample or Summary Report tables, double-click the first available cell in the Report Template Name column. A browse dialog box opens.

   Browse to the required template for a sample or summary report.

3. To select a sample or summary report:

   a. Click a cell in the Enable column. A check box appears.

   b. Select or clear the check box as required.

   c. Click outside the cell. If the report is enabled, the application displays Yes in the cell. If the report is unavailable, the cell is blank.

4. To change the Sample Report options for different sample types:
   a. Click the appropriate cell under Std, QC, Unk, or Other. A check box appears.
   b. Select or clear the check box as required.
   c. Click outside the cell. If the report is enabled for the Std, QC, or Other sample type, the application displays Yes in the cell. If the report is unavailable, the cell is blank.
5. To change the export options for a sample or summary report:
   a. Click the appropriate cell in the Save As column.
   b. Select from the available export formats: **None**, **Text**, **Doc**, **HTML**, or **PDF**.
   c. Click outside the cell. The cell displays the selected export format.
6. To insert a row in the Sample or Summary Report tables, double-click the row number where you want to insert a row. Right-click any cell in the row and choose **Insert Row** from the shortcut menu.
7. To delete a row in the Sample or Summary Report tables:
   - Double-click the row or rows you want to delete.
   - To delete a range of cells, drag across from the first to the last row in the range. Right-click any cell in the row and choose **Delete Rows** from the shortcut menu.
8. To save the new settings and close the dialog box, click **OK**.

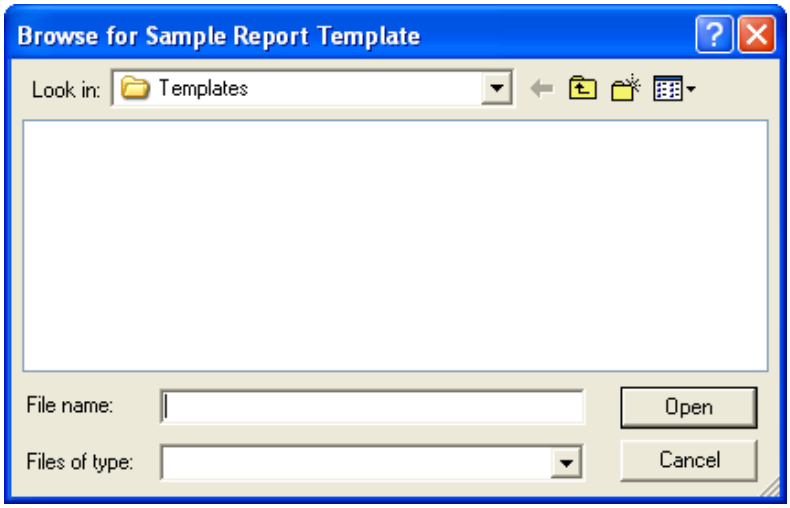
   To save the report list as the default option for new processing methods click **Save As Default**.

Selecting a Sample Report Template

❖ **To select a sample report template**

1. Choose **View > Reports** or click  in the View bar to display the Reports View.
2. In the Sample Reports area, double-click in the Report Template Name column. The Browse for Sample Report Template dialog box opens (see Figure 47).

   Figure 47. Browse for Sample Report Template dialog box

3. To select the required sample report template, click the template name. If it is not displayed, browse to the correct folder and select a template.

   The template name appears in the File Name box.

4. To close the dialog box and open the template, click **Open**.

Selecting a Summary Report Template

❖ **To select a summary report template**

1. Choose **View > Reports** or click  in the View bar to display the Reports View.
2. In the Summary Reports area, double-click in the Report Template Name column. The Browse for Summary Report Template dialog box opens.
3. To select the required summary report template, click the template name. If it is not displayed, browse to the correct folder.

   The template name appears in the File Name box.

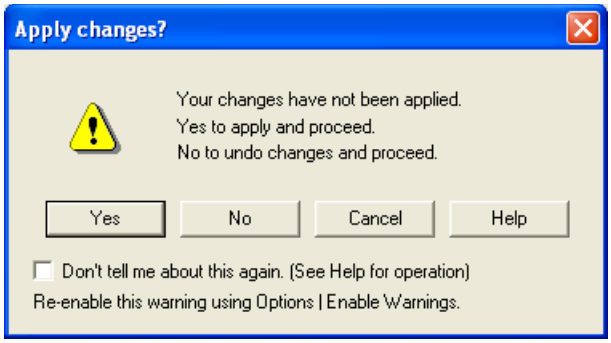
4. To close the dialog box and open a template, click **Open**.

Dealing with Unapplied Page Parameters

❖ To determine how the Xcalibur data system treats unapplied page parameters

When attempting a file operation, page or view change, or certain other action, you cannot proceed until the changes you have made to the parameters are applied. Unless you have selected the 'Don't Tell Me About This' check box, the Apply Changes? Dialog Box opens (see Figure 48).

Figure 48. Apply changes? dialog box



IMPORTANT Your next action affects the way in which the Xcalibur data system handles unapplied parameters in the future.

Choose from these options:

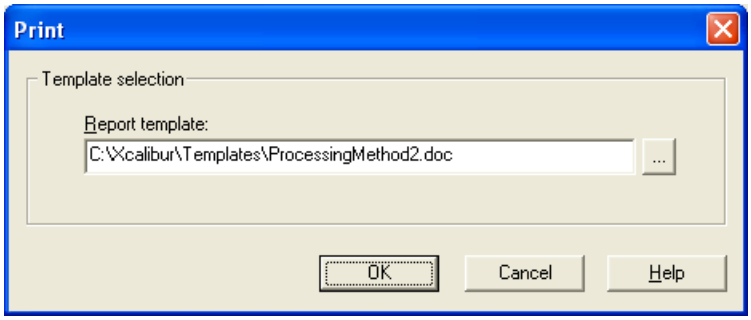
- To apply changes, click **Yes**. The data system applies changes automatically and, if appropriate, refreshes the previews. If validation succeeds, the data system applies the modifications and proceeds with your selected action. If validation fails, the application displays an error message. If an error exists, it stops the selected action and returns you to the Processing Setup view so that you can correct or undo the changes.
- To undo changes, click **No**. The data system discards changes automatically and without prompting whenever you select a page change, file operation, or other action requiring page validation. It continues with your selected action.
- To cancel the requested action, click **Cancel**. The data system returns you to the Processing Setup view without applying or discarding the changes. Clicking Cancel also clears the Don't Tell Me About This Again check box if you selected it.
- To suppress the display of the Apply Changes? dialog box, select the **Don't Tell Me About This Again** check box.
- To restore the Apply Changes? dialog box, choose **Options > Enable Warnings**.

Printing a Method

❖ **To print a report for the current processing method**

1. Choose **File > Print** or click  on the toolbar. The Print Dialog Box opens (see Figure 49).

   Figure 49. Print dialog box

2. To specify a template for the report, use the Report Template box.
3. Type the full path of the template or browse to locate the required template. For more information about selecting a template, see "Selecting a Sample Report Template" on page 75.
4. To save the new settings and close the dialog box, click **OK**. The hourglass cursor indicates that the processing method is being printed.

Working with Programs

See these topics to work with programs.

- Selecting a Program
- Setting Programs Parameters

Selecting a Program

❖ **To select a program**

1. To display the Programs View, choose **View > Programs** or click  in the View bar.
2. To open the Browse for Program dialog box, double-click a Program or Macro Name box. The Browse for Program dialog box opens.
3. To select the required program, click the program name. If it is not displayed, browse to the correct folder.

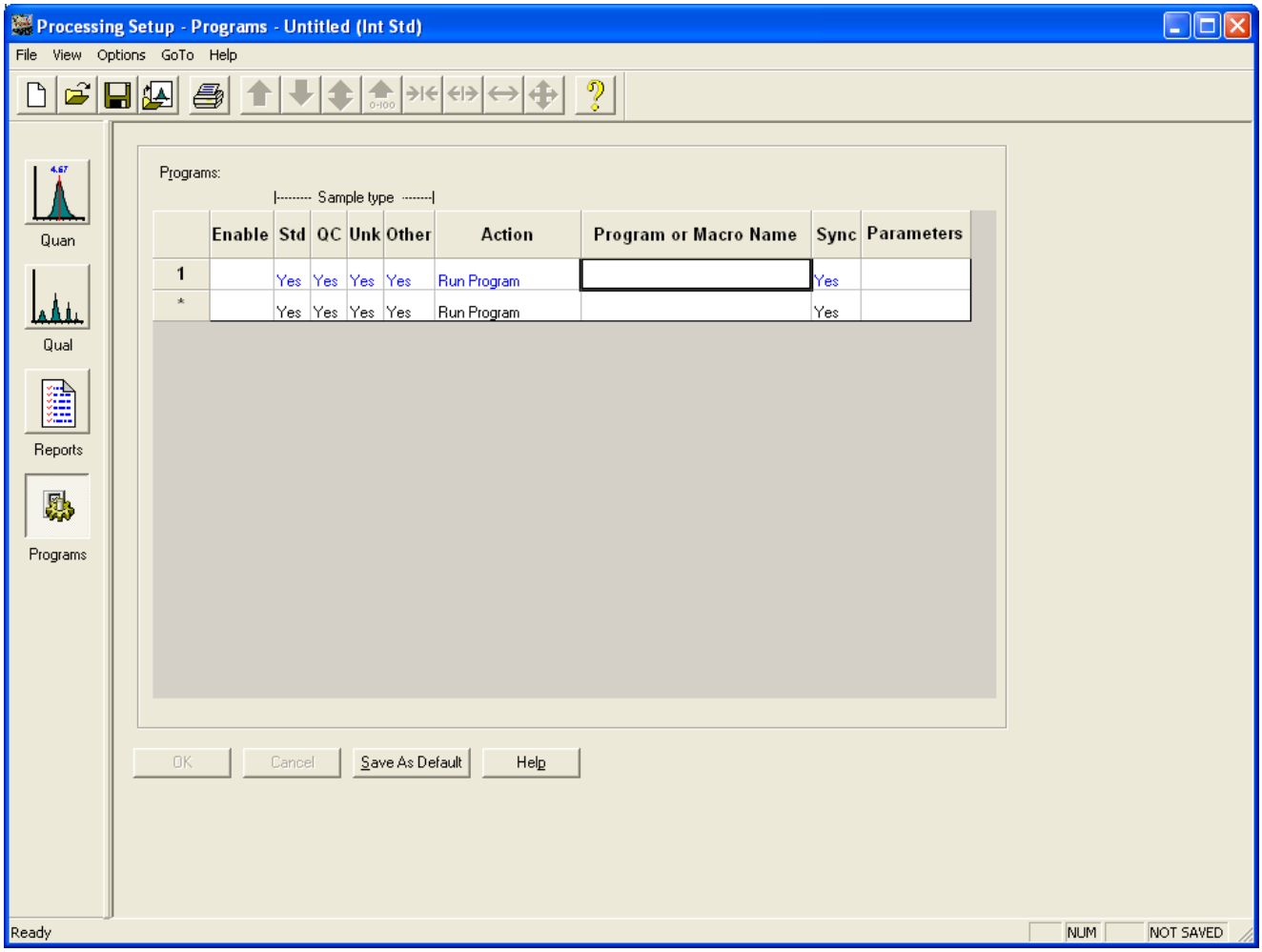
   The program name appears in the File Name box.
4. To close the dialog box, click **Open**.

Setting Programs Parameters

❖ To set programs parameters

1. Choose **View > Programs** or click  in the View bar to display the Programs View (see Figure 50).

Figure 50. Programs view



2. To add a program or macro to the Programs table, double-click the first available cell in the Program or Macro Name column and browse to the required program in the Browse for Program dialog box.

3. To enable a program or macro, click the associated cell in the Enable column. A check box appears. Select or clear the check box as required.

   Click outside the cell. If the program is enabled, the application displays Yes in the box. If the program is unavailable, the cell is blank.

4. To change the program options for different sample types, select the appropriate cell in the Other column. A check box appears. Select or clear the check box as required.

   Click outside the cell. If the program is available, the application displays Yes in the box. If the program is unavailable, the cell is blank.

5. To change the action for a program, select its corresponding cell in the Action column. Select from the list of available actions: **Run Excel Macro** or **Run Program**.

   Click outside the cell. The action for the program appears in the cell.

6. To change the Sync setting for a program, select its corresponding cell in the Sync column. A check box appears. Select or clear the check box as required.

   Click outside the cell. If synchronous program operation is available, the application displays Yes in the box. For asynchronous operation, the cell is blank.

7. To add command parameters for a program, select the corresponding cell in the Parameters column. Type the require commands.

8. To insert a row in the Programs table, double-click the row number where you want to insert a row.

   Right-click any cell in the row and choose **Insert Row** from the shortcut menu.

9. To delete a row in the Programs table, double-click the row or rows you want to delete.

   To delete a range of cells, drag across from the first to the last row in the range. Right-click any cell in the row and choose **Delete Rows** from the shortcut menu.

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

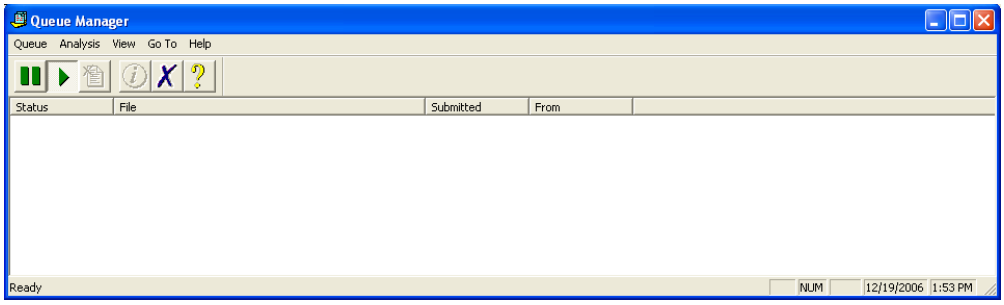
11. To save the report list as the default option for new processing methods, click **Save As Default**.

Managing the Xcalibur Processing Queue

❖ To manage the Xcalibur processing queue

1. From the Home Page window, choose **Tools > Queue Manager** (see Figure 51).

   Figure 51. Queue Manager view

2. Select processing queue options as desired:

   - To temporarily stop the processing queue, click in the toolbar or choose **Queue > Pause**.
   - To resume the processing queue when it is in Pause mode, click in the toolbar or choose **Queue > Resume**.
   - To update the display with current information, choose **View > Refresh**.
   - To remove a task from the queue, select the task to be removed and click in the toolbar or choose **Analysis > Remove from Queue**.
   - To remove all tasks from the queue, choose **Queue > Purge Queue**.
   - To view additional details, select the task in the queue and click in the toolbar or choose **Analysis > Details**.
   - To close the Processing Queue Manager window, press ALT+F4.

Processing Data

This chapter provides instructions for processing data. Whether you are processing or reprocessing the data, the results are the same. This guide refers to processed data whether the action is processing or reprocessing.

Contents

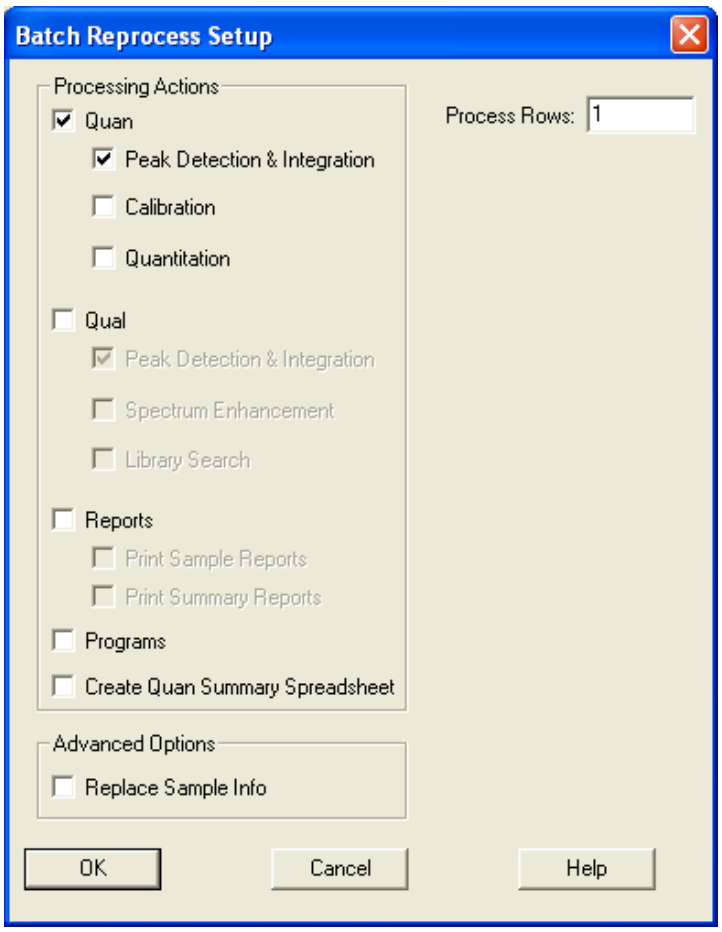
Processing a Batch of Samples

❖ To process samples selected from the current sequence

1. To select the rows for batch processing by the current sequence, drag in the far left column. The Xcalibur data system highlights the selected rows.

2. Click  in the Sequence Editor toolbar or choose **Actions > Batch Reprocess** in the Sequence Setup view. The Batch Reprocess Setup Dialog Box (see Figure 52) opens.

Figure 52. Batch Reprocess Setup dialog box



The application displays the sequence rows that you selected in step 1 in the Process Rows box.

3. To change the sample numbers that you entered in step 1, type the first and last row to be processed in the Process Rows box. The format is either *rownumber* for one sample or *firstrownumber–lastrownumber* for multiple samples.

4. In the Processing Actions area, select the following, and choose from displayed options.

   - the **Quan** check box: To activate Peak Detection & Integration, Calibration, and Quantitation processing, select the Quan check box.

- the **Qual** check box: To activate Peak Detection & Integration, Spectrum Enhancement, and Library Search processing, select the Qual check box.
- the **Reports** check box
- the **Programs** check box
- the **Create Quan Summary Spreadsheet** check box
- the **Replace Sample Info** check box in the Advanced Options area

For more information about options, see Batch Reprocess Setup Dialog Box.

5. To save the settings and close the dialog box, click **OK**. The application initiates batch processing of the selected samples.

Selecting a Calibration or QC Level

You must create and select a processing method with Calibration or QC levels before you can select one of the levels for a quality control sample type [QC] or standard update sample type [Std Update] to use in a sequence.

In the Sequence Setup view, the Level box displays the current calibration or QC level for the sequence row. This level is defined in the processing method displayed in the Processing Method box.

❖ To select or change a calibration or QC level for a sample

1. To open a list of levels from the Sequence Setup view for a sample of type Std Update or QC, select a processing method file that defines one or more levels.
2. To open a list of levels from the processing method, double-click the Level box.
3. To select the QC or calibration level, click the correct level for the sample.
4. To enter the settings into the Sequence Setup table, click away from the list to store the level. The data system displays the new level in the Level box for the sample.

Acquisition and Processing

The following table provides a workflow you can follow to do acquisition and processing automatically using the Xcalibur data system and the software that came with your hardware.

Workflow task	Reference
MS Tune Program: Develop a suitable acquisition method.	Refer to the tune guide that came with your hardware.
Instrument setup: Enter method parameters determined above.	See "Setting Up Instruments" on page 8
Prepare samples, standards, and so forth.	
Sequence setup: Acquire a raw file from a representative standard.	
Processing setup: Using the acquired raw files, create a product method.	See "Setting Quan Browser Process Parameters" on page 45 or "Setting Qual Browser Process Parameters" on page 65
Sequence setup: Create a sequence using New Sequence Template. Add an instrument method and a processing method.	See "Creating a Sequence Semi-Automatically" on page 23
Sequence setup: Run the sequence, acquire a set of data files. The application automatically processes data according to the processing method parameters.	See "Running a Sequence" on page 33
Quan Browser: Open the processed sequence. Review the integration of each chromatogram. Review the calibration curve for each target compound.	Refer to the *Quantitative Analysis User Guide*
Quan Browser or Processing setup: Adjust peak integration and calibration curve parameters as necessary.	Refer to the *Quantitative Analysis User Guide*
XReport: Preview representative files with the report templates until you find a template that suits your needs. Adjust the template and save as needed.	Refer to the *XReport User Guide*
Processing setup: Add the selected report template to the processing method.	See "Working with Reports" on page 72

Workflow task	Reference
Sequence setup: Batch process the sequence and print or save the appropriate reports.	See "Processing a Batch of Samples" on page 82
Perform subsequent quantitative analysis of the same compound by preparing the samples and creating a new sequence using the existing instrument method and processing method. The data system does acquisition, processing, and reporting automatically.	

Importing and Exporting Sequences

To import or export a sequence, do these procedures:

Checking Sequence Quality Before Importing

Before importing a sequence, check to see that the file type and format is correct and that the Xcalibur data system can read the column names of the sequence.

❖ **To verify that a sequence can be imported**

1. To open an example sequence file (.sld) into the Sequence Setup window, choose **File > Open** and click the file name.
2. To edit the file and save it, click row number 2 and drag your cursor to the last row number. Then, delete the rows. Choose **File > Save As** and save the sequence file.
3. Export the sequence, and name the file as a .csv file. See "Exporting a Sequence" on page 89 for more information.
4. Edit the .csv file in your spreadsheet or text editor application.

   The cell in the first column of the first row must contain the text Bracket Type=n, where n is a number from 1 to 4. Each number represents a particular bracket type. See "New Sequence Template Dialog Box" on page 109 for more information about bracket use.

   - 1: Overlapped
   - 2: None
   - 3: Non-Overlapped
   - 4: Open
5. Name and save the file as a .csv file.
6. Import the sequence. See "Importing a Sequence" on page 88 for more information.

Importing a Sequence

You can select the columns of a sequence to import and designate the path and file name of the imported file. The data system only reads comma-separated-value text files with a .csv file extension. This file format can be read by a text editor program or a spreadsheet program. The application generates an invalid file message if it attempts to import a sequence of any other file extension or file type.

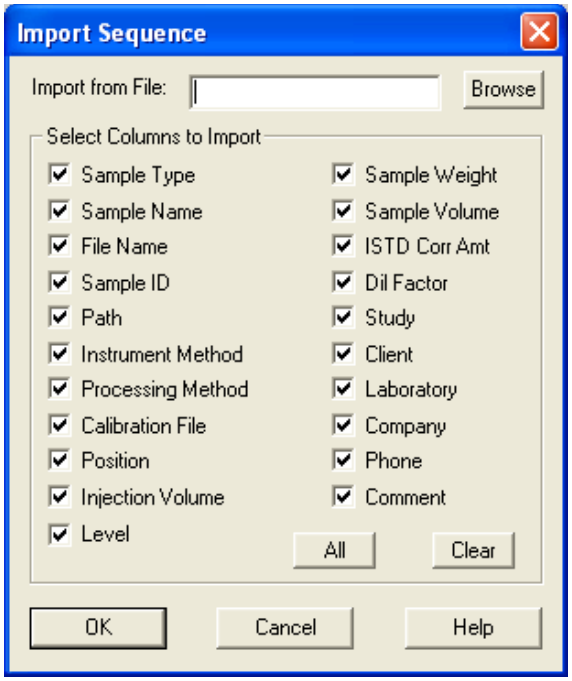
Note To make sure that the file type is correct and the column names of the sequence that you want to import can be read by the data system, use the following procedure: "Checking Sequence Quality Before Importing" on page 87.

The imported sequence file needs to contain the same list separator character that is set in your computer control panel. To change the list separator column in your system, use the following procedure: "Changing the List Separator Character" on page 19.

❖ To import a sequence

1. To open the Import Sequence Dialog Box, choose **File > Import Sequence** in the Sequence Setup view.

Figure 53. Import Sequence dialog box



2. To specify the path and file name of the file to be imported, enter the path and file name of the sequence file to be imported with a .cvs extension in the Import from File box or click **Browse** to select the path to the sequence file and select a file with a .csv extension.

   If you do not enter an extension, the application assigns a .csv extension for you. If you enter an extension other than .csv, it posts the following error message in step 4:

   Invalid file extension. File extension should be .csv.

3. To select sequence columns to be included in the imported file, use the check boxes in the Select Columns to Import area. Select the check boxes for the columns you want to include and clear the check boxes for the columns that you do not want to include in the imported file.

   - Click **All** to select all the column check boxes.
   - Click **Clear** to clear all the column check boxes.

4. To import the selected columns of the sequence you have specified, save the changes, and close the dialog box, click **OK**. The data system displays the imported file in the Sequence Setup view.

Exporting a Sequence

You can select the columns of a sequence to export and designate the path and file name of the exported file. The Xcalibur data system creates an exported comma-separated-value text file with a .csv file extension by inserting a column separator character between each sequence field. This file format can be read by a text editor program or a spreadsheet program.

The exported sequence file contains the current list separator character that is set in your computer control panel. To change the list separator column in your system, see "Changing the List Separator Character" on page 19.

❖ To export a sequence

1. To open the Export Sequence Dialog Box, choose **File > Export Sequence** in the Sequence Setup view.

2. To specify the path and file name of the file to export, enter a file name for the exported sequence file in the Export to File box or click **Browse** to select a path for storing the exported sequence file.

   Save the file as a .csv file. If you do not enter an extension, the application assigns a .csv extension for you. If you enter an extension other than .csv, the data system posts the following error message in step 4:

   Invalid file extension. File extension should be .csv.

3. To specify the sequence columns you want to export, select the sequence columns to be included in the exported file by using the check boxes in the Select Columns To Export area. Select check boxes for the columns you want to include and clear check boxes for the columns that you do not want to include in the exported file.
   - Click **All** to select all the column checkboxes.
   - Click **Clear** to clear all the column checkboxes.
4. To export the selected columns of the active sequence to the location that you have specified, click **OK**.
5. If you need to do so, return to "Checking Sequence Quality Before Importing" on page 87.

Sequence Setup Reference

Use the Sequence Setup view to set up a sequence containing unknown samples, calibration standard samples, quality control samples, and blank samples. You can also control your autosampler or syringe pump and run a sample, run a sequence of samples, or reprocess a batch of previously acquired raw data files.

Contents

For menu and toolbar information, see "Processing Setup Reference" on page 123.

Sequence Table

One row of the sequence corresponds to one sample injection. Each sample is defined by its sequence row settings. You can also manually inject samples from the front panel injector, as predefined in the sequence.

For quantitative analysis, a sequence can be generated semi-automatically based on a processing method. For example, Sequence Setup can divide up a large number of samples into smaller groups that are bracketed by calibration sets. The number of calibration levels in each calibration set is defined by your processing method; see Chapter 4, "Preparing for Processing." If required, calibration sets can be shared between brackets to make overlapping brackets. the Xcalibur data system supports sequences with no bracket, open brackets, overlapped brackets, or non-overlapped brackets.

Each sample is defined by the settings on its sequence row.

Table 1. Sequence table parameters (Sheet 1 of 6)

Parameter	Description
Sample Type	View or change the type of sample described by the sequence row. Different sets of sample types are presented for different bracket types. The sample type defines how the data system processes the sample data. Each sample must be classified as one of the following Xcalibur sample types: • Unknown • Blank • QC (quality control) • Standard Clear • Standard Update • Start Bracket • End Bracket • Standard Bracket ❖ **To change the sample type** 1. In the Sample Type column, click the arrow to display a list of sample type options. 2. Click to select a sample type. The application displays the new sample type in the Sample Type box.
File Name	View the name of the file that contains the sample data. The File Name is a combination of the Base File Name prefix assigned to a sequence and a sequential sequence number. • If you use the New File Template to create a sequence, the application defines the Base File Name and the Sequence Starting Number at that time. • If you do not change the default Sequence Starting Number 1, the suffix number is the same as the row number of the sequence: 001, 002, and so on. • If you change the default Sequence Starting Number to another number, then the first sample has the Starting Number and subsequent rows in the sequence are incremented by 001. For example, if the Starting Number is 100, the File Name for the first sample has 100 for a suffix, the second sample has 101 as a suffix, and so on. To edit this box after it is saved, select the cell and press F2 on your keyboard. The Xcalibur data system places the cursor to the right of the cell text. Delete the old file name and type a new file name.

Table 1. Sequence table parameters (Sheet 2 of 6)

Parameter	Description
Sample ID	View or change a unique identification (ID) number for each sample. To change the current ID number, type a new ID number in the Sample ID box. If you use the New File Template to create the sequence, you can use the Base Sample ID box to enter an alphanumeric prefix to the Sample ID that the data system applies to each sample in the new sequence. The application starts Sample ID numbering at 001. For example, if you type AB12 in the Base Sample ID box of the New File Template, the application assigns the following Sample IDs: AB12001, AB12002, AB12003, AB12004, AB12005. You can also choose to have the data system fill in the Sample ID boxes for calibration and quality control samples: in the New File Template dialog box, select both the Fill in Sample ID for Standards check box and Fill in Sample ID for QCs check box. To edit this box after it is saved, select the cell and press F2 on your keyboard. The Xcalibur application places the cursor to the right of the cell text. Delete the old sample ID and type a new sample ID.
Path	Enter the path to the raw file or files that the Xcalibur data system creates for the sample data. The application creates these files with a .raw extension. A path contains the drive and one or more folders. A typical path can look like: C:\Xcalibur\DATA. To find and select the path, double-click the Path box. The Select Directory dialog box opens. The application enters the path in the Path box. You can also type the path in the Path box.
Instrument Method	Enter the path and instrument method to be used to analyze the samples in the active sequence. A path contains the drive and one or more folders. A typical path for an instrument method file named ABC.meth can look like: C:\Xcalibur\methods\ABC.meth. To find and select the path and file name, double-click the Inst Meth box. The Select Instrument Method dialog box opens. The data system enters the path and file name in the Inst Meth box. You can also type the path and file name in the Inst Meth box.
Processing Method	Enter the path and processing method to be used to process the samples in the active sequence. A path contains the drive and one or more folders. A typical path for a processing method file named ABC.pmd can look like: C:\Xcalibur\methods\ABC.pmd. To find and select the path and file name, double-click the Processing Method box. The Select Processing Method dialog box opens. The application enters the path and file name in the Processing Method box. You can also type the path and file name in the Processing Method box.

Table 1. Sequence table parameters (Sheet 3 of 6)

Parameter	Description
Calibration File	View the path and file name of the Calibration Files to be used to process the samples in the current sequence using Bracket Type None. This column contains the full path and name of the current default calibration file. A path contains the drive and one or more directories. A typical path for a calibration file named ABC.xcal can look like this: C:\Xcalibur\methods\ABC.xcal. To find and select the path and file name, double-click the Calibration File box. The Select Calibration File dialog box opens. The application enters the path and file name in the Cal File box. You can also type the path and file name in the Cal File box.
Position	View or change the sample's position number in the autosampler. To change the position number, type a new position number in the Position box. If you use the New File Template to create your sequence, you can use the Initial Vial Position box to specify the first position number of the sequence that the data system assigns. You can also use the Re-Use Vial Positions check box to allow the data system to re-use or not re-use position numbers. To edit this box after it is saved, select the cell and press F2 on your keyboard. The application places the cursor to the right of the cell text. Delete the old vial position number and type a new vial position number.
Injection Volume	View or change the injection volume in microliters of sample to be injected. To change the volume, type the new volume in the Inj Vol box. If you are using an autosampler, you can set the default injection volume in the Autosampler dialog box in the Instrument Setup window. The minimum and maximum injection volumes that you can use depend on the autosampler you select. The usable range depends on the injection mode and might be smaller than the range displayed in the status bar. For more details, consult your autosampler manual. To edit this box after it is saved, select the cell and press F2 on your keyboard. The Xcalibur data system places the cursor to the right of the cell text. Delete the old injection volume and type the new injection volume.
Level	This box displays the word Level whenever the sequence row corresponds to a Calibration Sample or a Quality Control Sample with a defined level. To determine the current level for a sample, double-click the Level box for the sample. The Select Level dialog box opens, displaying the current level. To change the level, select the level from the list and click **OK**.

Table 1. Sequence table parameters (Sheet 4 of 6)

Parameter	Description
Sample Weight	View the amount of a component that has been placed in the sample. The unit for this sample weight is specified in the Processing Setup window and is only included in Xcalibur reports. The data system does not convert units. To change the sample weight, double-click the Sample Weight box. The cursor changes to the vertical bar cursor. Enter the correct sample weight. The cursor changes back to the original cursor when you click any other area of the view. If you have specified a processing method for your sequence, the application automatically enters the sample weights of the Calibration and/or Quality Control samples from the processing method settings. To edit this box after it is saved, select the cell and press F2 on your keyboard. The Xcalibur application places the cursor to the right of the cell text. Delete the old sample weight and type the new sample weight.
Sample Volume	View or change the volume of a component that has been placed in the sample. The unit for this volume is specified in the Processing Setup window and is only included in Xcalibur reports. The data system does not convert units. To change the sample volume, double-click the Sample Volume box. The cursor changes to the vertical bar cursor. Enter the correct sample volume. The cursor changes back to the original cursor when you click any other area of the view. If you have specified a processing method for your sequence, the data system automatically enters the units for the sample volume of the Calibration and/or Quality Control samples from the processing method settings. To edit this box after it is saved, select the cell and press F2 on your keyboard. The Xcalibur data system places the cursor to the right of the cell text. Delete the old sample volume and type the new sample volume.

Table 1. Sequence table parameters (Sheet 5 of 6)

Parameter	Description
ISTD Correction Amount	View or change the ISTD correction amount. If the value in this box is not 0.000, the value is used in an algorithm to automatically correct for the case where the internal standard amounts specified in the active processing method are correct, but where the amount of internal standard actually in one or more samples is different from the amount specified in the processing method. This correction eliminates the necessity of remaking the samples to the internal standard concentrations or amounts specified in the processing method and re-running the samples. For each component defined as an internal standard, a bulk adjustment factor can be applied to the base response of each internal standard defined in the processing method. If no correction is required, confirm that a value of 0.000 is entered in the Sequence Setup ISTD Corr Amt box. If a correction is required, enter the sum of all internal standard amounts or concentrations actually in the sample into the Sequence Setup ISTD Corr Amt box for the sample row or rows requiring adjustment. The value entered uses the same units as specified in the processing method. Do not type the units into the box. For example, for 20 ng, type 20. To edit this box after it is saved, select the cell and press F2 on your keyboard. The Xcalibur data system places the cursor to the right of the cell text. Delete the old ISTD correction amount and type the new ISTD correction amount.
Dilution Factor	View or change the dilution factor that was used to prepare the sample. The valid range is 0.000 to 10 000.000. The application interprets a value of 0.000 as no dilution. ❖ **To change this factor** 1. Double-click the Dil Factor box. The cursor changes to the vertical bar cursor. 2. Enter the correct factor. The cursor changes back to the original cursor when you click any other area of the view. If you have specified a processing method for the current sequence, The application automatically enters the Dil Factor value from the processing method settings. To edit this box after it is saved, select the cell and press F2 on your keyboard. The Xcalibur data system places the cursor to the right of the cell text. Delete the old dilution factor and type the new dilution factor.
Comment	View or change any comments that you have entered about the sample.
Sample Name	View the name that you assign to your sample.

Table 1. Sequence table parameters (Sheet 6 of 6)

Parameter	Description
Heading 1 [*Study*] Heading 2 [*Client*] Heading 3 [*Laboratory*] Heading 4 [*Company*] Heading 5 [*Phone*]	These boxes display information about a user-defined column heading that is pertinent to the active sample row in the sequence. You can use this field to convey information about this sample to others or as a reminder to yourself. ❖ **To change the Heading name** 1. Choose **Change > User Labels**. The User Labels dialog box opens. 2. Type the new column heading into one of the Heading boxes and click **OK**. The new Heading name appears with the Sequence Setup view column headings. If the new column heading does not appear in your sequence, choose **Change > Column Arrangement** to display the Column Arrangement Dialog Box. Select the new column heading in the Available Columns box. Click **Add** to move the new heading to the Displayed Columns box, and click **OK**. ❖ **To enter information about the column heading** Type the information in the new column heading box. You can edit this box after it is saved by selecting the cell and pressing F2 on your keyboard. The Xcalibur data system places a cursor in the box. You can then delete the old heading information and type the new heading information.

Dialog Boxes

- Batch Reprocess Setup Dialog Box
- Change Instruments In Use Dialog Box
- Column Arrangement Dialog Box
- Export Sequence Dialog Box
- Fill Down Dialog Box
- Go To Line Number Dialog Box
- Import Sequence Dialog Box
- New Sequence Template Dialog Box
- Run Sequence Dialog Box
- Transfer Row Information Dialog Box
- Tray Selection Dialog Box
- User Labels Dialog Box

Batch Reprocess Setup Dialog Box

Use this dialog box to select batch processing settings for the sequence rows displayed in the Process Rows box. You can use the check boxes to activate options that you have selected using the Processing Setup window. Whether you are processing or reprocessing the data, the results are the same. This guide refers to processed data whether the action is processing or reprocessing.

The Xcalibur data system requires that you select a valid processing method for each sample that you want to include in the batch reprocess. To change the processing method, double-click the Proc Meth [Processing Method] column for the sample row of interest. The Select Processing Method dialog box opens so that you can browse to and select a processing method for batch processing. If you do not select a valid processing method, the application posts a message describing the problem.

Table 2. Batch Reprocess Setup dialog box (Sheet 1 of 3)

Parameter	Description
Process Rows	
Process Rows	View or change the sequence rows that have been selected for batch processing. To change the range, either select the rows in the sequence before opening the Batch Reprocess Setup dialog box or type the sample (row number) or sample range (first row through last row) in the Process Rows box using the following format: *FirstRowNumber–LastRowNumber*. For example, to process sample rows 10 through 22, enter: 10–22.
Processing Actions	
Quan	Use quantitative processing functions. To activate Peak Detection & Integration, Calibration, and Quantitation processing, select the Quan check box. You can also activate these functions with the Quan processing actions of the Batch Reprocess Setup dialog box.
Peak Detection & Integration (Quan)	Perform peak detection and integration processing for the samples selected from the current sequence and displayed in the Process Rows box. Define peak detection and integration parameters on the Detection Page for Quan View in the Processing Setup window. Using this option requires a valid processing method and a valid raw file. To activate this batch processing option, select the Peak Detection & Integration check box.
Calibration (Quan)	Perform calibration processing for the samples selected from the current sequence and displayed in the Process Rows box. Define calibration parameters on the Calibration Page for Quan View in the Processing Setup window. Using this option requires a valid processing method and a valid raw file. To activate this batch processing option, select the Calibration check box.

Table 2. Batch Reprocess Setup dialog box (Sheet 2 of 3)

Parameter	Description
Quantitation (Quan)	Perform quantitation processing for the samples selected from the current sequence and displayed in the Process Rows box. Define quantitation parameters in the Quan view of the Processing Setup window. Using this option requires a valid processing method and a valid raw file. To activate this batch processing option, select the Quantitation check box.
Qual	Use qualitative processing functions. To activate Peak Detection & Integration, Spectrum Enhancement, and Library Search processing, select the Qual check box. You can also activate these functions with the Qual processing actions in the Batch Reprocess Setup dialog box.
Peak Detection & Integration (Qual)	Perform peak detection and integration batch processing for the samples selected from the current sequence and displayed in the Process Rows box. Define peak detection and integration parameters on the Identification Page for Qual View in the Processing Setup window. Using this option requires a valid processing method and a valid raw file. To activate this batch processing option, select the Peak Detection & Integration check box.
Spectrum Enhancement (Qual)	Perform spectrum enhancement batch processing for the samples selected from the current sequence and displayed in the Process Rows box. Define spectrum enhancement parameters on the Spectrum Enhancement Page for Qual View in the Processing Setup window. Using this option requires a valid processing method and a valid raw file. To activate this batch processing option, select the Spectrum Enhancement check box.
Library Search (Qual)	Perform library search batch processing for the samples selected from the current sequence and displayed in the Process Rows box. Define library search parameters on the Library Search Constraints Page for Qual View in the Processing Setup window. Using this option requires a valid processing method and a valid raw file. To activate this batch processing option, select the Library Search check box.
Reports	Print Sample Reports and Print Summary Reports. Select the Reports check box to enable both of these print functions. You can also activate these functions with the Reports processing actions in the Batch Reprocess Setup dialog box.

Table 2. Batch Reprocess Setup dialog box (Sheet 3 of 3)

Parameter	Description
Print Sample Reports	Print XReport Report Wizard sample reports for the samples selected from the current sequence and displayed in the Process Rows box. Define sample report parameters in the Reports view of the Processing Setup window. Using this option requires a valid processing method and a valid raw file. To activate this batch processing option, select the Print Sample Reports check box.
Print Summary Reports	Print XReport Report Wizard summary reports for the samples selected from the current sequence and displayed in the Process Rows box. Define summary report parameters in the Reports view of the Processing Setup window. Using this option requires a valid processing method and a valid raw file. To activate this batch processing option, select the Print Summary Reports check box.
Programs	Run programs. Select the Programs check box to run Programs. You can also activate these functions with the Programs processing actions of the Batch Reprocess Setup dialog box.
Create Quan Summary Spreadsheet	Create a quantitation summary for the samples selected from the current sequence and displayed in the Process Rows box. Define quantitation parameters in the Quan view of the Processing Setup window. Using this option requires a valid processing method and a valid raw file. To activate this batch processing option, select the Create Quan Summary Spreadsheet check box.
Advanced Options	
Replace Sample Info	Remove sequence data in the raw file and replace it with the active sequence data. Select the Replace Sample Info check box. To use the data in the current raw file, make sure the check box is clear.

Change Instruments In Use Dialog Box

Use this dialog box to select the instruments that you want to use to run the current sequence. For example, you might want to use one set of instruments to run sequence rows 1 through 10 and use a different set of instruments to run sequence rows 11 through 20.

Table 3. Change Instruments In Use dialog box parameters

Parameter	Description
Instrument	View or change the list of instruments that have been configured for operation as Xcalibur devices. ❖ **To add an instrument not on the list** 1. Click **Cancel** to close the Change Instruments In Use dialog box. 2. Close down all running Xcalibur programs. 3. Choose **Start > Programs > Thermo Foundation 1.0 > Instrument Configuration**. The Instrument Configuration view opens. 4. Select and configure the instrument. When you reopen the Change Instruments In Use dialog box, the newly configured instrument appears on the Instrument list.
In Use	View or change instrument status. The rows in this list display either Yes (in use) or a blank entry (not in use) to indicate instrument status. When you configure an instrument using the Instrument Configuration view, the default status of the instrument is Yes. If you do not want to use an instrument for the current sequence, click the Yes entry to change it to a blank entry. Instruments with a blank entry are not available for the current sequence. For example, if a sample is to be manually injected by syringe into a mass spectrometer or MS detector, the In Use entries for all instruments, except the mass spectrometer or MS detector, must be blank. For any sequence that you are about to submit for processing, make sure a Yes value appears for each instrument in the In Use area.
Start Instrument	Select an instrument from the Instrument list to be the Start Instrument. Click the Start Instrument list in the row of the instrument of choice to change the blank entry to Yes. This list can either have one Yes in one of the instrument rows or all blanks for all instrument rows (no Yes entries). The autosampler is usually selected to be the Start Instrument because this is the instrument that controls when a run starts. In this case, a Yes appears for all instruments to be used for the sequence submission, including the autosampler, because they are waiting for a contact closure event to start operation. When all devices used in the run achieve this status, the Start Instrument initiates the run.

Column Arrangement Dialog Box

Use this dialog box to select which columns are displayed and the position or order of the columns in the current sequence. Displayed columns are selected from the Available Columns list and added to the Displayed Columns list using the Add button.

Table 4. Column Arrangement dialog box parameters (Sheet 1 of 2)

Parameter	Description
Available Columns	View and change the columns that do not currently appear in the Sequence Setup table but that can be added. Possible columns include the following: • Sample Type • File Name • Sample ID • Path • Inst Meth • Proc Meth • Position • Inj Vol • Cal File • Level • Sample Wt • Sample Vol • ISTD Corr Amt • Dil Factor • Comment • SampleName • User Labels 1-5 To set User Labels, open the User Labels Dialog Box.
Displayed Columns	View the columns that currently appear in the Sequence Table. The left-to-right order of the columns for a particular sequence corresponds to the top-to-bottom order in the Displayed Columns list.
Buttons	
Add	To display a sequence column, select the column from the Available Columns list box. Click **Add** to move the column name to the Displayed Columns list. The application displays the columns that are listed in the Displayed Columns list.
Remove	To remove a sequence column from the current display, select the column from the Displayed Columns list box. Click **Remove** to move the column name to the Available Columns list.

Table 4. Column Arrangement dialog box parameters (Sheet 2 of 2)

Parameter	Description
Move Up	To change the column order in the current sequence, click **Move Up** and **Move Down**. To move a displayed column to the left in the sequence, select the column in the Displayed Columns list and click **Move Up**. The application displays only the columns that are listed in the Displayed Columns list. The left-to-right order of the columns for a particular sequence corresponds to the top-to-bottom order in the Displayed Columns list.
Move Down	To change the column order in the current sequence, click **Move Up** and **Move Down**. To move a displayed column to the right in the sequence, select the column in the Displayed Columns list and click **Move Down**. The application displays only the columns that are listed in the Displayed Columns list. The left-to-right order of the columns for a particular sequence corresponds to the top-to-bottom order in the Displayed Columns list.

Export Sequence Dialog Box

Use the Export Sequence dialog box to select the columns of the sequence that you want to export and to designate the path and file name of the exported file. The Xcalibur data system creates an exported comma-separated-value text file with a .csv file extension by inserting a column separator character between each sequence field. This file format can be read by a text editor program or a spreadsheet program.

The list separator character used for an exported sequence file is specified in the Regional Options page of the Settings Properties dialog box.

❖ To change the list separator character

1. Choose **Start > Settings > Control Panel**. The Control Panel window opens.
2. Double-click **Regional and Language Options.** The Regional and Language Options dialog box opens.
3. On the Regional Options page, click **Customize**. Click the **Numbers** tab.
4. Type a comma in the List Separator box.

Each country has a default list separator. For example, the list separator for United States is the comma. In this case, the application places a comma between each sequence field in the exported file. You can change the list separator to any alphanumeric character. However, avoid using characters that cannot be distinguished from characters used in the sequence text fields, such as alphabetic characters, because they result in unreadable (invalid) files. The most common list separators are the comma (,) and the semicolon (;).

Because you can modify the Study, Client, Laboratory, Company, and Phone columns using the User Labels dialog box, the application changes these fields in the exported file to User Label 1, User Label 2, User Label 3, User Label 4, and User Label 5, respectively.

The Export Sequence dialog box provides the following check boxes so that you can include or not include any or all of the sequence columns:

Table 5. Export Sequence dialog box parameters

Parameter	Description
Export to File	Designate the path and file name of the exported file. The file is saved with a .csv extension.
Select Columns to Export	This area contains check boxes that correspond to columns in the Sequence Table. To include the data in a column, select the corresponding check box. You can choose from the following columns: • Sample Type • File Name • Sample ID • Path • Inst Meth • Proc Meth • Position • Inj Vol • Level • Sample Wt • Sample Vol • ISTD Corr Amt • Dil Factor • Comment • Sample Name • User Labels 1-5
All	Click **All** to select all the check boxes.
Clear	Click **Clear** to clear all the check boxes.

Fill Down Dialog Box

Use this dialog box to fill selected rows of selected columns with duplicate text entries or appropriately sequenced number entries. First select the cells in the row that you want to copy from as well as all of the cell rows that you want to copy to. The Xcalibur data system highlights the cells you select.

Note The rows that you select must be contiguous (neighboring rows in the sequence). The row that you want to copy from must be the top row of the cells selected. The application then activates the Fill Down command on the Edit menu and the Fill Down button on the toolbar.

The data system performs its fill down function on any sequence columns or headings that you select.

Table 6. Fill Down dialog box parameters

Parameter	Description
Select Columns	Specify columns in the sequence. This area contains check boxes that correspond to columns in the Sequence Table. To include the data in a column, select the corresponding check box. You can choose from the following columns: • Sample Type • Sample Name • File Name • Sample ID • Path • Instrument Method • Processing Method • Calibration File • Position • Injection Volume • Level • Sample Weight • Sample Volume • ISTD Corr Amt • Dil Factor • Comment • User Labels 1-5
All	Click **All** to select all the check boxes.
Clear	Click **Clear** to clear all the check boxes.
Fill Rows *X* to __ using row *Y*	This box indicates which row you are using to fill down (*Y*), and which rows will be filled (*X* to the value that you enter).

Go To Line Number Dialog Box

Use the Go To Line Number dialog box to go to a specified row of the current sequence. This feature is extremely useful if you are reviewing or modifying a long sequence.

Table 7. Go To Line Number dialog box parameters

Parameter	Description
Row	Enter the row of the sequence that you want to display. To move to a specific row, type the row number (the number of the leftmost column of the sequence) in the Row box and click **OK**. The application selects the selected sequence row.

Import Sequence Dialog Box

Use the Import Sequence dialog box to select the columns of the sequence that you want to import and to designate the path and file name of the imported file. The Xcalibur data system only reads comma-separated-value text files with a .csv file extension. This file format can be read by a text editor program or a spreadsheet program. If you try to import any other file extension or file type, the application generates an invalid file message.

In addition, the list separator character used in the file that you import must be the same as the current list separator character set in your computer operating system.

IMPORTANT The list separator character used for an exported sequence file is specified on the Regional Options page of the Regional and Language Options dialog box.

❖ **To change the list separator character**

1. Choose **Start > Settings > Control Panel**. The Control Panel window opens.
2. Double-click **Regional and Language Options.** The Regional and Language Options dialog box opens.
3. On the Regional Options page, click **Customize**. Click the **Numbers** tab.
4. Type a comma in the List Separator box.

Each country has a default list separator. For example, the default list separator for United States is the comma. In this case, The application places a comma between each sequence field in the exported .csv file. You can change the list separator to any alphanumeric character. However, avoid using characters that cannot be distinguished from the characters used in the sequence text fields, such as alphabetic characters, because they result in unreadable (invalid) files. The most common list separators are the comma (,) and the semicolon (;).

Use the Import From File box or the Browse button to designate the path and file name of the imported sequence file.

The Import Sequence dialog box provides the following check boxes so that you can include or not include any or all of the sequence columns in the imported list. Click **All** to select all the column check boxes. Click **Clear** to clear all the column check boxes.

Table 8. Import Sequence dialog box parameters

Parameter	Description
Import From File	Designate the path and file name of the imported .csv file.
Select Columns to Import	This area contains check boxes that correspond to columns in the Sequence Table. To include the data in a column, select the corresponding check box. You can choose from the following columns: • Sample Type • Name • Sample ID • Path • Inst Meth • Proc Meth • Position • Inj Vol • Level • Sample Wt • Sample Vol • ISTD Corr Amt • Dil Factor • Comment • Sample Name • User Labels 1-5
All	Click **All** to select all the check boxes.
Clear	Click **Clear** to clear all the check boxes.

New Sequence Template Dialog Box

The New Sequence Template dialog box provides a quick and simple way to create a new sequence. Select the following options in the General, Samples, Bracket Type, Calibration, and QC areas. The Xcalibur data system creates a new sequence for you and displays it in the Sequence Setup view.

Table 9. New Sequence Template dialog box parameters (Sheet 1 of 7)

Parameter	Description
General	
Base File Name	Enter the base file name that the application uses when it creates the raw file for the sequence. The data system places additional information describing a specific sample at the end of this name so that each sample in your list has a unique identification. This file is stored in the location defined in the Path box. To assign a base file name that is used for all samples in the new sequence, type the name in the Base File Name box.
Starting Number	Type a number for the Xcalibur application to add as a suffix to the name you entered into the Base File Name box. This creates the File Name of the new sequence. For example, if the Base File Name is ABC and you enter 50 into the Starting Number box, the data system creates the new sequence with File Name ABC50 as the first file name.
Path	Enter the path to the raw files that the application creates for the sample data. Xcalibur creates these files with a .raw extension. A path contains the drive and one or more folders. A typical path can look like: C:\Xcalibur\DATA. To find and select the path, double-click Browse to the right of the Path box. The Select Data Directory dialog box opens. The Xcalibur application enters the path in the Path box. You can also type the path in the Path box.
Instrument Method	Enter the path and instrument method that you will use to analyze the samples in the active sequence. A path contains the drive and one or more folders. A typical path for an instrument method file named ABC can look like: C:\Xcalibur\methods\ABC. To find and select the path, double-click Browse to the right of the Instrument Method box. The Select Instrument Method dialog box opens. The data system enters the path and file name in the Inst Method box for you. You can also type the path and file name in the Instrument Method text box.
Processing Method	Enter the path and processing method for the Xcalibur data system to use to process the samples in the active sequence. A path contains the drive and one or more folders. A typical path for a processing method file named ABC can look like: C:\Xcalibur\methods\ABC. To find and select the path, double-click Browse to the right of the Processing Method box. The Select Processing Method dialog box opens. The application enters the path and file name in the Processing Method box. You can also type the path and file name in the Processing Method text box.

Table 9. New Sequence Template dialog box parameters (Sheet 2 of 7)

Parameter	Description
Calibration File	Enter the location for the calibration file. This box is only active if you select the None option in the Bracket Type area. If you select None as a bracket type, a Calibration File column is included in the sequence. This column contains the full path and name of the current default calibration file. A path contains the drive and one or more directories. A typical path for a calibration file named ABC can look like this: C:\Xcalibur\methods\ABC. Enter the path and file name of the calibration files that you will use to process the samples in the current sequence using bracket type None. • To append the new calibration data to a previously created calibration file, click Browse located to the right of the Calibration File box. The Select Calibration File dialog box opens. From this dialog box, browse to the calibration file. When you click OK, The data system enters the path and file name (without the .XCAL file extension) in the Calibration File box. When you create a new sequence, the application includes this path and calibration file name in the Calibration File column of the sequence. To display this column, choose Change > Column Arrangement and add the Calibration File column to the Columns Displayed box. • To create a new calibration file, type the path and calibration file name that you will use when the data system creates the calibration file during batch processing. Do not include the .XCAL file extension.
Samples	
Number of Samples	Select the number of Unknown samples for the Xcalibur application to include in the new sequence. The data system divides and orders these samples among the number of calibration sets or brackets that you select. For example, if you specify 2 calibration sets and 5 samples, The application orders the new sequence as follows: • Calibration Standard Samples (Set 1) • Unknowns (3 Samples) • Calibration Standard Samples (Set 2) • Unknowns (2 Samples)
Tray Type	View or change the tray type that must be installed in your autosampler when the current sequence is used. To change the tray type, click the arrow to display the list of vial tray type options. Select one of the vial tray types. The application displays your new selection in the Tray Type list.

Table 9. New Sequence Template dialog box parameters (Sheet 3 of 7)

Parameter	Description
Injections Per Sample	Type the number of replicate samples for the Xcalibur data system to include in the new sequence. The application divides and orders these samples among the number of calibration sets or brackets that you select. For example, if you specify 2 calibration sets, 5 samples, and 2 replicates per sample, the application orders the new sequence as follows: • Calibration Standard Samples (Set 1) – Unknown 1, Injection 1 – Unknown 1, Injection 2 – Unknown 2, Injection 1 – Unknown 2, Injection 2 – Unknown 3, Injection 1 – Unknown 3, Injection 2 • Calibration Standard Samples (Set 2) – Unknown 4, Injection 1 – Unknown 4, Injection 2 – Unknown 5, Injection 1 – Unknown 5, Injection 2
Initial Vial Position	Select the first vial position in the new sequence. The Xcalibur default first vial position is 1. To start at another position, type the position number into the Initial Vial Position box. For example, if you type 50, the data system numbers the first three vial positions as follows: • 50 • 51 • 52
Re-Use Vial Numbers	Define whether to reuse or not reuse vial positions for replicate samples. If you select the Re-Use Vial Positions check box, the data system creates a sequence where the replicate Calibration, QC, Blank, and Unknown samples are drawn from the same vial. If you clear the Re-Use Vial Positions check box, the application creates a sequence in which each sample is drawn from a different vial.

Table 9. New Sequence Template dialog box parameters (Sheet 4 of 7)

Parameter	Description
Base Sample ID	Type an alphanumeric prefix to the Sample ID that the data system applies to each sample in the new sequence. The data system starts Sample ID numbering at 001. For example, if you type AB12 in the Base Sample ID box, the application numbers the first five samples as follows: • AB12001 • AB12002 • AB12003 • AB12004 • AB12005
Bracket Type	
None	Select if the sequence contains no brackets. The Xcalibur data system processes the samples in the sequence in the order they are submitted. Real-time samples are processed before reprocessed samples. The application orders your Unknown, Blank (optional), Calibration (optional), and QC (optional) samples in the following repetitive sequence: • Calibration Blank Sample • Calibration Samples • Calibration Blank Sample • QC Samples • QC Blank Sample • Unknown Samples

Table 9. New Sequence Template dialog box parameters (Sheet 5 of 7)

Parameter	Description
Open	Select if the sequence contains one open bracket. You can place samples and calibrants in any order. Calibration samples are processed before Unknown and QC samples. The data system orders your Unknown, Blank (optional), Calibration (optional), and QC (optional) samples in the following repetitive sequence: • Blank Sample • Calibration Samples • Blank Sample • QC Samples • QC Blank Sample • Unknown Samples • Calibration Blank Sample • Calibration Samples • Calibration Blank Sample
Non-Overlapped	Select if the sequence contains one or more non-overlapped brackets. The data system orders your Unknown, Blank (optional), Calibration (optional), and QC (optional) samples in the following repetitive sequence: • Calibration Blank Sample • Calibration Samples • Calibration Blank Sample • QC Samples • QC Blank Sample • Unknown Samples • Calibration Blank Sample • Calibration Samples • Calibration Blank Sample

Table 9. New Sequence Template dialog box parameters (Sheet 6 of 7)

Parameter	Description
Overlapped	Select if the sequence contains one or more overlapped brackets. The data system orders your Unknown, Blank (optional), Calibration (optional), and QC (optional) samples in the following repetitive overlapping-bracket sequence: • Calibration Blank Sample [Bracket 1] • Calibration Samples [Bracket 1] • Calibration Blank Sample [Bracket 1] • QC Samples [Bracket 1] • QC Blank Sample [Bracket 1] • Unknown Samples [Bracket 1] • Calibration Blank Sample [Bracket 1, 2] • Calibration Samples [Bracket 1, 2] • Calibration Blank Sample [Bracket 1,2] • QC Samples [Bracket 2] • QC Blank Sample [Bracket 2] • Unknown Samples [Bracket 2] • Calibration Blank Sample [Bracket 2, 3] • Calibration Samples [Bracket 2, 3] • Calibration Blank Sample [Bracket 2, 3]....
Calibration	
Add Standards	Add calibration samples to the sequence. Define these samples in the processing method selected in the General area. Select a processing method before you include Calibration samples in the sequence. Click the Add Standards check box to activate the boxes and check boxes of the Calibration area.
Number of Calibration Sets	Enter the number of calibration sets that you want in your new sequence. This box is only active when you have selected Bracket Type: None. The valid range of values is 1 to 10.
Number of brackets	Enter the number of calibration sets that you want in your new sequence. This box is only active when you have selected Bracket Type: Non-Overlapped or Bracket Type: Overlapped. The valid range of values is 1 to 10.
Injections Per Level	Enter the number of replicate calibration standard samples that are to be run at each defined calibration level. The application groups replicate calibration samples in the new sequence. The valid range of values is 1 to 10.

Table 9. New Sequence Template dialog box parameters (Sheet 7 of 7)

Parameter	Description
Add Blanks	Add blanks to your sequence. If you select this check box, the data system places one blank before and one blank after each series of calibration standard samples in the new sequence.
Fill In Sample ID for Standards	Have the Xcalibur application fill in the Calibration Sample ID in the new sequence. This information is defined in the processing method for each calibration standard level.
QC	
Add QCs	Add quality control samples to the sequence. Define these samples in the processing method selected in the General area. You must select a processing method before you can include Quality Control samples in the sequence. Click the Add QCs check box to activate the options and check boxes of the QC area.
After First Calibration Only	Have the Xcalibur application add a quality control sample only after the first group of calibration samples in the new sequence. The data system does not follow subsequent calibration sample sets with a quality control sample. This option is only active if you select the Add QCs check box.
After Every Calibration	Have the Xcalibur application add a quality control sample after every calibration sample set in the new sequence. This option is only active if you select the Add QCs check box.
Add Blanks	Add Quality Control (QC) blanks to your sequence. If you select this check box, the data system places one blank after each series of quality control samples in the new sequence.
Fill In Sample ID for QCs	Have the Xcalibur data system fill in the Quality Control (QC) Sample ID in the new sequence. This information is defined in the processing method for each quality control level.

Run Sequence Dialog Box

Use this dialog box to select acquisition options and processing action options for the sequence. Finally, start the sequence.

The list of rows selected from the sequence must be consecutive. For example, you can run samples 1 through 10 by using the Run Sequence dialog box once. To skip sample 4, for example, run samples 1 through 3 and samples 5 through 10 by using the Run Sequence dialog box twice. The first time, select samples 1 through 3 and the second time, select samples 5 through 10.

Table 10. Run Sequence dialog box parameters (Sheet 1 of 5)

Parameter	Description
Acquisition Options	
Instrument	View all of the instruments that have been configured for operation as Xcalibur devices. ❖ **To add an instrument that is not on the list** 1. Click **Cancel** to close the Change Instruments In Use dialog box. 2. Close down all running Xcalibur programs. 3. Choose **Start > Programs > Thermo Foundation 1.0 > Instrument Configuration**. The Instrument Configuration view opens. 4. Select and configure the instrument. When you reopen the Change Instruments In Use dialog box, the newly configured instrument appears on the Instrument list.
Start Instrument	**Note** This read-only list can have either one "Yes" in one of the instrument rows or all blanks in all instrument rows (no "Yes" entries). The instrument that is usually chosen as the Start Instrument is the autosampler because this instrument controls when a run starts. In this case, all other instruments used for the sequence submission have a Yes value for In Use because these instruments are waiting for a contact closure event to start operation. When all devices used in the run receive this status, the Start Instrument initiates the run. To change the start instrument, click the Change Instrument button. The Change Instruments In Use dialog box opens.

Table 10. Run Sequence dialog box parameters (Sheet 2 of 5)

Parameter	Description
Start When Ready	Determine whether or not the Xcalibur data system starts the Run Sequence as soon as you do one of the following: Click OK in the Run Sequence dialog box, click  in the toolbar, or choose **Actions > Start Analysis** in the Home Page window. If you select the Start When Ready parameter, the data system places the sequence in the processing queue as soon as you click OK. If you select the Priority Sequence check box, the application runs the current sequence before the next sequence in the queue. If you clear the Priority Sequence check box, the application runs the current sequence after the last sequence in the queue. If you clear the Start When Ready parameter, the sequence is not put in the queue when you click OK. The application puts the sequence in the queue when you choose **Actions > Start Analysis**. If you select the Priority Sequence check box, it runs the current sequence run before the next sequence in the queue. If you clear the Priority Sequence check box, the application runs the current sequence after the last sequence in the queue.
Change Instruments	Change the status of Instruments In Use or select a different start instrument.
Instrument Method	
Start Up/Browse	Specify the instrument (.meth) file that will run at system startup.
Shut Down/Browse	Specify the instrument (.meth) file that will run at system shutdown.
Programs	
Pre Acquisition/ Browse	Specify the executable (.exe or .bat program) that will run before data acquisition.
Post Acquisition/ Browse	Specify the *.exe or .bat program that will run after data acquisition.
Run Synchronously	Run Pre Acquisition and Post Acquisition programs either synchronously (in series) or asynchronously (in parallel) with data collection. To run programs synchronously, the Run Manager waits until the program(s) can be run as a Pre Acquisition and/or Post Acquisition. To run programs asynchronously, the Xcalibur data system runs the program at the same time as data acquisition. For example, you can perform file conversions with XConvert.exe while you are taking data. In this case, the Pre Acquisition and Post Acquisition terminology does not apply.

Table 10. Run Sequence dialog box parameters (Sheet 3 of 5)

Parameter	Description
Pre Acquisition/ Post Acquisition	Run the Pre Acquisition program displayed in the Pre Acquisition box either synchronously (in series) or asynchronously (in parallel) with data collection. If you select the Pre Acquisition check box, the data system runs the program synchronously. In this case, the Run Manager waits until the Pre Acquisition program can be run prior to data acquisition. For example, to switch the divert valve before a run, you can select a synchronous Pre Acquisition program; or, to convert data from one data type to another data type while you are acquiring data, you can program and select a Post Acquisition program. If you clear the Pre Acquisition check box, the data system runs the program asynchronously. For example, you can use the XConvert.exe program to perform file conversions from one data type to another data type during processing. If the Post Acquisition check box is clear, the program displayed in the Post Acquisition box is run asynchronously. For example, you can perform operations that do not involve taking data. To change the current program or macro name in the command line, double-click the Program or Macro Name box to open the Open dialog box and select a program or macro. The application displays the new program or macro name. You can also type the command line. The sections below describe some of the macros that the Xcalibur data system understands. **Macro Arguments** You can use the following macros in the command line: %R: Provides the current raw file %I: Provides the instrument method name %S: Provides the sequence name %V: Provides the vial (or well) number in the Position column of the sequence %%: Provides a single % character in the run line

Table 10. Run Sequence dialog box parameters (Sheet 4 of 5)

Parameter	Description
Pre Acquisition/ Post Acquisition (continued)	Example using the XConvert.exe program: To convert the current file (myfile.raw) from Xcalibur (.raw) file format to ANDI (.cdf) file format and copy it to the current default data directory, use the following command line: Convert /DA /SL %R where: DA indicates that the destination file (D) is to be ANDI format (A) SL indicates that the source file (S) is an Xcalibur .raw file (L) %R is the macro argument for the current raw file Refer to the Command Line Format section for more examples. **Printing Raw Files and Layout Files**: You can include a command line argument that launches a program and prints a specified file to the default printer (/p) or a specified printer (/pt).
After Sequence Set System	
On	Select to leave the system in the On state when the current sequence is completed. Select the On state to run another sequence without waiting. All power and flows are maintained at operational levels. This option has the same effect as choosing Actions > Devices On from the Home Page window.
Standby	Put the system in the Standby state when the current sequence is completed. Select the Standby state to run another sequence with only a short delay of time. Depending on the instrument, this state turns gas and liquid flows off, but maintains heaters and other subsystems in an On state so that there is no warm-up time required when you change to the On state. This option has the same effect as choosing Actions > Devices Standby from the Home Page window.
Off	Put the system in the Off state when the current sequence is completed. The Off state indicates that all power to the instrument, which can be controlled by Xcalibur software, is turned off. This includes power to all heaters and most but not all subassemblies. This option has the same effect as choosing Actions > Devices Off from the Home Page window. **CAUTION** The Off state does not guarantee that all voltages are turned off, nor does it indicate that all heated components are at room temperature. To perform maintenance on an instrument, refer to the hardware manual for your instrument.

Table 10. Run Sequence dialog box parameters (Sheet 5 of 5)

Parameter	Description
User	Enter up to 24 alphanumeric characters that can be used for future reference to identify the operator who ran the sequence. To supply reference text that identifies the operator, type the text in the User box.
Run Rows	View or change the currently selected sequence rows that you want to run. You can change the range in the Run Rows box by closing the Run Sequence dialog box, selecting different sequence rows, and reopening the Run Sequence dialog box. You can also enter the range in the box.
Priority Sequence	Process the selected sequence as soon as possible or after the last sequence in the current queue. If the data system is processing a sample, the priority sequence is run next, ahead of all other samples in the processing queue. If the data system is not processing a sample, the priority sequence runs immediately. The application does not cancel a currently running sample or sequence to accommodate a priority sequence. When you open the Run Sequence dialog box, this check box is clear. To make sure the selected priority sequence runs as soon as possible, select the Priority Sequence check box.
Processing Actions	
Quan	Activate processing actions that you have defined in the Quan view of the Processing Setup window.
Qual	Activate processing actions that you have defined in the Qual view of the Processing Setup window.
Reports	Activate XReport Report Wizard processing actions that you have defined in the Reports view of the Processing Setup window.
Programs	Launch software programs for the samples selected from the current sequence and displayed in the Process Rows box. Define programs in the Programs view of the Processing Setup window. Using this option requires a valid processing method and a valid raw file. To activate this batch processing option, select the Programs check box.
Create Quan Summary	Print a summary of the quantitation data. Select the Create Quan Summary check box to print a summary. You can also activate these functions with the Create Quan Summary Spreadsheet processing actions of the Batch Reprocess Setup dialog box.

Transfer Row Information Dialog Box

Use the Transfer Row Information dialog box to copy information from one sample row of the sequence to other rows in the sequence that have either the same position in the autosampler tray or the same sample ID. The sequence list is scanned from top to bottom. When the Xcalibur data system finds repeated sample IDs or position numbers in the list, it copies the row information from the first occurrence of the sample ID or position to all rows with same sample ID or position number. The File Name and Sample Type columns are not affected.

Table 11. Transfer Row Information dialog box parameters

Parameter	Description
Match by Sample ID	Select this option to copy the row information from the first occurrence of a Sample ID to all rows that have the same Sample ID.
Match by Position	Select this option to copy the row information from the first occurrence of a position to all rows that have the same position.

Tray Selection Dialog Box

You can use the Fill Down Dialog Box to correct the vial position numbering sequence or to select the appropriate tray type. The tray types displayed in the list are all of those that are available for the currently configured autosampler.

Use the Tray Selection dialog box to select a tray for the currently configured autosampler.

Note If the configured autosampler does not provide a selection of sample trays, you will not see this dialog box; instead, the following message appears:

The configured autosampler does not offer any selection of trays.

Tray types are associated with and are a part of each sequence method. If you change your autosampler, you might obtain the following message:

Invalid autosampler vial position. A valid example vial position would be [ ].

The format inserted in the [ ] above corresponds to the currently configured autosampler.

Table 12. Tray Selection dialog box parameter

Parameter	Description
Select Tray Type with which to Validate Sequence	View or change the currently selected autosampler tray. To use a different tray, click the down arrow to display all available trays for the currently configured autosampler. Click the tray that you want to use to select it. The application displays the selected tray in the list box.

User Labels Dialog Box

Use the User Labels dialog box to define the caption labels of the five boxes that are located under the toolbar on the right side of the Sequence Setup view. These caption labels and the information entered in their respective boxes are stored with the sequence. In addition to the sequence heading labels, these heading labels also appear in the Export Sequence dialog box, Import Sequence dialog box, Fill Down dialog box, and Column Arrangement dialog box.

You can return the headings to their default values by clicking **Default Headings**. The default column headings are as follows:

- Heading 1: Study
- Heading 2: Client
- Heading 3: Laboratory
- Heading 4: Company
- Heading 5: Phone

To change a heading, select the current heading and type over it. If you don't want to use a heading, delete the text and leave the box blank. When all of the heading captions are correct, click **OK**.

C

Processing Setup Reference

Use Processing Setup to create a processing method for automated batch analysis. You can also modify existing methods, save method files, and restore existing method files.

Sequence Setup uses the processing method to initiate processing for qualitative and quantitative data, create reports, and run additional programs or macros (such as shutdown procedures).

Contents

Processing Setup

The Processing Setup window consists of a view bar, title bar, menu bar, toolbar, workspace, status bar, and access to Help.

Title Bar

Title bar components:

- The application name – Processing Setup
- The active view (Quan, Qual, Reports, or Programs)
- The active page (for example, Identification)
- The name of the opened method, or ‘Untitled’ if a new file has not yet been saved
- The selected type of calibration, internal or external standard

Processing Setup Toolbar

The toolbar contains shortcuts for frequently used menu commands. The Processing Setup toolbar buttons vary depending on the view currently displayed:

- Qual and Quan Views
- Reports and Programs Views

Qual and Quan Views

Table 13. Qual and Quan views

Button		Description
	New	Open a new file with the appropriate extension.
	Open	Find and open an existing file.
	Save	Enter audit information about the active file and select the location (disk and directory) where you want to save it.
	Open Raw File	Find and open a file with a .raw extension that already exists.
	Print	Select a report template for printing the processing method.
	Zoom Out Y	To show more data, zoom out on the Y-axis by a factor of two (2) to show more data. For example, you can change the Y-axis range from 0–25 to 0–50.
	Zoom In Y	To show more detail, zoom in on the Y-axis by a factor of two (2) from the current baseline to show more detail. For example, you can change the Y-axis range from 0–100 to 0–50.
	Auto Range	View the chromatogram, which is normalized from the minimum to the maximum signal. This option is suggested for PDA and UV data.
	Normalize	Normalize the intensity scale of the data display to a fixed range on the Y-axis. For example, from 0–25% to 0–100%.
	Zoom In X	To show more detail, zoom in on the X-axis by a factor of two (2) to show more detail. For example, you can change the X-axis range from 0–20 to 5–15.
	Zoom Out X	To show more data, zoom out on the X-axis by a factor of two (2) from the center to show more data. For example, you can change the X-axis range from 7–12.5 to 5–15.
	Display All Data	View all data on the X-axis or all text in a report. For example, you can change the X-axis range from 7.5–12.5 to 0–20.
	Reset Scaling to Full Scale	Reset chromatogram and spectrum scaling to the default values.
	Product Help	View Xcalibur Help and the Processing Setup window Help.

Reports and Programs Views

Table 14. Reports and Programs views

Button		Description
	New	Open a new file with the appropriate extension.
	Open	Find and open an existing file.
	Save	Enter audit information about the active file and select the location (disk and directory) where you want to save it.
	Open Raw File	Find and open an existing file (**.raw** extension).
	Print	Select a report template for printing the processing method.
	Product Help	View Xcalibur Help and Help for the Processing Setup window.

View Bar

From the View bar, located to the left of the window, click one of the four buttons to do the following:

View the Quan View.

View the Qual View.

View the Reports View.

View the Programs View.

Menus

Menus in the Processing Setup window:

- File Menu
- Zoom Menu (Qual and Quan views only)
- GoTo Menu
- View Menu
- Options Menu
- Help Menu

File Menu

Table 15. Processing Setup window – File menu

Command	Description
New 	Create a new file with an appropriate extension.
Open 	Open an existing file.
Save 	Update audit information, name a file, and specify file storage location (disk and directory).
Save As	View audit information about the active file, rename a file, and select a storage location (disk and directory).
Open Raw File 	Open an existing file (.raw extension).
Summary Information	Read, modify, or delete summary information about the active file.
Change Dataset Name	Select a dataset from a predefined list of names. The text of this menu item might be different if the administrator chose to use another name for a dataset. For example, this menu item might be *Change Job Name*.
Audit Trail	View all auditable events and changes made to data files in the current view.
Import Method	Locate (drive and directory) and open a stored method file.
Print Setup	Select the following printing options: printer, form, orientation, and one- or two-sided printing.
Print 	Select a report template for printing the processing method.
Most Recently Used Files	View the paths and names of the four most recently used files. These are located above the Exit command.
Exit	Close the active window. If you exit before clicking OK from an active dialog box, you receive a message about saving your changes.

GoTo Menu

Table 16. Processing Setup window – Go To menu

Command	Description
Instrument Setup	View and change setup details for the MS detector (mass spectrometer), LC, syringe pump, autosampler, divert valve, and Xcalibur analysis options.
Quan Browser	Reprocess raw files and create individual result files.
Qual Browser	Display and work with raw files containing spectra and chromatograms.
Library Browser	Display and work with reference spectra, spectra exported from Qual Browser, or spectra appended to libraries during qualitative processing.
Xcalibur Home Page	Open the Home Page window if it is closed or view the Home Page window if it is already open. This command closes the Instrument Setup window to make sure all instrument methods are closed when you run analyses that use these methods from the Home Page window. Use the Home Page window to access all Xcalibur functions and features.

Help Menu

Table 17. Processing Setup window – Help menu

Command	Description
Processing Setup Help	View Xcalibur Help and Help for the Processing Setup window.
View Help	View Xcalibur Help and Help for the current view.
Help On Current Item	View Help for the currently view or dialog box.
Xcalibur Help	View Xcalibur Help.
Glossary	View the glossary.
How To Use Help	View instructions on how to use the Help viewer.
About Processing Setup	View the installed version number of the Processing Setup program and the Thermo Fisher Scientific copyright notice.

Options Menu

Commands in the Options menu of the Processing Setup window vary depending on whether the current view is Quan, Qual, or Reports and Programs.

Table 18. Options menu for the Quan view

Command	Description
Identification	Choose void time and baseline parameters for peak identification purposes.
Masses	Change the default settings for mass tolerance and mass precision.
Standard Dilution	Enter calibration level information for non-internal standard components. This command appears in the menu only if you have defined at least one target compound on the Calibration page and you have the Levels page displayed.
Chromatography By	Choose between GC and LC detection modes. GC detection provides Ion Ratio confirmation options on the Quan Detection page.
Spectrum	Choose a low intensity cutoff percentage for peak detection purposes. This command appears in the menu only if you have selected the GC Chromatography mode in the Chromatography By dialog box and the Spectrum option (in the Peak Detection dialog box) on the Detection page.
Calibration By	Select internal or external calibration for the current processing method.
Delete [Component]	Remove a selected component from the processing method. The data system removes the component from the Components view.
Display	Change the style, color, labels, axes, and normalization of the Chromatogram and Spectrum Previews.
Settings	By default the application loads the most recently used method into Processing Setup at startup. You can change this option in the Settings dialog box and also configure the Xcalibur data system to display a raw file in the Chromatogram and Spectrum Previews at startup.
Enable Warnings	Turn on the display of warnings about operations and commands to change the processing method. To turn off warnings during a number of operations, select the **Don't Tell Me About This Again** check box in an information dialog box. If this menu command is unavailable, warnings are already enabled.

Table 19. Options menu for the Qual view

Command	Description
Identification	Choose void time and baseline parameters for peak identification purposes.
Masses	Change the default settings for mass tolerance and mass precision.
Display	Change the style, color, labels, axes, and normalization of the Chromatogram and Spectrum Previews.
Settings	By default the data system loads the most recently used method into Processing Setup at startup. You can change this option in the Settings dialog box and also configure the Xcalibur data system to display a raw file in the Chromatogram and Spectrum Previews at startup.
Enable Warnings	Turn on the display of warnings about operations and commands that change the processing method. To turn off warnings during a number of operations, select the **Don't Tell Me About This Again** check box in an information dialog box. If this menu command is unavailable, warnings are already enabled.

Table 20. Options menu for the Reports and Programs view

Command	Description
Settings	By default, the application loads the most recently used method into Processing Setup at startup. You can change this option in the Settings dialog box and also configure the data system to display a raw file in the Chromatogram and Spectrum Previews at startup.
Enable Warnings	Turn on the display of warnings about operations and commands that change the processing method. To turn off warnings during a number of operations, select the **Don't Tell Me About This Again** check box in an information dialog box. If the menu command is unavailable, warnings are already enabled.

View Menu

Table 21. Processing Setup window – View menu

Command	Description
Quan	View the Quan view in the Processing Setup window.
Qual	View the Qual view in the Processing Setup window.
Reports	View the Reports view in the Processing Setup window.
Programs	View the Programs view in the Processing Setup window.
View Bar	View or hide the View bar.
Component List	View or hide the Component List. This command is available only in the Quan view.
Toolbar	View or hide the toolbar.
Status Bar	View or hide the Status bar.

Zoom Menu

Table 22. Processing Setup window – Zoom menu

Command		Description
	Zoom In Y	To show more detail, zoom in on the Y-axis by a factor of two (2) from the current baseline to show more detail. For example, you can change the Y-axis range from 0 to 100 to 0 to 50.
	Zoom Out Y	To show more data, zoom out on the Y-axis by a factor of two (2) to show more data. For example, you can change the Y-axis range from 0 to 25 to 0 to 50.
	Normalize	Normalize the intensity scale of the data display to a fixed range on the Y-axis. For example, from 0 to 25% to 0 to 100%.
	Zoom In X	To show more detail, zoom in on the X-axis by a factor of two (2) to show more detail. For example, you can change the X-axis range from 0 to 20 to 5 to 15.
	Zoom Out X	To show more data, zoom out on the X-axis by a factor of two (2) from the center to show more data. For example, you can change the X-axis range from 7.5 to 12.5 to 5 to 15.
	Display All	View all data on the X-axis or all text in a report. For example, you can change the X-axis range from 7.5 to 12.5 to 0 to 20.
	Reset Scaling	Reset scaling to full scale display.

Processing Dialog Boxes

Apply Changes? Dialog Box

The Apply Changes? warning dialog box opens in the Processing Setup window when you have made changes to the current page and attempt one of the following actions without first clicking OK or Cancel:

- Switch to another page
- Switch to another component in Quan View
- Switch to another View, using either the buttons in the View bar or the options on the View menu
- Change chromatography type (Options > Chromatography By)
- Change calibration type (Options > Calibration By)
- Click Close on the title bar
- Choose one of the following menu items:

  File > Open
  File > <most recently used file list>
  File > Save
  File > Save As
  File > Exit
  File > Import Method
  File > New
  Options > Standard Dilution

Before proceeding with any of these actions, you must apply or undo the page modifications.

Table 23. Apply Changes? dialog box parameters (Sheet 1 of 2)

Parameter	Description
Don't Tell Me About This Again	Suppress the display of the Apply Changes? dialog box. In the future when the data system displays this dialog box, it will treat changes according to your final selection in the dialog box: • If you click Yes, the data system applies changes if validation is successful and continues with your selected action. If validation fails, the data system stops your intended action and returns you to Processing Setup to correct or discard changes made to the page. • If you click No, the data system discards all changes and continues with your selected action. To restore the dialog box, choose Options > Enable Warnings.

Table 23. Apply Changes? dialog box parameters (Sheet 2 of 2)

Parameter	Description
Buttons	
Yes	Apply changes to a Processing Setup page before proceeding with your selected action. When you click the button, the data system applies the changes and reports any errors. If an error occurs, the data system stops your intended action and returns you to Processing Setup so that you can correct or discard the changes. If you also select the Don't Tell Me About This Again check box, then in the future the data system • Does not display the Apply Changes? dialog box. • Applies changes automatically. • If a validation error occurs, stops your intended action and returns you to Processing Setup. If the validation is successful, the data system applies the changes and proceeds with your selected action.
No	Discard unapplied changes to a Processing Setup page before proceeding with your selected action. All changes are discarded, as though you pressed Cancel on the page. The Xcalibur application continues with your selected action. If you also select the Don't Tell Me About This Again check box, then in the future the data system • Does not display the Apply Changes? dialog box. • Always discards unapplied changes automatically and without prompting. • Proceeds with your intended action. You must click OK to apply changes made on a page; otherwise, they will be discarded.

Avalon Event List Dialog Box

Use the Avalon Event List dialog box to specify advanced component detection criteria in the Quan view or the Qual view of Processing Setup. Use these additional criteria if the standard detection criteria do not provide the desired results.

Table 24. Avalon Event List dialog box parameters (Sheet 1 of 3)

Parameter	Description
Event List	To detect peaks, Avalon uses the settings for initial events and user-defined timed events that are in the Event list. To calculate values for initial events, open a raw file, and then make the chromatogram view active. Click **Auto Calculate Initial Events** to update the Event list. ❖ **To change the settings in the Event list** 1. Click the row you want to change and enter any revised settings in the boxes below the list. 2. Click **Change** to automatically update the Event list, both here and on the Detection page, and automatically update the chromatogram display. There are seven initial entry integration events, identified by the initial value setting in the Time column. These are the default integration events that the Avalon integration algorithm requires. You can change the value of an initial entry integration event, but you cannot delete it or change its time value.
Time	View either the specified term initial value or a value of time in minutes. ❖ **To change the settings in the Event list** 1. Click the row you want to change and enter any revised settings in the boxes below the list. 2. Click **Change** to automatically update the Event list, both here and on the Detection page, and automatically update the chromatogram display.
Event	View descriptions of the detection parameters for initial events and timed events. You cannot change an event in the Event column associated with an initial value in the Time column. ❖ **To change a timed event in the Event column** 1. Highlight the row in the Event list and click the Event list box (below the Event list) to display the available events. 2. Select an event and Click **Change** to automatically update the Event list, both here and on the Detection page, and automatically update the chromatogram display.

Table 24. Avalon Event List dialog box parameters (Sheet 2 of 3)

Parameter	Description
Event (continued)	**Event Types** **Start/End Threshold**: Directly related to the RMS noise in the chromatogram, this parameter specifies the start and end threshold, the fundamental control used for peak detection. **Bunch Factor**: The number of points grouped together during peak detection. It controls the bunching of chromatographic points during integration and does not affect the final area calculation of the peak. The Bunch Factor must be an integer between 1 and 6; a larger bunch factor groups peaks into clusters. **Area Threshold**: Controls the area cutoff. The Xcalibur data system does not detect any peaks with a final area less than the area threshold. This control is in units of area for the data. **P-P Resolution**: The peak-to-peak resolution threshold controls how much peak overlap must be present before two or more adjacent peaks create a peak cluster. Peak clusters have a baseline drop instead of valley-to-valley baselines. This is specified as a percent of peak height overlap. **Negative Peaks**: Automatically resets after a negative peak has been found. **Tension**: Controls how closely the baseline should follow the overall shape of the chromatogram. A lower tension traces the baseline to follow changes in the chromatogram more closely. A high baseline tension follows the baseline less closely, over longer time intervals. Set in minutes. **Tangent Skim**: For fused peaks that are significantly different in size, the tangent skim method provides a method of allocating area to the various peaks. By default, the data system chooses the tallest peak in a cluster as the parent (solvent). You can also identify which peak in the cluster is the parent. The application detects tangent skim peaks on either side (or both sides) of the parent peak. Tangent skim automatically resets at the end of the peak cluster. The Threshold and Bunch Factor parameters are the most important ones in controlling peak detection.
Value	View values associated with initial events and timed events. The range of allowed values is specific to each event. To change a value in the Value column, select the row in the Event list and enter the revised setting in the Value box (below the Event list). Click **Change** to automatically update the Event list, both here and on the Detection page, and to automatically update the chromatogram display.

Table 24. Avalon Event List dialog box parameters (Sheet 3 of 3)

Parameter	Description
Event List Entry	
Time	View the currently highlighted entry from the Time column in the Event list. The time entry for events that are listed with an Initial Value cannot be changed. ❖ **To change a timed event in the Event column** 1. Highlight the row in the Event list and click the list below it to display the available events. 2. Select an event. Click **Change** to automatically update the Event list, both here and on the Detection page, and automatically update the chromatogram display.
Event	View the currently highlighted entry in the Event column of the Event list. You cannot change an event that is listed with an Initial Value in the Time column. To change the description of a timed event, select a description from the list. Click **Change** to automatically update the Event list, both here and on the Detection page, and automatically update the chromatogram display. Click here to view Event types.
Value	View the currently highlighted entry from the Value column of the Event list. The range of factors allowed for each value is specific to each event. To change the value setting for an event, enter the new factor in the box. Click **Change** to automatically update the Event list, both here and on the Detection page, and to automatically update the chromatogram display.
Buttons	
Add	Add a time/event/value entry for a timed event to the Event list. When you click Add, the data system automatically changes the peak detection results with the added specification in the currently selected chromatogram.
Delete	Remove a highlighted event from the Event list. You cannot delete initial values.
Change	Update a highlighted time/event/value entry in the Event list. When you click **Change**, the data system automatically changes the peak detection results with the added specification in the currently selected chromatogram. For initial events, you can change only the values (not the events).
Exit	Close the active window. If you exit before clicking **OK** from an active dialog box, the data system prompts you to save your changes.

Calibration and Quantitation Flags Dialog Box

Use the Calibration and Quantitation Flags dialog box to set the threshold values for calibration and quantitation flags. The Xcalibur data system reports these flags in results files, in printed reports, and in Quan Browser.

Table 25. Calibration and Quantitation Flags dialog box parameters

Parameter	Description
Calibration Flag	
R-Squared	Specify a flag threshold for the goodness of fit of the calibration curve. The application calculates a coefficient of determination (R-squared) whenever it computes a calibration curve. If the value is less than the R-squared threshold, the application sets the R-squared flag in the results file to true; otherwise it is set to false.
Quantitation Flags	
Detection Limit	Specify a flag threshold for the limit of detection. If the quantified component concentration is less than the Detection Limit threshold, the data system sets the Detection Limit flag in the results file to true; otherwise, it is set to false.
Linearity Limit	Specify a flag threshold for the linearity limit. If the quantified component concentration is less than the Linearity Limit threshold, the data system sets the Linearity Limit flag in the results file to true; otherwise, it is set to false.
Quantitation Limit	Specify a flag threshold for the limit of quantitation. If the quantified component concentration is less than the Quantitation Limit threshold, the data system sets the Quantitation Limit flag in the results file to true; otherwise, it is set to false.
Carry Over Limit	Specify a flag threshold for the carry over limit. If the quantified component concentration is less than the Carry Over Limit threshold, the data system sets the Carry Over Limit flag in the results file to true; otherwise, it is set to false.

Calibration Options Dialog Box

Use the Calibration Options dialog box to choose the calibration mode and method of calculating relative standard deviations. Your choice of calibration mode affects the options available on the Quan View Calibration page. The default calibration mode is Internal Standard.

Table 26. Calibration Options dialog box parameters

Parameter	Description
Calibration By	
Internal Standard	Configure the Xcalibur data system for internal standard calibration. If you select this option, the data system displays the ISTD options on the Calibration Page for Quan View.
External Standard	Configure the Xcalibur data system for external standard calibration. If you select this option, the data system hides the ISTD options on the Calibration Page for Quan View.
%RSD Calculation Method	
Use Calculated Amounts	Force the analysis routines to compute the standard deviation based on calculated amounts for each standard. This is the behavior of previous Xcalibur versions.
Use Response Values	Force the analysis routines to use the response value (area or height) for each sample when computing the standard deviation. When using response values in analyses, a change in the calibration curve has no effect on the standard deviation or the %RSD values since the response is not affected.

Chromatography Options Dialog Box

Use the Chromatography Options dialog box to choose the chromatography detection mode. Your choice affects the options available on the Quan View Detection page. the data system attempts to detect the type of instrument connected when you run the instrument for the first time and makes this the default type. If the application fails to determine the type of instrument, the system displays the Default Chromatography Type Dialog Box.

Table 27. Chromatography Options dialog box parameters

Parameter	Description
Chromatography By	
GC	Configure Quan view for GC chromatography peak detection to configure the Spectrum Option on the Detection page in Quan view.
LC	Configure Quan view for LC chromatography peak detection.

Correction for Isotope Contribution Dialog Box

Use the Correction for Isotope Contribution dialog box to correct for an impurity in the internal standard compound that elutes at the same time as the target compound or to correct for an impurity in the target compound that elutes at the same time as the internal standard.

Table 28. Correction for Isotope Contribution dialog box parameters (Sheet 1 of 2)

Parameter	Description
Contribution of ISTD to Target Compound (%)	This box displays the ratio: ISTD [impurity]/ISTD [pure] Where: ISTD [impurity] is an impurity compound in the internal standard reagent that elutes at the same time as the target compound. ISTD [pure] is the pure internal standard compound. To determine this ratio experimentally, analyze the ISTD reagent using the same method used for quantitation of the target compound. Use the respective peak areas or heights to determine the ratio of impurity to pure compound. The valid range is 0.00 to 100.00 percent. To change the impurity ratio, type a new value in the Contribution of ISTD to Target Compound box. The data system uses this ratio as the value x in the following impurity correction expressions: ISTD [corr] = [ISTD [obs] – y TM [obs]]/[1 – yx] TM [corr] = [TM [obs] – x ISTD [obs]]/[1 – yx] Where: ISTD [corr] is the corrected amount of internal standard. ISTD [obs] is the apparent amount of ISTD, as measured by the data system at the retention time for ISTD. This peak consists of ISTD [corr] + TM [impurity]. TM [corr] is the corrected amount of the target molecule. TM [obs] is the apparent amount of TM, as measured by the data system at the retention time for TM. This amount consists of TM [corr] + ISTD [impurity]. See Contribution of Target Compound to Internal Standard box for a complete description of the variable: y. For additional information, see “Correcting for Calibration Impurities” on page 61.

Table 28. Correction for Isotope Contribution dialog box parameters (Sheet 2 of 2)

Parameter	Description
Contribution of Target Compound to ISTD (%)	This box displays the ratio: TM [impurity]/TM [pure] Where: TM [impurity] is an impurity compound in the target molecule reagent that elutes at the same time as the internal standard. TM [pure] is the pure target compound. To determine this ratio experimentally, analyze the TM reagent using the method to be used for its quantitation. Use the respective peak areas or heights to determine the ratio of impurity to pure compound. The valid range is 0.00 to 100.00 percent. To change the impurity ratio, type a new value in the Contribution of Target Compound to Internal Standard box. The Xcalibur data system uses this ratio as the value y in the following impurity correction expressions: ISTD [corr] = [ISTD [obs] – y TM [obs]]/[1 – yx] TM [corr] = [TM [obs] – x ISTD [obs]]/[1 – yx] Where: ISTD [corr] is the corrected amount of internal standard. ISTD [obs] is the apparent amount of ISTD, as measured by the application at the retention time for ISTD [pure]. This peak consists of ISTD [corr] + TM [impurity]. TM [corr] is the corrected amount of the target molecule. TM [obs] is the apparent amount of TM, as measured by the application at the retention time for TM [pure]. This amount consists of TM [corr] + ISTD [impurity]. See Contribution of Internal Standard to Target Compound box for a complete description of the variable: x. For additional information, see "Correcting for Calibration Impurities" on page 61.

Data Flags Dialog Box

Use the Data Flags dialog box to set flags for peak area and height thresholds. Flags are reported as true or false in the results file. If you set a value to 0.0, the flag is always reported as false.

Table 29. Data Flags dialog box parameters

Parameter	Description
Area Threshold	Enter a value for the Area Threshold Data Flag. This is an absolute value of peak area (in counts ´ seconds). If a quantified peak has an area less than the threshold value, the Area Threshold flag is set to true.
Height Threshold	Enter a value for the Height Threshold Data Flag. This is an absolute value of peak height (in counts). If a quantified peak has a height less than the threshold value, the Height Threshold flag is set to true.

Default Chromatography Type Dialog Box

The first time you run Processing Setup, the Xcalibur application attempts to determine whether it is connected to an LC or GC instrument. If the data system fails to detect the type of instrument, the Default Chromatography Type dialog box opens where you can set the default chromatography detection mode. Your choice affects the options available on the Quan View Detection page:

- Select the GC option if you want GC detection modes in Quan View.
- Select the LC option if you want LC detection modes in Quan View.

You can change the chromatography type at any time using the Chromatography Options Dialog Box.

Table 30. Default Chromatography Type dialog box parameters

Parameter	Description
Chromatography By	
GC	Select this option to configure Quan view for GC chromatography peak detection. This turns on the Spectrum Option on the Detection page in Quan view.
LC	Select this option to configure Quan view for LC chromatography peak detection.

Details of Selected Analysis Dialog Box

Use the Details of Selected Analysis dialog box to review information for each task in the Processing Queue.

Table 31. Details of Selected Analysis dialog box parameters

Parameter	Description
File	View the file name you have selected from the Processing Queue Manager window. To change the selected file, click **Continue** to return to the Processing Queue Manager window so that you can select a different file. Then, choose **Analysis > Details** to reopen the Details of Selected Analysis dialog box with the new file selected.
Status	View Xcalibur processing status of the file in the File box. For example this box might display: Creating Summary. This box is read only.
Submitted	View the date as Month/Day/Year and time in hours:minutes:seconds that the file displayed in the File box was submitted for processing. For example this box might display: 02/22/99 16:24:15. This box is read only.
From	View the source of the batch processing task submission. For example this box might display: Reprocessing. This box is read only.
Actions	View the current Xcalibur actions and their status. For example the box might display: Create Summary, In Progress. This box is read only.
Continue	Close the Details of Selected Analysis dialog box and return to the Processing Queue Manager window. Then, you can select another file to review in the Details of Selected Analysis dialog box, or you can monitor the processing queue.

Genesis Advanced Detection Options Dialog Box

Use the Genesis Advanced Detection Options dialog box to specify advanced component detection criteria. Use these additional criteria if the standard detection criteria do not provide the desired results.

Table 32. Genesis Advanced Detection Options dialog box parameters (Sheet 1 of 2)

Parameter	Description
Peak Edge Detection	
Set a chromatogram peak edge detection criterion that uses the peak signal-to-noise cutoff value to assist in the detection of a peak edge. This test assumes an edge of a peak is found when the baseline adjusted height of the edge is less than the ratio of the baseline-adjusted apex height and the peak signal-to-noise cutoff ratio.	
Peak S/N Cutoff	View or change the signal-to-noise below which the data system defines the peak edge. For example, if the signal-to-noise at the apex is 500 and the Peak S/N Cutoff value is 200, the data system defines the right and left edges of the peak when the S/N reaches a value less than 200. The valid range is 50.0 to 10000.0. To change the cutoff value, type the new value in the Peak S/N Cutoff box. When you click **OK**, the data system applies the new peak detection parameter.
Report Noise As	
RMS	Calculate noise as RMS.
Peak To Peak	Calculate noise as peak-to-peak.
Valley Detection	
Use a valley detection approximation method to detect unresolved peaks. This method drops a vertical line from the apex of the valley between unresolved peaks to the baseline. The intersection of the vertical line and the baseline defines the end of the first peak and the beginning of the second peak.	
Rise (%)	View or change the percentage that the peak trace can rise above the baseline after passing through a minimum (before or after the peak). If the trace exceeds this rise percentage, the data system applies valley detection peak integration criteria. The data system applies this test to both the left and right edge of the peak. This criteria is useful for integrating peaks with long tails. The valid range is 0.1 to 500.0. To change the rise percentage, type the new value in the Rise Percentage box. When you click **OK**, the data system applies the new peak detection criteria.
Valley S/N	View or change the signal-to-noise criteria that the application uses for valley detection. The valid range is 1.0 to 100.0. To change the valley signal-to-noise criteria, type the new value in the Valley S/N box. When you click **OK**, the data system applies the new peak detection criteria.

Table 32. Genesis Advanced Detection Options dialog box parameters (Sheet 2 of 2)

Parameter	Description
Background Subtraction (For All Components)	
Minimize the contaminating effect of background on the peak identification process by performing background subtraction. The Xcalibur data system does the following: • Locates the lowest intensity scan in the Baseline and Noise window (as specified in the Identification Options dialog box) • Sums the specified Number of Scans in Background taken around the lowest scan • Normalizes this representative background spectrum • Subtracts the background spectrum from all scans in the detection window The data system periodically recalculates the representative background scan used for background subtraction to compensate for the possibility that the composition of the background can change over the course of a run.	
Number of Scans in Background	View or change the number of background scans used to determine the background. The valid range is 1 to 100. To change the number of background scans, type the new value in the Number of Scans in Background box. When you click **OK**, the data system applies the new baseline parameter.

Genesis Advanced Chromatogram Options Dialog Box

Use the Genesis Advanced Chromatogram Options dialog box to specify advanced criteria to detect your chromatographic peak. You can use these additional criteria if the standard detection criteria do not provide the desired results.

Table 33. Genesis Advanced Chromatogram Options dialog box parameters (Sheet 1 of 4)

Parameter	Description
Peak Identification	
Spectrum	Identify a peak using the maximizing masses technique. This technique is based on the assumption that each spectrum across a peak in a mass chromatogram contains one or more masses, *m/z* values, that are representative of the compound producing the peak. Assuming that there is no mass distortion across the apex of a peak, all masses rise, maximize, and fall in a consistent pattern. Noise by contrast is random: while noise at one *m/z* might increase, it is unlikely to occur consistently over multiple *m/z* values. You can then use this process to detect peaks in the presence of noise contamination. The Spectrum Option is only available when the selected Detector Type on the Qual Identification page is either MS or PDA. Also, if you have selected Spectrum detection and subsequently change the Detector Type to something other than MS or PDA, the data system automatically changes the detection mode to Highest Peak. If this option is selected, the data system keeps the setting only if the minimum number of masses is set to greater than one, or the minimum percentage of masses found is greater than zero.
Highest Peak	Specify using the highest peak for chromatogram peak identification. This option uses the Minimum Peak Height (S/N) parameter.
Minimum Mass Required	View or change the minimum number of masses that the data system should maximize simultaneously as a criteria for peak detection. The valid range is 1 to 999. To change the minimum number, type the new number in the Minimum Mass Required box.
Minimum Percent of Masses Found	View or change the minimum percent of masses that the data system should maximize simultaneously as a criteria for peak detection. The valid range is 0 to 100 percent. To change the minimum percent, type the new percent in the Minimum Percent of Masses Found box.
Minimum Peak Height	View or change the peak signal-to-noise criteria so that it is equal to or exceeds the criteria for peak detection. The application ignores all chromatogram peaks that have signal-to-noise values that are less than the Minimum Peak Height (S/N) value. To enter a peak signal-to-noise criteria, type the value in the Minimum Peak Height (S/N) box. The valid range is 0.0 (all peaks) to 999.0.

Table 33. Genesis Advanced Chromatogram Options dialog box parameters (Sheet 2 of 4)

Parameter	Description
Peak Edge Detection	
Peak Edge Detection	Set a chromatogram peak detection criteria that uses the peak signal-to-noise cutoff value to assist in peak edge detection. This test assumes an edge of a peak is found when the baseline adjusted height of the edge is less than the ratio of the baseline adjusted apex height and the peak signal-to-noise cutoff ratio.
Peak S/N Cutoff	View the signal-to-noise below which the data system defines the peak edge. For example, if the signal-to-noise at the apex is 500 and the Peak S/N Cutoff value is 200, the data system defines the right and left edges of the peak when the S/N reaches a value less than 200. The valid range is 50.0 to 10000.0. To change the cutoff value, type the new value in the Peak S/N Cutoff box. When you click **OK**, the data system applies the new peak detection parameter.
Report Noise As	
RMS	Specify that the Xcalibur application calculates noise as RMS.
Peak To Peak	Specify that the Xcalibur application calculates noise as peak-to-peak.
Peak Apex Detection	
Peak Apex Detection	The data system uses these parameters to detect multiple peaks. To detect multiple peaks, it slides a scan window across the chromatogram. The width of this window is specified in the number of scans in the Window Size box. When the maximizing masses conditions are met, the data system examines the region about this possible peak apex to determine whether or not the other peak identification criteria are satisfied. The Xcalibur application calculates a filter window to examine the corresponding scans for each scan window position as it slides along the mass chromatogram. Specify the width of the filter window in the Filter Width box.
Window Size	Enter a time window for the Refine spectrum enhancement method. The Refine algorithm applies the window across a chromatogram peak apex and uses it to search for the peak start and peak, end and to estimate the background noise. Set this parameter to the peak width.
Filter Width	View or change the number of scans included in the moving average across the peak apex detection Window Size parameter. A larger width tends to reduce the number of spurious peaks. The valid range is 1 to 3.

Table 33. Genesis Advanced Chromatogram Options dialog box parameters (Sheet 3 of 4)

Parameter	Description
Valley Detection	
Valley Detection	Use a valley detection approximation method to detect unresolved peaks. This method drops a vertical line from the apex of the valley between unresolved peaks to the baseline. The intersection of the vertical line and the baseline defines the end of the first peak and the beginning of the second peak.
Rise	View or change the percentage that the peak trace can rise above the baseline after passing through a minimum (before or after the peak). If the trace exceeds this rise percentage, the data system applies valley detection peak integration criteria. This test is applied to both the left and right edge of the peak. These criteria are useful for integrating peaks with long tails. The valid range is 0.1 to 500.0. To change the rise percentage, type a new value in the Rise Percentage box. When you click **OK**, the data system applies the new peak detection criteria.
Valley S/N	View or change the signal-to-noise criteria that the data system uses for valley detection. The valid range is 1.0 to 100.0. To change the valley signal-to-noise criteria, type the new value in the Valley S/N box. When you click **OK**, the data system applies the new peak detection criteria.
Background Subtraction	
Background Subtraction	Minimize the contaminating effect of background on the peak identification process. When you select background subtraction, the Xcalibur application: 1. Locates the lowest intensity scan in the Baseline and Noise window (as specified in the Identification Options dialog box). 2. Sums the specified Number of Scans in Background taken around the lowest scan. 3. Normalizes this representative background spectrum. 4. Subtracts the background spectrum from all scans in the detection window. The data system periodically recalculates the representative background scan used for background subtraction using the Background Recomputation Interval parameter. This is to compensate for the possibility that the composition of the background might change over the course of a run.
Background Recomputation Interval	To compensate for the possibility that the composition of the background might change over the course of a run, the data system periodically recalculates the representative background scan it uses for background subtraction. The Background Recomputation Interval is the time interval (in minutes) between these recalculations. To change the interval, type the new value in the Background Recomputation Interval box. The valid range is 0.5 to 10.0 minutes.

Table 33. Genesis Advanced Chromatogram Options dialog box parameters (Sheet 4 of 4)

Parameter	Description
Number of Scans in Background	View or change the number of background scans used to determine the background. The valid range is 1 to 100. To change the number of background scans, type the new value in the Number of Scans in Background box. When you click **OK**, the data system applies the new baseline parameter.

ICIS Advanced Parameters Dialog Box

Use the ICIS Advanced Parameters dialog box to specify advanced component detection criteria. Use these additional criteria if the standard detection criteria do not provide the desired results.

Table 34. ICIS Advanced Parameters dialog box parameters

Parameter	Description
Noise Method	
INCOS Noise	Use a single pass algorithm to determine the noise level. The ICIS peak detection algorithm uses this value.
Repetitive Noise	Use a multiple pass algorithm to determine the noise level. The ICIS peak detection algorithm uses this value. In general, this algorithm is more accurate in analyzing the noise than the INCOS Noise algorithm, but it takes longer.
RMS	Have the application calculate noise as RMS. By default, the data system uses Peak To Peak for the noise calculation. RMS is automatically selected if you determine the noise region manually.
Peak Parameters	
Min Peak Width	Type the minimum number of scans required in a peak. The valid range is 0 to 100 scans. The default value is 3 scans. The ICIS peak detection algorithm uses this value.
Multiple Resolution	Type the minimum separation in scans between the apexes of two potential peaks. This is a criterion to determine if two peaks are resolved. The valid range is 1 to 500 scans. The default value is 10 scans. The ICIS peak detection algorithm uses this value.
Area Tail Extension	Type the number of scans past the peak endpoint to use in averaging the intensity. The valid range is 0 to 100 scans. The default value is 5 scans. The ICIS peak detection algorithm uses this value.
Area Scan Window	Enter the number of scans on each side of the peak apex to be included in the area integration. The valid range is 0 to 100 scans. The default value of 0 scans specifies that all scans from peak start to peak end are to be included in the area integration. The ICIS peak detection algorithm uses this value.

Note This dialog box is available for a new processing method when ICIS is your current default. It is also available when Genesis or Avalon is your default, but the current processing method was previously created using the ICIS peak detection algorithm.

Identification Options Dialog Box

Use the Identification Options dialog box to adjust the parameters used by the Xcalibur data system to estimate baseline noise and to correct retention time assignments for void time.

Table 35. Identification Options dialog box parameters

Parameter	Description
Void Time	
Value	Type a value for the void time in minutes. The data system subtracts this time from the elution time of all recorded peaks to obtain the correct relative retention times.
First Peak	Select this option to set the void time to the retention time of the first detected peak. The data system processes data using the specified peak detection parameters to obtain the retention time of the first peak. This peak is assumed to be non-retained and its retention time is subsequently used as the void time. The application subtracts this time from the elution time for all remaining peaks to estimate the correct relative retention time.
Baseline	
Baseline and Noise Window	View the time range that the data system applies to each peak before calculating the baseline and baseline noise within it. If the window is too small, then the data system cannot calculate the baseline for a peak correctly because the baseline will be positioned up the sides of the peak. To ensure accurate noise calculation, the window should include the base width of the peak and an appreciable amount of baseline.
Baseline Noise Tolerance	View or change a value that controls how the baseline is drawn in the noise data. The higher the baseline noise tolerance value, the higher the baseline is drawn through the noise data. The valid range is 0.0 to 100.0. To change the baseline noise tolerance, type the new value in the Baseline Noise Tolerance box. When you click **OK**, the data system applies the new peak integration parameter.
Minimum Number of Scans in Baseline	View or change the minimum number of scans that the data system uses to calculate a baseline. A larger number includes more data in determining an averaged baseline. The valid range is 2 to 100.0. To change the minimum number of scans, type the new value in the Minimum Number of Scans in Baseline box. When you click **OK**, the data system applies the new baseline parameter.

Print Dialog Box

Use the Print dialog box to choose a report template for printing a processing method. Select a report template in the Report template box.

Note The Xcalibur data system prints a processing method using the name of the person who is currently logged in and requesting the print job, *not* the name of the person who developed the method. Similarly, the date and time on the printed report will be the time of the print job, not the time that the method was created.

Table 36. Print dialog box parameter

Parameter	Description
Report Template	This box displays the pathname of the default processing method report template, for example: c:\xcalibur\templates\default processing method report.doc. You can specify a new template, either by typing directly in the box or by browsing using the browse button. If you select a new template and then click **OK** on the Print dialog box, the template becomes the new default processing method report template.

Search List Dialog Box

Use the Search List dialog box to specify the names and search order of libraries used by the processing method.

Table 37. Search List dialog box parameters (Sheet 1 of 2)

Parameter	Description
Library Lists	
Available Libraries	View the libraries that are currently excluded from searching during processing. the application regenerates this list when you open the dialog box.
Selected Libraries	View the libraries that are currently included in searches during processing. The order of the libraries defines the order in which they are searched by the application. The application generates the Available Libraries list dynamically so this box always lists the libraries stored on your system. The Selected Libraries list is contained in the processing method and might contain libraries that are not present on your system. When you click OK, the application checks the Selected Libraries list and displays a warning dialog box if any of these are not available on your system.

Table 37. Search List dialog box parameters (Sheet 2 of 2)

Parameter	Description
Buttons	
Add	Transfer a library from the Available Libraries list box to the Selected Libraries list box. This appends the library in the search list.
Remove	Transfer a library from the Selected Libraries list box to the Available Libraries list box.
Top	Move a library in the Selected Libraries list box to the top of the list (first in the search order).
Up	Move a library in the Selected Libraries list box up one position (earlier in the search order).
Down	Move a library in the Selected Libraries list box down one position (later in the search order).
Bottom	Move a library in the Selected Libraries list box to the final position (last in the search order).

Settings Dialog Box

Use the Settings dialog box to customize Processing Setup. By default, the Xcalibur data system loads the most recently used method into Processing Setup at startup. You can change this option and also configure the application to open a raw file in the Chromatogram and Spectrum previews when you open a processing method.

Table 38. Settings dialog box parameters

Parameter	Description
Startup Mode	
Startup Mode	Specify whether Processing Setup opens with a new method or with the most recently used method.
Load Last Processing Method	Specify that the application will load the most recently used method when you start a Processing Setup session.
Create New Processing Method	Specify that the application will start a new method when you begin a Processing Setup session.
Auto-Open Raw File	
Auto-Open Raw File	Specify whether or not Processing Setup opens a raw file in the chromatogram and spectrum cells when you open a method. For this feature to operate, a raw file must be associated with the method. This association occurs when the method is saved—if a raw file is present, it is saved with the method.
On	Configure Processing Setup so that a raw file is automatically opened with each method. The data system populates the chromatogram and spectrum cells with the raw file associated with the method when it was last saved.
Off	Configure Processing Setup so that no raw file is opened when you open a method.

Spectrum Options Dialog Box

Use the Spectrum Options dialog box to set a low intensity cutoff (%) value for use in Spectrum detection mode.

Table 39. Spectrum Options dialog box parameter

Parameter	Description
Low Intensity Cutoff (%)	View the intensity cutoff value used by the Spectrum detection method. If you use a spectrum from a raw file to generate the Spectrum *m/z* – intensity (%) grid, the data system discards any ions in the selected range that have an intensity below the cutoff value. The data system only activates the Spectrum menu option and Spectrum Options dialog box when you select the Spectrum radio button on the Detection page in GC chromatography mode.

Standard Dilution Dialog Box

Use the Standard Dilution dialog box to enter calibration level information for all target components.

Table 40. Standard Dilution dialog box parameters (Sheet 1 of 2)

Parameter	Description
Target Compound Components	View the total number of target compound components defined in the processing method, including ISTD and non-ISTD component types.
Selected Components	View the selected number of non-ISTD components for Standard Dilution.
Base Amounts	
Component	View the names of all the defined target components included in the standard dilution, calibration level calculations in your method.
Amount	View or change the calibration amounts of the target components used for each target compound. To enter a calibration amount, type the value in the Amount box at the appropriate level. You must provide a value for each listed Component for the data system to be able to calculate the calibration levels.
Dilution Factors	
Cal Level	View or change defined calibration levels. The Xcalibur application can accommodate up to 50 calibration levels. To enter a calibration level, type the new name in the appropriate Cal Level box (32 characters maximum). To delete a Cal Level row, click the numbered tile to the left of the row. The application highlights the row. Press **DELETE**. The application transfers these Cal Level values to the Cal Level column of the Calibration Levels table on the Levels page for each component.

Table 40. Standard Dilution dialog box parameters (Sheet 2 of 2)

Parameter	Description
Dilution	View or change the stock dilution factors for each calibration level. To enter a dilution factor, type the value in the appropriate Dilution box. The value must be greater than 0.00000001 and less than or equal to 1. In calculating the calibration level amount for each component, the data system multiplies the Dilution factor with the Base Amount value. The result is transferred to the corresponding Amount box in the Calibration Levels table on the Levels page for the component. The application repeats this procedure for all Calibration Levels and all components.

Processing Views

Click the appropriate link for information about processing views.

- Qual View
  - Identification Page for Qual View
  - Spectrum Enhancement Page for Qual View
  - Library Search Options Page for Qual View
  - Library Search Constraints Page for Qual View
  - Peak Purity Page for Qual View
- Quan View
  - Identification Page for Quan View
  - Detection Page for Quan View
  - Calibration Page for Quan View
  - Levels Page for Quan View
  - System Suitability Page for Quan View
  - Peak Purity Page for Quan View
- Programs View
- Reports View

Qual View

Use the Qual view of the Processing Setup window to set up a method for qualitative processing. For processing qualitative data, the Xcalibur data system identifies peaks and can submit a representative mass spectrum of each chromatogram peak to the Library Browser (NIST MS Search) for matching against reference spectra. You can choose various spectrum enhancement and library search options.

The Qual view consists of a Menu bar, Toolbar, and Qual view pages. This view also provides access to Xcalibur Help.

Menus

File Menu | View Menu | Zoom Menu
Options Menu | GoTo Menu | Help Menu

Toolbar

Processing Setup Toolbar

Qual View Pages

- Identification Page for Qual View
  - Avalon Identification Page for Qual View
  - ICIS Identification Page for Qual View
  - Genesis Identification Page for Qual View
- Spectrum Enhancement Page for Qual View
- Library Search Options Page for Qual View
- Library Search Constraints Page for Qual View
- Peak Purity Page for Qual View

Buttons

Qual view pages feature OK and Cancel buttons. These are enabled only if you change one or more parameters on the page; otherwise, they are unavailable. When you change or edit a parameter, do one of the following:

- To apply the changes to the current processing method, click **OK**. The data system reports any validation errors.
- To undo all changes made to the page and revert to the previously applied values, click **Cancel**.

Note that these actions do not affect the saved version of the processing method. This can only be modified by choosing **File > Save**.

The application displays the Apply Changes? Dialog Box if you attempt to change pages, views, or programs without applying or discarding changes. Use this dialog box to apply or discard the changes before continuing with your intended action.

Chromatogram and Spectrum Previews

The Chromatogram and Spectrum previews display the chromatogram and spectrum from the currently opened raw file. Initially, the application displays the spectrum corresponding to the apex scan of the first detected peak. If no peak has been detected in the Chromatogram preview, the spectrum for the first scan in the raw file appears.

These previews are available on the following pages:

- Identification, Detection, and Peak Purity pages for Quan View
- Identification, Spectrum Enhancement, and Peak Purity pages for Qual View

You can use the Chromatogram preview, together with the Spectrum preview, to assess the effects of processing parameters. You can also use the Chromatogram preview to set the retention time Range window in the Identification page for Qual View. You can also use the Spectrum preview in the Qual view to do the following:

- Set Mass Ranges on the Identification page
- Combine parameters on the Spectrum Enhancement page

Methods of rescaling the chromatogram displayed in the preview:

- Toolbar buttons
- Zoom menu commands
- The cursor

Important points to note:

- The cursor action is always applied to the pinned cell.
- Within an active cell, cursor actions rescale the chromatogram shown in the preview.

Identification Page for Qual View

Use the Identification page for Qual View to specify the type of chromatogram the processing method uses during qualitative processing. You can also adjust peak detection and identification criteria.

The application displays the version of this page (ICIS, Genesis, or Avalon) that corresponds to your current default peak detection algorithm: ICIS, Genesis, or Avalon.

Avalon Identification Page for Qual View

Use the Avalon Identification page for Qual View to specify the type of chromatogram to be used by the processing method during qualitative processing. You can also adjust peak detection and identification criteria for the Avalon peak detection algorithm.

Table 41. Avalon Identification page for Qual view parameters (Sheet 1 of 8)

Parameter	Description
Detector	
Type	View or change the currently selected detector type: • MS • Analog • A/D Card • PDA • UV To change the detector type, click the arrow to display the list of detector types. Click the required detector type.
Peak Detect	View or change the Xcalibur peak detection algorithms. ❖ **To select an algorithm** 1. Enter a name in the **Name** box. 2. Click the **Peak Detect** list to display the algorithm names. 3. Select an algorithm and click **OK**. The application recalculates the current data using the specified algorithm. It changes the default parameters for peak detection to those specific to that algorithm.
Delay	Enter a delay time (in minutes) to synchronize analog or digital data with MS scans. The Delay value compensates for any difference (negative or positive) in the arrival time of eluents at the UV and MS detectors. The valid range is –5.0 to +5.0 minutes.

Table 41. Avalon Identification page for Qual view parameters (Sheet 2 of 8)

Parameter	Description
Filter	View or change the current scan filter for the active file of extension .raw. You can use a scan filter to specify that processing is to be applied to a subset of the scans in a raw file. To apply a different scan filter, select a new filter from the scan filter list (most common method), select a new filter from the list and edit the scan filter, or type a new scan filter command string in the box using the scan filter format. To select from the list of scan filters used to create the raw file, click the arrow on the box to display the scan filter options. Click one of the scan filters. The data system displays the scan filter in the Filter box. This scan filter example: c full ms [26.8–251] finds all scans in a raw file that have the following properties: centroid data Scan Mode: Full Scan Power: MS Product Ion Mass Range: *m/z* 26.81 to 251.00

Table 41. Avalon Identification page for Qual view parameters (Sheet 3 of 8)

Parameter	Description
Trace	From the three Trace lists, to specify the type of chromatogram you want to use for data processing, select 1. A basic chromatogram type, for example, TIC, from the first list. 2. A logical operator: + or – from the second list. Your selection of an operator activates. 3. The third list for you to select a second chromatogram type to add to, or subtract from, the first type. For example, Mass Range. The list includes the valid remaining trace types. You can use trace combinations to subtract from a chromatogram the contributions from a solvent or noise. Combinations are limited to traces of the same type. For MS scans, valid trace types are TIC, Mass Range, and Base Peak. For Analog data, the application supports up to four channels (labeled Analog 1–4). For data from an A/D Card, the application supports four channels (labeled A/D Card Ch 1–4). For PDA data, valid trace types are Wavelength Range, Total Scan, or Spectrum Maximum. For UV detector data, the application supports four channels (labeled Channel A–D). Click the following for valid combinations. • Valid MS Trace Combinations • Valid Analog Trace Combinations • Valid A/D Card Trace Combinations • Valid PDA Trace Combinations • Valid UV Trace Combinations
Mass	View or change the mass range for the Mass Range trace type. the application displays this box when you select a Mass Range trace type or a TIC ± Mass Range trace combination for an MS detector type. To change the range or to add a new range, type the range in the box. The valid range depends on the configured detector. The format is *LowMass–HighMass*. For example, for the range *m/z* 123 through 456, type **123–456**. You can sum up to 50 mass ranges by entering mass ranges or single mass values separated by your computer list separator character. To view or set the list separator character, see "Changing the List Separator Character."

Table 41. Avalon Identification page for Qual view parameters (Sheet 4 of 8)

Parameter	Description
Mass 1	View or change the mass range for the first trace type. The application displays this box when you select a Mass Range ± Mass Range trace combination for an MS detector type. To change the range or to add a new range, type the range in the box. The valid range depends on the configured detector. The format is *LowMass–HighMass*. For example, for the range *m/z* 123 through 456, type **123–456**. You can sum up to 50 mass ranges by entering mass ranges or single mass values separated by your computer list separator character. To view or set the list separator character, see "Changing the List Separator Character."
[Mass] 2	View or change the mass range for the second trace type. The application displays this box when you select a Mass Range ± Mass Range trace combination for an MS detector type. To change the range or to add a new range, type the range in the box. The format is *LowMass–HighMass*. For example, for the range *m/z* 123 through 456, type **123–456**. You can sum up to 50 mass ranges by entering mass ranges or single mass values separated by your computer list separator character. To view or set the list separator character, see "Changing the List Separator Character."
BP	View or change the mass value for the base peak. The application displays this box when you select a Base Peak trace for an MS detector type. To change the base peak mass, type the value in the box.
MR	View or change the mass range for the second Mass Range trace type. The application displays this box when you select a Base Peak ± Mass Range trace combination for an MS detector type. To change the range or to add a new range, type the range in the box. The format is *LowMass–HighMass*. For example, for the range *m/z* 123 through 456, type **123–456.**

Table 41. Avalon Identification page for Qual view parameters (Sheet 5 of 8)

Parameter	Description
Wavelength	View or change the wavelength range for the Wavelength Range or Spectrum Maximum trace type. Xcalibur displays this box when you select one of the following trace combinations for a PDA detector type: • Spectrum Maximum • Wavelength Range • Total Scan – Wavelength Range To change the range or to add a new range, type the range in the box. The valid range depends on the configured detector. The format is *LowWavelength–HighWavelength*. For example, for the range *m/z* 123 through 456, type **123–456**. You can sum up to 50 wavelength ranges by entering ranges or single values separated by your computer list separator character. To view or set the list separator character, see "Changing the List Separator Character."
Wavelength 1	View or change the wavelength or wavelength range for the first trace type. The application displays this box when you select one of the following trace combinations for a PDA detector type: • Wavelength Range ± Wavelength Range • Spectrum Maximum ± Wavelength Range To change the range or to add a new range, type the range in the box. The valid range depends on the configured detector. The format is *LowWavelength–HighWavelength*. For example, for the range *m/z* 123 through 456, type **123–456**. You can sum up to 50 wavelength ranges by entering ranges or single values separated by your computer list separator character. To view or set the list separator character, see "Changing the List Separator Character."
[Wavelength] 2	View or change the wavelength or wavelength range for the second trace type. The application displays this box when you select one of the following trace combinations for a PDA detector type: • Wavelength Range ± Wavelength Range • Spectrum Maximum ± Wavelength Range To change the range or to add a new range, type the range in the box. The valid range depends on the configured detector. The format is *LowWavelength–HighWavelength*. For example, for the range *m/z* 123 through 456, type **123–456**. You can sum up to 50 wavelength ranges by entering ranges or single values separated by your computer list separator character. To view or set the list separator character, see "Changing the List Separator Character."

Table 41. Avalon Identification page for Qual view parameters (Sheet 6 of 8)

Parameter	Description
Selected Retention Time Window	
Selected Retention Time Window	Use the Ranges box to define the detection window for qualitative processing.
Range	Enter a time span to limit qualitative processing. Qual processes a peak only if its apex retention time lies in the range. The valid range is 0.1 to 999.0 minutes. To change the time window or to enter a new time window, type the number of seconds in the Range box. Type an asterisk (*) to represent the full chromatogram range of the active raw file.
Avalon Peak Integration	
Avalon Peak Integration	View or change peak integration criteria. These parameters are used by the Avalon peak detection algorithm. To change the settings in the Event list, click **Advanced** to display the Avalon Event List Dialog Box.
Smoothing Points	Determine the degree of data smoothing to be performed on the active component peak prior to peak detection and integration. The valid range is any odd value from 1 (no smoothing) through 15 (maximum smoothing). To smooth your component peak data prior to integration, type a value in the Smoothing Points box. See also the "Avalon Detection Page for Quan View" on page 201 and the "Genesis Detection Page for Quan View" on page 208.
Event List	
Event List	To detect peaks, Avalon uses the settings for initial events and user-defined timed events that are in the Event list. To calculate values for initial events, open a raw file, and then make the chromatogram view active. Click **Auto Calculate Initial Events** to update the Event list. ❖ **To change the settings in the Event list** 1. Click **Advanced** to display the Avalon Event List Dialog Box, containing an Event list that you can edit. 2. Highlight the row you want to change and enter any revised settings in the boxes below the list. 3. Click **Change** to automatically update the Event list, both here and on the Detection page, and automatically update the chromatogram display. There are seven initial entry integration events, identified by the initial value setting in the Time column. These are the default integration events required by the Avalon integration algorithm. You can change the value of an initial entry integration event, but you cannot delete it or change its Time value.

Table 41. Avalon Identification page for Qual view parameters (Sheet 7 of 8)

Parameter	Description
Time	This column contains either the term *initial value* or a value of time in minutes. ❖ **To change the time of a timed event** 1. Click **Advanced** to display the Avalon Event List Dialog Box, containing an Event list that you can edit. 2. Highlight the row in the Event list and enter the revised setting in the Time box (below the Event list). 3. Click **Change** to automatically update the Event list, both here and on the Detection page, and automatically update the chromatogram display.
Event	View or change descriptions of the detection parameters for initial events and timed events. You cannot change an event in the Event column associated with an initial value in the Time column. ❖ **To change a timed event in the Event column** 1. Click **Advanced** to display the Avalon Event List Dialog Box, containing an Event list that you can edit. 2. Highlight the row in the Event list, and click the Event list to display the events options. 3. Select an event, and then Click **Change** to automatically update the Event list, both here and on the Detection page, and automatically update the chromatogram display.
Value	View or change values associated with initial events and timed events. The range of allowed values is specific to each event. ❖ **To change a value in the Value column** 1. Click **Advanced** to display the Avalon Event List Dialog Box, containing an Event list that you can edit. 2. Highlight the row in the Event list, and enter the revised setting in the Value box (below the Event list). 3. Click **Change** to automatically update the Event list, both here and on the Detection page, and automatically update the chromatogram display.

Table 41. Avalon Identification page for Qual view parameters (Sheet 8 of 8)

Parameter	Description
Auto Calculate Initial Events	Automatically estimate the initial values for peak detection. Open a raw file to select this button with the Event list of the Avalon peak detection algorithm. When you click the button, Avalon automatically estimates the initial values for the detection of peaks based on the data in the current raw file and displays those initial values in the Event list. Use this button to force Avalon to search for the best values of initial events that detect peaks in the data. The application does not change any timed event in the Event list when you click this button. Auto Calculate Initial Events determines initial values for the following events only: Start Threshold, End Threshold, Area Threshold, P-P [Resolution] Threshold, Bunch Factor, Negative Peaks, and Tension. You can also specify timed events for these events in the same Event list.
Limit Peaks	
Select Top Peaks	
Enable	Limit peak detection to a specified number based on either peak area or peak height.
Select by Area	Select the Area option to restrict detection to the most significant peaks based on area rather than height.
Select by Height	Restrict detection to the most significant peaks based on height rather than area.
Num to Select	Set the maximum number of peaks to be detected. The application selects the largest peaks based on intensity (height) or area.
Rel Peak Height Threshold	
Enable	Limit the list of detected chromatogram peaks to those exceeding the specified value, entered as a percentage of the most intense peak in the chromatogram.
% of Highest Peak	Enter a percentage threshold to limit the number of peaks submitted for further processing. The application discards any detected peaks with an intensity less than the threshold percentage of the most intense peak.
Buttons	
Save As Default	Validate and save the settings on the current page as default settings. The application uses these settings for all new processing methods. The software writes over the previous default values and cannot recover them.
Advanced	Set advanced peak identification and detection parameters. The Avalon peak detection algorithm uses these parameters, displayed in the Event list on the Detection page.

Valid MS Trace Combinations

This table shows the valid trace combinations available on the Trace lists. Your choice of combination affects other controls on the page as described in the Resulting Controls column.

Table 42. Valid MS trace combinations parameters

Trace 1	Operator	Trace 2	Resulting Controls
Mass Range	[blank]	[unavailable]	Mass (*m/z*) box
Mass Range	–	Mass Range	Mass1 (*m/z*) box 2 text box
Mass Range	+	Mass Range	Mass1 (*m/z*) box 2 text box
TIC	[blank]	[unavailable]	none
TIC	–	Mass Range	Mass (*m/z*) box
TIC	–	Base Peak	Mass (*m/z*) box
Base Peak	[blank]	[unavailable]	Mass (*m/z*) box
Base Peak	–	Mass Range	BP box MR text box
Base Peak	+	Mass Range	BP box MR text box
Neutral Fragment (MS/MS data only)	[unavailable]	[unavailable]	Mass

Valid Analog Trace Combinations

This table shows the valid trace combinations available in the Trace lists. The Mass Range/Wavelength Range control is unavailable.

Table 43. Valid Analog trace combinations parameters

Trace 1	Operator	Trace 2	Resulting Controls
Analog n ($1 \leq n \leq 4$)	[blank]	[unavailable]	None
Analog n ($1 \leq n \leq 4$)	–	Analog m ($1 \leq m \leq 4$, m /= n)	None
Analog n ($1 \leq n \leq 4$)	+	Analog m ($1 \leq m \leq 4$, m /= n)	None

Valid A/D Card Trace Combinations

This table shows the valid trace combinations available in the Trace lists when you have selected an A/D Card detector type. The Mass Range/Wavelength Range control is unavailable.

Table 44. Valid A/D Card trace combinations parameters

Trace 1	Operator	Trace 2	Resulting Controls
A/D Card Channel n ($1 \leq n \leq 4$)	[blank]	[unavailable]	None
A/D Card Channel n ($1 \leq n \leq 4$)	–	A/D Card Channel m ($1 \leq m \leq 4$, m /= n)	None
A/D Card Channel n ($1 \leq n \leq 4$)	+	A/D Card Channel m ($1 \leq m \leq 4$, m /= n)	None

Valid PDA Trace Combinations

This table shows the valid trace combinations available in the Trace lists when you have selected a PDA detector type in the Type list box on the Identification page of Qual or Quan views. Your choice of combination affects other controls on the page as described in the Resulting Controls column.

Table 45. Valid PDA trace combinations parameters

Trace 1	Operator	Trace 2	Resulting Controls
Wavelength Range	[blank]	[unavailable]	Wavelength (nm) box
Wavelength Range	+	Wavelength Range	Wavelength1 (nm) box 2 text box
Wavelength Range	–	Wavelength Range	Wavelength1 (nm) box 2 text box
Total Scan	[blank]	[unavailable]	None
Total Scan	–	Wavelength Range	Wavelength (nm) box
Total Scan	–	Spectrum Maximum	Wavelength (nm) box
Spectrum Maximum	[blank]	[unavailable]	Wavelength (nm) box
Spectrum Maximum	+	Wavelength Range	Wavelength1 (nm) box 2 text box
Spectrum Maximum	–	Wavelength Range	Wavelength1 (nm) box 2 text box

Valid UV Trace Combinations

This table lists the valid trace combinations available in the Trace lists for UV detectors. The Mass Range/Wavelength Range control is unavailable.

Table 46. Valid UV trace combinations parameters

Trace 1	Operator	Trace 2	Resulting Controls
Channel n (A ≤ n ≤ D)	[blank]	[unavailable]	None
Channel n (A ≤ n ≤ D)	–	Channel m (A ≤ m ≤ D, m /= n)	None
Channel n (A ≤ n ≤ D)	+	Channel m (A ≤ m ≤ D, m /= n)	None

ICIS Identification Page for Qual View

Use the ICIS Identification page for Qual View to specify the type of chromatogram to be used by the processing method during qualitative processing. You can also adjust peak detection and identification criteria for the ICIS peak detection algorithm.

Table 47. ICIS Identification page for Qual view parameters (Sheet 1 of 7)

Parameter	Description
Detector	
Type	View or change the currently selected detector type: • MS • Analog • A/D Card • PDA • UV To change the detector type, click the arrow to display the list of detector types, and then click the required detector type.
Peak Detect	Select an Xcalibur peak detection algorithm. ❖ **To select an algorithm** 1. Click the **Peak Detect** list to display the algorithm names. 2. Select an algorithm and click **OK** to recalculate the data using that algorithm. The application changes the default parameters for peak detection to those specific to that algorithm.

Table 47. ICIS Identification page for Qual view parameters (Sheet 2 of 7)

Parameter	Description
Delay	Type a delay time (in minutes) to synchronize analog or digital data with MS scans. The Delay value compensates for any difference (negative or positive) in the arrival time of eluents at the UV and MS detectors. The valid range is –5.0 to +5.0 minutes.
Filter	View or change the current scan filter for the active file of extension .raw. You can use a scan filter to specify that processing is to be applied to a subset of the scans in a raw file. To apply a different scan filter, select a new filter from the scan filter list (most common method), select a new filter from the list and edit the scan filter, or type a new scan filter command string into the box using the scan filter format. To select from the list of scan filters used to create the raw file, click the arrow on the box to display the list. Click one of the scan filters. The application displays the scan filter in the Filter box. This scan filter example: c full ms [26.81–251] finds all scans in a raw file that have the following properties: centroid data Scan Mode: Full Scan Power: MS Product Ion Mass Range: *m/z* 26.81 to 251.00

Table 47. ICIS Identification page for Qual view parameters (Sheet 3 of 7)

Parameter	Description
Trace	Specify the type of chromatogram you want to use for data processing. From the three Trace lists, you can select: 1. A basic chromatogram type, for example, TIC, from the first list. 2. A logical operator: + or – from the second list. Your selection of an operator activates. 3. The third list for you to select a second chromatogram type to add to, or subtract from, the first type. For example, Mass Range. The list includes the valid remaining trace types. You can use trace combinations to subtract the contributions from a solvent or noise from a chromatogram. Combinations are limited to traces of the same type. For MS scans, valid trace types are TIC, Mass Range, and Base Peak. For Analog data, the application supports up to four channels (labeled Analog 1–4). For data from an A/D Card, the application supports four channels (labeled A/D Card Ch 1–4). For PDA data, valid trace types are Wavelength Range, Total Scan, or Spectrum Maximum. For UV detector data, the application supports four channels (labeled Channel A–D). Valid MS trace combinations. Click the following links for valid trace combinations: • Valid MS Trace Combinations • Valid Analog Trace Combinations • Valid A/D Card Trace Combinations • Valid PDA Trace Combinations • Valid UV Trace Combinations
Mass *(m/z)*	View or change the mass range for the Mass Range trace type. The application displays this box when you select a Mass Range trace type or a TIC ± Mass Range trace combination for an MS detector type. To change the range or to add a new range, type the range in the box. The valid range depends on the configured detector. The format is *LowMass–HighMass*. For example, for the range *m/z* 123 through 456, type **123–456**. You can sum up to 50 mass ranges by entering mass ranges or single mass values separated by your computer list separator character. To view or set the list separator character, see "Changing the List Separator Character."

Table 47. ICIS Identification page for Qual view parameters (Sheet 4 of 7)

Parameter	Description
Mass 1 (*m/z*)	View or change the mass range for the first trace type. The application displays this box when you select a Mass Range ± Mass Range trace combination for an MS detector type. To change the range or to add a new range, type the range in the box. The valid range depends on the configured detector. The format is *LowMass–HighMass*. For example, for the range *m/z* 123 through 456, type **123–456**. You can sum up to 50 mass ranges by entering mass ranges or single mass values separated by your computer list separator character. To view or set the list separator character, see "Changing the List Separator Character."
[Mass] 2 (*m/z*)	View or change the mass range for the second trace type. The application displays this box when you select a Mass Range ± Mass Range trace combination for an MS detector type. To change the range or to add a new range, type the range in the box. The format is *LowMass–HighMass*. For example, for the range *m/z* 123 through 456, type **123–456**. You can sum up to 50 mass ranges by entering mass ranges or single mass values separated by your computer list separator character. To view or set the list separator character, see "Changing the List Separator Character."
BP	View or change the mass value for the base peak. The application displays this box when you select a Base Peak trace for an MS detector type. To change the base peak mass, type the value in the box.
MR	View or change the mass range for the second trace type, Mass Range. The application displays this box when you select a Base Peak ± Mass Range trace combination for an MS detector type. To change the range or to add a new range, type the range in the box. The format is *LowMass–HighMass*. For example, for the range *m/z* 123 through 456, type **123–456**.

Table 47. ICIS Identification page for Qual view parameters (Sheet 5 of 7)

Parameter	Description
Wavelength (nm)	View or change the wavelength range for the Wavelength Range or Spectrum Maximum trace type. Xcalibur displays this box when you select one of the following trace combinations for a PDA detector type: • Spectrum Maximum • Wavelength Range • Total Scan – Wavelength Range To change the range or to add a new range, type the range in the box. The valid range depends on the configured detector. The format is *LowWavelength–HighWavelength.* For example, for the range *m/z* 123 through 456, type **123–456**. You can sum up to 50 wavelength ranges by entering ranges or single values separated by your computer list separator character. To view or set the list separator character, see "Changing the List Separator Character."
Wavelength 1 (nm)	View or change the wavelength or wavelength range for the first trace type. The application displays this box when you select one of the following trace combinations for a PDA detector type: • Wavelength Range ± Wavelength Range • Spectrum Maximum ± Wavelength Range To change the range or to add a new range, type the range in the box. The valid range depends on the configured detector. The format is *LowWavelength–HighWavelength*. For example, for the range *m/z* 123 through 456, type **123–456**. You can sum up to 50 wavelength ranges by entering ranges or single values separated by your computer list separator character. To view or set the list separator character, see "Changing the List Separator Character."
[Wavelength] 2 (nm)	View or change the wavelength or wavelength range for the second trace type. The application displays this box when you select one of the following trace combinations for a PDA detector type: • Wavelength Range ± Wavelength Range • Spectrum Maximum ± Wavelength Range To change the range or to add a new range, type the range in the box. The format is *Low Wavelength–HighWavelength*. For example, for the range *m/z* 123 through 456, type the following: 123–456. You can sum up to 50 wavelength ranges by entering ranges or single values separated by your computer list separator character. To view or set the list separator character, see "Changing the List Separator Character."

Table 47. ICIS Identification page for Qual view parameters (Sheet 6 of 7)

Parameter	Description
Selected Retention Time Window	
Range	Enter a time span to limit qualitative processing. Qual processes a peak only if its apex retention time lies in the range. The valid range is 0.1 to 999.0 minutes. To change the time window or to enter a new time window, type the number of seconds in the Range box. Type an asterisk (*) to represent the full chromatogram range of the active raw file.
ICIS Peak Integration	
Smoothing Points	Enter the number of points used in the moving average used to smooth the data. The valid range is any odd value from 1 through 15 points. The default value is 1 point. The ICIS peak detection algorithm uses this value.
Baseline Window	Specify the number of scans to review to look for a local minima. The valid range is 1 through 500. The default value is 40 scans. The ICIS peak detection algorithm uses this value.
Area Noise Factor	Specify the noise level multiplier used to determine the peak edge after the location of the possible peak. The valid multiplier range is 1 through 500. The default multiplier is 5. The ICIS peak detection algorithm uses this value.
Peak Noise Factor	Specify the noise level multiplier used to determine the potential peak signal threshold. The valid multiplier range is 1 through 1000. The default multiplier is 10. The ICIS peak detection algorithm uses this value.
Constrain Peak Width	Limit the peak width of a component during peak integration of a chromatogram. You can then set values that control when peak integration is turned on and off by specifying a peak height threshold and a tailing factor. To limit a peak width, select the Constrain Peak Width check box. The Peak Height (%) box and the Tailing Factor box appear.
Peak Height	View or change the percent of the total peak height (100%) that a signal must be above the baseline before integration is turned on or off. Select the Constrain Peak Width check box to activate this box. The valid range is 0.0 to 100.0%. To enter this height, type the appropriate value in the Peak Height (%) box.
Tailing Factor	View or change a factor that controls how the Xcalibur application integrates the tail of a peak. This factor is the maximum ratio of the trailing edge to the leading side of a constrained peak. Select the Constrain Peak Width check box to activate this box. The valid range is 0.5 through 9.0.
Min	View a representative drawing of a low value of the active parameter. The cursor location defines the active parameter. The number in the upper left corner of the graphic is a representative low value of the active parameter. This number is not the current low value of the range of the active parameter. For example, if you click the Smoothing Points box, the graphic shows the typical result obtained with a low number of smoothing points: a peak with reduced noise.

Table 47. ICIS Identification page for Qual view parameters (Sheet 7 of 7)

Parameter	Description
Max	View a representative drawing of a high value of the active parameter. The cursor location defines the active parameter. The number in the upper left corner of the graphic is a representative high value of the active parameter. This number is not the current high value of the range of the active parameter. For example, if you click the Smoothing Points box, the graphic shows the typical result obtained with a high number of smoothing points: a peak without noise.
Limit Peaks	
Select Top Peaks	
Enable	Limit peak detection to a specified number based on either peak area or peak height.
Select by Area	Select the Area option to restrict detection to the most significant peaks based on area rather than height.
Select by Height	Select the Height option to restrict detection to the most significant peaks based on height rather than area.
Num to Select	Enter the maximum number of peaks to be detected. The application selects the largest peaks based on intensity (height) or area.
Rel Peak Height Threshold	
Enable	Limit the list of detected chromatogram peaks to those exceeding the specified value, entered as a percentage of the most intense peak in the chromatogram.
% of Highest Peak	Enter a percentage threshold to limit the number of peaks submitted for further processing. The application discards any detected peaks with an intensity less than the threshold percentage of the most intense peak.
Buttons	
Save As Default	Validate and save the settings on the current page as default settings. The application uses these settings for all new processing methods. The software writes over the previous default values and cannot recover them.
Advanced	Set advanced peak identification and detection parameters in the ICIS Advanced Parameters Dialog Box. These parameters are used by the ICIS peak detection algorithm.

Genesis Identification Page for Qual View

Use the Genesis Identification page for Qual View to specify the type of chromatogram the processing method uses during qualitative processing. You can also adjust peak detection and identification criteria for the Genesis peak detection algorithm.

Table 48. Genesis Identification page for Qual view parameters (Sheet 1 of 8)

Parameter	Description
Detector	
Type	View or change the currently selected detector type: • MS • Analog • A/D Card • PDA • UV To change the detector type, click the arrow to display the list of detector types, and then click the required detector type.
Peak Detect	Select one of the Xcalibur peak detection algorithms. ❖ **To select an algorithm** 1. Enter a name in the **Name** box. 2. Click the **Peak Detect** list to display the algorithm names. 3. Select an algorithm and click **OK**. The application recalculates the current data using the specified algorithm. The application changes the default parameters for peak detection to those specific to that algorithm.
Delay	Enter a delay time (in minutes) to synchronize analog or digital data with MS scans. The Delay value compensates for any difference (negative or positive) in the arrival time of eluents at the UV and MS detectors. The valid range is –5.0 to +5.0 minutes.

Table 48. Genesis Identification page for Qual view parameters (Sheet 2 of 8)

Parameter	Description
Filter	View or change the current scan filter for the active .raw file. You can use a scan filter to specify that processing is to be applied to a subset of the scans in a raw file. To apply a different scan filter, select a new filter from the scan filter list (most common method), select a new filter from the list and edit the scan filter, or type a new scan filter command string into the box using the scan filter format. To select from the list of scan filters used to create the raw file, click the arrow to display the list. Click one of the scan filters. The application displays the scan filter in the Filter box. This scan filter example: c full ms [26.81–251] finds all scans in a raw file that have the following properties: centroid data Scan Mode: Full Scan Power: MS Product Ion Mass Range: *m/z* 26.81 to 251.00

Table 48. Genesis Identification page for Qual view parameters (Sheet 3 of 8)

Parameter	Description
Trace	Specify the type of chromatogram you want to use for data processing. From the three Trace lists, select: 1. A basic chromatogram type, for example, TIC, from the first list. 2. A logical operator: + or – from the second list. Your selection of an operator activates. 3. The third list for you to select a second chromatogram type to add to, or subtract from, the first type. For example, Mass Range. The list includes the valid remaining trace types. You can use trace combinations for subtracting the contributions from a solvent or noise from a chromatogram. Combinations are limited to traces of the same type. For MS scans, valid trace types are TIC, Mass Range, and Base Peak. For Analog data, the application supports up to four channels (labeled Analog 1–4). For data from an A/D Card, the application supports four channels (labeled A/D Card Ch 1–4). For PDA data, valid trace types are Wavelength Range, Total Scan, or Spectrum Maximum. For UV detector data, the application supports four channels (labeled Channel A–D). Click the following for valid trace combinations: • Valid MS Trace Combinations • Valid Analog Trace Combinations • Valid A/D Card Trace Combinations • Valid PDA Trace Combinations • Valid UV Trace Combinations
Mass	View or change the mass range for the Mass Range trace type. The application displays this box when you select a Mass Range trace type or a TIC ± Mass Range trace combination for an MS detector type. To change the range or to add a new range, type the range in the box. The valid range depends on the configured detector. The format is *LowMass–HighMass*. For example, for the range *m/z* 123 through 456, type **123–456**. You can sum up to 50 mass ranges by entering mass ranges or single mass values separated by your computer list separator character. To view or set the list separator character, see "Changing the List Separator Character."

Table 48. Genesis Identification page for Qual view parameters (Sheet 4 of 8)

Parameter	Description
Mass 1	View or change the mass range for the first trace type. The application displays this box when you select a Mass Range ± Mass Range trace combination for an MS detector type. To change the range or to add a new range, type the range in the box. The valid range depends on the configured detector. The format is *LowMass–HighMass*. For example, for the range *m/z* 123 through 456, type **123–456**. You can sum up to 50 mass ranges by entering mass ranges or single mass values separated by your computer list separator character. To view or set the list separator character, see "Changing the List Separator Character."
[Mass] 2	View or change the mass range for the second trace type. The application displays this box when you select a Mass Range ± Mass Range trace combination for an MS detector type. To change the range or to add a new range, type the range in the box. The format is *LowMass–HighMass*. For example, for the range *m/z* 123 through 456, type **123–456**. You can sum up to 50 mass ranges by entering mass ranges or single mass values separated by your computer list separator character. To view or set the list separator character, see "Changing the List Separator Character."
BP	View or change the mass value for the base peak. The application displays this box when you select a Base Peak trace for an MS detector type. To change the base peak mass, type the value in the box.
MR	View or change the mass range for the second trace type, Mass Range. The application displays this box when you select a Base Peak ± Mass Range trace combination for an MS detector type. To change the range or to add a new range, type the range in the box. The format is *LowMass–HighMass*. For example, for the range *m/z* 123 through 456, type **123–456**.

Table 48. Genesis Identification page for Qual view parameters (Sheet 5 of 8)

Parameter	Description
Wavelength	View or change the wavelength range for the Wavelength Range or Spectrum Maximum trace type. The application displays this box when you select one of the following trace combinations for a PDA detector type: • Spectrum Maximum • Wavelength Range • Total Scan – Wavelength Range To change the range or to add a new range, type the range in the box. The valid range depends on the configured detector. The format is *LowWavelength–HighWavelength*. For example, for the range *m/z* 123 through 456, type **123 –456**. You can sum up to 50 wavelength ranges by entering ranges or single values separated by your computer list separator character. To view or set the list separator character, see "Changing the List Separator Character."
Wavelength 1	View or change the wavelength or wavelength range for the first trace type. The application displays this box when you select one of the following trace combinations for a PDA detector type: • Wavelength Range ± Wavelength Range • Spectrum Maximum ± Wavelength Range To change the range or to add a new range, type the range in the box. The valid range depends on the configured detector. The format is *LowWavelength–HighWavelength*. For example, for the range *m/z* 123 through 456, type **123–456**. You can sum up to 50 wavelength ranges by entering ranges or single values separated by your computer list separator character. To view or set the list separator character, see "Changing the List Separator Character."

Table 48. Genesis Identification page for Qual view parameters (Sheet 6 of 8)

Parameter	Description
[Wavelength] 2	View or change the wavelength or wavelength range for the second trace type. The application displays this box when you select one of the following trace combinations for a PDA detector type: • Wavelength Range ± Wavelength Range • Spectrum Maximum ± Wavelength Range To change the range or to add a new range, type the range in the box. The format is *LowWavelength–HighWavelength.* For example, for the range *m/z* 123 through 456, type **123–456**. You can sum up to 50 wavelength ranges by entering ranges or single values separated by your computer list separator character. To view or set the list separator character, see "Changing the List Separator Character."
Selected Retention Time Window	
Range	Enter a time span to limit qualitative processing. Qual processes a peak only if its apex retention time lies in the range. The valid range is 0.1 to 999.0 minutes. To change the time window or to enter a new time window, type the number of seconds in the Range box. Type an asterisk (*) to represent the full chromatogram range of the active raw file.
Genesis Peak Integration	
Smoothing Points	Determine the degree of data smoothing to be performed on the active component peak prior to peak detection and integration. The valid range is any odd value from 1 (no smoothing) through 15 (maximum smoothing). To smooth your component peak data prior to integration, type a value in the Smoothing Points box.
S/N Threshold	View or change the current signal-to-noise threshold for peak integration. The application only integrates peaks with signal-to-noise greater than this value. Peaks with signal-to-noise less than this value are not integrated. The valid range is 0.0 to 999.0. To change the current value, type a new value in the S/N Threshold box.
Enable Valley Detection	Use the Xcalibur valley detection approximation method to detect unresolved peaks. This method drops a vertical line from the apex of the valley between unresolved peaks to the baseline. The intersection of the vertical line and the baseline defines the end of the first peak and the beginning of the second peak. To turn this method on, select the Valley Detection check box. To turn this method off, clear the check box.

Table 48. Genesis Identification page for Qual view parameters (Sheet 7 of 8)

Parameter	Description
Expected Width	View or change the expected peak width parameter (in seconds). This controls the minimum width that a peak is expected to have if valley detection is enabled. With valley detection enabled, any valley points nearer than the [expected width]/2 to the top of the peak are ignored. If a valley point is found outside the expected peak width, the application terminates the peak at that point. It always terminates a peak when the signal reaches the baseline, independent of the value set for the expected peak width. The valid range is 0.0 to 999.0 seconds. To change the current value, type a new width in the Expected Width box.
Constrain Peak Width	Limit the peak width of a component during peak integration of a chromatogram. You can then set values that control when peak integration is turned on and off by specifying a peak height threshold and a tailing factor. To limit a peak width, select the Constrain Peak Width check box. The Peak Height (%) box and the Tailing Factor box appear.
Peak Height	View or change the percent of the total peak height (100%) that a signal must be above the baseline before integration is turned on or off. Select the Constrain Peak Width check box to activate this box. The valid range is 0.0 to 100.0%. To enter this height, type the appropriate value in the Peak Height (%)box.
Tailing Factor	View or change a factor that controls how the data system integrates the tail of a peak. This factor is the maximum ratio of the trailing edge to the leading side of a constrained peak. Select the Constrain Peak Width check box to activate this box. The valid range is 0.5 through 9.0.
Min	View a representative drawing of a low value of the active parameter. The cursor location defines the active parameter. For example, if you click the Smoothing Points box, the graphic shows the typical result obtained with a low number of smoothing points: a peak with reduced noise. The number in the upper left corner of the graphic is a representative low value of the active parameter. This number is not the current low value of the range of the active parameter.
Max	View a representative drawing of a high value of the active parameter. The cursor location defines the active parameter. For example, if you click the Smoothing Points box, the graphic shows the typical result obtained with a high number of smoothing points: a peak without noise. The number in the upper left corner of the graphic is a representative high value of the active parameter. This number is not the current high value of the range of the active parameter.

Table 48. Genesis Identification page for Qual view parameters (Sheet 8 of 8)

Parameter	Description
Limit Peaks	
Select Top Peaks	
Enable	Limit peak detection to a specified number based on either peak area or peak height.
Select by Area	Select the Area option to restrict detection to the most significant peaks based on area rather than height.
Select by Height	Select the Height option to restrict detection to the most significant peaks based on height rather than area.
Num to Select	Enter the maximum number of peaks to be detected. The application selects the largest peaks based on intensity (height) or area.
Rel Peak Height Threshold	
Enable	Limit the list of detected chromatogram peaks to those exceeding the specified value, entered as a percentage of the most intense peak in the chromatogram.
% of Highest Peak	Enter a percentage threshold to limit the number of peaks submitted for further processing. The application discards any detected peaks with an intensity less than the threshold percentage of the most intense peak.
Buttons	
Save As Default	Validate and save the settings on the current page as default settings. The application uses these settings for all new processing methods. The software writes over the previous default values and cannot recover them.
Advanced	Set advanced peak identification and detection parameters in the Genesis Advanced Detection Options Dialog Box. The Genesis peak detection algorithm uses these parameters.

Library Search Constraints Page for Qual View

Use the Library Search Constraints page for Qual View to limit a library search to increase processing efficiency. For example, you might want to exclude certain high intensity ions that appear in many compounds or that are present in the spectrum background. You can target a search to a particular range of molecular weights or to compounds containing certain elements.

Table 49. Library Search Constraints page for Qual view parameters (Sheet 1 of 6)

Parameter	Description
Molecular Weight	
Enable	Limit the library search to compounds with a specific molecular weight or molecular weight range.
Range	Type a molecular weight or molecular weight range in the box (for example, 200–250). During a search, the data system only compares processed spectra with reference data derived from compounds with a molecular weight inside the specified range.
Other Databases	
Enable	Limit the library search to entries in the NIST library that are also featured in other databases. Each entry in the NIST library contains a list of other commercial databases containing information about the compound. The application reports search results featured in one or more of the selected databases. (A search result does not have to feature in all the selected databases.)
Fine	Report search results from reference compounds or spectra also to be found in commercially available Fine Chemical Index.
TSCA	Report search results from reference compounds or spectra also to be found in the Toxic Substances Control Act Inventory (TSCA).
RTECS	Report search results from reference compounds or spectra also to be found in the Registry of Toxic Effects of Chemical Substances (RTECS).
EPA	Report search results from reference compounds or spectra also to be found in the Environmental Protection Agency (EPA) Environmental Monitoring Methods Index.
USP	Report search results from reference compounds or spectra also to be found in the US Pharmacopoeia (USP)/U.S.A.N.
HODOC	Report search results from reference compounds or spectra also to be found in the CRC Handbook of Data of Organic Compounds (HODOC).
NIH	Report search results from reference compounds or spectra also to be found in the NIH-NCI Inventory File.
EINECS	Report search results from reference compounds or spectra also to be found in the European Index of Commercial Chemical Substances (EINECS).
IR	Report search results from reference compounds or spectra also to be found in the NIST/EPA Gas Phase IR Database.

Table 49. Library Search Constraints page for Qual view parameters (Sheet 2 of 6)

Parameter	Description
Clear All	Clear all the check boxes in the Other Databases area.
Name Fragment	
Enable	Limit the library search results to compounds with a specific name or name fragment.
Name	Enter a text string (up to 39 characters) to represent a fragment of a compound name, for example, “cyclo”. During the library search, the application filters search results and only returns those containing the specified text in their names. Note that the entry is case insensitive: “CYCLO” returns compounds containing the fragments “cyclo”, “Cyclo”, and “CYCLO”.
Element Constraints	
Enable	Limit the library search to compounds containing specific elements using the Individual Element and/or Elements in Compound methods. You can use the two types of elemental limits together, but you must make sure there are no contradictions. For example, you might put “C=0” in the Individual Element group and then list “C” in the Elements in Compound box. When a contradiction occurs, the data system displays a warning dialog box.
Individual Element	
Individual Element table	Set specific criteria about the elements required in a library search result. Each row in the table represents an element limit. There are three parts to each limit: • Element, a IUPAC approved abbreviation for an element, for example “Cl” for chlorine. • Condition, a mathematical operator, < (less than), > (greater than) or = (equals). • Value, a numerical value representing the number of atoms of the specified element required to satisfy the limit. | | Element | Condition | Value | | 1 | F | > | 5 | | 2 | Cl | = | 3 | In the example shown here, the application would only return search results for compounds that contain • More than five fluorine atoms • Exactly three chlorine atoms You do not need to provide a complete elemental profile. The library search returns compounds if they satisfy all the specified criteria regardless of any other elements present.
[Row Number]	Each numbered row represents an item in the table. The asterisk symbol indicates the last unused row in the table. Use this row to enter a new item.

Table 49. Library Search Constraints page for Qual view parameters (Sheet 3 of 6)

Parameter	Description
Element	Enter the IUPAC approved abbreviation for the element you want to use an element limit. It is used in conjunction with the Condition list and Value box in the same row of the Individual Element table. To enter an element limit, click the box and type the required abbreviation. For example, to apply carbon as an element limit, type **C**. The application adds a new row to the table for further entries.
Condition	Enter a condition for an element limit. The application uses this value together with the Condition list and Value box in the same row of the Individual Element table. Valid conditions are • < (less than) • > (greater than) • = (equals) To enter an element limit condition, click the box to activate the list. Click the down arrow and select the required abbreviation.
Value	Enter a numerical value for an element limit. It is used in conjunction with the Condition list and Value box in the same row of the Individual Element table. The value represents the number of atoms of the specified element required by library compounds to satisfy the limit. To enter an element limit value, click the box and then type the required number. The valid range is 0 to 99.
Elements in Compound	
Elements	Specify a list of elements that must be present in returned search results. To enter an element list, click the box and type the IUPAC approved abbreviation for each element. Separate each element in the list (of up to 30 characters) by a comma.
All	Specify that the data system returns search results containing all, and only, the listed elements. For example “C, H, O” would return HCHO but not CO2, CH4, or CH2Cl2. Compare with the Some option.
Some	Specify that the data system returns search results that contain at least one of the specified elements and no elements that are unlisted. For example, “C, H, O” would return CO2, CH4, HCHO but not CH2Cl2. Compare with the All option.
Clear	Delete the text in the Elements in Compounds box.

Table 49. Library Search Constraints page for Qual view parameters (Sheet 4 of 6)

Parameter	Description
Mass Spectral Peak Constraints	
Enable	Build a profile of ions and ion abundances to be matched against library entries during the search. The search algorithm only returns search results matching the specified limits.
Mass Spectral Peak Constraints table	Set specific criteria about the mass spectral peaks required in a library search result. Each row in the table represents an individual mass spectral peak limit. There are four components to each limit represented by the table columns: **Type**: Normal, Loss, Rank, or Maxmass ***m/z***: For a Normal, Rank, or Maxmass type limit, use this box to enter the *m/z* value of the mass spectral peak to be constrained. In a Loss type limit, use this box to enter the value of a neutral loss. **From**: For a Normal, Loss, or Maxmass type limit, use this box to enter the minimum abundance of the constrained mass spectral peak. In a Rank type limit, use this box to enter the lowest position of the ion in an intensity ordered list of spectral peaks. **To**: For a Normal, Loss, or Maxmass type limit, use this box to enter the maximum abundance of the constrained mass spectral peak. In a Rank type limit, use this box to enter the highest position of the ion in an intensity ordered list of spectral peaks.
[Row Number]	Each numbered row represents an item in the table. The asterisk (*) indicates the last unused row in the table. Use this row to enter a new item.

Table 49. Library Search Constraints page for Qual view parameters (Sheet 5 of 6)

Parameter	Description
Type	Specify the type of ion limit. **Normal**: This limit applies to a specific ion represented by its *m/z* value. The 'From' and 'To' values represent the abundance of the ion. **Loss**: This limit describes a neutral loss from a molecular ion. In this case, the *m/z* value (limited to 64) represents the mass of the 'lost' neutral group, for example, for methyl *m/z* = 15. For this limit to be matched, a library spectrum must contain • A fragment ion at an *m/z* value 15 less than the molecular ion • An abundance in the specified 'From' and 'To' range **Rank**: This limit tests the order of an ion in the spectrum in terms of relative abundance. Ions are ranked from the largest (the base peak) to the 16th largest. A compound matches a Rank limit if its library spectrum contains a mass spectral peak • At the specified *m/z* value • Ranked between the specified 'From' and 'To' rank positions If you specify the same number in both fields, the designated ion must have that rank in the retrieved spectrum. **Maxmass**: Maxmass sets a limit on the *m/z* value of the most significant high mass ion. Library search results must feature • An ion at the specified *m/z* value • No significantly larger masses at higher *m/z* values • An abundance in the specified 'From' and 'To' range
m/z	Enter the *m/z* value of the mass spectral peak to be constrained in a Normal, Rank, or Maxmass type limit. The application discards a library search result if it does not contain a mass spectral peak at the specified *m/z* value. For a Loss type limit, use this box to enter the value of a neutral loss. The application discards a library search result if it does not feature a fragment ion at an *m/z* value appropriate to the specified neutral loss (in relation to the molecular ion).
From	For a Normal, Loss, or Maxmass type limit, use this box to enter the minimum abundance of the constrained mass spectral peak. For a Rank type limit, use this box to enter the lowest position of the ion in an intensity ordered list of spectral peaks. You can specify the same number in both From and To boxes. In this case, the application discards a library search result unless the designated mass spectral peak is present in exactly the specified abundance or rank in the retrieved spectrum.

Table 49. Library Search Constraints page for Qual view parameters (Sheet 6 of 6)

Parameter	Description
To	For a Normal, Loss, or Maxmass type limit, use this box to enter the maximum abundance of the constrained mass spectral peak. For a Rank type limit, use this box to enter the highest position of the ion in an intensity ordered list of spectral peaks. You can specify the same number in both From and To boxes. In this case, the application discards a library search result unless the designated mass spectral peak is present in exactly the specified abundance or rank in the retrieved spectrum.
Absolute	Set the Absolute and Relative options to specify how the data system applies the From and To parameters in the Mass Spectral Peak Constraints table. Select the Absolute option if you want the application to evaluate all table entries as a percentage of the base (largest) ion in the spectrum. Values must be between 0 and 100%. For example, if you enter 10 and 50 in the From and To fields of a Normal type limit, the application discards any search results in which the specified mass spectral peak is not present at an abundance of between 10 and 50%. For Normal and Loss type limits, the abundance values can also be relative.
Relative	Set the Absolute and Relative options to specify how the data system applies the From and To parameters in the Mass Spectral Peak Constraints table. Select the Relative option if you want the data system to treat the first entry as an absolute Normal or Loss type. It then considers subsequent entries in the table relative to the first. In the following example, library search results must contain • An ion at *m/z* 125 with an abundance between 10 and 50% of the base ion • An ion at *m/z* 250 with an intensity between 50 and 999% of the observed intensity of the first ion in the list Relative mode is not available for Rank or Maxmass types.
Button	
Save As Default	Validate and save the settings on the current page as default settings. The application uses these settings for all new processing methods. The software writes over the previous default values and cannot recover them.

Library Search Options Page for Qual View

The Library Search Options page consists of the parameters to define a comparison search of your compound to published compound data. It consists of three main areas: Search Type, Options, and Append to User Library.

Use the Library Search Options page to view and select search criteria that are defined for the active processing method. See the next table.

Table 50. Library Search Options page for Qual view parameters (Sheet 1 of 4)

Parameter	Description
Search Type	
Identity	Apply an identity search algorithm for library matching of spectra. A normal identity search is the default option.
Normal	Apply a normal identity search algorithm for library matching of spectra. This is the default option. A normal identity search is suited to low quality or unusual spectra. The search algorithm uses a standard pre-screen search filter.
Quick	Apply a quick identity search algorithm for library matching of spectra. Use this option when you are sure the spectrum or compound exists in the library. The search algorithm uses a fast pre-screen search filter.
Penalize Rare Compounds	Reduce the match factor of rare compounds. This option is effective only when you have selected one or more of the NIST databases (such as MAINLIB). It has no effect on spectra in user libraries or other commercial libraries. Each reference spectrum in a NIST library contains a record of other commercial databases containing information about the compound. A compound is considered rare if it is present in a limited number of these databases. If you select the Penalize Rare Compounds option, search match compounds in few, or no other databases other than the NIST libraries have their match factors reduced (the maximum penalty is 50 out of 1000). This limitation, in effect, leads to a relative increase in the match factors of common compounds, placing them higher on the library search result list (search result list) than exotic isomers with near identical spectra.
Similarity	Apply a Similarity search algorithm for library matching of spectra.
Simple	Apply a simple similarity search algorithm for library matching of spectra. This option finds a large set of spectra to compare with the submitted spectrum, and is generally slower than an identity search. Use a simple similarity search in either of these cases: • You know that the unknown spectrum is not in the library. • The spectrum is of poor quality so that a reliable match is unlikely.

Table 50. Library Search Options page for Qual view parameters (Sheet 2 of 4)

Parameter	Description
Hybrid	Apply a hybrid similarity search algorithm for library matching of spectra. This option uses a combination of the simple and neutral loss search strategies. The neutral loss search requires an estimate of the unknown's molecular weight. If the unknown compound contains chemical structures that generate both characteristic ions and neutral loss patterns, the search result list from this search can identify these structures.
Neutral Loss	Apply a neutral loss similarity search algorithm for library matching of spectra. The neutral losses in a spectrum are the mass differences between the molecular ion and other major ions in the spectrum. For certain classes of compound, neutral losses can be very characteristic spectral features. In a neutral loss search, the data system examines the submitted spectrum and identifies the molecular ion. The application submits the mass value of the molecular ion to the search along with the spectrum. The search algorithm calculates the significant neutral losses and compares them with library data. Search results are returned according to matches of the molecular ion and its neutral losses.
Options	
Maximum Number of Hits	View or change the maximum number of search results to be returned by a library search and reported in the results file. The application selects the search results with the highest matching factors. The default limit is 5.
Reverse Search	Select this check box if you want search results—matching library spectra—to be sorted by the Reverse Search Match Factor. By default, the data system sorts search results by the Forward Match Factor.
Search with MW =	Restrict the search to library entries with a particular molecular weight. Use the associated box to enter the molecular weight.
Append to User Library	
Enable	Add processed spectra to a specified user library. Spectra are added to the specified user library in these situations. • The library search produces no search results. • The top search result fails to exceed one or more of the match factors. With the match factors you can select new or unusual spectra and avoid duplicate entries.
User Library	View or change the name of the user library used to store spectra. To select a user library, click the arrow to display the list of Xcalibur user libraries. Click a user library in the list.

Table 50. Library Search Options page for Qual view parameters (Sheet 3 of 4)

Parameter	Description
Thresholds	
Match Factor	Set a forward match factor threshold for spectra subject to the Append to User Library option. The application submits the spectrum from each identified peak to a library search as determined by the other parameters on the Library Search Options page. If the top search result (hit) from a library search exceeds the Match Factor threshold or any of the other threshold values, the application records the search result list in the results file and the spectrum is not appended to the specified library. If the top search result fails to match any of the threshold values, the data system discards the search result list and appends the spectrum to the specified library. The match is scored on a scale of 0 to 999.
Reverse Match Factor	Set a Reverse Match Factor threshold for spectra subject to the Append to User Library option. The application submits the spectrum from each identified peak to a library search as determined by the other parameters on the Library Search Options page. If the top search result from a library search exceeds the Reverse Match Factor threshold or any of the other threshold values, the application records the search result list in the results file and the spectrum is not appended to the specified library. If the top search result fails to match any of the threshold values, the application discards the search result list and appends the spectrum to the specified library. The match is scored on a scale of 0 to 999.
Probability	Set a Probability threshold for spectra subject to the Append to User Library option. The application submits the spectrum from each identified peak to a library search as determined by the other parameters on the Library Search Options page. If the top search result from a library search exceeds the Probability threshold or any of the other threshold values, the application records the search result list in the results file and the spectrum is not appended to the specified library. If the top search result fails to match any of the threshold values, the Xcalibur application discards the search result list and appends the spectrum to the specified library. The limits of probability are 0 to 100.

Table 50. Library Search Options page for Qual view parameters (Sheet 4 of 4)

Parameter	Description
Mass Defect	
Enable	Include mass defect values for library searches in a processing method.
Defect	Specify values (in millimass units) for mass defect to correct for the differences between the actual masses and the nominal integer masses of the atoms in a molecule. Assign a larger value (in millimass units) for mass defect to larger molecules because, in general, they are composed of more atoms than smaller molecules; larger molecules need a larger correction factor to approximate the linear function that the Xcalibur data system uses to calculate masses. Specify a smaller value for lower mass ranges in the first box and specify a larger value for higher mass ranges in the second box.
At Mass	Specify the masses at which the data system applies specified mass defect values to calculations of mass. Specify a smaller mass value in the first box, and specify a larger mass value in the second box.
Buttons	
Save As Default	Validate and save the settings on the current page as default settings. The application uses these settings for all new processing methods. The software writes over the previous default values and cannot recover them.
Search List	Open the Search List Dialog Box.

Peak Purity Page for Qual View

Use the Peak Purity page for Qual view to specify the values of the peak purity parameters to be included in a qualitative processing method for the PDA detector type only. After you specify the processing method in a sequence, you can apply the parameters to your qualitative PDA analysis as you acquire data. Use a raw file of PDA data in Qual Browser to determine which peak purity parameter values you want to use in the processing method.

Table 51. Peak Purity page for Qual view parameters

Parameter	Description
Purity Parameters	
Enable	Activate Peak Purity parameters for PDA chromatograms in an active chromatogram cell to calculate peak purity results. Peak detection occurs automatically prior to the peak purity calculation.
Scan Threshold	Specify a minimum value of intensity for wavelength scans in milliabsorbance units (mAU). A Peak Purity computation using scan threshold starts with the scan at the apex of the peak and then collects wavelength data from scans on both sides of the apex until the scan threshold is reached. Use scan threshold for either symmetrical or asymmetrical peaks. The default value for scan threshold is 3 mAU. The range of possible values is 0 to 1000 mAU (or 1 AU). In a sample with high background or noise, you might start with a value for scan threshold of 40 mAU.
Peak Coverage	Specify a maximum percent value of the width of the integrated peak. A Peak Purity computation using peak coverage starts with the scan at the apex of the peak and then collects wavelength data from scans on both sides of the apex until the percent peak coverage is reached. Use peak coverage for symmetrical peaks. The default value for peak coverage is 95% of the integrated peak width.
Limit Scan Wavelength	Limit the number of wavelengths to include in the Peak Purity computation. Enter a range in the Wavelength Range box.
[Wavelength] Range	Specify a range of UV scans (in nanometers) that include the wavelengths of your peak(s) of interest. A Peak Purity computation using wavelength range starts with the scan at the apex of a peak and then collects wavelength data from scans on both sides of the apex until all the wavelengths in the range are included. Use wavelength range for either symmetrical or asymmetrical peaks. Select the Limit Scan Wavelength check box to activate this box. The default wavelength range is the full width of the scan.

Spectrum Enhancement Page for Qual View

Use the Spectrum Enhancement page for Qual View to select an option for enhancing spectra. If you select the check box, the Xcalibur data system displays one of three options:

- Refine Option in the Spectrum Enhancement Page for Qual View
- Combine Option in the Spectrum Enhancement Page for Qual View
- Threshold Option in the Spectrum Enhancement Page for Qual View

Refine Option in the Spectrum Enhancement Page for Qual View

Use the Refine option to specify the Refine spectrum enhancement method. The Refine algorithm determines which ions in the selected spectrum derive from a constant chromatography background and then removes them to produce a refined spectrum.

Refine requires two parameters that you can set and test interactively: Window Size (sec) and Noise Threshold.

The Refine algorithm examines the mass chromatogram of each ion contributing to the apex scan:

1. It discards masses without a peak maximum within ±1 scan of the defined chromatogram peak apex.
2. It then searches for a minimum in the specified Window Size range on either side of the peak apex. These points define the peak start and peak end.
3. Using scans at and beyond the peak start and peak end, Refine measures the background noise level in the mass chromatogram.
4. Refine uses extrapolation to estimate the contribution of noise to the scan at the peak apex. Refine adjusts the mass intensity of the apex scan accordingly.
5. Finally, Refine uses the Noise Threshold parameter to determine whether the adjusted intensity is significant in comparison to the background noise. If:

   Adjusted Intensity < Noise Threshold × Background Noise

   the mass is discarded from the final spectrum.

Table 52. Spectrum Enhancement page for Qual view parameters

Parameter	Description
Enhancement Options	
Refine	
Window Size	Enter a time window for the Refine spectrum enhancement method. The Refine algorithm applies the window across a chromatogram peak apex and uses it to search for the peak start and peak end and to estimate the background noise. Set this parameter to the peak width.
Noise Threshold	Enter a value for the Noise Threshold parameter. The Refine algorithm uses the Noise Threshold parameter to determine whether adjusted ion intensities are significant in comparison to the background noise. The parameter is actually a factor rather than a threshold. For example, with a Noise Threshold value of 2, ions are discarded from the enhanced spectrum unless their intensities are twice the measured background noise.
Button	
Save As Default	Validate and save the settings on the current page as default settings. The application uses these settings for all new processing methods. The software writes over the previous default values and cannot recover them.

❖ **To display this page and option**

1. From the Qual view of the Processing Setup window, click the **Spectrum Enhancement** tab.
2. Select the **Enable** check box.
3. Select the **Refine** option.

Combine Option in the Spectrum Enhancement Page for Qual View

Use the Combine option to specify the Combine spectrum enhancement method. The Combine algorithm produces a single enhanced spectrum for each detected peak by

- Averaging all the scans across each peak top
- Subtracting background contributions (averaged from a number of scans and scaled appropriately) assessed from baseline regions on either side of each peak.

Combine requires six parameters that you can set and test interactively. The algorithm is applied to all detected chromatogram peaks in the specified Retention Time field. You might need to examine the peaks in a reference chromatogram carefully to make sure the Combine settings are appropriate for all the peaks of interest.

In setting up Combine, you might find it helpful to display scan numbers in the chromatogram cell. To do this, open a raw file and activate Scan Numbers in the Chromatogram Labels page of the Display Options dialog box.

Table 53. Combine Option in the Spectrum Enhancement page for Qual view parameters

Parameter	Description
Enhancement Options	
Background Subtraction Left Region	
Region Width (points)	Enter the number of scans to average in the analysis of the background spectrum in the Left region. The Combine algorithm uses this, together with a similar region from the right of each peak, for background analysis.
Region End	
Peak Start	Select this option to use the peak start time to define the end time of the left background subtraction region.
Points Before Peak Top	Select this option to define the left region start point as a specific number of scans before the peak top. Use the associated box to enter the number of scans.
Peak Top Region	
Peak Top Region	Determine the number of scans used by the Combine algorithm.
Width (points)	Enter the number of scans to average across the apex of the peak. Examine the chromatogram peak and estimate the number of good scans across the peak apex.
Chromatogram Peak diagram	
Chromatogram Peak diagram	View a schematic diagram that illustrates the three regions of a chromatogram peak used by the Combine spectrum enhancement method: Peak Top, Left, and Right.
Background Subtraction Right Region	
Region Width (points)	Enter the number of scans to average in the analysis of the background spectrum in the Left region. The Combine algorithm uses this, together with a similar region from the left of each peak, for background analysis.
Region Start	
Peak End	Activate this option to use the peak end time. This is the default option.
Points After Peak Top	Select this option to define the right region end point as a specific number of scans after the peak top. Use the associated box to enter the number of scans.
Button	
Save As Default	Validate and save the settings on the current page as default settings. The application uses these settings for all new processing methods. The software writes over the previous default values and cannot recover them.

❖ To display this page and option

1. From the Qual view of the Processing Setup window, click the **Spectrum Enhancement** tab.
2. Select the **Enable** check box.
3. Select the **Combine** option.

Threshold Option in the Spectrum Enhancement Page for Qual View

Use the Threshold option to specify the threshold spectrum enhancement method. This method limits the number of ions in the final spectrum prior to library searching by applying an intensity threshold. If the intensity of an ion is below the specified threshold, the ion is discarded from the spectrum.

Table 54. Threshold option in the Spectrum Enhancement page for Qual view parameters

Parameter	Description
Enhancement Options	
Threshold	
Cutoff Threshold (%)	Enter a limiting intensity value as a percentage of the most intense mass. The application produces an enhanced spectrum by discarding any ions with an intensity below the specified threshold.
Button	
Save As Default	Validate and save the settings on the current page as default settings. The application uses these settings for all new processing methods. The software writes over the previous default values and cannot recover them.

❖ To display this page and option

1. From the Qual view of the Processing Setup window, click the **Spectrum Enhancement** tab.
2. Select the **Enable** check box.
3. Select the **Threshold** option.

Quan View

Use the Quan view of the Processing Setup window to set up a method for quantitative processing. For processing quantitative data, you can identify multiple target compounds and give each its own calibration with unique amounts and curve fitting. Xcalibur quantitative processing supports multiple internal standards with individual amount corrections if required.

For quantitative analysis, you can use Sequence Setup to generate a sequence semi-automatically, based on a processing method.

The Quan view consists of a Menu bar, Toolbar, and Quan view pages. This view also provides access to Xcalibur Help.

Menus

Processing Setup window menus:

File Menu	View Menu	Zoom Menu
Options Menu	GoTo Menu	Help Menu

Toolbar

Processing Setup Toolbar

Quan View Pages

The Quan view has the following pages:

- Identification Page for Quan View
- Detection Page for Quan View
  - Avalon Detection Page for Quan View
  - Genesis Detection Page for Quan View
  - ICIS Detection Page for Quan View
- Calibration Page for Quan View
- Levels Page for Quan View
- System Suitability Page for Quan View
- Peak Purity Page for Quan View

Buttons

Each of the Quan view pages feature OK and Cancel buttons. These are active only if you change one or more parameters on the page. Otherwise, they are unavailable. When you have changed or edited a parameter, do the following:

- To apply the changes to the current processing method, click **OK**. The application reports any validation errors.
- To undo all changes made to the page and revert to the previously applied values, click **Cancel**.

Note that these actions do not affect the saved version of the processing method. The saved version can only be modified by using the **File > Save** command.

The application displays the Apply Changes? Dialog Box if you attempt to change pages, views, or applications without applying or discarding changes. Use this dialog box to apply or discard the changes before you continue with your intended action.

Chromatogram and Spectrum Previews

The Chromatogram and Spectrum previews display the chromatogram and spectrum from the currently opened raw file. Initially, the spectrum shown is the one corresponding to the apex scan of the first detected peak. If no peak has been detected in the Chromatogram preview, the spectrum for the first scan in the raw file appears.

These previews are available on the following pages:

- Identification, Detection, and Peak Purity pages for Quan View
- Identification, Spectrum Enhancement, and Peak Purity pages for Qual View

You can use the Chromatogram preview, in conjunction with the Spectrum preview, to assess the effects of processing parameters. You can also use the Chromatogram preview to set the retention time Range window on the Identification page for Qual View. You can also use the Spectrum preview in the Qual view to do the following:

- Set Mass Ranges on the Identification page
- Combine parameters on the Spectrum Enhancement page

You can rescale the chromatogram displayed in the preview by using toolbar buttons, Zoom menu commands, or the cursor.

Important points to note are as follows:

- The cursor action is always applied to the pinned cell.
- Within an active cell, cursor actions rescale the chromatogram shown in the preview.

Calibration Page for Quan View

The Calibration page consists of a Calibration settings page and a Components list:

- The Calibration settings page consists of Component Type, Target Compounds, Internal Standard, Weighting, Origin, and Response.
- The Components list is located at the far right of the page where you can view and select component names that are defined for the active processing method.

Table 55. Calibration page for Quan view parameters (Sheet 1 of 4)

Parameter	Description
Component Type	
Target Compound	Specify that the selected component is a target compound. This button is only active if you have defined at least one component as an internal standard and selected another component as Component Type: Target Compound. ❖ **To select a component as a target compound type** 1. Select a component. 2. Select the **Target Compound** option and click **OK**. The application activates the options in the Target Compound area.
ISTD	Specify that the selected component is an internal standard. ❖ **To select a component as an internal standard compound type** 1. Select a component. 2. Select the **Internal Standard** option and click **OK**. When you choose the ISTD option: • The ISTD area becomes active. • The Target Compounds area is unavailable. • The Levels page becomes unavailable. The ISTD option is unavailable if you have selected the External Standard option in the Calibration Options Dialog Box.
ISTD	
Amount	View the amount of the selected component that is added to each sample to provide an internal standard. You can enter mounts with up to three decimals of precision. Select the ISTD Component Type to activate this box.
Units	View the units used for the internal standard amount. For example, ng. Select the ISTD Component Type to activate this box.

Table 55. Calibration page for Quan view parameters (Sheet 2 of 4)

Parameter	Description
Target Compounds	
Target Compounds	View or change target compounds. These settings are active only if you have defined at least one component as an internal standard and selected another component as a Target compound.
ISTD	View or change the selected internal standard component to be used for calibration of the target compound. ❖ **To select a different internal standard component** 1. Click the arrow to display a list of all previously entered internal standard components. 2. Click a component in the list.
Isotope % button	Make calibration corrections for isotope contributions of the internal standard to the target compound and the target compound to the internal standard using the Correction for Isotope Contribution dialog box.
Calibration Curve	View or change the selected calibration curve type. To select a calibration curve type, click the arrow to display a list of Xcalibur calibration curve types. Then, click a component in the list. Available curve types: • linear curve • quadratic curve • linear log-log calibration curve [quantitation] • quadratic log-log calibration curve [quantitation] • average response factor (RF) curve • point-to-point curve • cubic spline curve • locally weighted curve
Units	View or change the label used for the x-coordinate in the calibration curve plot when it appears on the Calibration page of the Quan view. Enter any alphanumeric string.
Weighting	
Equal	Weight all calibration data points equally during the least-squares regression calculation of the calibration curve.
1/X	Specify a weighting of 1/X for all calibration data points during the least-squares regression calculation of the calibration curve. Calibrants are weighted by the inverse of their quantity.
1/X^2	Specify a weighting of 1/X^2 for all calibration data points during the least-squares regression calculation of the calibration curve. Calibrants are weighted by the inverse of the square of their quantity.

Table 55. Calibration page for Quan view parameters (Sheet 3 of 4)

Parameter	Description
1/Y	Specify a weighting of 1/Y for all calibration data points during the least-squares regression calculation of the calibration curve. Calibrants are weighted by the inverse of their response (or response ratio).
1/Y^2	Specify a weighting of 1/Y^2 for all calibration data points during the least-squares regression calculation of the calibration curve. Calibrants are weighted by the inverse of the square of their response (or response ratio).
1/s^2	Specify a weighting of 1/s^2 for all calibration data points during the least-squares regression calculation of the calibration curve. Calibrants at a given level are weighted by the inverse of the standard deviation of their responses (or response ratios). For this weighting factor to be used, there must be two or more replicates at each level. If only one calibrant is available for any level, 1/s^2 weighting cannot be used.
Origin	
Ignore	Exclude the origin as a valid point in your calibration curve. If you select this option, the calibration curve might or might not pass through the origin.
Force	Make sure that the calibration curve passes through the origin of the data point plot.
Include	Include the origin as a single data point in the calculation of the calibration curve. If you select this option, the calibration curve might or might not pass through the origin.
Response	
Area	Specify that the data system use the area of the target compound peak to acquire the data used for the calibration.
Height	Specify that the data system use the height of the target compound peak to acquire the data used for the calibration.
Component	
Component List	View or change component names for the active processing method. This list is located in the Components pane at the far right of the Processing Method window and contains all of the component names that have been defined for the active processing method. ❖ **To add a new component to the list** 1. Replace NEW in the Name box with the name of the component. 2. Click **OK**. The new component name appears in the Name box and Component List. ❖ **To delete a component from the list** 1. Click the component name in the Component List. 2. Choose **Options > Delete Component**.

Table 55. Calibration page for Quan view parameters (Sheet 4 of 4)

Parameter	Description
Buttons	
Save As Default	Validate and save the settings on the current page as default settings. The application uses these settings for all new processing methods. This option guarantees that the settings for the component are consistent and valid. These default settings will be used for all new components. The software writes over the previous default values and cannot recover them.
Flags	Set peak area and peak height threshold values in the Data Flags Dialog Box. The application reports these data flags in results files, printed reports, and Quan Browser.

Detection Page for Quan View

Use the Detection page to specify peak integration and detection criteria.

Based on your selected default peak detection algorithm, the data system displays the corresponding version of this page (ICIS Detection Page for Quan View, Genesis Detection Page for Quan View, or Avalon Detection Page for Quan View).

Avalon Detection Page for Quan View

On the Identification page of the Quan view, you can choose from among the ICIS, Genesis, and Avalon Xcalibur peak detection algorithms.

Note Click **Advanced** to display a dialog box to change parameters in the Event list.

Use the Avalon Detection page to view or specify the peak detection and integration criteria for the Avalon peak detection algorithm.

Table 56. Avalon Detection page for Quan view parameters (Sheet 1 of 8)

Parameter	Description
Avalon Peak Integration	
Avalon Peak Integration	View or change peak integration criteria. The Avalon peak detection algorithm uses these parameters. To change the settings in the Event list, click **Advanced** to display the Avalon Event List Dialog Box.
Smoothing Points	Determine the degree of data smoothing to be performed on the active component peak prior to peak detection and integration. The valid range is any odd value from 1 (no smoothing) through 15 (maximum smoothing). To smooth your component peak data prior to integration, enter a value in the Smoothing Points box.

Table 56. Avalon Detection page for Quan view parameters (Sheet 2 of 8)

Parameter	Description
Event List	
Event List	View the list of events and highlight the row you want to change. Enter any revised settings in the boxes below the list. Click **Change** to automatically update the Event list, both here and on the Detection page and automatically update the chromatogram display. To detect peaks, Avalon uses the settings for initial events and user-defined timed events that are in the Event list. There are seven initial entry integration events that are identified by the initial value setting in the Time column. These are the default integration events required by the Avalon integration algorithm. You can change the value of an initial entry integration event, but you cannot delete it or change its time value. ❖ **To calculate values for initial events** 1. Open a raw file and make the chromatogram view active. 2. Click **Auto Calculate Initial Events** to update the Event list. 3. Change the settings in the Event list by clicking on **Advanced**. The Avalon Event List Dialog Box opens, containing an Event list that you can edit.
Time	Change the time of a timed event. This column contains either the term *initial value* or a value of time in minutes. ❖ **To change the time** 1. Click **Advanced**. The Avalon Event List Dialog Box opens, containing an Event list that you can edit. 2. Highlight the row in the Event list and enter the revised setting in the Time box (below the Event list). 3. Click **Change** to automatically update the Event list, both here and on the Detection page and automatically update the chromatogram display.
Event	View or change descriptions of the detection parameters for initial events and timed events. You cannot change an event in the Event column associated with an initial value in the Time column. ❖ **To change a timed event in the Event column** 1. Click **Advanced**. The Avalon Event List Dialog Box opens, containing an Event list that you can edit. 2. Highlight the row in the Event list, and click the **Event** list (below the Event list) to display the available events. 3. Select an event. Click **Change** to automatically update the Event list, both here and on the Detection page, and automatically update the chromatogram display.

Table 56. Avalon Detection page for Quan view parameters (Sheet 3 of 8)

Parameter	Description
Value	View or change values associated with initial events and timed events. The range of allowed values is specific to each event. ❖ **To change a value in the Value column** 1. Click **Advanced**. The Avalon Event List Dialog Box opens, containing an Event list that you can edit. 2. Highlight the row in the Event list and enter the revised setting in the Value box (below the Event list). 3. Click **Change** to automatically update the Event list, both here and on the Detection page, and automatically update the chromatogram display.
Auto Calculate Initial Events	Select to have Avalon automatically estimate the initial values for the detection of peaks based on the data in the current raw file and then display those initial values in the Event list. This button is active with the Event list of the Avalon peak detection algorithm only if a raw file is open. Use this button to force Avalon to search for the best values of initial events that detect peaks in the data. Any timed event in the Event list is unchanged when you click this button. Auto Calculate Initial Events determines initial values for these events only: Start Threshold, End Threshold, Area Threshold, P-P [Resolution] Threshold, Bunch Factor, Negative Peaks, and Tension. You can also specify timed events for these events in the same Event list.

Table 56. Avalon Detection page for Quan view parameters (Sheet 4 of 8)

Parameter	Description
Avalon Peak Detection	
Spectrum	Use a reference spectrum defined in the processing method for component identification. The application attempts to match the reference spectrum with a series of unknown spectra and calculates a score value for each comparison. This option is only available in Xcalibur GC chromatography mode (set in the Chromatography Options Dialog Box). If you select the Spectrum option, the following parameters appear: **Spectrum Peak Detection**: View spectrum peak detection only in Xcalibur GC Chromatography mode when you select the **Spectrum** option. You must also have selected the MS detector type on the Identification page. **Peak Identification Table**: Enter mass/charge [*m/z*] and intensity data for up to 50 spectrum peaks. The application uses this data to identify the active component in the Find algorithm. It displays this table only when you select the Spectrum option in its GC Chromatography mode. ***m/z**:* View or change the mass/charge [*m/z*] value for one peak in the reference spectrum. The intensity for this *m/z* value is given in the adjacent Intensity table box. Use other rows of the table to enter as many as 50 *m/z* values. The application uses this data to identify the active component the Find algorithm. It displays this table only when you select the Spectrum option in its GC Chromatography mode. **Intensity**: Enter intensity data for one peak in the reference spectrum. The *m/z* value for this intensity is given in the adjacent *m/z* Table box. Use other rows of the table to enter as many as 50 intensity values. The application uses this data to identify the active component the Find algorithm. It displays this table only when you select the Spectrum option in its GC Chromatography mode.

Table 56. Avalon Detection page for Quan view parameters (Sheet 5 of 8)

Parameter	Description
Thresholds	**Forward**: Set a threshold value for forward comparisons between the reference spectrum and candidates in the chromatogram. A forward search is a direct matching algorithm comparing unknowns against the reference spectrum in the peak identification table. The match is scored on a scale of 0 to 999. A perfect match results in a score of 999. As a general guide, 900 or greater is an excellent match; 800 to 900, a good match; 700 to 800, a fair match. Less than 600 is a poor match. Unknown spectra with many peaks tend to score lower than similar spectra with fewer peaks. **Reverse**: Set a threshold value for reverse comparisons between the reference spectrum and candidates in the chromatogram. A reverse search ignores any peaks in the unknown that are not in the reference spectrum in the peak identification table. The match is scored on a scale of 0 to 999. A perfect match results in a score of 999. As a general guide, 900 or greater is an excellent match; 800 to 900, a good match; 700 to 800, a fair match. Less than 600 is a poor match. A spectrum with many peaks tends to score more highly in a reverse match than a forward match. **Match**: Set a threshold value for match comparisons between the reference spectrum and candidates in the chromatogram. Match is scored on a scale of 0 to 999. The match algorithm is a complex probability factor based on the differences between the forward factors of all the candidates. If one candidate has a forward matching factor of 900 and the next best is only 300, the probability of the component being correctly identified is high and so the match factor is scored highly for the first candidate. If the forward factors for all the candidates are similar, whether high or low, the match factor is low.
Highest Peak	Use the highest peak in the chromatogram for component identification.
Nearest RT	Use the peak with the nearest retention time in the chromatogram for component identification.

Table 56. Avalon Detection page for Quan view parameters (Sheet 6 of 8)

Parameter	Description
Options for Highest Peak or Nearest RT	If you are in GC mode and you select the Highest Peak or Nearest RT options, the following parameters appear: **Ion Ratio Confirmation**: View spectrum peak detection only in Xcalibur GC Chromatography mode when you select either the **Highest Peak** or **Nearest RT** option. You must also have selected the MS detector type on the Identification page. Use the settings in this area to specify up to five qualifier ions to confirm the detection of a target analyte. You can also set the coelution window and select a method for calculating the target ion ratio window and tolerance. **Enable**: This check box indicates whether or not Ion Ratio Confirmation is enabled. **Ion Ratio Using**: **Area or Height** This readback shows the currently selected peak quantitation method: area or height. The application uses the same method to calculate the qualifier ion peak response and then the target ratio. You can change this parameter by selecting the Area or Height options in the Response area on the Calibration page. **Qualifier Ion Table**: Use this table to enter mass/charge [*m/z*] and target ratio tolerances [Window ± %] data for up to 5 qualifier ions. If you select Area response, the application integrates each qualifier ion peak and calculates a ratio using the integrated qualifier ion peak and the quantitation peak area. It then compares this ratio with your specified target ratio. If the calculated ratio is outside of the target ratio by more than your specified tolerance (Window ± %), the quantitation peak is rejected. If you select Height response, the application calculates a ratio using the qualifier ion peak height with the height of the quantitation peak. It then compares this ratio with your specified target ratio. If the calculated ratio is outside of the target ratio by more than your specified tolerance (Window ± %), the quantitation peak is rejected. ***m/z****:* View the mass/charge [*m/z*] value for a qualifier ion. The target ratio tolerance for this *m/z* value appears in the adjacent Window ± % table box. Use other rows of the table to enter data for 5 qualifier ions. The application uses this data to confirm the identity of a quantitation peak by comparing the relative responses of qualifier ion and quantitation peaks with predetermined values. **Target Ratio**: View the Target Ratio (%) value for a qualifier ion. The *m/z* value and target ratio tolerance for the qualifier ion are given in the adjacent *m/z* and Window ± % table boxes. Use other rows of the table to enter data for 5 qualifier ions. The application uses this data to confirm the identity of a quantitation peak by comparing the relative responses of qualifier ion and quantitation peaks with predetermined values.

Table 56. Avalon Detection page for Quan view parameters (Sheet 7 of 8)

Parameter	Description
Options for Highest Peak or Nearest RT (continued)	**Window**: Specify the Target Ratio tolerance for a qualifier ion. Use other rows of the table to enter data for 5 qualifier ions. The application uses this data to confirm the identity of a quantitation peak by comparing the relative responses of qualifier ion and quantitation peaks with the specified values. **Qualifier Ion Coelution**: Set the Qualifier Ion Coelution window. Prior to ion ratio confirmation, the application generates a mass chromatogram for each specified qualifier ion. Each of these chromatograms must feature a peak matching that of the quantitation mass or masses. If the retention time of the qualifier ion peak apex lies outside of the Qualifier Ion Coelution window (centered on the quantitation peak), the application rejects the quantitation peak. The application tests quantitation peaks with matching qualifier ion peaks (in the Coelution window) for ion ratio confirmation.
Window	
Relative	Specify that the target ratio tolerance values in the Window ± % column of the qualifier ion table are relative values. For example, if you set the target ratio to 50% and the Window ± % parameter to 20%, the expected target ion ratio range is 40 to 60%. (With the Absolute option this range would be 30 to 70%.) If the ion ratio is outside this range, the ion ratio confirmation test has failed, and the application sets the IRC Flag to false. If the qualifier ion peak/quantitation peak ratio is within range, the ion ratio confirmation test is passed and the data system sets the IRC Flag to true. The response of all specified qualifier ions must be inside the respective ratio ranges for IRC to succeed. In assessing a target ion ratio range, the data system truncates the range at 0% to avoid negative values.
Absolute	Specify that the target ratio tolerance values in the Window ± % column of the qualifier ion table are absolute values. For example, if you set the target ratio to 50% and the Window ± % parameter to 20%, the expected target ion ratio range is 30 to 70%. (With the Relative option this range would be 40 to 60%.) If the qualifier ion peak/quantitation peak ratio is outside this range, the ion ratio confirmation test has failed and the application sets the IRC Flag to false. If the qualifier ion peak/quantitation peak ratio is within range, the ion ratio confirmation test is passed and the application sets the IRC Flag to true. The response of all specified qualifier ions must be inside the respective ratio ranges for IRC to succeed. In assessing a target ion ratio range, the Xcalibur application truncates the range at 0% to avoid negative values.

Table 56. Avalon Detection page for Quan view parameters (Sheet 8 of 8)

Parameter	Description
Buttons	
Save As Default	Validate and save the settings on the current page as default settings. The application uses these settings for all new processing methods. This option guarantees that the settings for the component are consistent and valid. These default settings are then used for all new components. The software writes over the previous default values and cannot recover them.
Advanced	Set advanced peak identification and detection parameters. The Avalon peak detection algorithm uses these parameters, which are displayed in the Event list on the Detection page.
Flags	Set peak area and peak height threshold values in the Data Flags Dialog Box. The application reports these data flags in results files, printed reports, and Quan Browser.

Genesis Detection Page for Quan View

On the Identification page for Quan view, you can choose from among the ICIS, Genesis, and Avalon Xcalibur peak detection algorithms.

Use the Genesis Detection page to specify peak integration and detection criteria for the Genesis peak detection algorithm.

Table 57. Genesis Detection page for Quan view parameters (Sheet 1 of 7)

Parameter	Description
Genesis Peak Integration	
Smoothing Points	Determine the degree of data smoothing to be performed on the active component peak prior to peak detection and integration. The valid range is any odd value from 1 (no smoothing) through 15 (maximum smoothing). To smooth your component peak data prior to integration, enter a value in the Smoothing Points box.
S/N Detection	View or change the current signal-to-noise threshold for peak integration. The application only integrates peaks with signal-to-noise greater than this value. Peaks with signal-to-noise less than this value are not integrated. The valid range is 0.0 to 999.0. To change the current value, enter a new value in the S/N Threshold box.
Enable Valley Detection	Choose the Xcalibur valley detection approximation method to detect unresolved peaks. This method drops a vertical line from the apex of the valley between unresolved peaks to the baseline. The intersection of the vertical line and the baseline defines the end of the first peak and the beginning of the second peak. To turn this method on, select the Valley Detection check box. To turn this method off, clear the check box.

Table 57. Genesis Detection page for Quan view parameters (Sheet 2 of 7)

Parameter	Description
Expected Width	View or change the expected peak width parameter (in seconds). This controls the minimum width that a peak is expected to have if valley detection is enabled. With valley detection enabled, any valley points nearer than the [expected width]/2 to the top of the peak are ignored. If a valley point is found outside the expected peak width, the data system terminates the peak at that point. The application always terminates a peak when the signal reaches the baseline, independent of the value set for the expected peak width. The valid range is 0.0 to 999.0 seconds. To change the current value, type a new width in the Expected Width box.
Constrain Peak Width	Limit the peak width of a component during peak integration of a chromatogram. You can then set values that control when peak integration is turned on and off by specifying a peak height threshold and a tailing factor. To limit a peak width, select the Constrain Peak Width check box. The Peak Height (%) box and the Tailing Factor box appear.
Peak Height	View or change the percent of the total peak height (100%) that a signal must be above the baseline before integration is turned on or off. Select the Constrain the Peak Width check box to activate this box. The valid range is 0.0 to 100.0%. To enter this height, type the appropriate value in the Peak Height (%) box.
Tailing Factor	View or change a factor that controls how the data system integrates the tail of a peak. This factor is the maximum ratio of the trailing edge to the leading side of a constrained peak. Select the Constrain the Peak Width check box to activate this box. The valid range is 0.5 through 9.0.
Min	View a representative drawing of a low value of the active parameter. The active parameter is defined by the current location of the cursor. For example, if you click the Smoothing Points box, the graphic shows the typical result obtained with a low number of smoothing points: a peak with reduced noise. The number in the upper left corner of the graphic is a representative low value of the active parameter. This number is not the current low value of the range of the active parameter.
Max	View a representative drawing of a high value of the active parameter. The active parameter is defined by the current location of the cursor. For example, if you click the Smoothing Points box, the graphic shows the typical result obtained with a high number of smoothing points: a peak without noise. The number in the upper left corner of the graphic is a representative high value of the active parameter. This number is not the current high value of the range of the active parameter.

Table 57. Genesis Detection page for Quan view parameters (Sheet 3 of 7)

Parameter	Description
Genesis Peak Detection	
Spectrum	Select a reference spectrum defined in the processing method for component identification. The application attempts to match the reference spectrum with a series of unknown spectra and calculates a score value for each comparison. This option is only available in Xcalibur GC chromatography mode (set in the Chromatography Options Dialog Box). If you select the Spectrum option, the following parameters appear: **Spectrum Peak Detection**: View spectrum peak detection only in Xcalibur GC Chromatography mode when you select the Spectrum option. You must also have selected the MS detector type on the Identification page. **Peak Identification Table**: Use this table to enter mass/charge [*m/z*] and intensity data for up to 50 spectrum peaks. The application uses this data to identify the active component the Find algorithm. It displays this table only when you select the Spectrum option in its GC Chromatography mode. ***m/z***: Use this box in the Spectrum Peak Identification table to view the mass/charge [*m/z*] value for one peak in the reference spectrum. The intensity for this *m/z* value is given in the adjacent Intensity table box. Use other rows of the table to enter as many as 50 *m/z* values. The application uses this data to identify the active component the Find algorithm. It displays this table only when you select the Spectrum option in its GC Chromatography mode. **Intensity**: Use this box in the Spectrum Peak Identification table to enter intensity data for one peak in the reference spectrum. The *m/z* value for this intensity is given in the adjacent *m/z* Table box. Use other rows of the table to enter as many as 50 intensity values. The application uses this data to identify the active component the Find algorithm. It displays this table only when you select the Spectrum option in its GC Chromatography mode.

Table 57. Genesis Detection page for Quan view parameters (Sheet 4 of 7)

Parameter	Description
Thresholds	**Forward**: Set a threshold value for forward comparisons between the reference spectrum and candidates in the chromatogram. A forward search is a direct matching algorithm comparing unknowns against the reference spectrum in the peak identification table. The match is scored on a scale of 0 to 999. A perfect match results in a score of 999. As a general guide, 900 or greater is an excellent match; 800 to 900, a good match; 700 to 800, a fair match. Less than 600 is a poor match. Unknown spectra with many peaks tend to score lower than similar spectra with fewer peaks. **Reverse**: Set a threshold value for reverse comparisons between the reference spectrum and candidates in the chromatogram. A reverse search ignores any peaks in the unknown that are not in the reference spectrum in the peak identification table. The match is scored on a scale of 0 to 999. A perfect match results in a score of 999. As a general guide, 900 or greater is an excellent match; 800 to 900, a good match; 700 to 800, a fair match. Less than 600 is a poor match. A spectrum with many peaks tends to score more highly in a reverse match than a forward match. **Match**: Set a threshold value for match comparisons between the reference spectrum and candidates in the chromatogram. Match is scored on a scale of 0 to 999. The match algorithm is a complex probability factor based on the differences between the forward factors of all the candidates. If one candidate has a forward matching factor of 900 and the next best is only 300, the probability of the component being correctly identified is high. This means that the match factor will be scored highly for the first candidate. If the forward factors for all the candidates are similar, whether high or low, the match factor will be low.
Highest Peak	Use the highest peak in the chromatogram for component identification.
Nearest RT	Use the peak with the nearest retention time in the chromatogram for component identification.

Table 57. Genesis Detection page for Quan view parameters (Sheet 5 of 7)

Parameter	Description
Options for Highest Peak or Nearest RT	If you are in GC mode and you select the Highest Peak or Nearest RT options, the following parameters appear: **Ion Ratio Confirmation**: View spectrum peak detection only in Xcalibur GC Chromatography mode when you select either the Highest Peak or Nearest RT option. You must also have selected the MS detector type on the Identification page. Use the settings in this area to specify up to five qualifier ions to confirm the detection of a target analyte. You can also set the coelution window and select a method for calculating the target ion ratio window and tolerance. **Enable**: This check box indicates whether or not Ion Ratio Confirmation is activated. **Ion Ratio Using**: **Area or Height** This readback shows the currently selected peak quantitation method: area or height. The application uses the same method to calculate the qualifier ion peak response and then the target ratio. You can change this parameter by selecting the Area or Height options in the Response area on the Calibration page. **Qualifier Ion Table**: Use this table to enter mass/charge [*m/z*] and target ratio tolerances [Window ± %] data for up to 5 qualifier ions. If you select Area response, the application integrates each qualifier ion peak and calculates a ratio using the integrated qualifier ion peak and the quantitation peak area. The application then compares this ratio with your specified target ratio. If the calculated ratio is outside of the target ratio by more than your specified tolerance (Window ± %), the quantitation peak is rejected. If you select Height response, the application calculates a ratio using the qualifier ion peak height with the height of the quantitation peak. The application then compares this ratio with your specified target ratio. If the calculated ratio is outside of the target ratio by more than your specified tolerance (Window ± %), the quantitation peak is rejected. ***m/z****:* View the mass/charge [*m/z*] value for a qualifier ion. The target ratio tolerance for this *m/z* value appears in the adjacent Window ± % table box. Use other rows of the table to enter data for 5 qualifier ions. The application uses this data to confirm the identity of a quantitation peak by comparing the relative responses of qualifier ion and quantitation peaks with predetermined values. **Target Ratio**: View the Target Ratio (%) value for a qualifier ion. The *m/z* value and target ratio tolerance for the qualifier ion are given in the adjacent *m/z* and Window ± % table boxes. Use other rows of the table to enter data for 5 qualifier ions. The application uses this data to confirm the identity of a quantitation peak by comparing the relative responses of qualifier ion and quantitation peaks with predetermined values.

Table 57. Genesis Detection page for Quan view parameters (Sheet 6 of 7)

Parameter	Description
Options for Highest Peak or Nearest RT (continued)	**Window**: Use this box in the Qualifier Ion table to specify the Target Ratio tolerance for a qualifier ion. Use other rows of the table to enter data for 5 qualifier ions. The application uses this data to confirm the identity of a quantitation peak by comparing the relative responses of qualifier ion and quantitation peaks with the specified values. **Qualifier Ion Coelution**: Use this box to set the Qualifier Ion Coelution window. Prior to ion ratio confirmation, the data system generates a mass chromatogram for each specified qualifier ion. Each of these chromatograms must feature a peak matching that of the quantitation mass(es). If the retention time of the qualifier ion peak apex lies outside of the Qualifier Ion Coelution window (centered on the quantitation peak), the data system rejects the quantitation peak. The application tests quantitation peaks with matching qualifier ion peaks (inside the Coelution window) for ion ratio confirmation.
Window	
Relative	Specify that the target ratio tolerance values in the Window ± % column of the qualifier ion table are relative values. For example, if you set the target ratio to 50% and the Window ± % parameter to 20%, the expected target ion ratio range is 40 to 60% (with the Absolute option this would be 30 to 70%). If the ion ratio is outside this range, the ion ratio confirmation test has failed and the data system sets the IRC flag to false. If the qualifier ion peak/quantitation peak ratio is within range, the ion ratio confirmation test is passed and the data system sets the IRC Flag to true. The response of all specified qualifier ions must be inside the respective ratio ranges for IRC to succeed. In assessing a target ion ratio range, the application truncates the range at 0% to avoid negative values.
Absolute	Specify that the target ratio tolerance values in the Window ± % column of the qualifier ion table are absolute values. For example, if you set the target ratio to 50% and the Window ± % parameter to 20%, the expected target ion ratio range is 30 to 70% (with the Relative option this would be 40 to 60%). If the qualifier ion peak/quantitation peak ratio is outside this range, the ion ratio confirmation test has failed and the data system sets the IRC Flag to false. If the qualifier ion peak/quantitation peak ratio is within range, the ion ratio confirmation test is passed and the data system sets the IRC Flag to true. The response of all specified qualifier ions must be inside the respective ratio ranges for IRC to succeed. In assessing a target ion ratio range, the application truncates the range at 0% to avoid negative values.

Table 57. Genesis Detection page for Quan view parameters (Sheet 7 of 7)

Parameter	Description
Minimum Peak Height	View the peak signal-to-noise values or change them to equal or exceed so that the data system uses the Nearest RT Peak Identification criteria. For Component Identification purposes, the application ignores all chromatogram peaks that have signal-to-noise values that are less than the S/N Threshold value. The valid range is 0.0 (all peaks) through 999.0.
Buttons	
Save As Default	Validate and save the settings on the current page as default settings. The application uses these settings for all new processing methods. This option guarantees that the settings for the component are consistent and valid. These default settings will be used for all new components. The software writes over the previous default values and cannot recover them.
Advanced	Set advanced peak identification and detection parameters in the Genesis Advanced Detection Options Dialog Box. The Genesis peak detection algorithm uses these parameters.
Flags	Set peak area and peak height threshold values in the Data Flags Dialog Box. The application reports these data flags in results files, printed reports and Quan Browser.

ICIS Detection Page for Quan View

On the Identification page of the Quan view, you can choose from among the ICIS, Genesis, and Avalon Xcalibur peak detection algorithms.

Use the ICIS Detection page to specify peak integration and detection criteria for the ICIS peak detection algorithm.

Table 58. ICIS Detection page for Quan view parameters (Sheet 1 of 7)

Parameter	Description
ICIS Peak Integration	
ICIS Peak Integration	Specify peak integration criteria. These parameters are used by the ICIS peak detection and integration algorithm.
Smoothing Points	Enter the number of points used in the moving average used to smooth the data. The valid range is any odd value from 1 through 15 points. The default value is 1 point. The ICIS peak detection algorithm uses this value.
Baseline Window	Specify the number of scans to review for a local minima. The valid range is 1 through 500. The default value is 40 scans. The ICIS peak detection algorithm uses this value.
Area Noise Factor	Specify the noise level multiplier used to determine the peak edge after the location of the possible peak. The valid multiplier range is 1 through 500. The default multiplier is 5. The ICIS peak detection algorithm uses this value.
Peak Noise Factor	Specify the noise level multiplier used to determine the potential peak signal threshold. The valid multiplier range is 1 through 1000. The default multiplier is 10. The ICIS peak detection algorithm uses this value.

Table 58. ICIS Detection page for Quan view parameters (Sheet 2 of 7)

Parameter	Description
Constrain Peak Width	Limit the peak width of a component during peak integration of a chromatogram. You can then set values that control when peak integration is turned on and off by specifying a peak height threshold and a tailing factor. To limit a peak width, select the Constrain Peak Width check box. The Peak Height (%) box and the Tailing Factor box appear.
Peak Height	View or change the percent of the total peak height (100%) that a signal must be above the baseline before integration is turned on or off. Select the Constrain Peak Width check box to activate this box. The valid range is 0.0 to 100.0%. To enter this height, type the appropriate value in the Peak Height (%) box.
Tailing Factor	View or change a tailing factor that controls how the data system integrates the tail of a peak. This factor is the maximum ratio of the trailing edge to the leading side of a constrained peak. Select the Constrain Peak Width check box to activate this box. The valid range is 0.5 through 9.0.
Min	View a representative drawing of a low value of the active parameter. The active parameter is defined by the current location of the cursor. For example, if you click the Smoothing Points box, the graphic shows the typical result obtained with a low number of smoothing points: a peak with reduced noise. The number in the upper left corner of the graphic is a representative low value of the active parameter. This number is not the current low value of the range of the active parameter.
Max	View a representative drawing of a high value of the active parameter. The active parameter is defined by the current location of the cursor. For example, if you click the Smoothing Points box, the graphic shows the typical result obtained with a high number of smoothing points: a peak without noise. The number in the upper left corner of the graphic is a representative high value of the active parameter. This number is not the current high value of the range of the active parameter.

Table 58. ICIS Detection page for Quan view parameters (Sheet 3 of 7)

Parameter	Description
ICIS Peak Detection	
Spectrum	Use a reference spectrum defined in the processing method for component identification. The application attempts to match the reference spectrum with a series of unknown spectra and calculates a score value for each comparison. This option is only available in Xcalibur GC chromatography mode (set in the Chromatography Options Dialog Box). If you select the Spectrum option, the following parameters appear: **Spectrum Peak Detection**: View spectrum peak detection only in Xcalibur GC Chromatography mode when you select the Spectrum option. You must also select the MS detector type on the Identification page. **Peak Identification Table**: Use this table to enter mass/charge [*m/z*] and intensity data for up to 50 spectrum peaks. The application uses this data to identify the active component the Find algorithm. It displays this table only when you select the Spectrum option in its GC Chromatography mode. ***m/z***: Use this box in the Spectrum Peak Identification table to view the mass/charge (*m/z*) value for one peak in the reference spectrum. The intensity for this *m/z* value is given in the adjacent Intensity table box. Use other rows of the table to enter as many as 50 *m/z* values. The application uses this data to identify the active component the Find algorithm. It displays this table only when you select the Spectrum option in its GC Chromatography mode. **Intensity**: Use this box in the Spectrum Peak Identification table to enter intensity data for one peak in the reference spectrum. The *m/z* value for this intensity is given in the adjacent *m/z* Table box. Use other rows of the table to enter as many as 50 intensity values. The application uses this data to identify the active component the Find algorithm. It displays this table only when you select the Spectrum option in its GC Chromatography mode.

Table 58. ICIS Detection page for Quan view parameters (Sheet 4 of 7)

Parameter	Description
Thresholds	**Forward**: Set a threshold value for forward comparisons between the reference spectrum and candidates in the chromatogram. A forward search is a direct matching algorithm comparing unknowns against the reference spectrum in the peak identification table. The match is scored on a scale of 0 to 999. A perfect match results in a score of 999. As a general guide, 900 or greater is an excellent match; 800 to 900 a good match; 700 to 800 a fair match. Less than 600 is a poor match. Unknown spectra with many peaks tends to score lower scores than similar spectra with fewer peaks. **Reverse**: Set a threshold value for reverse comparisons between the reference spectrum and candidates in the chromatogram. A reverse search ignores any peaks in the unknown that are not in the reference spectrum in the peak identification table. The match is scored on a scale of 0 to 999. A perfect match results in a score of 999. As a general guide, 900 or greater is an excellent match; 800 to 900 a good match; 700 to 800 a fair match. Less than 600 is a poor match. A spectrum with many peaks tends to score more highly in a reverse match than a forward match. **Match**: Set a threshold value for match comparisons between the reference spectrum and candidates in the chromatogram. Match is scored on a scale of 0 to 999. The match algorithm is a complex probability factor based on the differences between the forward factors of all the candidates. If one candidate has a forward matching factor of 900 and the next best is only 300, the probability of the component being correctly identified is high and so the match factor will be scored highly for the first candidate. If the forward factors for all the candidates are similar, whether high or low, the match factor will be low.
Highest Peak	Use the highest peak in the chromatogram for component identification.
Nearest RT	Use the peak with the nearest retention time in the chromatogram for component identification.

Table 58. ICIS Detection page for Quan view parameters (Sheet 5 of 7)

Parameter	Description
Options for Highest Peak or Nearest RT	If you are in GC mode and you select the Highest Peak or Nearest RT options, the following parameters appear: **Ion Ratio Confirmation**: View spectrum peak detection only in Xcalibur GC Chromatography mode when you select either the Highest Peak or Nearest RT option. You must also have selected the MS detector type on the Identification page. Use the settings in this area to specify up to five qualifier ions to confirm the detection of a target analyte. You can also set the coelution window and select a method for calculating the target ion ratio window and tolerance. **Enable**: This check box indicates whether or not you selected the Ion Ratio Confirmation option. **Ion Ratio Using: Area or Height** This readback shows the currently selected peak quantitation method: area or height. The application uses the same method to calculate the qualifier ion peak response and then the target ratio. You can change this parameter by selecting the **Area** or **Height** options in the Response area on the Calibration page. **Qualifier Ion Table**: Use this table to enter mass/charge [*m/z*] and target ratio tolerances [Window ± %] data for up to 5 qualifier ions. If you select Area response, the application integrates each qualifier ion peak and calculates a ratio using the integrated qualifier ion peak and the quantitation peak area. The application then compares this ratio with your specified target ratio. If the calculated ratio is outside of the target ratio by more than your specified tolerance (Window ± %), the quantitation peak is rejected. If you select Height response, the application calculates a ratio using the qualifier ion peak height with the height of the quantitation peak. It then compares this ratio with your specified target ratio. If the calculated ratio is outside of the target ratio by more than your specified tolerance (Window ± %), the quantitation peak is rejected. ***m/z***: View or change the mass/charge [*m/z*] value for a qualifier ion. The target ratio tolerance for this *m/z* value appears in the adjacent Window ± % table box. Use other rows of the table to enter data for 5 qualifier ions. The application uses this data to confirm the identity of a quantitation peak by comparing the relative responses of the qualifier ion and quantitation peaks with predetermined values. **Target Ratio**: View or change the Target Ratio (%) value for a qualifier ion. The *m/z* value and target ratio tolerance for the qualifier ion are given in the adjacent *m/z* and Window ± % table boxes. Use other rows of the table to enter data for 5 qualifier ions. The application uses this data to confirm the identity of a quantitation peak by comparing the relative responses of the qualifier ion and quantitation peaks with predetermined values.

Table 58. ICIS Detection page for Quan view parameters (Sheet 6 of 7)

Parameter	Description
Options for Highest Peak or Nearest RT (continued)	**Window**: Specify the Target Ratio tolerance for a qualifier ion. Use other rows of the table to enter data for 5 qualifier ions. The application uses this data to confirm the identity of a quantitation peak by comparing the relative responses of the qualifier ion and quantitation peaks with the specified values. **Qualifier Ion Coelution**: Set the Qualifier Ion Coelution window. Prior to ion ratio confirmation, the application generates a mass chromatogram for each specified qualifier ion. Each of these chromatograms must feature a peak matching that of the quantitation mass(es). If the retention time of the qualifier ion peak apex lies outside of the Qualifier Ion Coelution window (centered on the quantitation peak), the application rejects the quantitation peak. The data system tests quantitation peaks with matching qualifier ion peaks (in the Coelution window) for ion ratio confirmation.
Window	
Relative	Specify that the target ratio tolerance values in the Window ± % column of the qualifier ion table are relative values. For example, if you set the target ratio to 50% and the Window ± % parameter to 20%, the expected target ion ratio range is 40 to 60% (with the Absolute option this would be 30 to 70%). If the ion ratio is outside this range, the ion ratio confirmation test has failed and the data system sets the IRC Flag to false. If the qualifier ion peak/quantitation peak ratio is within range, the ion ratio confirmation test is passed and the data system sets the IRC Flag to true. The response of all specified qualifier ions must be inside the respective ratio ranges for IRC to succeed. In assessing a target ion ratio range, the application truncates the range at 0% to avoid negative values.
Absolute	Specify that the target ratio tolerance values in the Window ± % column of the qualifier ion table are absolute values. For example, if you set the target ratio to 50% and the Window ± % parameter to 20%, the expected target ion ratio range is 30 to 70% (with the Relative option this would be 40 to 60%). If the qualifier ion peak/quantitation peak ratio is outside this range, the ion ratio confirmation test has failed and the data system sets the IRC Flag to false. If the qualifier ion peak/quantitation peak ratio is within range, the ion ratio confirmation test is passed and the data system sets the IRC Flag to true. The response of all specified qualifier ions must be inside the respective ratio ranges for IRC to succeed. In assessing a target ion ratio range, the application truncates the range at 0% to avoid negative values.

Table 58. ICIS Detection page for Quan view parameters (Sheet 7 of 7)

Parameter	Description
Minimum Peak Height	View the peak signal-to-noise values or change them to equal or exceed so that the data system uses the Nearest RT Peak Identification criteria. For Component Identification purposes, the application ignores all chromatogram peaks that have signal-to-noise values that are less than the S/N Threshold value. The valid range is 0.0 (all peaks) through 999.0.
Buttons	
Save As Default	Validate and save the settings on the current page as default settings. The application uses these settings for all new processing methods. This option guarantees that the settings for the component are consistent and valid. These default settings are used for all new components. The software writes over the previous default values and cannot recover them.
Advanced	View or change advanced peak identification and detection parameters in the ICIS Advanced Parameters Dialog Box. These parameters are used by the ICIS peak detection algorithm.
Flags	View or change peak area and peak height threshold values in the Data Flags Dialog Box. The application reports these data flags in results files, printed reports, and Quan Browser.

Identification Page for Quan View

Use the Identification page to name components and specify retention time, detector type, and peak identification, detection, and integration criteria.

Table 59. Identification page for Quan view parameters (Sheet 1 of 7)

Parameter	Description
Name	This box displays a list of component names for the active processing method. To display the component identification settings for a component on the list, click the name of the component in the Component Name box. To add a new component to the component list, replace the <New> entry in the Component Name box with the name of the new component. Press **ENTER** or click **OK** to enter the new component. The new component appears in the Component list in the Components pane.
Detector Type	View or change the currently selected detector type: • MS • Analog • A/D Card • PDA • UV To change the detector type, click the arrow to display the list of detector types. Click the required detector type.

Table 59. Identification page for Quan view parameters (Sheet 2 of 7)

Parameter	Description
Peak Detect	View and change Xcalibur peak detection algorithm options to recalculate the data using that algorithm. ❖ **To select an algorithm** 1. Enter a name in the Name box. 2. Click the **Peak Detect** list to display the algorithm names. 3. Select an algorithm and click **OK**. The application recalculates the current data using the specified algorithm. It changes the default parameters for peak detection to those specific to that algorithm.
Scan Filter	This box displays the current scan filter for the active file with extension .raw. You can use a scan filter to specify that processing is to be applied to a subset of the scans in a raw file. To apply a different scan filter, select a new filter from the scan filter list (most common method), select a new filter from a list and edit the scan filter, or type a new scan filter command string into the box using the scan filter format. To select from the list of scan filters used to create the raw file, click the arrow on the box to display the list. Click one of the scan filters. The application displays the scan filter in the Filter box. This scan filter example: c full ms [26.81–251] finds all scans in a raw file that have the following properties: centroid data Scan Mode: Full Scan Power: MS Product Ion Mass Range: *m/z* 26.81 to 251.00

Table 59. Identification page for Quan view parameters (Sheet 3 of 7)

Parameter	Description
Trace	From the three Trace lists, choose the type of chromatogram you want to use for data processing. Select: 1. A basic chromatogram type, for example, TIC, from the first list. 2. A logical operator: + or – from the second list. Your selection of an operator activates: 3. The third list for you to select a second chromatogram type to add to, or subtract from, the first type. For example, Mass Range. The list includes the valid remaining trace types. You can use trace combinations to subtract from a chromatogram the contributions from a solvent or noise. Combinations are limited to traces of the same type. • For MS scans, valid trace types are TIC, Mass Range, and Base Peak • For Analog data, up to four channels are supported (labeled Analog 1–4) • For data from an A/D Card, four channels are supported (labeled A/D Card Ch 1–4) • For PDA data, valid trace types are Wavelength Range, Total Scan, or Spectrum Maximum • For UV detector data, four channels are supported (labeled Channel A–D). Valid MS trace combinations Click the following links for valid combinations. – Valid MS Trace Combinations – Valid Analog Trace Combinations – Valid A/D Card Trace Combinations – Valid PDA Trace Combinations – Valid UV Trace Combinations

Table 59. Identification page for Quan view parameters (Sheet 4 of 7)

Parameter	Description
For MS detector type:	
Mass	View or change the mass range for the Mass Range trace type. The application displays this box when you select a Mass Range trace type or a TIC ± Mass Range trace combination for an MS detector type. To change the range or to add a new range, type the range in the box. The valid range depends on the configured detector. The format is *LowMass–HighMass*. For example, for the range *m/z* 123 through 456, type **123–456**. You can sum up to 50 mass ranges by entering mass ranges or single mass values separated by your computer list separator character. To view or set the list separator character, see "Changing the List Separator Character."
Mass1	View or change the mass range for the first trace type. The application displays this box when you select a Mass Range ± Mass Range trace combination for an MS detector type. To change the range or to add a new range, type the range in the box. The valid range depends on the configured detector. The format is *LowMass–HighMass*. For example, for the range *m/z* 123 through 456, type **123–456**. You can sum up to 50 mass ranges by entering mass ranges or single mass values separated by your computer list separator character. To view or set the list separator character, see "Changing the List Separator Character."
[Mass] 2	View or change the mass range for the second trace type. The application displays this box when you select a Mass Range ± Mass Range trace combination for an MS detector type. To change the range or to add a new range, type the range in the box. The format is *LowMass–HighMass*. For example, for the range *m/z* 123 through 456, type **123–456**. You can sum up to 50 mass ranges by entering mass ranges or single mass values separated by your computer list separator character. To view or set the list separator character, see "Changing the List Separator Character."
BP	View or change the range to search for the highest peak. The application displays this box when you select a Base Peak trace for an MS detector type. If you enter a single *m/z* value in this box, that *m/z* value defines the base peak. To change the base peak mass range, type the value in the box. A mass range from *m/z*=A to *m/z*=B is entered in the format A–B.
MR	View or change the mass range for the second Mass Range trace type. The application displays this box when you select a Base Peak ± Mass Range trace combination for an MS detector type. To change the range or to add a new range, type the range in the box. The format is *Low Mass–HighMass*. For example, for the range *m/z* 123 through 456, type **123–456**.

Table 59. Identification page for Quan view parameters (Sheet 5 of 7)

Parameter	Description
For PDA detector type:	
Wavelength	View or change the wavelength range for the Wavelength Range or Spectrum Maximum trace type. The application displays this box when you select one of the following trace combinations for a PDA detector type: • Spectrum Maximum • Wavelength Range • Total Scan – Wavelength Range To change the range or to add a new range, type the range in the box. The valid range depends on the configured detector. The format is *LowWavelength–HighWavelength*. For example, for the range *m/z* 123 through 456, type **123–456**. You can sum up to 50 wavelength ranges by entering ranges or single values separated by your computer list separator character. To view or set the list separator character, see "Changing the List Separator Character."
Wavelength 1	View or change the wavelength or wavelength range for the first trace type. The application displays this box when you select one of the following trace combinations for a PDA detector type: • Wavelength Range ± Wavelength Range • Spectrum Maximum ± Wavelength Range To change the range or to add a new range, type the range in the box. The valid range depends on the configured detector. The format is *LowWavelength–HighWavelength*. For example, for the range *m/z* 123 through 456, type **123–456**. You can sum up to 50 wavelength ranges by entering ranges or single values separated by your computer list separator character. To view or set the list separator character, see "Changing the List Separator Character."

Table 59. Identification page for Quan view parameters (Sheet 6 of 7)

Parameter	Description
[Wavelength] 2	View or change the wavelength or wavelength range for the second trace type. The application displays this box when you select one of the following trace combinations for a PDA detector type: • Wavelength Range ± Wavelength Range • Spectrum Maximum ± Wavelength Range To change the range or to add a new range, type the range in the box. The format is *LowWavelength–HighWavelength*. For example, for the range *m/z* 123 through 456, type **123–456**. You can sum up to 50 wavelength ranges by entering ranges or single values separated by your computer list separator character. To view or set the list separator character, see "Changing the List Separator Character."
Keys	View or change comments about the analysis. The box holds up to 50 characters and is case sensitive for alphabetic characters (for example, "abc" is recognized as being different from "Abc").
Retention Time	
Expected	View or change the anticipated retention time for the data system to detect the selected component. The valid range depends on the configured hardware. To change the time or to enter a new time, type the number of minutes in the Expected (retention time) box.
Window	View or change the allowable retention time window for the elution of the selected component. The valid range is 1.0 to 999.0 seconds. To change the time window or to enter a new time window, type the number of seconds in the (retention time) Window box.
Use as RT Reference	Select whether to use the actual retention time (RT) of the active component (displayed in the Name box in the same view) to adjust the expected retention time of another component. To use the active component as an RT Reference (retention time reference), select this check box. If you do not want to use this component as an RT reference, clear this check box. All RT References appear in the Adjust Using list.
View Width	View or change the current view width (in minutes). The valid range depends on the configured hardware. To change the view width, enter the desired time in the View Width box.
Adjust Using check box	Select whether to adjust the expected retention time (RT) of the active component (displayed in the Name box in the same view) using the actual retention time of the RT Reference, such as an internal standard. The application displays the RT Reference in the Adjust Using list to the right of this check box. There must be at least one RT Reference in the processing method for this check box to be active. RT References are created if you select the Use As RT Reference check box when the component is active.

Table 59. Identification page for Quan view parameters (Sheet 7 of 7)

Parameter	Description
Adjust Using list	View or change the retention reference component that the data system uses to adjust the expected retention time of the active component (displayed in the Name box in the same view). This list is only active if you select the Adjust Using check box to the left of this list. To change the RT Reference component, click the arrow to display the list of RT Reference components. The application uses the actual retention time of the RT Reference component to correct the retention time of the active component. It provides the following correction to the expected retention time: Adjusted RT Component Expected = [RT Component Expected] - [RT Reference Actual] / [RT Reference Expected].
Components	
Component list	View all of the component names that have been defined for the active processing method. This list is located in the Components pane at the far right of the Processing Method window. ❖ **To add a new component to the list** 1. Replace <New> in the Name box with the name of the component. 2. Click **OK**. The new component name appears in the Name box and Component list. ❖ **To delete a component from the list** 1. Click the name of the component to delete from the Component list. 2. Choose **Options > Delete Component**.
Buttons	
Save as Default	Validate and save the settings on the current page as default settings. The application uses these settings for all new processing methods. This option guarantees that the settings for the component are consistent and valid. These default settings are used for all new components. The software writes over the previous default values and cannot recover them. Those settings that you are likely to change, such as Name, Expected Retention Time, Trace Type, and so on, are not stored as default settings.

Levels Page for Quan View

Use the Levels page to define Calibration and QC levels for Target compounds. You can use the Standard Dilution Dialog Box to create calibration level information for all components quickly and easily. This page is not available for ISTD component types.

Table 60. Levels page for Quan view parameters (Sheet 1 of 2)

Parameter	Description
Readback	
Units	View the units set on the Calibration page. The units are also used in reports and in Quan Browser.
Calibration Levels	
Calibration Levels Shortcut Menu	Insert a new row in the Calibration Levels table. From the Levels page of the Processing Setup Quan window, right-click the **Cal Levels** table to display this menu containing the following commands: **Delete Rows**: This command deletes the currently selected row of the QC Levels table. **Insert Rows**: This command inserts a new row in the QC Levels table. **Copy Levels to All Target Components**: This command copies the current QC Levels table to all target components. This action ensures that all target components contain exact duplicates of the current components table.
Calibration Levels Table	View calibration level names and calibration level amounts.
Cal Level	View or change the calibration levels for the selected component. The application can accommodate up to 50 calibration levels. To enter a calibration level, type the new value in the appropriate Cal Level box. To delete a Cal level row, click to the left of the row. The application highlights the row. Then press DELETE.
Amount	View or change the amounts of the target compound used for each calibration level. You can enter amounts with up to three decimals of precision. To enter a calibration amount, type the value in the Amount box at the appropriate level.
QC Levels	
QC Levels Shortcut Menu	Make changes to the QC Levels table. From the Levels page of the Processing Setup Quan window, right-click the QC Levels table to display this menu containing the following commands: **Delete Rows**: This command deletes the currently selected row of the QC Levels table. **Insert Rows**: This command inserts a new row in the QC Levels table. **Copy Levels to All Target Components**: This command copies the current QC Levels table to all target components. This action ensures that all target components contain exact duplicates of the current components table.

Table 60. Levels page for Quan view parameters (Sheet 2 of 2)

Parameter	Description
QC Levels Table	View QC (quality control) level names, quality control level amounts, and % test values. Use QC samples containing known amounts of a component to check the accuracy of an analysis. The application measures the quantity of the QC component in the same manner as unknown components. The measured quantity is then compared with a user-defined expected quantity and a user-defined percent test.
QC Level	View the quality control levels for the selected component. The application can accommodate up to 50 QC levels. To enter a quality control level, type the value in the appropriate QC Level box. The default level amount value changes from 0.000 to 0.010 when you enter a value for a QC level. To delete a QC level row, click to the left of the row. The application highlights the row. Then press DELETE**.**
Amount	View the amount that the data system calculates was injected for each QC level for the selected calibration component, based on the calibration curve. The application uses the least-squares calibration curve for all levels to determine the amount (X-axis) that corresponds to the experimental response (Y-axis).
% Test	View a value for the acceptable difference (as a percent) between the known amount and calculated (measured) amount of each QC level.
Buttons	
Save As Default	Validate and save the settings on the current page as default settings. The application uses these settings for all new processing methods. This option guarantees that the settings for the component are consistent and valid. These default settings are used for all new components. The software writes over the previous default values and cannot recover them.

Peak Purity Page for Quan View

Use the Peak Purity page to specify the values of the peak purity parameters to include in a quantitative processing method for the PDA detector type only. When you specify the processing method in a sequence, you can then apply the parameters to your quantitative PDA analysis as you acquire data. Use a raw file of PDA data in Quan Browser to specify the values for peak purity parameters that you want to use in the processing method.

Table 61. Peak Purity page for Quan view parameters

Parameter	Description
Purity Parameters	
Enable	View or change Peak Purity parameters for PDA chromatograms in an active chromatogram cell. To view or change Peak Purity parameters and calculate peak purity results, select the Enable check box. Peak detection occurs automatically prior to the peak purity calculation.
Scan Threshold	Specify a minimum value of intensity for wavelength scans in milliabsorbance units (mAU). A Peak Purity computation using scan threshold starts with the scan at the apex of the peak, and then collects wavelength data from scans on both sides of the apex until the scan threshold is reached. Use scan threshold for either symmetrical or asymmetrical peaks. The default value for scan threshold is 3 mAU. The range of possible values is 0 to 1000 mAU (or 1 AU). In a sample with high background or noise, you might start with a value for scan threshold of 40 mAU.
Peak Coverage	Specify a maximum percent value of the width of the integrated peak. A Peak Purity computation using peak coverage starts with the scan at the apex of the peak and then collects wavelength data from scans on both sides of the apex until the percent peak coverage is reached. Use peak coverage for symmetrical peaks. The default value for peak coverage is 95% of the integrated peak width.
Limit Scan Wavelength	View or change the Wavelength Range box. Select this check box to limit the number of wavelengths to include in the Peak Purity computation. Then enter a range in the Wavelength Range box.
[Wavelength] Range	Specify a range of UV scans (in nanometers) that include the wavelengths of your peak or peaks of interest. A Peak Purity computation using wavelength range starts with the scan at the apex of a peak and collects wavelength data from scans on both sides of the apex until all the wavelengths in the range are included. Use wavelength range for either symmetrical or asymmetrical peaks. To activate this box, select the Limit Scan Wavelength check box. The default wavelength range is the full width of the scan.

System Suitability Page for Quan View

Use the System Suitability page to carry out a sequence of automated chromatographic checks that assign a pass or fail qualification to a target peak. These checks are based on an analysis of the quantitation peak and, if ion ratio confirmation is enabled, all qualifier ion peaks in the retention time window. System suitability flags are reported in Sample and Summary reports and in Quan Browser.

Table 62. System Suitability page for Quan view parameters (Sheet 1 of 4)

Parameter	Description
Resolution Parameters	
Enable	Specify system suitability checks on the resolution of quantitation peaks. Resolution testing is based on a comparison of the peak height with adjacent valley height in the quantitation window. If the endpoint of a peak is not detected as a valley, the peak always passes the Resolution Threshold test, regardless of the set threshold value or the presence of overlapping peaks.
Resolution Threshold (%)	View or change the resolution threshold. The default value is 90% and the valid range is 0 to 100%. Resolution threshold is defined as the ratio: 100 × V/P where: V = the horizontal asymptote extended from the target peak's apex to the lowest point in the valley between the target peak and a neighboring peak P = the height of the target peak
Symmetry Parameters	
Enable	Specify system suitability checks for the symmetry of quantitation peaks. Symmetry is determined at a specified peak height and is a measure of how even-sided a peak is about a perpendicular dropped from its apex. If the end point of a peak is not detected as a valley, the peak always passes the Resolution Threshold test, regardless of the set threshold value or the presence of overlapping peaks.
Peak Height (%)	View or change the Peak Height where the data system measures the symmetry of target peaks. The default value is 50%. You can enter any value in the range 0 to 100%.

Table 62. System Suitability page for Quan view parameters (Sheet 2 of 4)

Parameter	Description
Symmetry Threshold (%)	View or change the Symmetry Threshold value. The defined Symmetry Threshold is > 70% at 50% peak height. This value represents a realistic practical tolerance for capillary GC data. You can enter any value in the range 0% to 100%. The default value is 80% at 50% peak height. The application determines symmetry at the peak height specified in the Peak Height % box. For the purposes of the test, a peak is considered symmetrical if: (Lesser of L and R) × 100 / (Greater of L and R) > Symmetry Threshold % where: L = the distance from the left side of the peak to the perpendicular, dropped from the peak apex R = the distance from the right side of the peak to the perpendicular, dropped from the peak apex Measurements of L and R are taken from the raw file without smoothing.
Peak Classification Parameters	
Enable	Specify system suitability checks for the classification of quantitation peaks.
Detect Peak Width	
Peak Height (%)	View or change the Peak Height where the data system tests the width of target peaks. You can enter any value in the range 0 to 100%. The default value is 50%.
Min Peak Width	View or change the minimum peak width at the specified peak height for the peak width suitability test. The default value is 0.6. You can set any value from 0 to 30 seconds.
Max Peak Width	View or change the maximum peak width at the specified peak height for the peak width suitability test. The default value is 0.6. You can set any value from 0 to 30 seconds.

Table 62. System Suitability page for Quan view parameters (Sheet 3 of 4)

Parameter	Description
Detect Tailing	
Peak Height (%)	View or change the Peak Height where the data system measures the tailing of target peaks. The default value is 10%. Enter any value from 0 to 100%.
Failure Threshold	View or change the failure threshold for the tailing suitability test. The default defined failure threshold is < 2 at 10% peak height. The valid range is 1 to 50. Tailing is calculated at the value defined in the Peak Height (%) box. For the purposes of the test, a peak is considered to be excessively tailed if: R / L > Failure Threshold % where: L = the distance from the left side of the peak to the perpendicular, dropped from the peak apex R = the distance from the right side of the peak to the perpendicular, dropped from the peak apex Measurements of L and R are taken from the raw file without smoothing.
Detect Column Overload	
Peak Height (%)	View or change the Peak Height at which the data system measures column overloading. The default value is 50%. Enter any value from 0 to 100%.
Failure Threshold	View or change the failure threshold value for the column overload suitability test. The default defined threshold is 1.5 at 50% peak height. The valid range is 1 to 20. A peak is considered to be overloaded if: L / R > Failure Threshold % where: L = the distance from the left side of the peak to the perpendicular, dropped from the peak apex R = the distance from the right side of the peak to the perpendicular, dropped from the peak apex Measurements of L and R are taken from the raw file without smoothing.

Table 62. System Suitability page for Quan view parameters (Sheet 4 of 4)

Parameter	Description
Detect Baseline Clipping	
Number of Peak Width for Noise Detection	View or change the Number of Peak Widths for Noise Detection testing parameter for the baseline clipping system suitability test. The default value is 1.0 and the valid values are from 0.1 to 10. A peak is considered to be baseline clipped if there is no signal (zero intensity) on either side of the peak in the specified number of peak widths. The range is truncated to the quantitation window if the specified number of peak widths extends beyond the window's edge.
Detect Minimum Signal-To-Noise Ratio	
Signal-To-Noise Ratio	View or change the threshold for system suitability testing of the signal-to-noise ratio. The default value is 20 and the permitted range is 1 to 500. The application calculates the signal-to-noise ratio in the quantitation window using only the baseline signal. Any extraneous, minor, detected peaks are excluded from the calculation.
Buttons	
Save As Default	Validate and save the settings on the current page as default settings. The application uses these settings for all new processing methods. This option guarantees that the settings for the component are consistent and valid. These default settings are used for all new components. The software writes over the previous default values and cannot recover them.

Programs View

Use the Programs view of the Processing Setup window to compile a list of programs or macros to be run by the application after the analysis of a sample and the processing of the resulting data. The application runs the programs in the listed order.

The Programs view features a Menu bar, a Toolbar, and the Programs table. This view also provides access to Xcalibur Help.

Menus

Processing Setup window menus:

File Menu | View Menu | Options Menu
GoTo Menu | Help Menu

Toolbar

Processing Setup Toolbar

Table

The Programs Table lists the programs to be run by the application during post processing.

Table 63. Programs table (Sheet 1 of 2)

Parameter	Description
Programs	
Programs	Specify post processing programs or macros to be run after the processing of a bracketed or non-bracketed sequence. Each row in the Programs table consists of eight columns.
[Row Number]	Each numbered row represents an item in the table. The asterisk (*) indicates the last unused row in the table. Use this row to enter a new item.
Enable	View the availability of the program or macro. If the program or macro is available, the box displays a Yes value. If it is unavailable, the box is blank. When you click the box, a check box appears and you can change the status.
Sample Type	
Std	View the availability of the report for Standard Sample types. If the report is available, the box displays a Yes value. If it is unavailable, the box is blank. When you click the box, a check box appears and you can change the status.
QC	View the availability of the report for QC sample types. If the report is available, the box displays a Yes value. If it is unavailable, the box is blank. When you click the box, a check box appears and you can change the status.

Table 63. Programs table (Sheet 2 of 2)

Parameter	Description
Unk	View the availability of the report for Unknown sample types. If the report is available, the box displays a Yes value. If it is unavailable, the box is blank. When you click the box, a check box appears and you can change the status.
Other	View the availability of the report for sample types other than Standard, QC, or Unknown. If the report is available, the box displays a Yes value. If it is unavailable, the box is blank. When you click the box, a check box appears and you can change the status.
Action	View the action that occurs when a program is run. To change the current action, click the Action list to display the action options. Then select one of the following actions: Run Excel Macro or Run Program.
Program or Macro Name	View or change the full path of the program or macro that the application uses during post processing. You can type the full path in the box or browse for the program or macro in the Browse for Program dialog box. Double-click the Program or Macro Name box to display the Browse for Program dialog box. Or right-click the cell and select Browse from the context menu. To change the current program or macro name in the command line, double-click the Program or Macro Name box to activate the Open dialog box so that you can select your program or macro. The application displays the new program or macro name. You can also type the command line. Example using the XConvert.exe program: To convert the current file (myfile.raw) from Xcalibur (.raw) file format to ANDI (.cdf) file format and copy it to the current default data directory, use the following command line: Convert /DA /SL %R in which DA indicates that the destination file (D) is to be ANDI format (A) SL indicates that the source file (S) is an LCQ raw file (L) %R is the macro argument for the current raw file Refer also to the *Xcalibur System and 21 CFR Part 11 Compliance Administrator Guide* for more examples.
Sync	Specify if the selected program is to be run synchronously or asynchronously. The application initiates asynchronous programs simultaneously but starts synchronous programs only when the previous program is finished. To change the current action, click the box and then select or clear the check box as required.
Parameters	Specify any command parameters for the selected program. See the Program or Macro Name box for examples.

Column Headings

This table lists column headings in the Programs table and their use.

Table 64. Column headings in the Programs table

Column heading	Use
Enable	Enables a program.
Save As	Provides you with various options for exporting the specified summary report.
Std	Determines whether the application runs a program after a Standard sample analysis.
QC	Determines whether the application runs the program after a QC sample analysis.
Unk	Determines whether the application runs the program after an Unknown sample analysis.
Other	Determines whether the application runs the program after any other type of sample analysis.
Action	Provides two options: Run Program or Run Excel Macro.
Program Name	Displays the full path of the program or macro to be run by the data system during post processing.
Sync	Determines whether the selected program runs synchronously or asynchronously. The application initiates asynchronous programs simultaneously. A synchronous program starts only when the previous program is terminated.
Parameters	Specifies any command parameters for the selected program. If an Export Only action is selected, the cell lists the available export file types: .xls, .txt, or .csv. The application exports a Report File formatted according to the selected file extension.

Macro Arguments

You can use the following macros in the command line:

Macro arguments	Macro parameter replacement
%R	Provides the current raw file.
%F	Provides the current result file.
%%	Provides a single % character in the run line.
%X	If the previous custom report was generated using Actions > Export Only, the %X macro provides the result file name with the extension that was selected from the Export Type list. If you convert a file and select an .xls extension, the application uses the converted raw file with a .crf extension. It does not change the extension if you select a .txt or .csv extension. If the previous custom report was generated using Actions: Run Excel Macro, the %X macro provides the result file name with an .xls extension.
%S	Passes the current .sld file and the current row number. The row number is zero based: 0 denotes the first sample, 1 refers to the second sample, and so on.

Printing Raw Files and Layout Files

You can include a command line argument that launches an application and prints a specified file to the default printer (/p) or a specified printer (/pt).

Buttons

Reports View features OK, Cancel, and Save As Default buttons. The OK and Cancel buttons are activated only if you change one or more parameters in the Reports tables; otherwise, they are unavailable. When you change or edit a parameter:

- To apply the changes to the current processing method, click **OK**. The application reports any validation errors.
- To undo all changes made to the tables and revert to the previously applied values, click **Cancel**.

Note that these actions do not affect the saved version of the processing method. This can only be modified by using the **File > Save** command.

To validate and save the settings on the current page as default settings, click **Save As Default**. These settings are then used for all new processing methods. The previous default values are overridden and cannot be recovered.

If you attempt to change views or applications without applying or discarding changes, the application displays the Apply Changes? Dialog Box. Use this dialog box to apply or discard the changes before continuing with your intended action.

Reports View

Use the Reports view of the Processing Setup window to specify how the data system produces reports for samples and sequences. The application provides several standard report formats. You can also design custom reports in XReport, the Xcalibur report designer. The application exports results in a number of file formats including XLS and HTML.

The Reports view consists of a Menu bar, a Toolbar, and two reports tables. This view also provides access to Xcalibur Help.

Menus

Processing Setup window menus:

File Menu | View Menu | Options Menu
GoTo Menu | Help Menu

Toolbar

Processing Setup Toolbar

Tables

The Reports view displays two tables:

- Sample Reports list the reports to be produced for processed samples in a sequence.
- Summary Reports list the reports to be produced for sequences or brackets.

Table 65. Reports view tables (Sheet 1 of 2)

Parameter	Description
Sample Reports	Specify Sample reports to be issued for each sample in a sequence. Each row in the Sample Reports table consists of seven columns. Refer to the *XReports User Guide* for more information about generating reports.
Row Number	Each numbered row represents an item in the table. The asterisk (*) indicates the last unused row in the table. Use this row to enter a new item.
Enable	View or change report status. If the report is available, the box displays a Yes value. If it is unavailable, the box is blank. When you click the box, a check box appears and you can change the enable status.
Sample Type	
Std	View or change report availability for Standard Sample types. If the report is available, the box displays a Yes value. If it is unavailable, the box is blank. When you click the box, a check box appears and you can change the status.
QC	View or change report availability for QC sample types. If the report is available, the box displays a Yes value. If it is unavailable, the box is blank. When you click the box, a check box appears and you can change the status.
Unk	View or change report availability for Unknown sample types. If the report is available, the box displays a Yes value. If it is unavailable, the box is blank. When you click the box, a check box appears and you can change the status.
Other	View or change report availability for sample types other than Standard, QC, or Unknown. If the report is available, the box displays a Yes value. If it is unavailable, the box is blank. When you click the box, a check box appears and you can change the status.
Save As	View the selected file export option for the sample report. The application saves the exported file with the sample file name and the correct extension in the Data folder where result files are stored.
Report Template Name	View or change the full path of the template that the application will use to generate the report. You can type the full path in the box or browse for the template in the Browse for Sample Report Template dialog box. Double-click a Report Template Name box to display the Browse for Sample Report Template dialog box. Or right-click the cell and select Browse from the context menu.

Table 65. Reports view tables (Sheet 2 of 2)

Parameter	Description
Summary Reports	
Summary Reports	Specify Summary reports to be issued after processing of a bracketed or non-bracketed sequence. Each row in the Sample Reports table consists of three columns.
Row Number	Each numbered row represents an item in the table. The asterisk (*) indicates the last unused row in the table. Use this row to enter a new item.
Enable	View or change report status. If the report status is available, the box displays a Yes value. If it is unavailable, the box is blank. When you click the box, a check box appears and you can change the status.
Save As	View or change the selected file export option for the sample report. The application saves the exported file with the sample file name and the appropriate extension in the data folder where result files are stored.
Report Template Name	View or change the full path of the template that the application uses when generating the summary report. You can type the full path in the box or browse for the template in the Browse for Summary Report Template dialog box. Double-click a Report Template Name box to display the Browse for Summary Report Template dialog box. Or right-click the cell and select Browse from the context menu.

The following table defines columns for sample reports.

Column heading	Use
Enable	Enable a sample report.
Std	Specify the report for a Standard sample type.
QC	Specify the report for a QC sample type.
Unk	Specify the report for an Unknown sample type.
Other	Specify the report for all other sample types.
Save As	View or change various options for exporting the specified sample report.
Report Template Name	View or change the full path of the template that the application uses in generating the sample report.

The following table defines columns for summary reports.

Column heading	Use
Enable	Enable a summary report.
Save As	View or change various options for exporting the specified summary report.
Report Template Name	View or change the full path of the template that the application uses in generating the summary report.

Valid file types

The following table lists the valid files types.

Export type	Description
None	print only, no exported file
Text	ASCII text file (*.txt)
Doc	Microsoft™ Word™ file (*.doc)
HTML	HTML file (*.html)
PDF	Adobe™ Acrobat™ file (*.pdf)
RTF	rich text format (*.rtf)
XLS	Microsoft Excel file (*.xls)

Buttons

Reports View features OK, Cancel, and Save As Default buttons. You can only select the OK and Cancel buttons if you change one or more parameters in the Reports tables; otherwise, they are unavailable. When you change or edit a parameter:

- To apply the changes to the current processing method, click **OK**. The application reports any validation errors.
- To undo all changes made to the tables and revert to the previously applied values, click **Cancel**.

Note that these actions do not affect the saved version of the processing method. This version can only be modified by using the **File > Save** command.

Click **Save As Default** to validate and save the settings on the current page as default settings. The application uses these settings for all new processing methods. The software writes over the previous default values and cannot recover them.

If you attempt to change views or applications without applying or discarding changes, the application displays the Apply Changes? dialog box. Use this dialog box to apply or discard the changes before continuing with your intended action.

Processing Queue Manager Window

Use the Processing Queue Manager window to control the Xcalibur processing queue. Each time you select Processing options in Run This Sample, Run Sequence, or Batch Reprocess in the Sequence Setup window, a queue service starts in the background. When the Run Manager program finishes an analysis, it sends the data to the queue for processing. Processings are submitted using a first-in first-out queue priority. You can pause processing, resume processing, purge the queue, and obtain information about processing.

To control the Xcalibur processing queue, use these menu commands and toolbar buttons:

Table 66. Processing Queue Manager window parameters (Sheet 1 of 2)

Command	Description
Queue	
Pause 	Pause all processing operations temporarily and puts Xcalibur processing in Standby mode.
Resume 	Change Xcalibur operation status from Standby (as a result of a pause command) to Run status.
Purge Queue	Remove all processing requests from the Processing Queue Manager. This command can be used during troubleshooting to clear the application of all processing tasks.
Exit	Close the Processing Queue Manager window.
Analysis	
Remove From Queue 	Remove all selected processing requests from the Processing Queue Manager. This command can be used during troubleshooting to clear the application of all processing tasks.
Details 	Open the Details of Selected Analysis Dialog Box so that you can view additional information about a selected processing task.
View	
Toolbar	Display or hide the toolbar. The toolbar appears if it was previously hidden or hides if it is currently displayed.
Status Bar	Display or hide the status bar. The status bar appears if it was previously hidden or hides if it is currently displayed. The status bar is a horizontal box at the bottom of the Processing Queue Manager window.
Refresh	Update the Xcalibur processing queue with the most current information.
GoTo	
Xcalibur Home Page	Return you to the Roadmap view of the Home Page window.

Table 66. Processing Queue Manager window parameters (Sheet 2 of 2)

Command	Description
Help	
Queue Manager Help 	Open Help for the Processing Queue Manager.
Xcalibur Help	Open Xcalibur Help.
Glossary	Open the glossary.
How To Use Help	Open Help that describes how to use the Help viewer.
About Queue Manager	Open the About Processing Queue Manager dialog box. This dialog box displays the installed version number of the Processing Queue Manager program and the Thermo Fisher Scientific copyright notice.

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