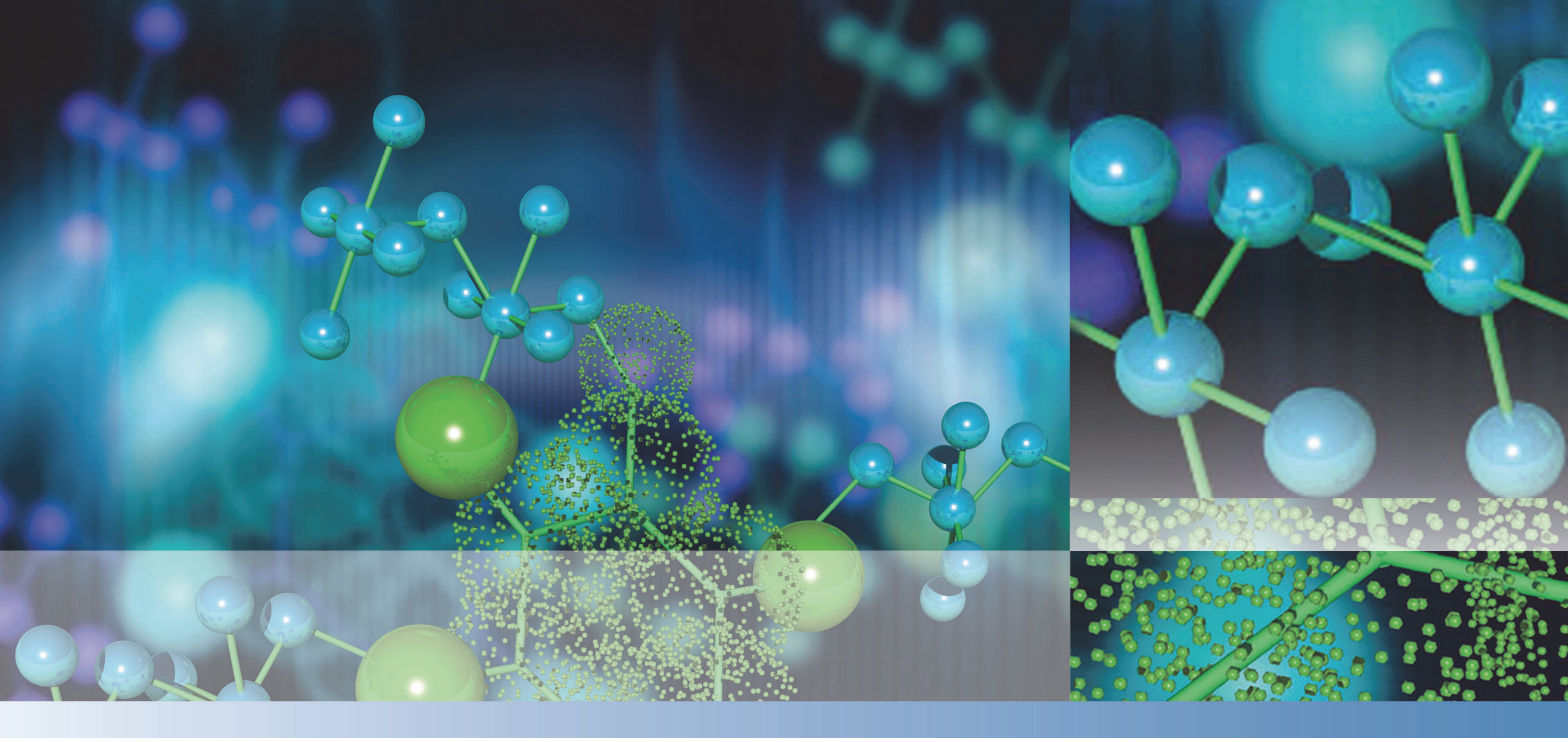

Thermo

Xcalibur Data Acquisition and Processing

User Guide

Software Version 3.0

XCALI-97549 Revision A June 2013

DOCUMENTATION
SURVEY

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Release history: Revision A, June 2013

Software version: Thermo Xcalibur 3.0 and later

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Preface

This manual describes how to use the Xcalibur data system to acquire and process data.

Contents

- Related Documentation
- Special Notices
- Contacting Us

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

DOCUMENTATION
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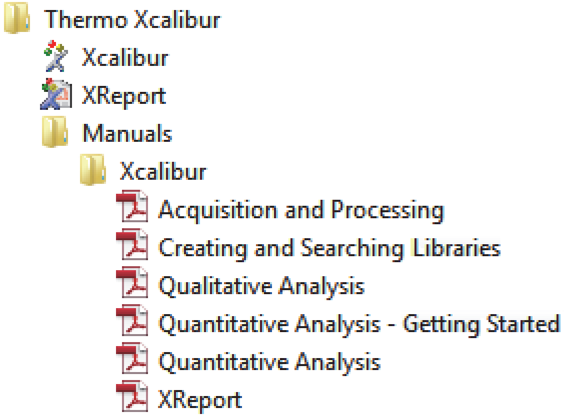
Related Documentation

In addition to this guide, which provides information about data acquisition and processing, Thermo Fisher Scientific provides the following documentation for the Xcalibur data system:

- *Xcalibur Quantitative Analysis Getting Stared Guide*—Contains tutorials that guide you through post-acquisition processing of quantitation data.
- *Xcalibur Quan Browser User Guide*—Describes how to use the Quan Browser window to review and print reports for quantitation data.
- *Xcalibur Qual Browser User Guide*—Describes how to use the Qual Browser window to review qualitative data.
- *Xcalibur Library Browser User Guide*—Describes how to create and search mass spectral libraries.
- *XReport User Guide*—Describes how to use the XReport application to create custom report templates.
- Help from within the software

You can access manuals (as PDF files) for the Xcalibur data system and instruments controlled by the Xcalibur data system from the data system computer and the Internet.

- To access the Xcalibur manual set from the computer taskbar, choose **Start > All Programs** (or **Programs**) **> Thermo Xcalibur > Manuals > Xcalibur**.



Thermo Xcalibur
  Xcalibur
  XReport
  Manuals
    Xcalibur
      Acquisition and Processing
      Creating and Searching Libraries
      Qualitative Analysis
      Quantitative Analysis - Getting Started
      Quantitative Analysis
      XReport

- To access the manual set for the Thermo Scientific mass spectrometer from the computer taskbar, choose **Start > All Programs** (or **Programs**) **> Thermo Instruments > Manuals >** ***mass spectrometer***.
- To access the manual set for the LC system from the computer taskbar, choose **Start > All Programs** (or **Programs**) **> Thermo Instruments > Manuals > LC Devices >** ***Thermo Scientific brand*** or ***third-party manufacturer***.

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 Fisher Scientific for the information you need.

❖ To contact Technical Support

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

Find software updates and utilities to download at mssupport.thermo.com.

❖ To contact Customer Service for ordering information

Phone	800-532-4752
Fax	561-688-8731
E-mail	us.customer-support.analyze@thermofisher.com
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Go to mssupport.thermo.com, agree to the Terms and Conditions, and then click **Customer Manuals** in the left margin of the window.

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- Fill out a reader survey online at www.surveymonkey.com/s/PQM6P62.
- Send an e-mail message to the Technical Publications Editor at techpubs-lcms@thermofisher.com.

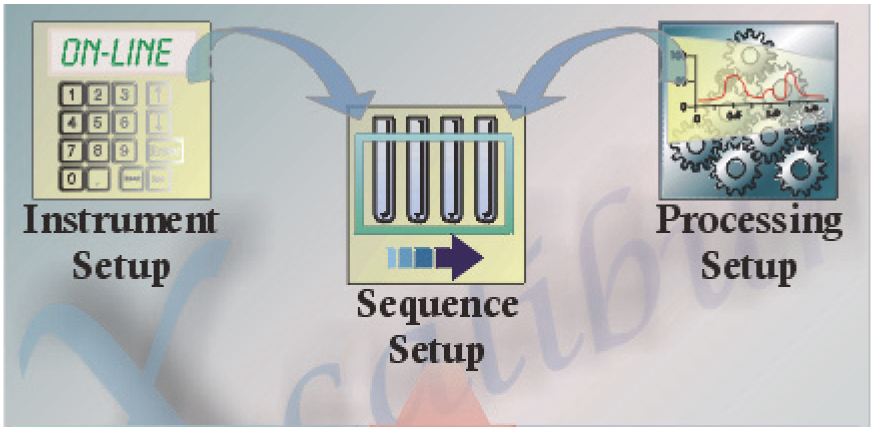
Introduction

This guide describes how to acquire and process data with the Xcalibur data system.

This chapter describes the core portion of the Xcalibur data system, where you create instrument methods for data acquisition, sequences for data acquisition and processing, and processing methods to analyze the raw data and generate reports.

Figure 1 shows the data acquisition and processing portions of the Xcalibur data system. The Instrument Setup window, Processing Setup window, and Sequence Setup view form the core of the Xcalibur data system.

Figure 1. Xcalibur Homepage Roadmap view (top portion)



Contents

- Home Page Overview
- Instrument Setup Overview
- Sequence Setup View Overview
- Processing Setup Overview
- Data Acquisition and Processing Workflow

Home Page Overview

When you start the Xcalibur data system, it opens to the Roadmap view of the Home Page window.

The Home Page window consists of the Info view, which appears on the left side of the window when it is not hidden, and one of these three views: the Roadmap view, the Sequence Setup view, or the Real-Time Plot view.

- Use the Info view to check the status of your instrument and the acquisition queue.
- Use the Roadmap view to access the other Xcalibur data system windows.
- Use the Sequence Setup view to create and run acquisition and processing sequences.
- Use the Real-Time Plot view to monitor data acquisition after you submit an acquisition sequence.

Instrument Setup Overview

Use the Instrument Setup window to do the following:

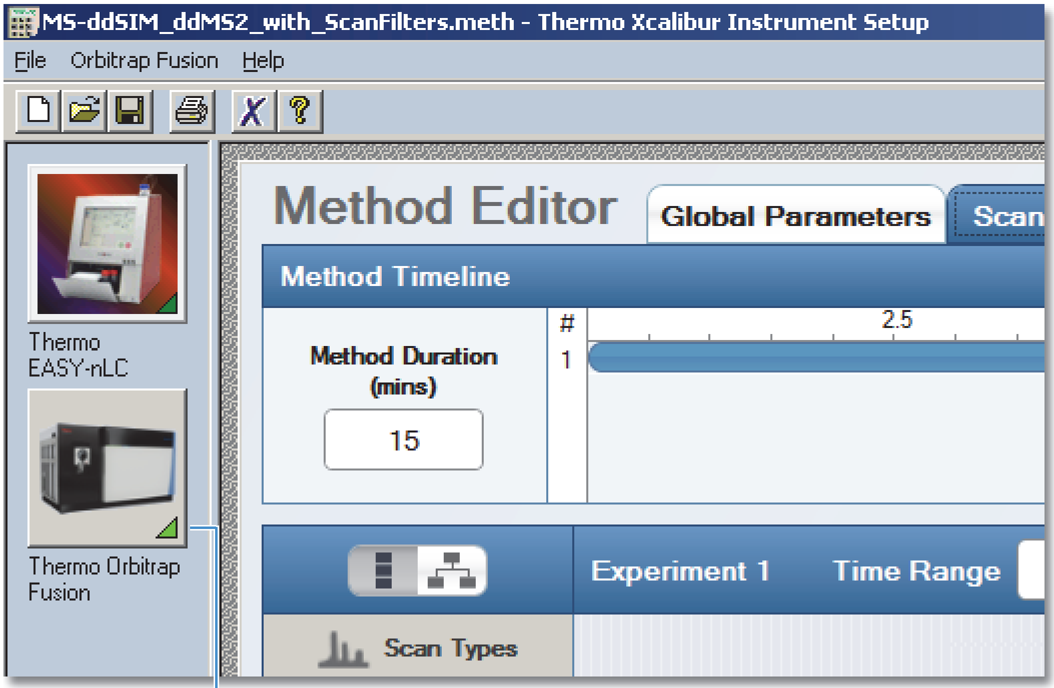
- Create instrument methods that contain the parameters for all of the devices that make up your instrument (see "Creating an Instrument Method" on page 13).
- Directly control the individual devices that make up your instrument (see "Accessing the Direct Controls or Menu Options for Each Device" on page 14).

The Instrument Setup window provides access to the individual views for the configured devices of your instrument. If the instrument configuration is not set up in the Thermo Foundation Instrument Configuration window, the devices do not appear in the Instrument Setup view.

Note For more information about the Instrument Setup window, see Appendix B, "Instrument Setup." For more information about setting up the instrument configuration for your instrument, see "Setting Up the Instrument Configuration in the Foundation Platform" on page 147.

Figure 2 shows the Instrument Setup window for an LC/MS instrument with the EASY-nLC™ nanoflow liquid chromatography instrument and LTQ Orbitrap™ mass spectrometer. Clicking the Orbitrap Fusion™ icon on the View bar opens the Orbitrap Fusion Method Editor view. The bright green triangle in the bottom right corner of the Orbitrap Fusion icon indicates that the active view displays the instrument method parameters for the Orbitrap Fusion mass spectrometer.

Figure 2. Orbitrap Fusion Method Editor view in the Instrument Setup window

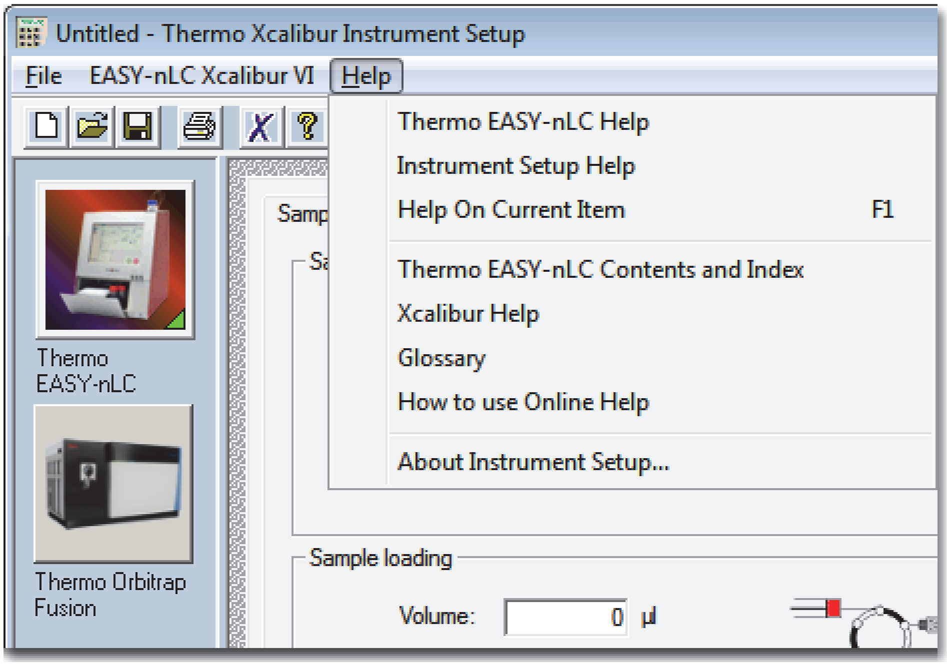


Method Duration (mins): 15

Bright green triangle

Each instrument view in the Instrument Setup window has its own Help menu (Figure 3).

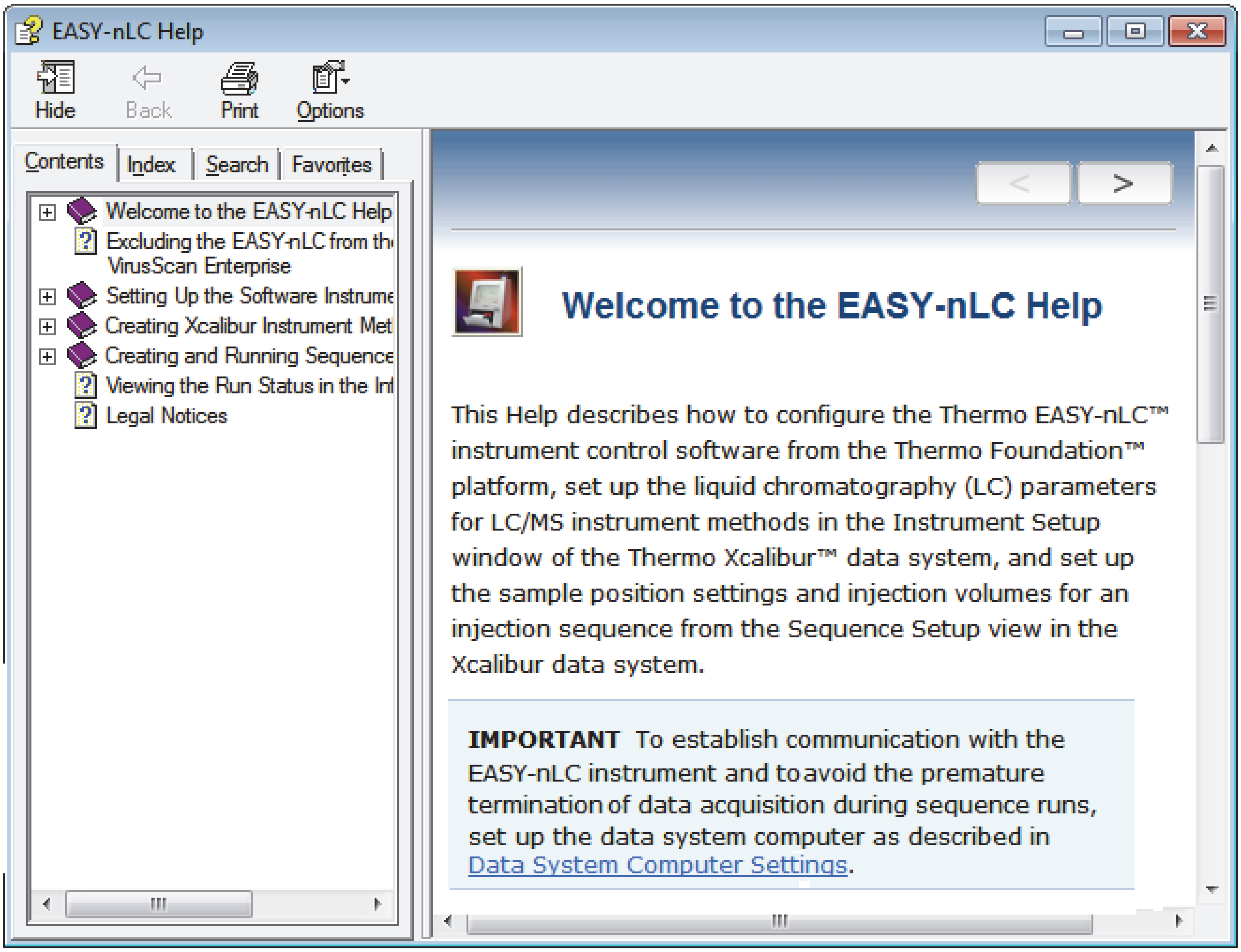
Figure 3. Help menu for the EASY-nLC nanoflow LC instrument



Volume: 0 µl

Choosing Help >Thermo EASY-nLC Help in the EASY-nLC instrument view opens the Help for the EASY-nLC instrument (Figure 4).

Figure 4. Welcome page of the EASY-nLC Help system



Welcome to the EASY-nLC Help

This Help describes how to configure the Thermo EASY-nLC™ instrument control software from the Thermo Foundation™ platform, set up the liquid chromatography (LC) parameters for LC/MS instrument methods in the Instrument Setup window of the Thermo Xcalibur™ data system, and set up the sample position settings and injection volumes for an injection sequence from the Sequence Setup view in the Xcalibur data system.

IMPORTANT To establish communication with the EASY-nLC instrument and to avoid the premature termination of data acquisition during sequence runs, set up the data system computer as described in Data System Computer Settings.

Like the Xcalibur Help, the instrument Help has a navigation pane with the following pages:

- Contents page, where you can quickly navigate the Help
- Index page, where you can look up specific terms
- Search page, where you can search for terms and concepts
- Favorites page, where you can add links to the most frequently used topics

The Help systems provided with the LC device drivers on the LC Devices DVD describe how to set up the device configuration in the Foundation platform and the method parameters in the Xcalibur Instrument Setup window. The Help systems provided with Thermo Scientific mass spectrometers describe how to Tune the instrument and how to set up the method parameters in the Instrument Setup window. For an LC/MS system, an instrument method contains the method parameters for all of the system instruments.

Sequence Setup View Overview

Use the Sequence Setup view to do the following:

- Create a sequence that describes how the data is to be acquired, how the data is to be processed, or both.
- Run a single sample or a sample set and acquire a set of unprocessed data files.
- Run a single sample or a sample set and process the data files as they are acquired.
- Batch reprocess previously acquired data files.

Note For more information about the Sequence Setup view, see Appendix C, "Sequence Setup."

Sequence files have the .sld file extension whether they contain only instrument methods, only processing methods, or both types of methods.

When you submit a single sample run (made by selecting one sequence row) or a sequence run to the acquisition queue, the Xcalibur data system checks for a valid instrument method.

When you batch reprocess a sequence, the Xcalibur data system checks for valid data files and a processing method.

You can use a sequence to automate injections from either an autosampler or the mass spectrometer's syringe pump. Whether you use an autosampler or the mass spectrometer's syringe pump, you must create an instrument method to acquire data files. If you are using an autosampler, the sequence must specify the sample positions (in the autosampler tray compartment) of the samples that you want to inject.

For information about making automated injections with the syringe pump, refer to the Getting Started Guide for the mass spectrometer and the Help topic for the Syringe Pump page in the mass spectrometer's device view of the Instrument Setup window.

Figure 5 shows a 5-row sequence that can be used to acquire data by injecting samples with an autosampler or a syringe pump. Each row of the sequence corresponds to one sample injection and each injection is defined by the settings in its sequence row.

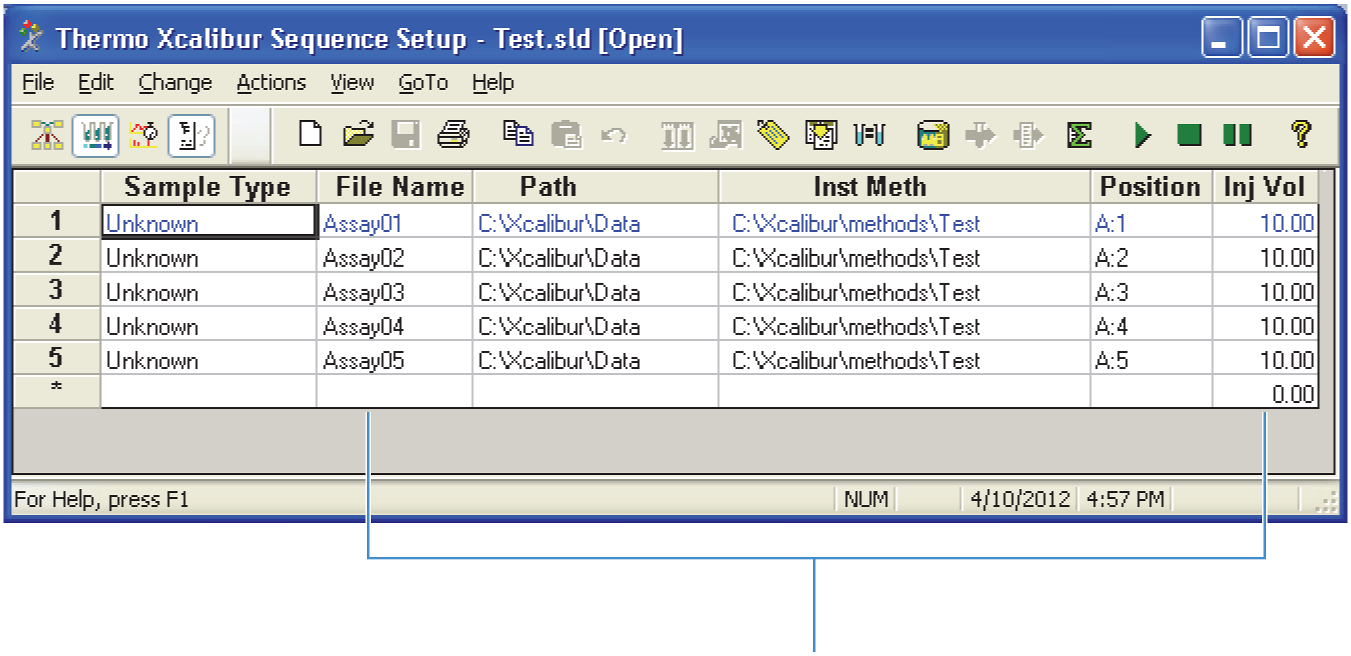
Note The title bar of the Sequence Setup view lists the name of the current sequence.

Figure 5 shows the sequence columns required to acquire raw data files:

- File Name: Contains the data file names.
- Path: Specifies where the data system is to store the data files as it acquires them.
- Inst Meth: Contains the name and location of the instrument method that specifies the data acquisition and chromatography settings for each injection. Each data file is associated with one instrument method. A sequence can contain more than one instrument method.
- Position: Contains the positions of the sample vials in the autosampler tray compartment. The position notation depends on the autosampler model and tray type.
- Inj Vol: Contains the injection volume for each injection. This volume overrides the injection volume (if available) in the instrument method. The default injection volume is 10 µL.

The Sample Type sequence column is not required for data acquisition.

Figure 5. Sequence Setup view with the Info view of the Home Page window hidden



	Sample Type	File Name	Path	Inst Meth	Position	Inj Vol
1	Unknown	Assay01	C:\Xcalibur\Data	C:\Xcalibur\methods\Test	A:1	10.00
2	Unknown	Assay02	C:\Xcalibur\Data	C:\Xcalibur\methods\Test	A:2	10.00
3	Unknown	Assay03	C:\Xcalibur\Data	C:\Xcalibur\methods\Test	A:3	10.00
4	Unknown	Assay04	C:\Xcalibur\Data	C:\Xcalibur\methods\Test	A:4	10.00
5	Unknown	Assay05	C:\Xcalibur\Data	C:\Xcalibur\methods\Test	A:5	10.00
*						0.00

Information required for data acquisition

Processing Setup Overview

Use the Processing Setup window to do the following:

- Create a new processing method that provides qualitative results, quantitative results, or both. Processing methods are saved as a .pmd file type.
- Modify existing processing methods.

You can add a processing method to a sequence before or after you acquire data files.

The Processing Setup window consists of these elements. You can hide or show the view bar, toolbar, and status bar.

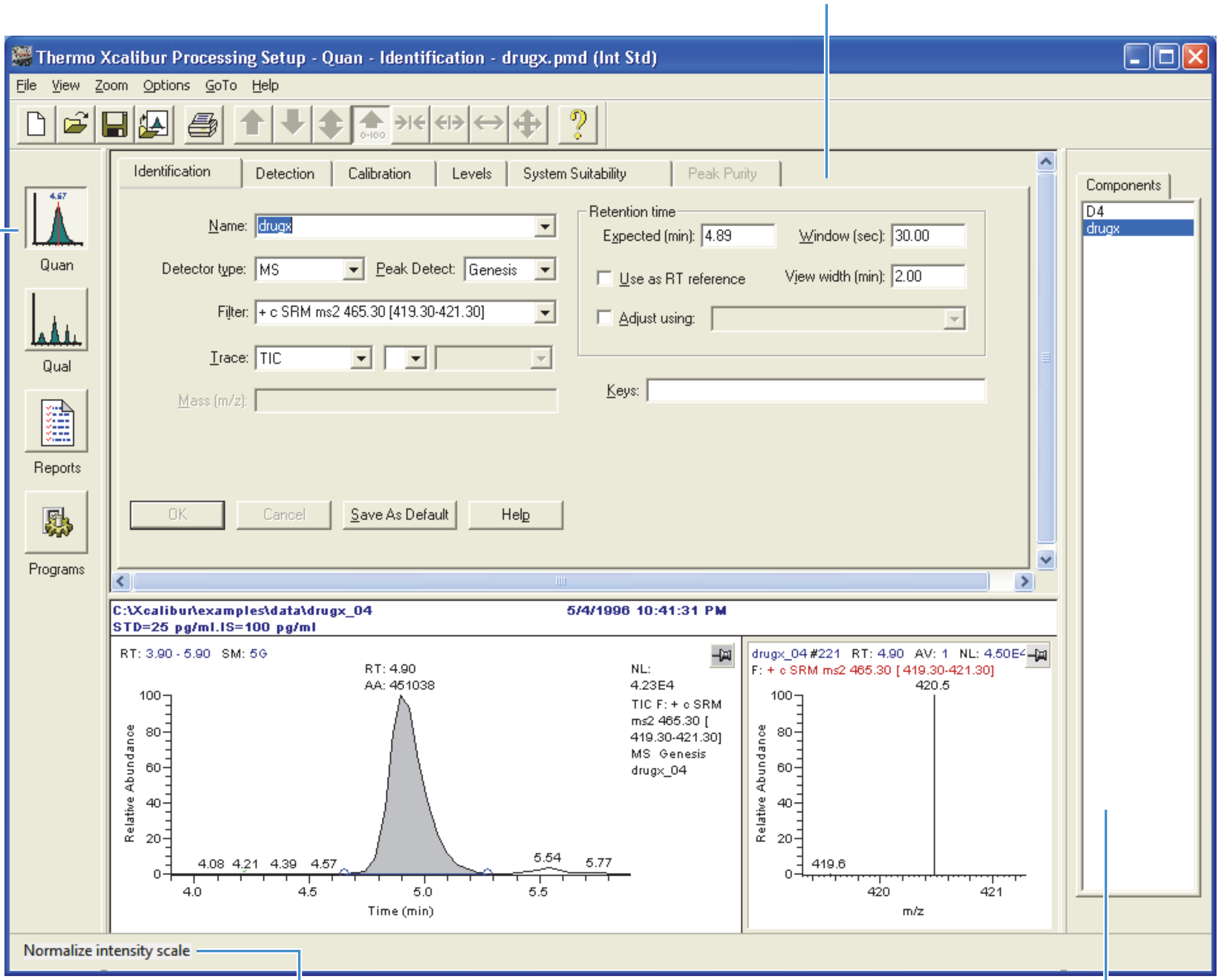
Element	Function
Title bar	Lists the current window, view, page, processing method, and calibration mode (internal standard or external standard).
Menu bar	Provides commands to hide or show window elements, access to optional dialog boxes for the current view, access to other Xcalibur windows, and access to Xcalibur data system Help, the Processing Setup window Help, the current view Help, and the current page or dialog box Help.
Toolbar	Provides commands for the current view and access to the current page or dialog box Help.
View bar	Contains an icon for each of the four sections of a processing method. The parameters for a processing method are divided into the Quan, Qual, Reports, and Programs views.
Workspace	Provides data entry boxes, check boxes, and option buttons for the parameter settings. • The Quan view is divided into three sections: the parameters section, the user-generated components list, and the raw data display with a chromatogram cell and a spectrum cell. • The Qual view is divided into two sections: the parameters section and the raw data display with a chromatogram cell and a spectrum cell. • The Reports view contains two selection tables: one for individual sample reports and one for sequence summary reports. • The Programs view contains a selection table where you specify post-acquisition programs and macros.
Status bar	The left side of the bar displays a functional description of the selected toolbar icon or menu command. The right side of the bar displays Not Saved until you save the current processing method.

The view within the Processing Setup window changes depending on which icon you click on the View bar. The Quan view contains six tabbed pages (Figure 6).

Figure 6. Processing Setup – Quan view – Identification page

View bar

Workspace area



Thermo Xcalibur Processing Setup - Quan - Identification - drugx.pmd (Int Std)

Name: drugx

Detector type: MS

Peak Detect: Genesis

Filter: + c SRM ms2 465.30 [419.30-421.30]

Trace: TIC

Mass (m/z):

Retention time

Expected (min): 4.89

Window (sec): 30.00

☐ Use as RT reference

View width (min): 2.00

☐ Adjust using:

Keys:

Components: D4, drugx

C:\Xcalibur\examples\data\drugx_04
STD=25 pg/ml.IS=100 pg/ml
5/4/1998 10:41:31 PM

Functional description of currently selected toolbar icon

Named components

To create a processing method that provides qualitative results, quantitative results, or both, follow these procedures:

- "Setting Up the Quantitative Processing Parameters" on page 21
- "Setting Up the Qualitative Processing Parameters" on page 50
- "Adding Report Templates to Processing Methods" on page 59
- "Adding Programs or Macros to Processing Methods" on page 64

For information about searching libraries, refer to the *Xcalibur Library Browser User Guide*.

Data Acquisition and Processing Workflow

Table 1 provides a workflow that you can follow to acquire and process data automatically using the Xcalibur data system and the instrument control software.

Table 1. Data acquisition and processing workflow (Sheet 1 of 2)

Workflow task	Reference
MS Tune program—Determine the data acquisition settings for the MS detector. Save the ion source settings for the MS detector in a tune method.	Refer to the Tune Help or the Getting Started Guide for the Thermo Scientific mass spectrometer.
Instrument Setup window—Import the stored tune method into the instrument method, and then enter the remaining instrument method settings for the LC/MS or GC/MS system.	See Chapter 2, “Creating Instrument Methods and Using the Direct Controls.”
Prepare samples, standards, and so forth. Load the samples into the autosampler.	For information about loading samples into the autosampler, refer to the Help provided with the autosampler’s instrument control software.
Sequence Setup window—Create a sequence with one row and acquire a raw file from a representative sample or standard.	See “Creating a Sequence Semi-Automatically” on page 69.
Processing Setup window—Open the acquired raw file and create a processing method.	See “Setting Up the Quantitative Processing Parameters” on page 21, “Setting Up the Qualitative Processing Parameters” on page 50, or both topics.
Sequence Setup window—Use the New Sequence Template dialog box to create a new sequence with the instrument method and the processing method.	See “Creating a Sequence Semi-Automatically” on page 69.
Sequence Setup window—Run the sequence and acquire a set of data files. The data system uses the instrument method, position, and injection volume to acquire the data files and the processing method to process the data.	See “Running a Single Sample or Multiple Samples” on page 101.
Quan Browser window—Open the processed sequence. Review the integration of each chromatogram. Review the calibration curve for each target compound.	Refer to the *Xcalibur Quan Browser User Guide.*
Quan Browser or Processing Setup windows—Adjust the peak integration and calibration curve parameters as necessary.	Refer to the *Xcalibur Quan Browser User Guide.*
XReport application—Preview representative files with the report templates until you find a sample template and summary templates that suit the analysis. Adjust the template or templates and save as needed.	Refer to the *XReport User Guide.*

Table 1. Data acquisition and processing workflow (Sheet 2 of 2)

Workflow task	Reference
Processing Setup window—Add the selected report template or templates to the processing method.	See "Adding Report Templates to Processing Methods" on page 59.
Sequence Setup window—Batch reprocess the sequence and print or save the appropriate reports.	See "Batch Reprocessing a Sequence" on page 116.
Perform subsequent analyses by preparing the samples and creating a new sequence with the existing instrument and processing methods.	

2

Creating Instrument Methods and Using the Direct Controls

Use the Instrument Setup window to create instrument methods and to prepare the instrument devices for daily operation. An instrument method contains the settings for your chromatographic method and the data acquisition settings for the mass spectrometer. To prepare the LC or GC devices for daily operation, use the direct controls that are available from the individual device views.

> **Tip** Before you start a sample run, use the controls provided in the Instrument Setup window to remove air from the LC system and to equilibrate the chromatographic column.
>
> For information about the direct controls for the chromatographic devices, refer to the Help provided with each device. You can access manuals for devices controlled by the Xcalibur data system from the Windows™ Start menu by choosing **Start** > **Programs** (or **All Programs**) > **Thermo Instruments** > **Manuals**.

Contents

- Opening the Instrument Setup Window
- Creating an Instrument Method
- Accessing the Direct Controls or Menu Options for Each Device

For more information about the Instrument Setup window, see Appendix B, "Instrument Setup."

Opening the Instrument Setup Window

Use the Instrument Setup window to create instrument methods and to access additional controls for the configured devices of your LC/MS or GC/MS system.

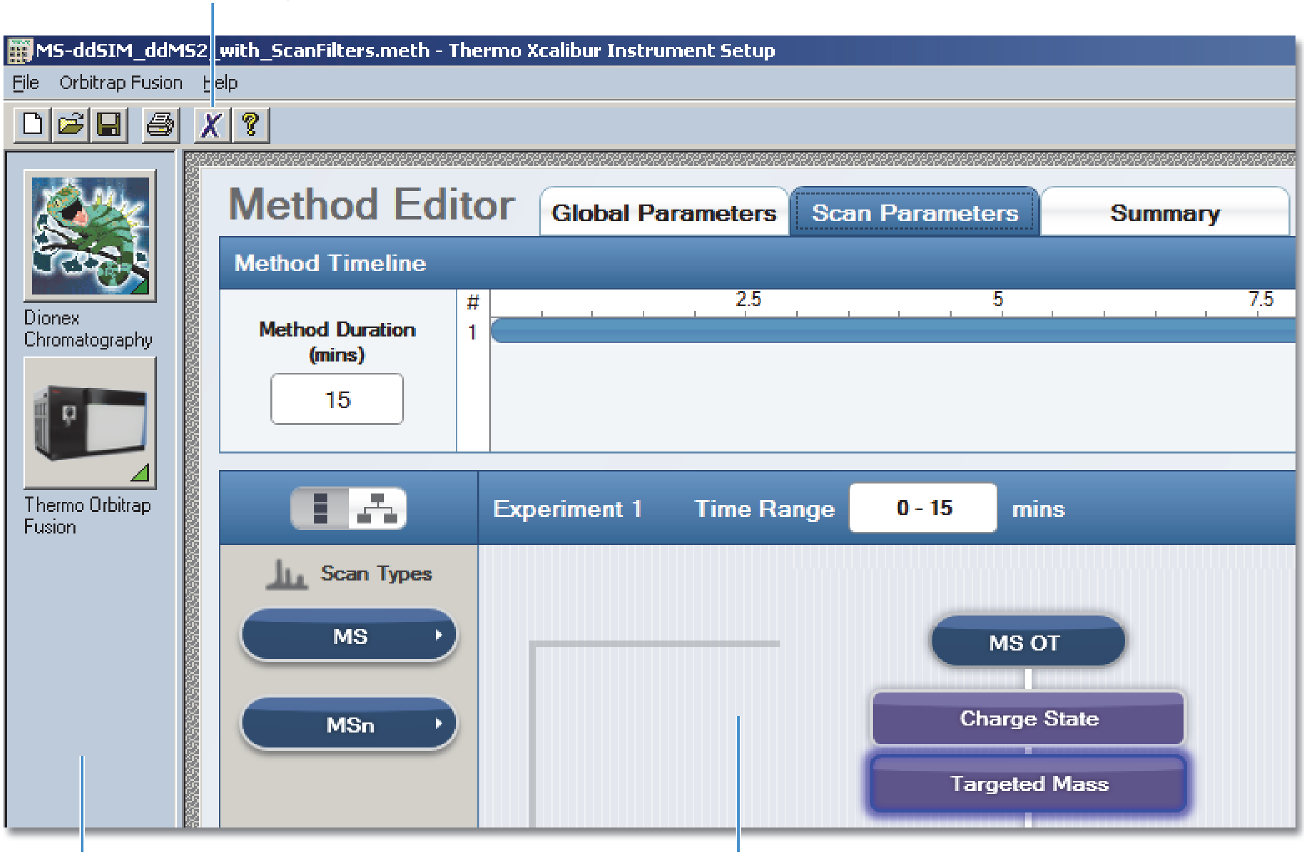
❖ To open the Instrument Setup window

From the Processing Setup, Quan Browser, or Home Page window, choose **GoTo > Instrument Setup** from the menu bar.

The Instrument Setup window opens (Figure 7). For more information about the Instrument Setup window, see Appendix B, “Instrument Setup.”

Figure 7. Instrument Setup window showing the Orbitrap Fusion view

Home Page icon



View bar

Orbitrap Fusion view

The left side of the window contains the View bar with icons for all of the configured devices. The right side of the window displays the view for the device currently selected in the View bar. The icon for the currently selected device has a green triangle in its lower right corner.

❖ To return to the Home Page window

On the Instrument Setup window toolbar, click the **Home Page** icon, X.

Creating an Instrument Method

Instrument methods contain the chromatographic and data acquisition parameters required for sample runs. To create an instrument method, you must specify the appropriate settings for each device of your instrument that is controlled by the Xcalibur data system.

❖ To create an instrument method

1. Open the Instrument Setup window (see “Opening the Instrument Setup Window” on page 12).

2. To enter the instrument method settings, do the following for each device in the View bar:

   a. Click the device icon.

      The view for the specific device appears on the right side of the Instrument Setup window.

      Note For information about customizing the device view for the mass spectrometer, see “Accessing the Direct Controls or Menu Options for Each Device” on page 14.

   b. Enter the appropriate settings for the device as follows:

      - For the chromatography devices, enter the chromatographic conditions.
      - For the mass spectrometer, enter the data acquisition parameters. Depending on the mass spectrometer, you might need to import the appropriate Tune method into the instrument method.

      Note Almost every page or dialog box that is available in the device view for a chromatographic device or the mass spectrometer has an associated Help topic.

      To open the Help topic for the page or dialog box that is currently open, choose **Help > Help on Current Item**.

3. To save the instrument method, choose **File > Save As**.

   The Save As dialog box opens.

4. In the Save In list, browse to the folder where you want to store the instrument method.

5. In the File Name box, enter the instrument method name, and then click **Save**.

   The File Summary Information dialog box opens.

6. Click **OK**.

   The instrument method file is saved in the specified location and has a .meth file extension.

7. To close the Instrument Setup window, choose **File > Exit**.

Accessing the Direct Controls or Menu Options for Each Device

Most of the chromatography devices controlled by the Xcalibur data system have a set of direct controls that you can use to prepare the system for daily operation.

The device view for the mass spectrometer has a menu that provides additional options for the view.

❖ To access the direct controls or menu options for a device

1. Open the Instrument Setup window (see "Opening the Instrument Setup Window" on page 12).
2. To open the view for a particular device, click its device icon on the View bar.
3. To open the Direct Control dialog box for a chromatography device, choose ***Device Name*** > **Direct Control** from the menu bar in the device view.

   Tip You can use the direct controls for the LC pump to start an isocratic mobile phase and equilibrate the LC column to the starting conditions in the instrument method. If the autosampler has temperature-controlled zones or the LC system includes a separate temperature-controlled module, such as a column compartment, you can use the direct controls to turn on the autosampler's built-in column oven or the temperature-controlled module and equilibrate the LC column to the temperature in the instrument method.

4. To open the menu options for the mass spectrometer's device view, choose ***Device Name*** and an additional menu selection.

3

Creating Processing Methods

To set up the workflow options for the Processing Setup window and to create processing methods to analyze your data and print reports, follow these procedures.

Contents

- Opening the Processing Setup Window
- Setting Up the Workflow Options for the Processing Setup Window
- Setting Up the Void Time and Baseline Identification Options
- Setting Up the Quantitative Processing Parameters
- Setting Up the Qualitative Processing Parameters
- Adding Report Templates to Processing Methods
- Adding Programs or Macros to Processing Methods

When you finish setting up the parameters for a processing method in the Processing Setup window, use the Save or Save As commands to save the method. Processing methods have a .pmd file extension.

Opening the Processing Setup Window

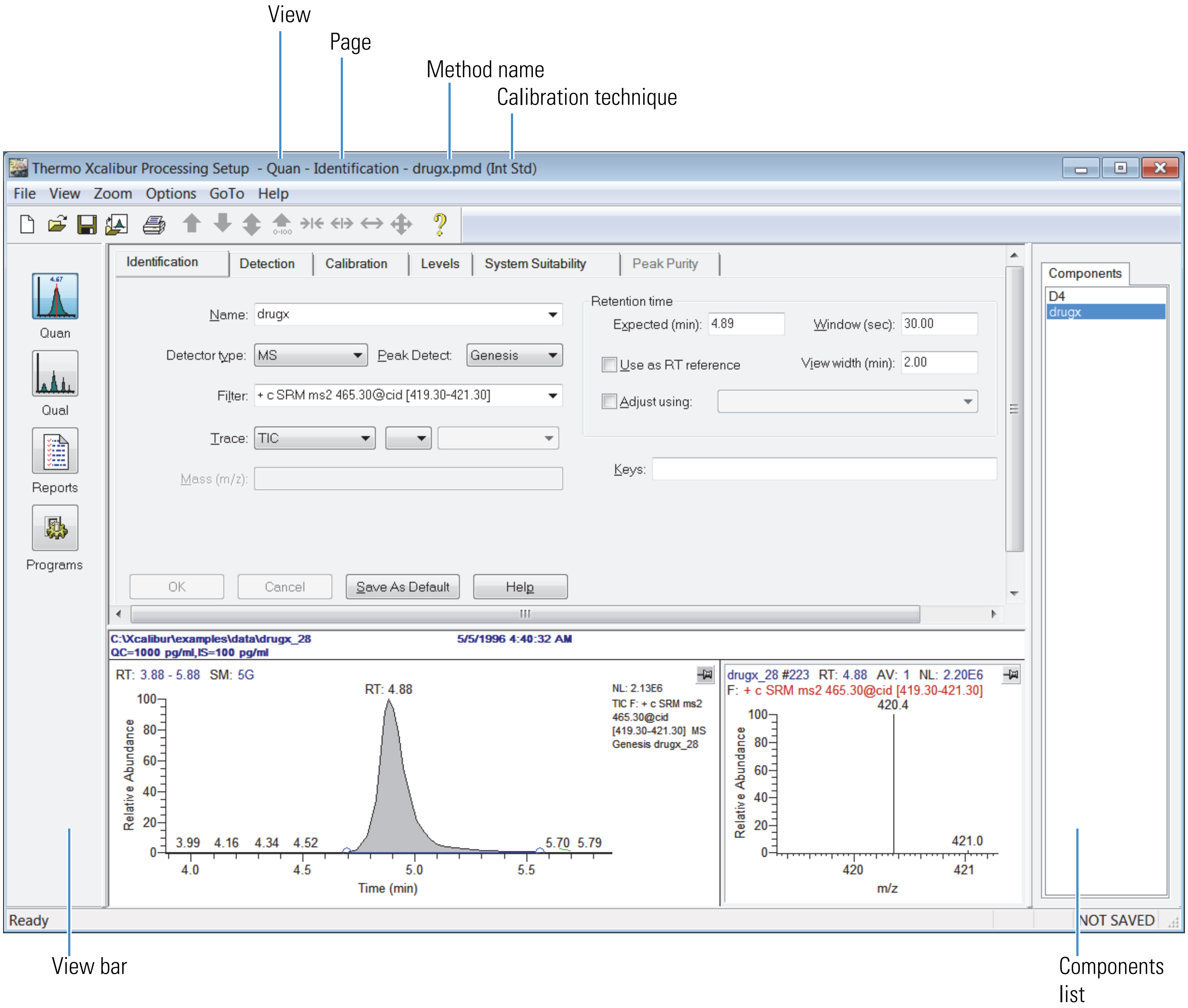
Use the Processing Setup window to create quantitative and qualitative processing methods. Before you create a processing method,

You can open the Processing Setup window in these ways:

- From the HomePage – Roadmap view, click the **Processing Setup** icon, , on the Roadmap.
- From the Home Page, Instrument Setup, Quan Browser, or Library Browser window, choose **GoTo > Processing Setup** from the menu bar.
- In the sequence table of the Sequence Setup view, select a processing method in the Processing Method column, and then choose **Actions > Open File** from the menu bar.

The window’s title bar lists the current *view*, *page*, *study* (if enabled), and *processing method name* (Figure 8). The Processing Setup window has four views that you can navigate by using the View bar or the View menu. If the View bar is hidden, choose **View > View Bar** to display it on the left side of the window.

Figure 8. Processing Setup window with View bar displayed



View

Page

Method name

Calibration technique

View bar

Components list

Thermo Xcalibur Processing Setup - Quan - Identification - drugx.pmd (Int Std)

Name: drugx

Detector type: MS

Peak Detect: Genesis

Filter: + c SRM ms2 465.30@cid [419.30-421.30]

Trace: TIC

Mass (m/z):

Retention time

Expected (min): 4.89

Window (sec): 30.00

☐ Use as RT reference

View width (min): 2.00

☐ Adjust using:

Keys:

C:\Xcalibur\examples\data\drugx_28 5/5/1996 4:40:32 AM
QC=1000 pg/ml,IS=100 pg/ml

Components
D4
drugx

Ready

NOT SAVED

If you have not already set up the workflow options for the Processing Setup window, do so now as described in the next topic, “Setting Up the Workflow Options for the Processing Setup Window” on page 17.

Setting Up the Workflow Options for the Processing Setup Window

Follow these procedures to set up the workflow options for the Processing Setup window:

- Setting Up the Startup Options
- Dealing with Unapplied Page Parameters

Setting Up the Startup Options

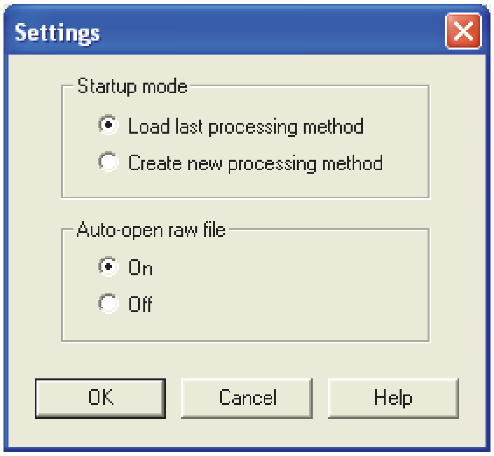
You can set up the Processing Setup window to open with either the last processing method or the untitled processing method template. You can also set up the Processing Setup window to populate the chromatogram and spectrum cells with data from the raw data file that is associated with the processing method.

❖ To set up the startup options for the Processing Setup window

1. From the Processing Setup window menu bar, choose **Options > Settings**.

   The Settings dialog box opens (Figure 9). For more information about the parameters for this dialog box, see "Settings Dialog Box" on page 290.

   Figure 9. Settings dialog box

   Startup mode
   ● Load last processing method
   ○ Create new processing method

   Auto-open raw file
   ● On
   ○ Off

2. In the Startup Mode area, select the appropriate startup option as follows:

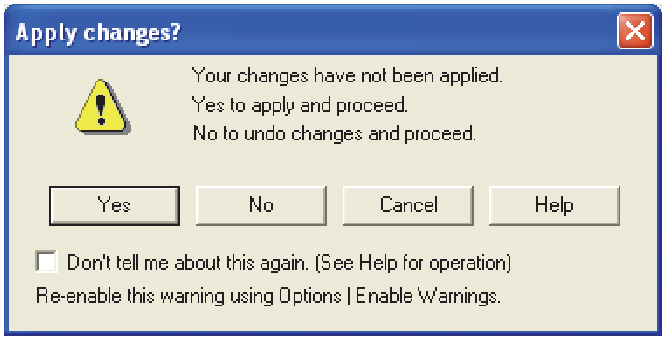
   - To load the last used processing method at startup, select the **Load Last Processing Method** option.
   - To start each new session with a new processing method, select the **Create New Processing Method** option.

3. In the Auto-open Raw File area, select whether the chromatogram and spectrum cells are populated when you open a processing method as follows:
    - To open processing methods with the chromatogram and spectrum cells populated with their associated raw files, select the **On** option.
    - To open processing 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**.

Dealing with Unapplied Page Parameters

The default setting for the Enable Warnings option is Enabled (Activated), which means that when you attempt a file operation, page or view change, or certain other actions, the Apply Changes? Dialog Box opens and you cannot proceed until you apply or undo the changes (Figure 10).

Figure 10. Apply changes? dialog box



Apply changes?

Your changes have not been applied.
Yes to apply and proceed.
No to undo changes and proceed.

☐ Don't tell me about this again. (See Help for operation)
Re-enable this warning using Options | Enable Warnings.

❖ To apply the changes you made on the current page or view

In the Apply Changes dialog box, click **Yes**.

The data system applies changes automatically and, if appropriate, refreshes the chromatogram and spectrum views. 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 window so that you can correct or undo the changes.

❖ To undo the changes you made on the current page or view

In the Apply Changes dialog box, 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

In the Apply Changes dialog box, click **Cancel**.

The data system returns you to the Processing Setup window 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 turn off the Enable Warnings feature

In the Apply Changes dialog box, select the **Don't Tell Me About This Again** check box.

IMPORTANT Turning off the Enable Warnings feature changes the way in which the Xcalibur data system handles unapplied parameters.

❖ To enable the warnings feature

Choose **Options** > **Enable Warnings**.

Note If you are setting up an internal standard calibration, another dialog box appears when you click the Levels tab. This dialog box contains the following warning: This component is an ISTD and does not have any levels, so the Levels page will be empty. To turn off this warning, select the Don't Tell Me About This Again check box.

Setting Up the Void Time and Baseline Identification Options

Use the Identification Options dialog box to specify the void time and baseline settings for the analyses to be processed with the current processing method or to change the default settings for these parameters.

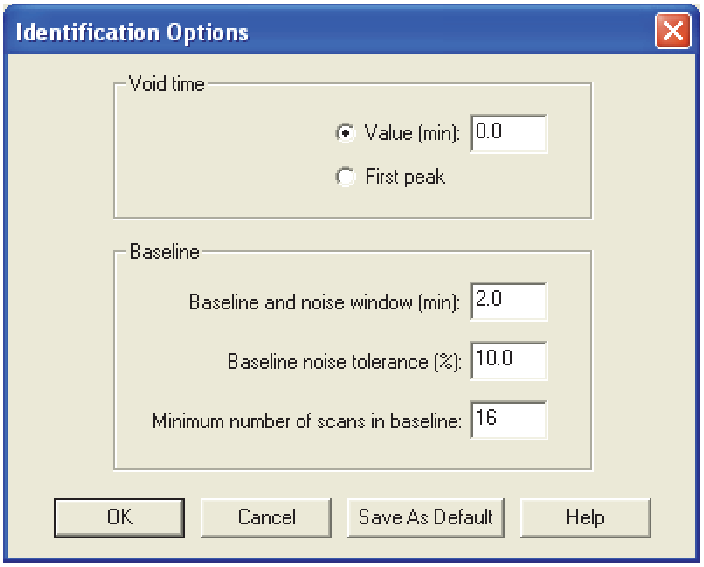
The void time is the elution time of an unretained peak. The Xcalibur data system uses the void time to calculate the relative retention times of the chromatographic peaks.

❖ To set the identification options for the current processing method

1. Choose **Options** > **Identification** from either the Quan view or the Qual view of the Processing Setup window.

   The Identification Options dialog box opens (Figure 11). For parameter descriptions, see "Identification Options Dialog Box" on page 286.

Figure 11. Identification Options dialog box



● Value (min): 0.0

○ First peak

Baseline and noise window (min): 2.0

Baseline noise tolerance (%): 10.0

Minimum number of scans in baseline: 16

2. To specify the void time, do one of the following:

    - To specify an absolute void time, select the **Value (min)** option, and then type a value from **0.0** to **100.0** minutes in the associated box.

    –or–

    - To specify a relative void time that is based on the retention time of the first detected peak, select the **First Peak** option.

3. To adjust the Baseline parameters, do the following:

    - In the Baseline and Noise Window (min) box, type a value from **0.1** to **1000.0** for the baseline and noise window.

      The data system uses this window to calculate the baseline noise.

    - In the Baseline Noise Tolerance % box, type a value from **0.0** to **100.0**.

    - In the Minimum Number of Scans in Baseline box, type an integer from **2** to **100**.

4. To save your settings with the current processing method, click **OK**.

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

Setting Up the Quantitative Processing Parameters

Use the Quan view of the Processing Setup window to set up the quantitative processing parameters for a processing method. The Quan view contains the following pages: Identification, Detection, Calibration, Levels, System Suitability, and Peak Purity (for PDA data only).

Before you enter the Quan view settings for the processing method, do the following:

- Specify whether the data is from a GC/MS system or an LC/MS system.
- Specify whether the processing method uses an external standard calibration or an internal standard calibration.

❖ To open the Quan view of the Processing Setup window

From the Processing Setup window, do one of the following:

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

–or–

- On the View bar, click the **Quan** icon, .

To set up the quantitative parameters for a processing method, follow these procedures:

- "Changing the Chromatography Mode" on page 22
- "Changing the Calibration Mode" on page 23
- "Setting Up the Quan View Identification Parameters" on page 24
- "Setting Up the Quan View Integration and Detection Parameters" on page 26
- "Setting Up the Calibration Parameters" on page 39
- "Setting Up the Calibration and Quantitation Flags" on page 42
- "Correcting for Calibration Impurities" on page 44
- "Setting Up the Calibration and QC Levels" on page 45
- "Setting Up the System Suitability Parameters" on page 48

Changing the Chromatography Mode

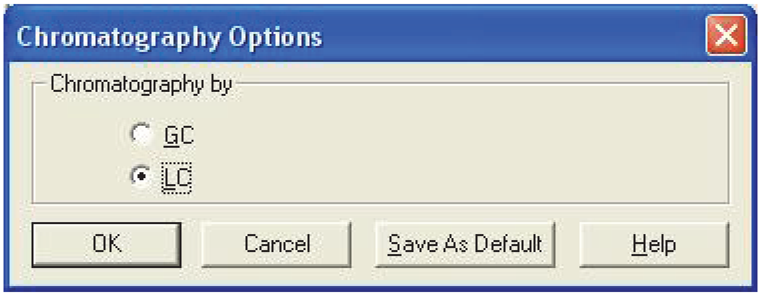
Use the Chromatography Options dialog box to specify the inlet (liquid or gas chromatography) used to acquire the raw data files.

❖ To change the chromatography detection mode

1. In the Quan view of Processing Setup, choose **Options > Chromatography By**.

   The Chromatography Options Dialog Box opens (Figure 12).

   Figure 12. Chromatography Options dialog box

2. Select a detection mode as follows:

   - To choose the GC detection mode, including the Spectrum detection option, select the **GC** option.

   - To choose the LC detection mode, 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 the Calibration Mode

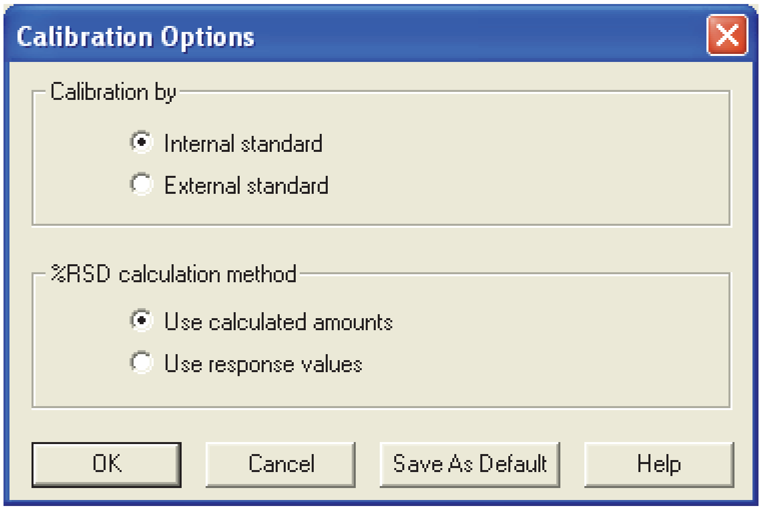
Use the Calibration Options dialog box to change the calibration mode. For parameter descriptions, see "Calibration Options Dialog Box" on page 270.

❖ To change the calibration mode

1. In the Quan view of Processing Setup, choose **Options > Calibration Options.**

   The Calibration Options dialog box opens (Figure 13).

   Figure 13. Calibration Options dialog box



Calibration Options

Calibration by
● Internal standard
○ External standard

%RSD calculation method
● Use calculated amounts
○ Use response values

2. Select the calibration mode as follows:
   - For an internal standard calibration, select the **Internal Standard** option.
   - For an 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**.

Setting Up the Quan View Identification Parameters

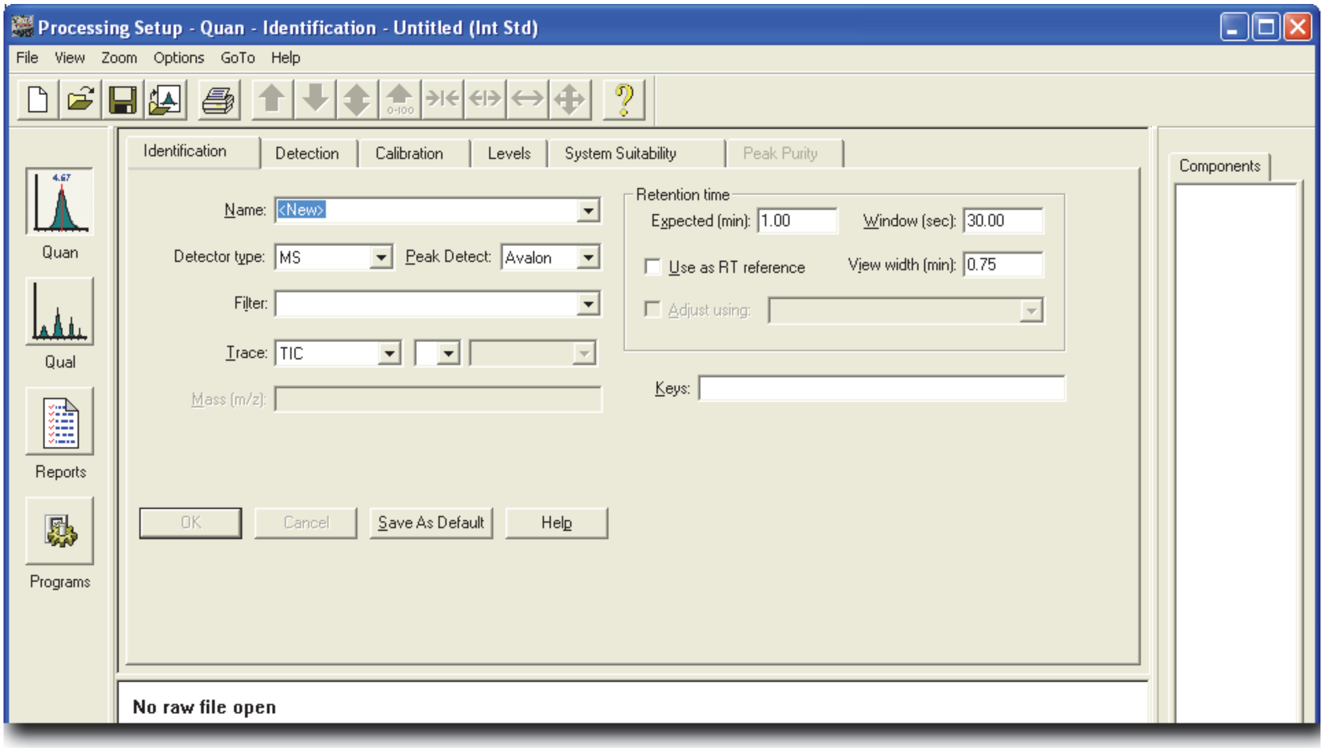
Use the Identification Page for Quan View to set up the identification parameters for each analyte (component) in your sample mixture.

For parameter descriptions, see "Identification Page for Quan View" on page 343.

❖ To set the identification parameters

1. From the Quan view of the Processing Setup window, click the **Identification** tab (Figure 14).

Figure 14. Identification page for Quan view



Processing Setup - Quan - Identification - Untitled (Int Std)

Name: <New>
Detector type: MS
Peak Detect: Avalon
Filter:
Trace: TIC
Mass (m/z):
Retention time
Expected (min): 1.00
Window (sec): 30.00
☐ Use as RT reference
View width (min): 0.75
☐ Adjust using:
Keys:

No raw file open

2. For each component (analyte) that you want to identify, do the following:
   a. In the Name box, do the following:
      i. Select **<New>**.
      ii. Type the name of the component.

   > **Note** For each component that you add to the Components list, you must select New in the list box, and then type the name of the component.

   b. From the Detector Type list, select the detector type: **MS**, **Analog**, **A/D card**, **PDA**, or **UV**.

   c. From the Peak Detect list, select a peak detection algorithm: **Genesis**, **ICIS**, or **Avalon**.

   d. 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.

      Tip To select a scan filter from a list, you must first open an example raw data file. To open a raw file, choose **File > Open Raw File**. The Open Raw File dialog box opens. Select a raw file and click **Open**.

      For information about the nomenclature for scan filters, refer to the *Xcalibur Qual Browser User Guide*.

   e. Select a Trace type or Trace combination in the three Trace lists as follows:

      i. Select a Trace type from the first Trace list.

      ii. To use a Trace type combination, select an operator (+ or –) in the second Trace list.

      iii. Select the second Trace type in the third list.

   f. If needed, type the mass range or wavelength range of the selected component in the Mass or Wavelength box.

   g. Type a text comment in the Keys box.

   h. In the Retention Time area, type the expected retention time of the selected component in the Expected (min) box.

   i. Type the allowable time deviation for the expected retention time (the window for the retention time) in the Window (sec) box.

   j. Specify whether the retention time of the selected component is to be used as a reference time for other components:

      i. To use the selected component for a retention time reference, select the **Use As RT Reference** check box.

      ii. 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.

3. To apply the settings for the selected component, click **OK**.

   The component name appears in the Components list on the right side of the Quan view. The Identification page remains open, and the other tabs become available.

4. To remove a component from the Components list, do the following:

   a. Select the component in the Components list.

   b. Choose **Options > Delete *component name***.

      A dialog box appears with the following query: Confirm delete “*component name*”?

   c. Click **OK** to delete the component from the component list and close the dialog box.

Setting Up the Quan View Integration and Detection Parameters

Use the Detection page of the Quan view to specify the integration and peak detection settings for the processing method.

The Detection page contains two areas: Peak Integration and Peak Detection. The available parameters in both the Peak Integration and Peak Detection areas depend on the peak detection algorithm selected on the Identification page of the Quan view. The three peak detection algorithms are Genesis, ICIS, and Avalon. The available Peak Detection parameters also depend on whether the data is from a GC/MS system or an LC/MS system.

These procedures show you how to set up the integration and detection parameters. Begin with the procedure for the peak detection algorithm that you selected on the Identification page of the Quan view.

- “Setting Up the Genesis Detection Parameters in the Quan View,” on this page
- “Setting Up the ICIS Detection Parameters in the Quan View” on page 29
- “Setting Up the Avalon Detection Parameters in the Quan View” on page 31
- “Setting Up the Peak Detection Parameters for Chromatography by GC” on page 34
- “Setting Up the Detection Data Flags in Quan View” on page 38

Setting Up the Genesis Detection Parameters in the Quan View

This procedure describes how to set up the parameters for the Genesis peak detection algorithm.

When you select the Genesis peak detection algorithm for a component, the two areas on the Detection page of the Quan view are labeled Genesis Peak Integration and Genesis Peak Detection.

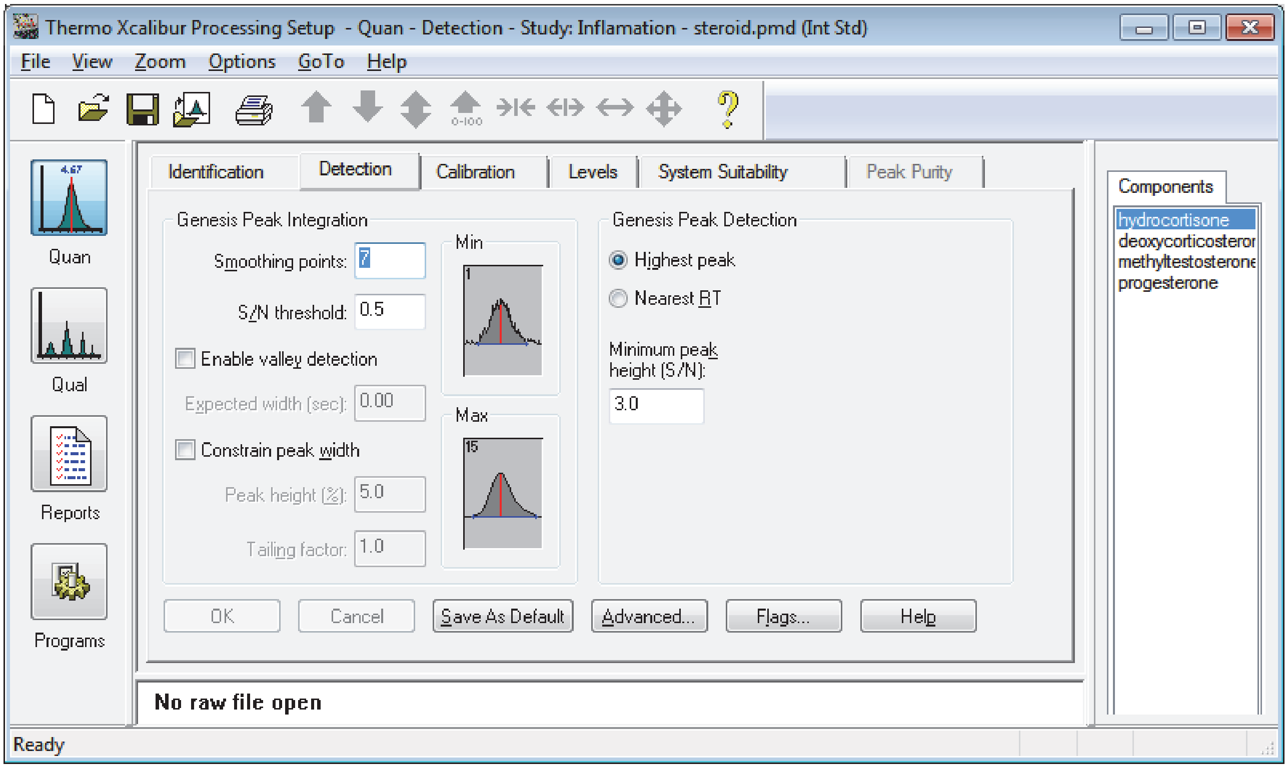
For information about the parameters for the Genesis peak detection algorithm, see “Genesis Detection Page for Quan View” on page 359.

❖ To set up the Genesis detection parameters for a component

1. In the Quan view, click the **Detection** tab.

   If you selected Genesis in the Peak Detect list on the Identification Page for Quan View for the component highlighted in the Components list on the right side of the window, the Genesis Detection Page appears (Figure 15).

Figure 15. Genesis Detection page for Quan view



Thermo Xcalibur Processing Setup - Quan - Detection - Study: Inflamation - steroid.pmd (Int Std)

Genesis Peak Integration

Smoothing points: 7

S/N threshold: 0.5

☐ Enable valley detection

Expected width (sec): 0.00

☐ Constrain peak width

Peak height (%): 5.0

Tailing factor: 1.0

Genesis Peak Detection

● Highest peak

○ Nearest RT

Minimum peak height (S/N): 3.0

Components

hydrocortisone
deoxycorticosteror
methyltestosterone
progesterone

No raw file open

Ready

2. Set up the integration parameters in the Genesis Peak Integration area as follows:

   - To enter the smoothing level that the data system applies to the chromatogram before peak integration, type a value in the Smoothing Points box in the Genesis Peak Integration area.

   - To enter a signal-to-noise ratio threshold value, type a value in the S/N Threshold box.

     The data system 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.

   - 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.

   - To apply peak height and tailing factor integration criteria, select the **Constrain Peak Width** check box. Then type the start integration setting in the Peak Height (%) box and the stop integration setting in the Tailing Factor box.

3. To specify peak detection criteria, select one of the following component identification options:
   - For an LC/MS system, select one of these two options:
     - To choose the highest peak in the chromatogram, select the **Highest Peak** option.
     - To choose the peak with the nearest retention time, select the **Nearest RT** option.
   - For a GC/MS system, select one of these three options:
     - To use a reference spectrum, select the **Spectrum** option. Then, make the appropriate entries in the spectrum and Thresholds tables.

       For more information, see "Setting Up the Spectrum Detection Parameters for Chromatography by GC" on page 35.
     - To choose the highest peak in the chromatogram, select the **Highest Peak** option.
     - To choose the peak with the nearest retention time, select the **Nearest RT** option.

       When you select either the Highest Peak or Nearest RT option, the Ion Ratio Confirmation parameters become available.
       - To use ion ratio confirmation, select the **Enable** check box in the Ion Ratio Confirmation area. Then, make the appropriate entries in the table.
       - In the Window% area, select **Relative** or **Absolute**.
       - In the Qualifier Ion Coelution area, type a value, in minutes, in the box.

       For more information, see "Setting Up Ion Ratio Confirmation for Chromatography by GC" on page 37.
4. To enter a signal-to-noise ratio threshold, type a value in the Minimum Peak Height (S/N) box.

   The data system ignores all chromatogram peaks that have a signal-to-noise value less than this parameter value.
5. To use the advanced detection options for the Genesis peak detection algorithm, do the following:

   a. Click **Advanced**.

      The Genesis Advanced Detection Options dialog box opens. For information about the parameters in this dialog box, see "Genesis Advanced Detection Options Dialog Box" on page 281.

   b. Make the appropriate entries and click **OK**.
6. To save the settings on the Detection page, click **OK**.

Setting Up the ICIS Detection Parameters in the Quan View

This procedure describes how to set up the parameters for the ICIS peak detection algorithm.

When you select the ICIS peak detection algorithm for a component, the two areas on the Detection page of the Quan view are labeled ICIS Peak Integration and ICIS Peak Detection.

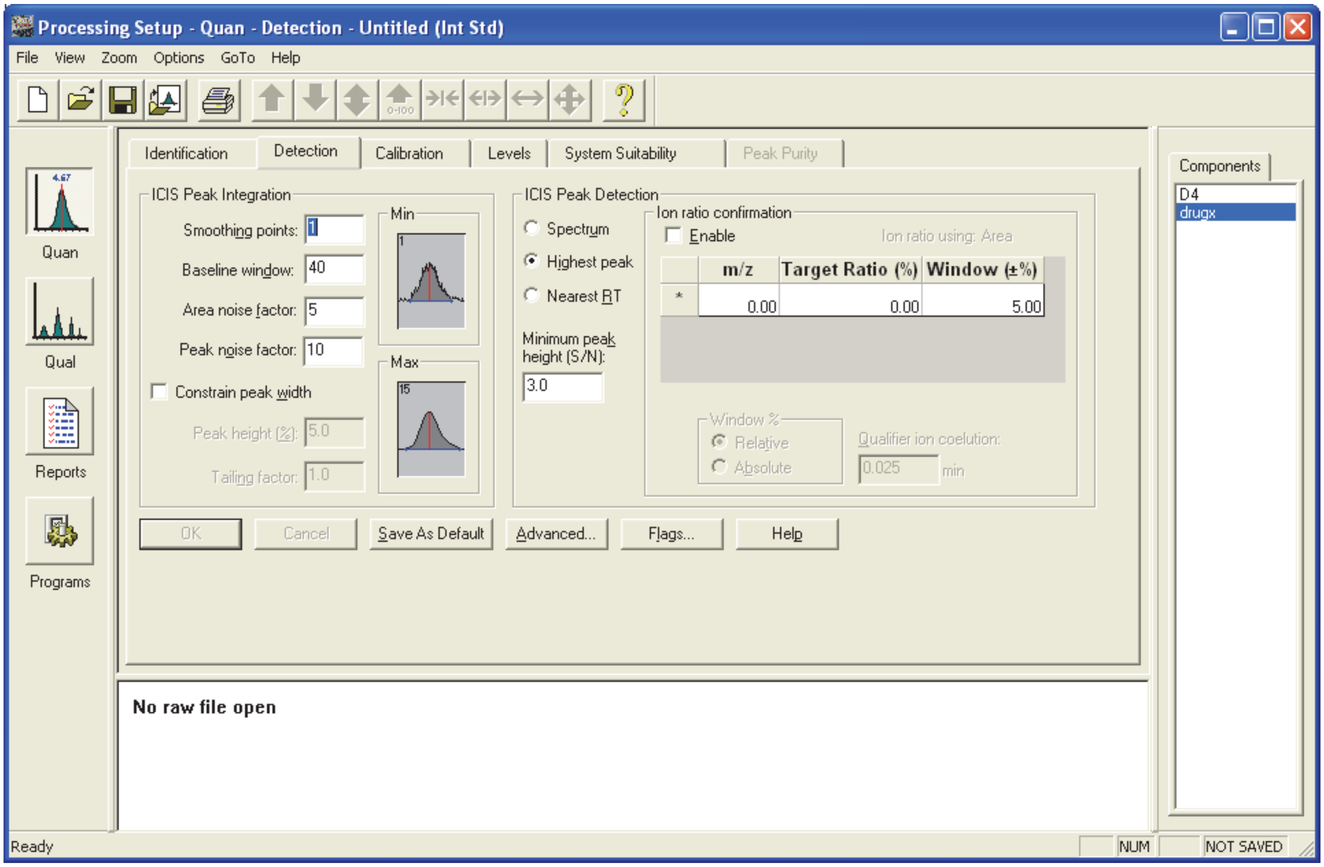
For more information about the parameters on the ICIS Detection page in the Quan view, see “ICIS Detection Page for Quan View” on page 369.

❖ To set up the ICIS detection parameters for a component

1. In the Quan view, click the **Detection** tab.

   If you selected ICIS in the Peak Detect list on the Identification page for the component highlighted in the Components list on the right side of the window, the ICIS Detection page appears (Figure 16).

Figure 16. ICIS Detection page for Quan view (GC mode)



ICIS Peak Integration
Smoothing points: 1
Baseline window: 40
Area noise factor: 5
Peak noise factor: 10
☐ Constrain peak width
Peak height (%): 5.0
Tailing factor: 1.0
Min 1
Max 15

ICIS Peak Detection
○ Spectrum
● Highest peak
○ Nearest RT
Minimum peak height (S/N): 3.0

Ion ratio confirmation
☐ Enable
Ion ratio using: Area

	m/z	Target Ratio (%)	Window (±%)
*	0.00	0.00	5.00

Window %
● Relative
○ Absolute
Qualifier ion coelution: 0.025 min

Components
D4
drugx

No raw file open

Ready
NUM
NOT SAVED

2. Set up the integration parameters in the ICIS Peak Integration area as follows:
    - To set the smoothing level that the application applies to the chromatogram before peak integration, type a value in the Smoothing Points box.
    - To set the baseline window parameter, type a value in the Baseline Window box.
    - To set the area noise factor, type a value in the Area Noise Factor box.
    - To set the peak noise factor, type a value in the Peak Noise Factor box.
    - 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 criterion, type a value in the Tailing Factor box.
3. To specify peak detection criteria, select one of the following component identification options:
    - For an LC/MS system, select one of these two options:
        - To choose the highest peak in the chromatogram, select the **Highest Peak** option.
        - To choose the peak with the nearest retention time, select the **Nearest RT** option.
    - For a GC/MS system, select one of these three options:
        - To use a reference spectrum, select the **Spectrum** option. Then, make the appropriate entries in the spectrum and Thresholds tables.

          For more information, see "Setting Up the Spectrum Detection Parameters for Chromatography by GC" on page 35.
        - To choose the highest peak in the chromatogram, select the **Highest Peak** option.
        - To choose the peak with the nearest retention time, select the **Nearest RT** option.

          When you select either the Highest Peak or Nearest RT option, the Ion Ratio Confirmation parameters become available.
            - To use ion ratio confirmation, select the **Enable** check box in the Ion Ratio Confirmation area. Then, make the appropriate entries in the table.
            - In the Window% area, select **Relative** or **Absolute**.
            - In the Qualifier Ion Coelution area, type a value, in minutes, in the box.

          For more information, see "Setting Up Ion Ratio Confirmation for Chromatography by GC" on page 37.

4. To enter a signal-to-noise ratio threshold, type a value in the Minimum Peak Height (S/N) box.

   The data system ignores all chromatogram peaks that have a signal-to-noise value less than this parameter value.

5. To modify the advanced detection options for the ICIS peak detection algorithm, do the following:

   a. Click **Advanced**.

      The ICIS Advanced Detection Options dialog box opens. For information about the parameters in this dialog box, see "ICIS Advanced Parameters Dialog Box" on page 284.

   b. Make the appropriate entries and click **OK** to save the new settings and close the dialog box.

6. To save the settings on the Detection page, click **OK**.

Setting Up the Avalon Detection Parameters in the Quan View

This procedure describes how to set up the parameters for the Avalon peak detection algorithm on the Detection page of the Processing Setup – Quan view.

When you select the Avalon peak detection algorithm for a component, the two areas on the Detection page of the Quan view are labeled Avalon Peak Integration and Avalon Peak Detection.

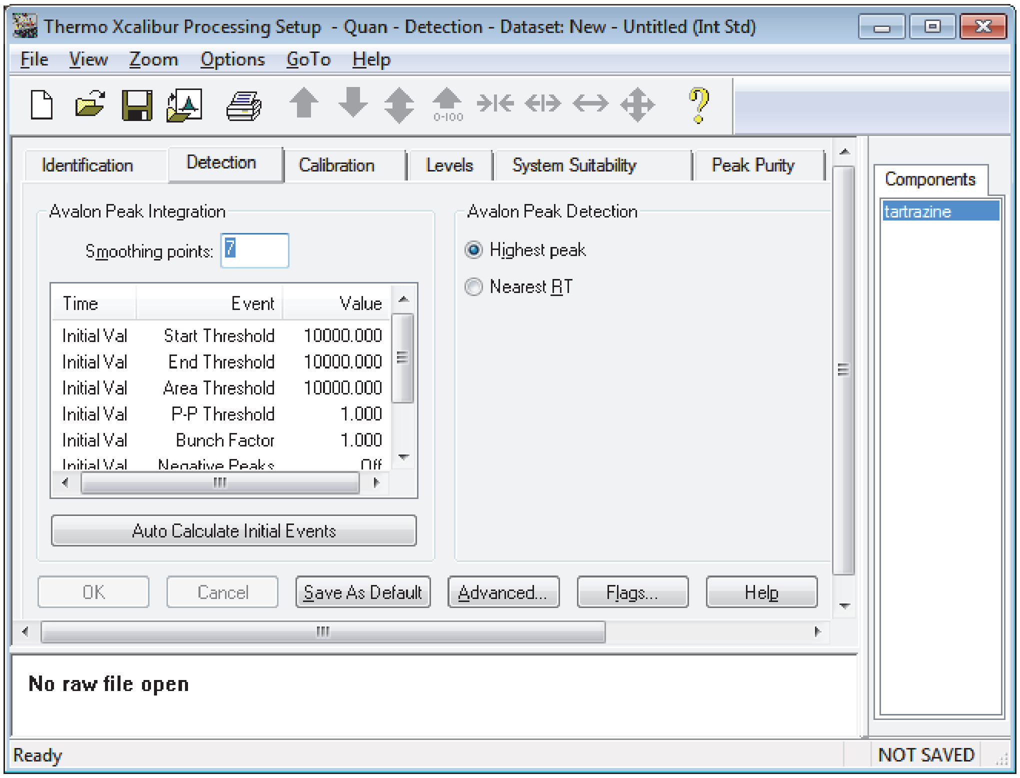
For more information about the parameters on the Avalon Detection page, see "Avalon Detection Page for Quan View" on page 351.

❖ To set up the Avalon detection parameters for a component

1. In the Quan view, click the **Detection** tab.

   The Avalon Detection page for Quan View appears (Figure 17).

Figure 17. Avalon Detection page



Avalon Peak Integration

Smoothing points: 7

Time	Event	Value
Initial Val	Start Threshold	10000.000
Initial Val	End Threshold	10000.000
Initial Val	Area Threshold	10000.000
Initial Val	P-P Threshold	1.000
Initial Val	Bunch Factor	1.000
Initial Val	Negative Peaks	Off

Avalon Peak Detection

● Highest peak

○ Nearest RT

Components: tartrazine

No raw file open

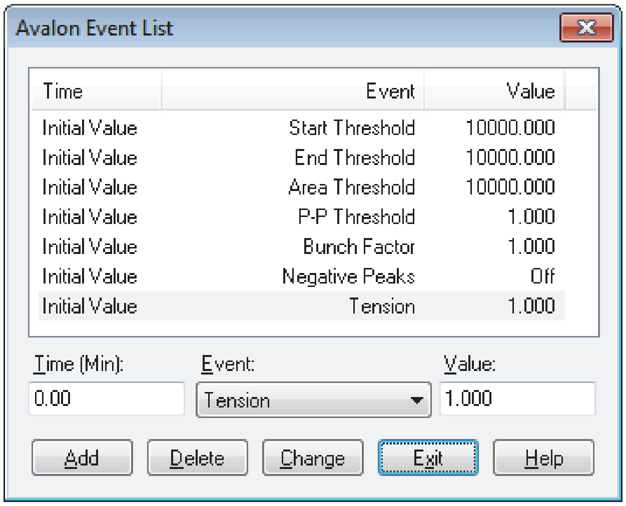
2. To enter the smoothing level that the application applies to the chromatogram before peak integration, type a value in the Smoothing Points box in the Avalon Peak Integration area.

3. To edit the events table, do the following:

   a. Click **Advanced**.

      The Avalon Event List dialog box opens (Figure 18).

Figure 18. Avalon Event List dialog box



Time	Event	Value
Initial Value	Start Threshold	10000.000
Initial Value	End Threshold	10000.000
Initial Value	Area Threshold	10000.000
Initial Value	P-P Threshold	1.000
Initial Value	Bunch Factor	1.000
Initial Value	Negative Peaks	Off
Initial Value	Tension	1.000

Time (Min): 0.00

Event: Tension

Value: 1.000

b. To edit the Event list, highlight the row you that want to change, one row at a time, and enter the revised settings in the boxes. Click **Change**.

c. To save the new settings and close the dialog box, click **Exit**.

4. To specify peak detection criteria, select one of the following component identification options:

   - For an LC/MS system, select one of these two options:
     - To choose the highest peak in the chromatogram, select the **Highest Peak** option.
     - To choose the peak with the nearest retention time, select the **Nearest RT** option.
   - For a GC/MS system, select one of these three options:
     - To use a reference spectrum, select the **Spectrum** option. Then, make the appropriate entries in the spectrum and Thresholds tables.

       For more information, see "Setting Up the Spectrum Detection Parameters for Chromatography by GC" on page 35.
     - To choose the highest peak in the chromatogram, select the **Highest Peak** option.
     - To choose the peak with the nearest retention time, select the **Nearest RT** option.

       When you select either the Highest Peak or Nearest RT option, the Ion Ratio Confirmation parameters become available.
       - To use ion ratio confirmation, select the **Enable** check box in the Ion Ratio Confirmation area. Then, make the appropriate entries in the table.
       - In the Window% area, select **Relative** or **Absolute**.
       - In the Qualifier Ion Coelution area, type a value, in minutes, in the box.

       For more information, see "Setting Up Ion Ratio Confirmation for Chromatography by GC" on page 37.

5. To save the settings on the Detection page, click **OK**.

Setting Up the Peak Detection Parameters for Chromatography by GC

For GC/MS data, the Xcalibur data system provides two confirmation techniques for peak detection: spectrum and ion ratio confirmation.

These procedures describe how to set the parameters for the confirmation techniques:

- Setting Up the Spectrum Options for Chromatography by GC
- Setting Up the Spectrum Detection Parameters for Chromatography by GC
- Setting Up Ion Ratio Confirmation for Chromatography by GC

Setting Up the Spectrum Options for Chromatography by GC

For a GC/MS system, you can set up a low-intensity cutoff for the spectral data.

❖ To change the low intensity cutoff threshold for spectrum detection

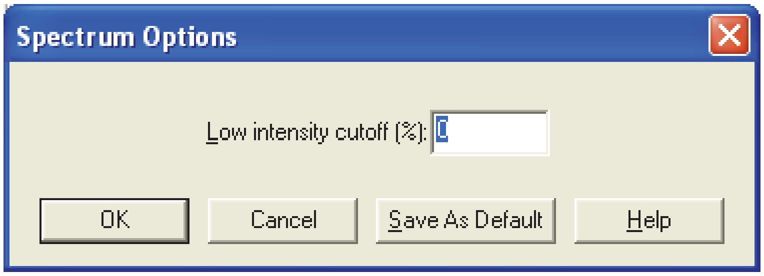
1. If you have not already done so, set up the processing method for data produced by a GC/MS system as follows:
   a. Choose **Options > Chromatography By**.

      The Calibration Options Dialog Box opens (see Figure 12 on page 22).

   b. Select the **GC** option.
   c. Click **OK** to accept the new setting and close the dialog box.
2. In the Quan view, click the **Detection** tab.
3. In the Peak Detection area, select the **Spectrum** option.
4. From the menu bar, choose **Options > Spectrum**.

   The Spectrum Options Dialog Box opens (Figure 19).

Figure 19. Spectrum Options dialog box



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

Setting Up the Spectrum Detection Parameters for Chromatography by GC

For GC/MS data, follow these procedures to set up the spectrum detection parameters for a component on the Detection page of the Quan view in the Processing Setup window.

❖ To select the spectrum detection options for a component

1. If you have not already set up the data system to process the data from a GC/MS system, do the following:
    a. In the Quan view of the Processing Setup window, choose **Options > Chromatography By**.

       The Chromatography Options dialog box opens (see Figure 12 on page 22).

    b. Select the **GC** option

    c. Click **OK** to accept the new setting and close the dialog box.

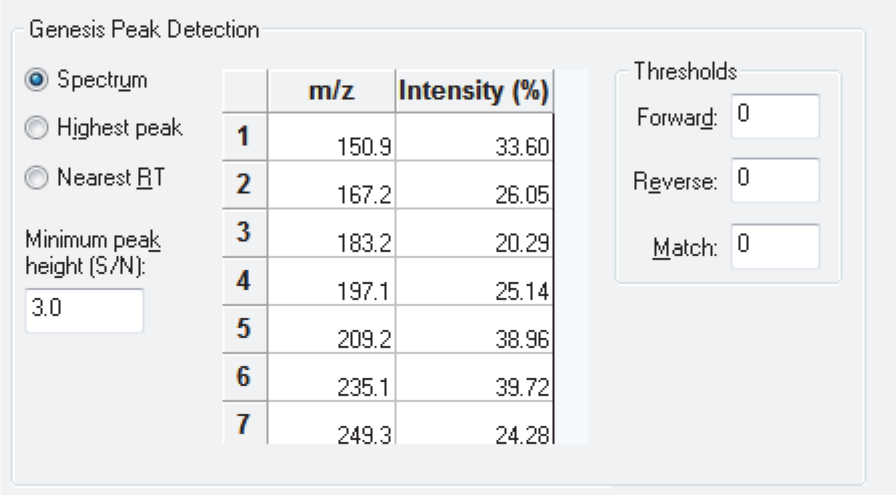
2. In the Quan view, click the **Detection** tab (Figure 15 on page 27).

3. To display the spectrum options in the Peak Detection area, select the **Spectrum** option.

4. Enter the mass-to-charge [*m/z*] and intensity data for up to 50 spectrum peaks in the spectrum peak identification table (Figure 20).

    - To manually enter the peak data, see "To enter data manually in the spectrum table."
    - To interactively enter the peak data, see "To enter data in the spectrum table by using an open raw file."

Figure 20. Spectrum peak identification table



Genesis Peak Detection

● Spectrum
○ Highest peak
○ Nearest RT

Minimum peak height (S/N): 3.0

	m/z	Intensity (%)
1	150.9	33.60
2	167.2	26.05
3	183.2	20.29
4	197.1	25.14
5	209.2	38.96
6	235.1	39.72
7	249.3	24.28

Thresholds
Forward: 0
Reverse: 0
Match: 0

❖ To enter data manually in the spectrum table

1. For all the ions in the reference spectrum (up to a maximum of 50), do the following:
   - 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.
2. To edit the table, do the following:
   - 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.
   - To delete a range of rows, drag the cursor from the first to the final row in the selected range. Then right-click and select **Delete Rows**.

❖ To enter data in the spectrum table by using an open raw file

1. Set the low-intensity cutoff as described in "Setting Up the Spectrum Options for Chromatography by GC" on page 34.
2. Pin the spectrum cell.
3. Click the appropriate component peak in the chromatogram cell.

   The data system displays the spectrum from the selected time point in the spectrum cell and copies the *m/z* and intensity values of the ions in the mass spectrum to the peak identification table. It discards any ions with intensities below the Low Intensity Cutoff % parameter in the Spectrum Options Dialog Box.
4. To set threshold values for spectrum matching in the Thresholds area.
   - In the Forward box, type an integer from **0** to **1000**.
   - In the Reverse box, type a value from **0** to **1000**.
   - In the Match box, type a value from **0** to **100**.

     For more information about the settings for these parameters, see "Detection Page for Quan View" on page 351.
5. To save the settings, click **OK**.

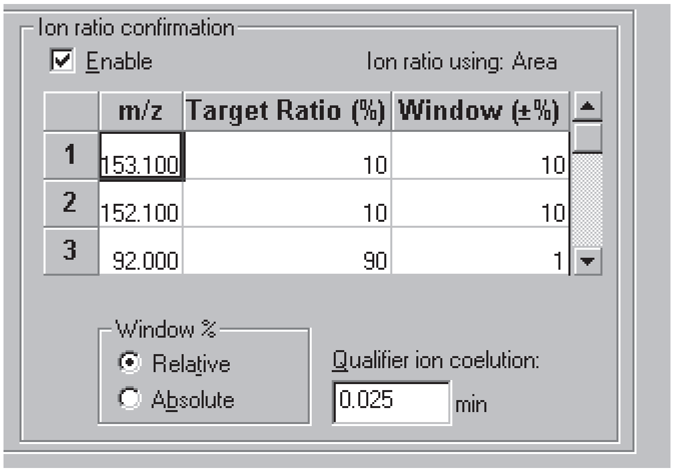
Setting Up Ion Ratio Confirmation for Chromatography by GC

This procedure for setting up the ion ratio confirmation parameters applies only to GC/MS data.

❖ To set up ion ratio confirmation for a component

1. In the Quan view of the Processing Setup window, click the **Detection** tab.
2. Select the **Highest Peak** option or the **Nearest RT** option in the Peak Detection area.
3. To turn on the ion ratio confirmation feature, select the **Enable** check box in the Ion Ratio Confirmation area (Figure 21).

Figure 21. Ion ratio confirmation area



Ion ratio confirmation

☑ Enable

Ion ratio using: Area

	m/z	Target Ratio (%)	Window (±%)
1	153.100	10	10
2	152.100	10	10
3	92.000	90	1

Window %

● Relative

○ Absolute

Qualifier ion coelution: 0.025 min

4. To enter the information for up to four qualifier ions for the current component, do the following for each ion:
   - 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.
5. To edit the table, do the following:
   - 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.
   - To delete a range of rows, drag the cursor from the first to the final row in the selected range. Then right-click and select **Delete Rows**.

6. Set the Window% mode as follows:
   - 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.
7. To set a value, in minutes, for the qualifier ion coelution window, type a value in the Qualifier Ion Coelution box.
8. To save the settings, click **OK**.

Setting Up the Detection Data Flags in Quan View

Use the Data Flags dialog box to set up the data flags. You can access the Data Flags dialog box from the Quan view – Detection page. For more information about the Data Flags dialog box, see "Data Flags Dialog Box" on page 274.

❖ To set up the data flag settings

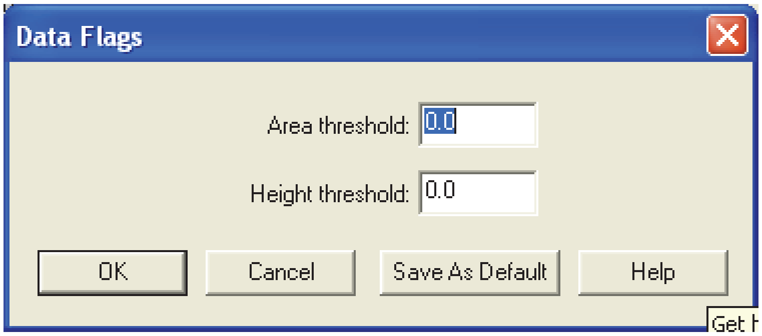
1. In the Quan view of the Processing Setup window, click the **Detection** tab.

   The Detection page opens (see Figure 16 on page 29).

2. Click **Flags**.

   The Data Flags dialog box opens (Figure 22).

Figure 22. Data Flags dialog box



Area threshold: 0.0

Height threshold: 0.0

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 Up the Calibration Parameters

Use the Calibration page of the Quan view to set up the calibration information for a quantitative analysis.

If you selected the External Standard calibration option, the parameters for internal standards are not available. For an external standard calibration, one calibration curve is associated with each target compound.

If you selected the Internal Standard calibration option, the parameters for both the internal standards and the target components are available. The component list must include at least one internal standard. One calibration curve is associated with each target component. For an internal standard calibration, each target compound must have an associated internal standard component.

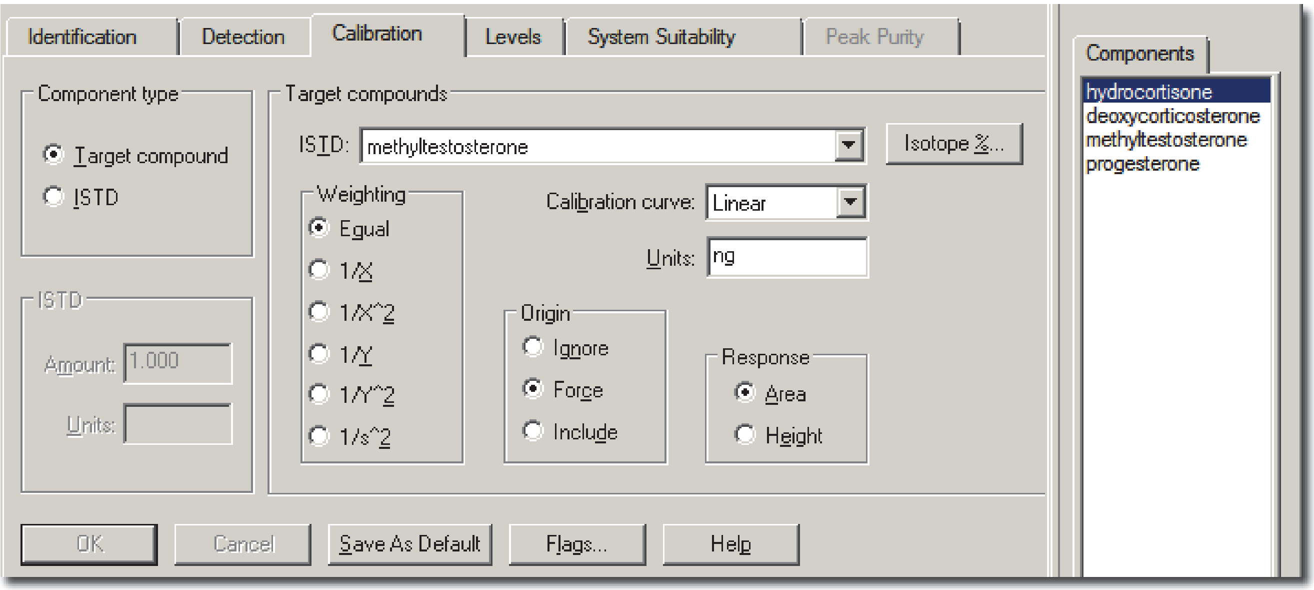
For more information about the parameters on the Calibration page, see “Calibration Page for Quan View” on page 378.

❖ To define the calibration curve parameters and the internal standard component for target components and the amount for internal standard components

1. In the Quan view of the Processing Setup window, click the **Calibration** tab.

   The Calibration page opens (Figure 23).

   Figure 23. Calibration page



Component type
- ● Target compound
- ○ ISTD

ISTD
- Amount: 1.000
- Units:

Target compounds
- ISTD: methyltestosterone
- Weighting: ● Equal ○ 1/X ○ 1/X^2 ○ 1/Y ○ 1/Y^2 ○ 1/s^2
- Calibration curve: Linear
- Units: ng
- Origin: ○ Ignore ● Force ○ Include
- Response: ● Area ○ Height

Components
- hydrocortisone
- deoxycorticosterone
- methyltestosterone
- progesterone

2. Depending on the calibration technique, do one of the following:

   - For an internal standard calibration, go to step 3.
   - For an external standard calibration, go to step 4.

3. For an internal standard calibration, do the following:
    a. For each internal standard component, do the following:
        i. Select the component in the Component list on the right side of the Processing Setup window.
        ii. In the Component Type area, select the **ISTD** option.
        iii. In the ISTD area, type the amount for the selected internal standard in the Amount box.

    > **Note** For an internal standard calibration, you must assign the ISTD type to at least one component before you can assign the Target Compound type to other components.

    b. For each target compound, do the following:
        i. Select the component in the Component list.
        ii. Select the **Target Compound** option.
        iii. In the ISTD list, select the internal standard component that you added to the target compound standard.
        iv. To correct for isotope contributions, click **Isotope %**.

            The Correction for Isotope Contribution dialog box opens. See "Correcting for Calibration Impurities" on page 44 for information about entering values into this box.

        v. Make the appropriate entries.
        vi. Click **OK** to accept the entries and close the dialog box.
        vii. Go to step 5.
4. For an external standard calibration, do the following:
    a. Select the component in the Components list.
    b. Select the **Target Compound** option.
5. For both calibration techniques, do the following for each target compound:
    a. Select the component in the Components list.
    b. In the Calibration Curve list, select the curve type:

        - Linear
        - Quadratic
        - Linear log-log
        - Quadratic log-log
        - Average response factor (RF)
        - Point-to-point
        - Cubic spline
        - Locally weighted

c. For the Linear and Quadratic curve types, select an option in the Weighting area.

   If you select any of the other curve types, the Weighting area is not available.

   For more information about the curve types and the weighting options, see "Calibration Page for Quan View" on page 378.

d. For the Linear, Quadratic, Point-to-Point, or Cubic Spline curve types, in the Origin area select how the data system treats the origin in the calibration curve calculation as follows:

   - Select the **Ignore** option to exclude the origin from the calibration curve calculation.
   - Select the **Force** option to require that the calibration curve pass through the origin.
   - Select the **Include** option to include the origin as one data point.

e. To select the units to be displayed on graphs and reports, type the appropriate units in the Units box.

f. In the Response area, define the basis for the quantitation:

   - To quantitate on the basis of the integrated area of component peaks, select the **Area** option.
   - To quantitate on the basis of the calculated height of component peaks, select the **Height** option.

Setting Up the Calibration and Quantitation Flags

Use the Calibration and Quantitation Flags dialog box to set up calibration and quantitation flags for the processing method. You can access this dialog box from the Calibration page of the Quan view.

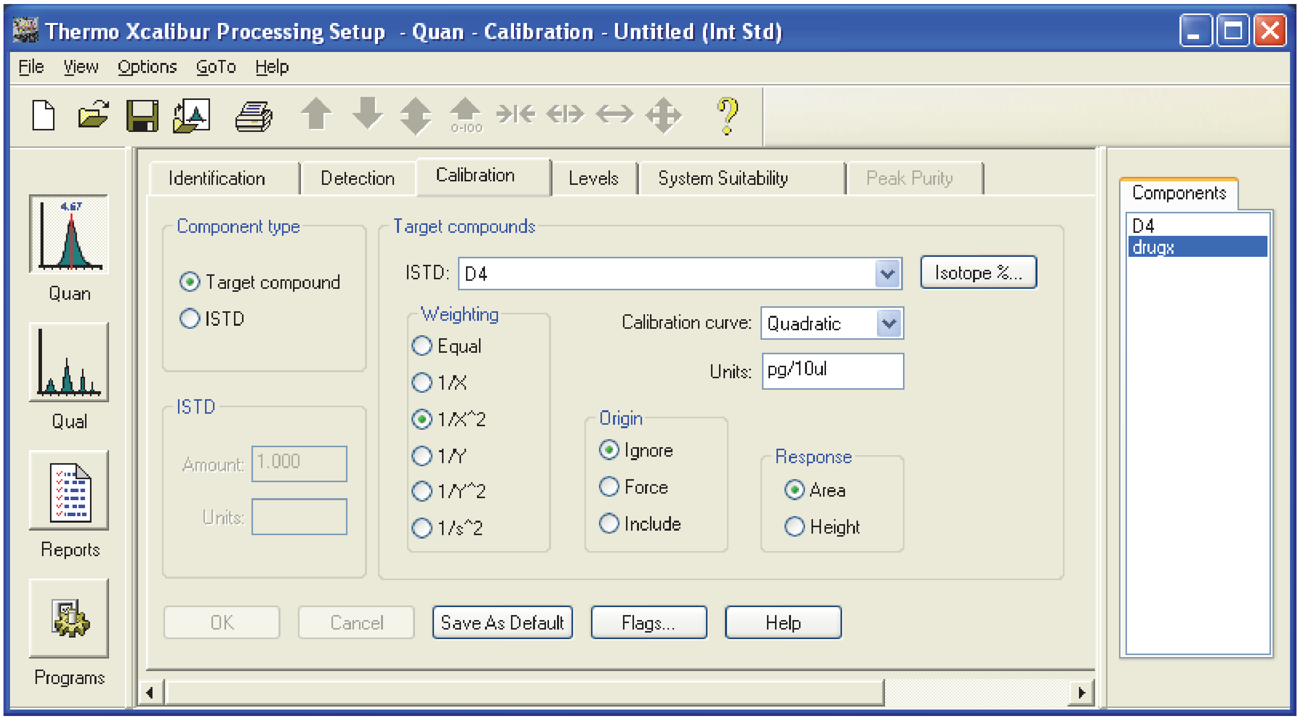
For more information about the Calibration and Quantitation Flags dialog box, see "Calibration and Quantitation Flags Dialog Box" on page 269.

❖ To set up calibration and quantitation flags

1. From the Quan view of the Processing Setup window, click the **Calibration** tab.

   The Calibration page opens (Figure 24).

Figure 24. Calibration page for the Quan view of the Processing Setup window



Thermo Xcalibur Processing Setup - Quan - Calibration - Untitled (Int Std)

Component type
● Target compound
○ ISTD

ISTD
Amount: 1.000
Units:

Target compounds
ISTD: D4
Calibration curve: Quadratic
Units: pg/10ul

Weighting
○ Equal
○ 1/X
● 1/X^2
○ 1/Y
○ 1/Y^2
○ 1/s^2

Origin
● Ignore
○ Force
○ Include

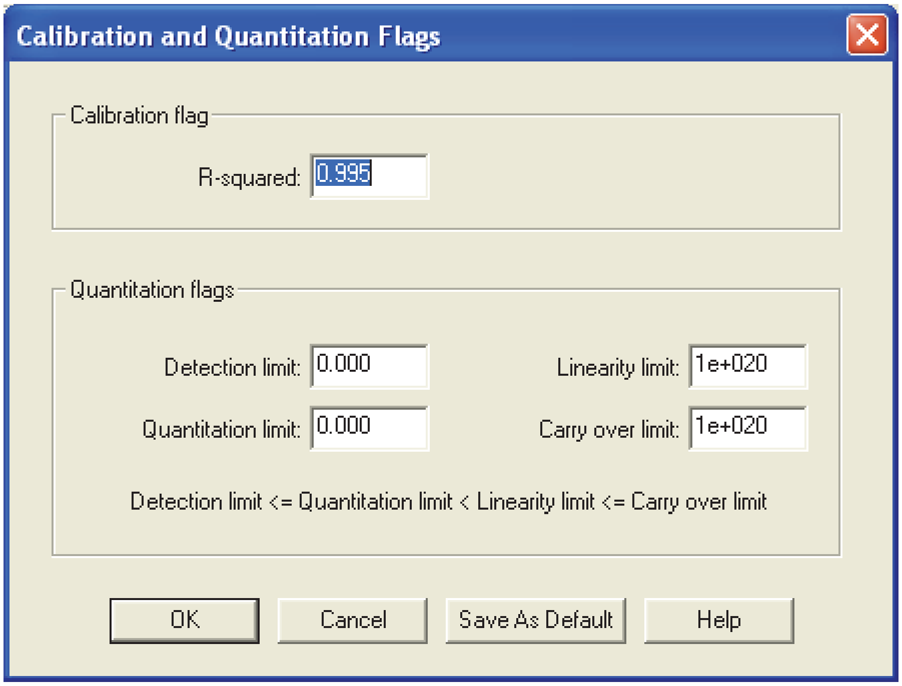
Response
● Area
○ Height

Components
D4
drugx

2. Click **Flags**.

   The Calibration and Quantitation Flags dialog box opens (Figure 25).

Figure 25. Calibration and Quantitation Flags dialog box



R-squared: 0.995

Detection limit: 0.000

Quantitation limit: 0.000

Linearity limit: 1e+020

Carry over limit: 1e+020

Detection limit <= Quantitation limit < Linearity limit <= Carry over limit

3. In the Calibration Flag area, type a value from 0.000 to 1.000 in the R-squared box to specify the calibration flag threshold.

4. In the Quantitation Flags area, do the following:

   - 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 that elutes at the same time as the target compound reagent [TM], or to correct for an impurity in the target compound reagent TM [impurity] that elutes at the same time as the internal standard reagent [ISTD], or to correct for impurities in both reagents.

❖ To correct for calibration impurities

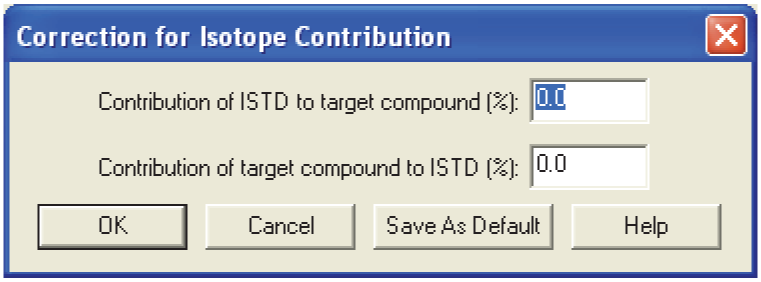
1. From the Quan view of the Processing Setup window, click the **Calibration** tab.

   The Calibration Page opens (see Figure 24 on page 42).

2. Click **Isotope %**.

   The Correction for Isotope Contribution dialog box opens (Figure 26).

   Figure 26. Correction for Isotope Contribution dialog box

   Contribution of ISTD to target compound (%): 0.0

   Contribution of target compound to ISTD (%): 0.0

3. Make the following entries:

   - If you have an impurity in your internal standard that elutes at the same time as the target compound, 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 this step, the data system corrects for the ISTD [impurity] or TM [impurity] and reports the corrected amounts of ISTD and TM.

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

Setting Up the Calibration and QC Levels

Use the Levels page of the Processing Setup – Quan view to set up the levels for the calibration standards and QC samples in the processing method.

You can set up the level information for the calibration standards in two ways: by manual entry on the Levels page or semi-automatically by using the Standard Dilutions dialog box. You can only set up the level information for the QC samples manually.

To set up the levels for the calibration standards and QC samples, follow these topics:

- Setting Up the Levels for the Calibration and QC Standards
- Using the Standard Dilutions Dialog Box to Set Up the Calibration Levels

Setting Up the Levels for the Calibration and QC Standards

You can set up the calibration standard levels in the processing method either manually or by using the Standard Dilutions dialog box. You can only enter the QC levels manually.

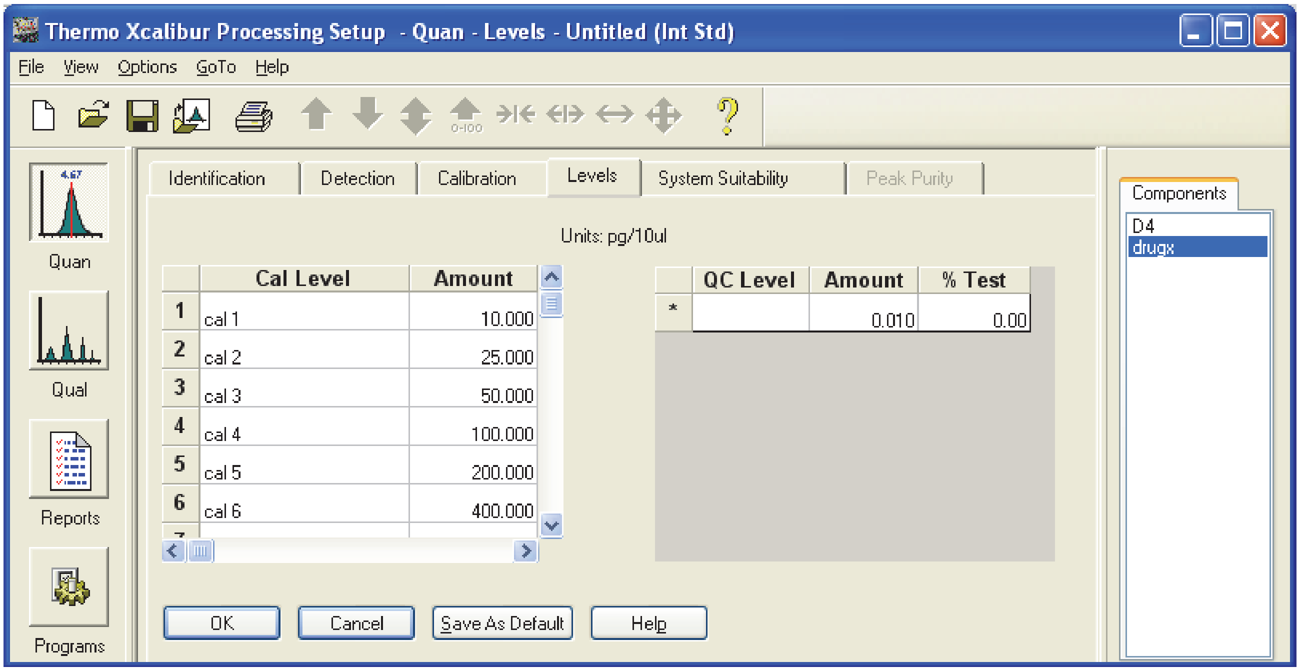
For more information about the Levels page, see "Levels Page for Quan View" on page 383.

❖ To set up the calibration and QC levels for the target components

1. From the Quan view of the Processing Setup window, click the **Levels** tab.

   The Levels page opens (Figure 27).

Figure 27. Levels page for Quan view



Units: pg/10ul

	Cal Level	Amount
1	cal 1	10.000
2	cal 2	25.000
3	cal 3	50.000
4	cal 4	100.000
5	cal 5	200.000
6	cal 6	400.000

	QC Level	Amount	% Test
*		0.010	0.00

Components:
D4
drugx

2. To select a component, click a target component in the Components list on the right side of the Processing Setup window.

   The Levels page is not available for ISTD components.

3. To set up the calibration levels for all the target components, do one of the following:

   - Use the Standard Dilution Dialog Box (see “Using the Standard Dilutions Dialog Box to Set Up the Calibration Levels” on page 46).

   –or–

   - Select a target component, and then type the settings for the selected component in the Calibration Levels table:
     - To enter the calibration levels for a component, type alphanumeric text to identify the levels in the Cal Level boxes.
     - To enter the amount of the target component for each level, type numeric values in the Amount boxes.

   > **Note** Enter the amount of the internal standard spiked into each sample and each calibration standard in the Internal Standard area on the Calibration page. Every sample and standard must have the same spiked amount of the internal standard associated with the target component.

4. For each target component, enter information about the quality control samples in the QC Levels table:

   - To enter the quality control levels, type alphanumeric text to identify the levels in the QC Level boxes.
   - To enter the amount of the target component added at each level, type numeric values in the Amount boxes.
   - To enter the acceptable difference (as a percentage) between the known amount and the calculated amount for each QC level, type numeric values in the % Test boxes.

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

Using the Standard Dilutions Dialog Box to Set Up the Calibration Levels

To simplify data entry, use the Standard Dilution dialog box to enter the calibration standard and QC levels in the processing method.

For more information about the Standard Dilution dialog box, see “Standard Dilution Dialog Box” on page 292.

❖ To enter the calibration levels for the target components

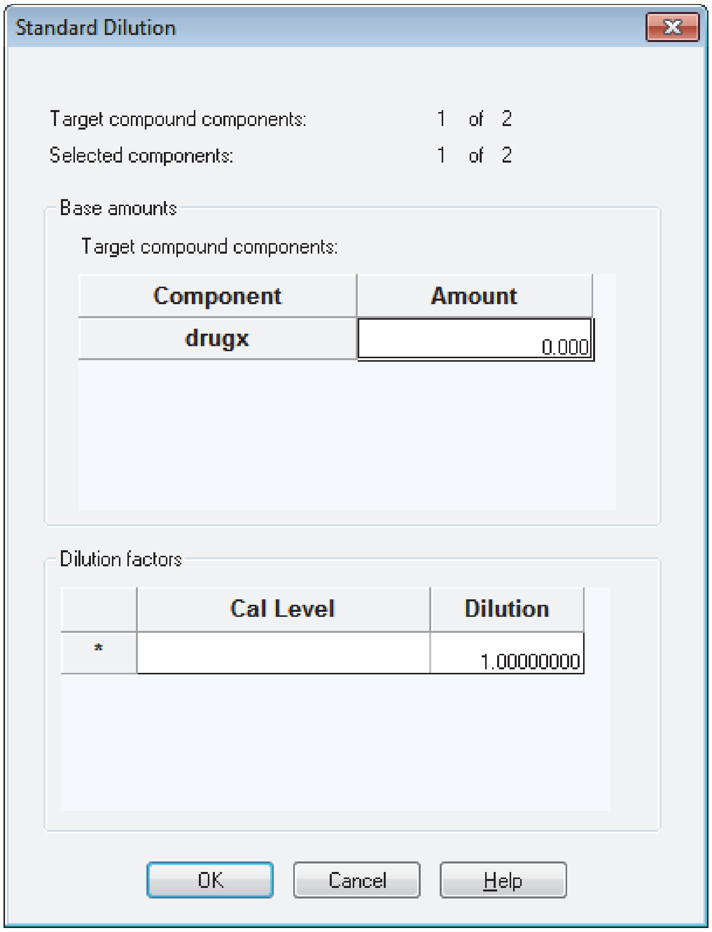
1. From the Quan view of the Processing Setup window, click the **Levels** tab.

   The Levels page opens.

2. Choose **Options > Standard Dilution** from the menu bar.

   The Standard Dilution dialog box opens (Figure 28).

   Figure 28. Standard Dilution dialog box



Target compound components: 1 of 2
Selected components: 1 of 2

Target compound components:

Component	Amount
drugx	0.000

	Cal Level	Dilution
*		1.00000000

3. For each target component, type the undiluted amount in the Amount box in the Base Amounts table. Then, press ENTER.

4. For each calibration level, enter the dilution information in the Dilution Factors table:

   - Type alphanumeric text for the calibration level in the Cal Level column.
   - Type the dilution factor (from 0.00000001 to 1) for the calibration level in the Dilution column.

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

   The data system uses the settings to calculate the calibration level amounts for all the target components defined in the processing method.

Setting Up the System Suitability Parameters

Use the System Suitability page of the Processing Setup – Quan view to set up the system suitability parameters for your chromatographic analysis.

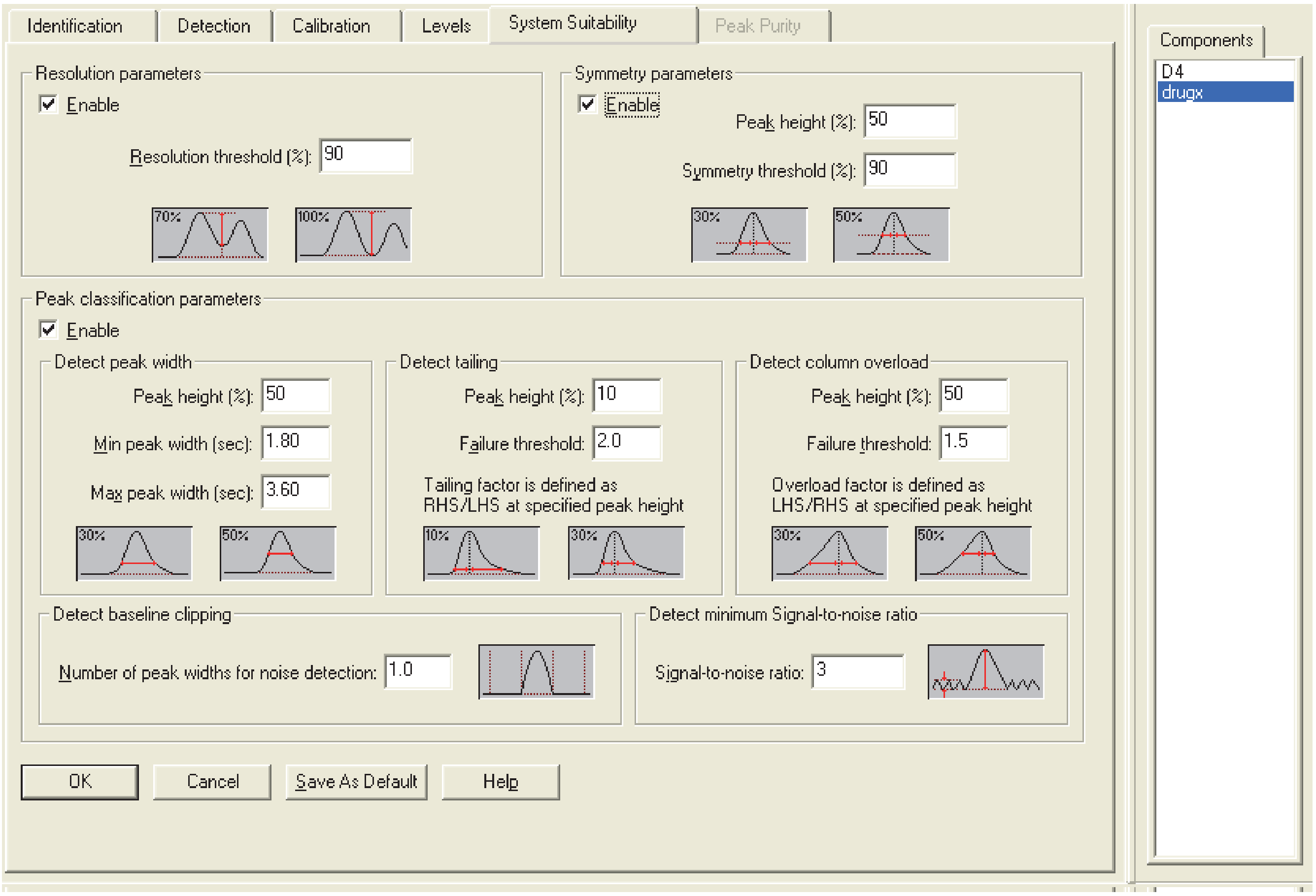
For more information about the system suitability parameters, see “System Suitability Page for Quan View” on page 385.

❖ To set up the system suitability parameters

1. From the Quan view of the Processing Setup window, click the **System Suitability** tab.

   The System Suitability page opens (Figure 29).

Figure 29. System Suitability page of the Processing Setup window – Quan view



Resolution parameters
☑ Enable
Resolution threshold (%): 90

Symmetry parameters
☑ Enable
Peak height (%): 50
Symmetry threshold (%): 90

Peak classification parameters
☑ Enable

Detect peak width
Peak height (%): 50
Min peak width (sec): 1.80
Max peak width (sec): 3.60

Detect tailing
Peak height (%): 10
Failure threshold: 2.0
Tailing factor is defined as RHS/LHS at specified peak height

Detect column overload
Peak height (%): 50
Failure threshold: 1.5
Overload factor is defined as LHS/RHS at specified peak height

Detect baseline clipping
Number of peak widths for noise detection: 1.0

Detect minimum Signal-to-noise ratio
Signal-to-noise ratio: 3

D4
drugx

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 Up the Qualitative Processing Parameters

The Qual view of the Processing Setup window has five pages: Identification, Spectrum Enhancement, Library Search Options, Library Search Constraints, and Peak Purity (for PDA data only). This section describes the Identification and Spectrum Enhancement pages. Refer to the *Creating and Searching Libraries User Guide* for information about using libraries to search for spectra.

❖ To open the Qual view of the Processing Setup window

From the Processing Setup window, do one of the following:

- On the View bar, click the **Qual** icon, .

–or–

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

To set up the qualitative parameters for a processing method, follow these procedures:

- "Setting Up the Qual View Identification Parameters," on this page
- "Setting Up the Qual View Spectrum Enhancement Parameters" on page 55

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

Setting Up the Qual View Identification Parameters

Use the Identification page of the Processing Setup – Qual view to specify the type of chromatogram that the processing method uses during qualitative processing. You can also adjust peak detection and identification criteria.

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

For parameter descriptions, see these topics:

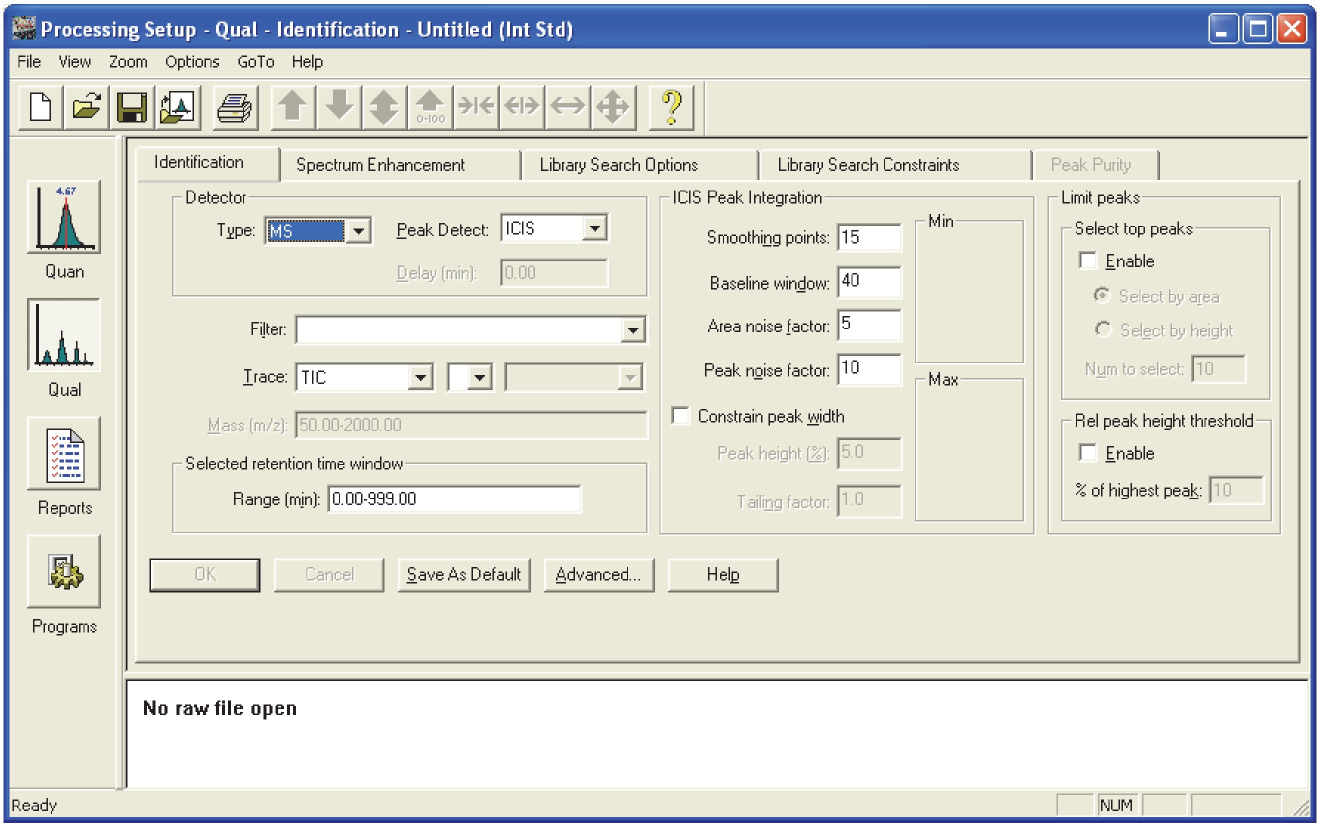
- "Avalon Identification Page for Qual View" on page 299
- "ICIS Identification Page for Qual View" on page 306
- "Genesis Identification Page for Qual View" on page 314

❖ To set up the Qual view identification parameters

1. From the Qual view of the Processing Setup window, click the **Identification** tab.

   The Identification page for the Qual view opens (Figure 30).

Figure 30. Identification page for the Qual view



Detector
Type: MS
Peak Detect: ICIS
Delay (min): 0.00
Filter:
Trace: TIC
Mass (m/z): 50.00-2000.00
Selected retention time window
Range (min): 0.00-999.00

ICIS Peak Integration
Smoothing points: 15
Baseline window: 40
Area noise factor: 5
Peak noise factor: 10
☐ Constrain peak width
Peak height (%): 5.0
Tailing factor: 1.0
Min
Max

Limit peaks
Select top peaks
☐ Enable
● Select by area
○ Select by height
Num to select: 10
Rel peak height threshold
☐ Enable
% of highest peak: 10

No raw file open

2. To open a raw file, do the following:
   a. Choose **File > Open Raw File**.

      The Open Raw File dialog box opens.

   b. Select a raw file to analyze.
   c. Click **Open**.
3. In the Detector area, do the following:
   a. Select a detector from the Type list.

      Valid detector types are MS, Analog, A/D Card, PDA, or UV.

   b. If you select a non-MS detector 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.

c. In the Peak Detect list, select the peak detection algorithm that you want the data system to use to identify and integrate peaks.

   The selections are ICIS, Genesis, and Avalon.

   > **Note** Select the appropriate peak detection algorithm on the basis of these criteria:
   >
   > - The Genesis peak detection algorithm supports backward compatibility with Xcalibur 1.0 studies.
   > - The ICIS peak detection algorithm is designed for MS data and has superior peak detection efficiency at low MS signal levels.
   > - The Avalon peak detection algorithm is designed for UV data. Avalon also supports negative peaks.

4. 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.
5. 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.
6. 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.
7. To specify a retention time window of the chromatogram for qualitative processing, do one of the following:
   - Type the time range in the Range box (for example, 0.30–1.55).

     –or–

   - Using a representative raw file, interactively select the retention time window in the chromatogram cell as follows:

     a. If you have not already done so, open a representative raw file.

     b. Pin the spectrum cell.

     c. In the chromatogram cell, drag the cursor horizontally across the peak in the chromatogram cell.

        The data system updates the Range (min) box with a time span centered on the apex of the dragged peak.

8. Select from among these peak integration options: Genesis, ICIS, Avalon.

   Table 2 describes the peak integration options.

Table 2. Peak integration options (Sheet 1 of 2)

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 an odd integer from 3 (minimum smoothing) to 15 (maximum smoothing).
	• In the S/N Threshold box, type the signal-to-noise threshold value.
	• 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. For information about the parameters in this dialog box, see "Genesis Advanced Chromatogram Options Dialog Box" on page 276
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**. The ICIS Advanced Parameters dialog box opens. For information about the parameters in this dialog box, see "ICIS Advanced Parameters Dialog Box" on page 284.

Table 2. Peak integration options (Sheet 2 of 2)

Peak detect	Peak integration options
Avalon	• In the Smoothing Points box, type the number for the amount of smoothing that the data system applies before integration. The valid values are odd integers from 3 (minimum smoothing) to 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, do the following: a. Click **Advanced**. The Avalon Event List dialog box opens. For information about this dialog box, see "Avalon Event List Dialog Box" on page 265. b. 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. c. After editing the peak detection settings, click **Exit** to close the dialog box.

9. 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 on the basis of the peak areas, select the **By Area** option.

      - To restrict processing to the most significant peaks on the basis of the peak heights, 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.

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

Setting Up the Qual View Spectrum Enhancement Parameters

Use the Spectrum Enhancement page of the Processing Setup – Qual View to select an option for enhancing spectra.

To set up the spectrum enhancement parameters, follow the appropriate procedure:

- "Using the Combine Option for Spectrum Enhancement" on page 55
- "Using the Refine Option for Spectrum Enhancement" on page 57
- "Using the Threshold Option for Spectrum Enhancement" on page 58

Using the Combine Option for Spectrum Enhancement

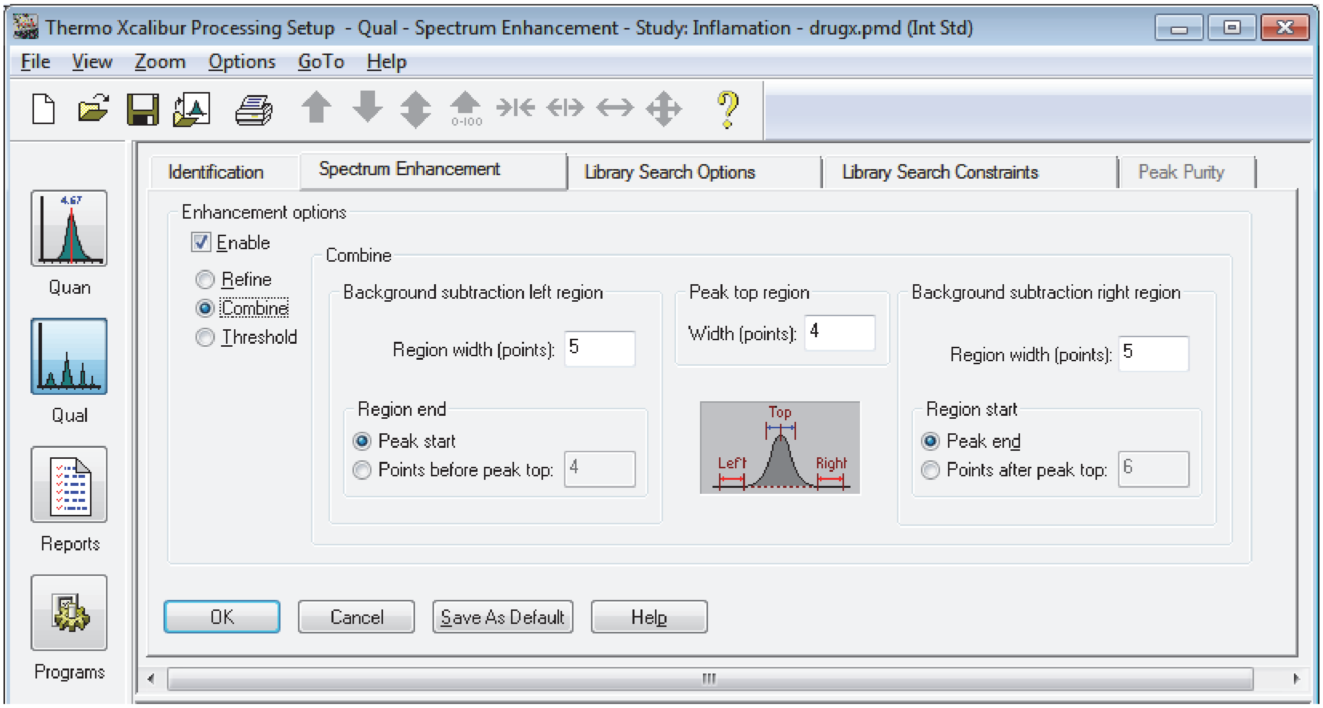
For information about the parameters in the Combine area on the Spectrum Enhancement page of the Processing Setup – Qual view, see "Spectrum Enhancement Page for Qual View" on page 322.

❖ To use the Combine option for spectrum enhancement

1. From the Qual view of the Processing Setup window, click the **Spectrum Enhancement** tab.

   The Spectrum Enhancement page opens. Figure 31 shows the parameters for the Combine option.

Figure 31. Spectrum Enhancement page of the Qual view with the Combine option selected



Thermo Xcalibur Processing Setup - Qual - Spectrum Enhancement - Study: Inflamation - drugx.pmd (Int Std)

Enhancement options
☑ Enable
○ Refine
● Combine
○ Threshold

Combine
Background subtraction left region
Region width (points): 5
Region end
● Peak start
○ Points before peak top: 4

Peak top region
Width (points): 4

Background subtraction right region
Region width (points): 5
Region start
● Peak end
○ Points after peak top: 6

2. To display the Spectrum Enhancement options, select the **Enable** check box.
3. To 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 as follows:
    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 as follows:
        - 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. Then, 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 as follows:
    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. Then, type the number of scans in the associated Points After Peak Top box.
7. To save your settings, click **OK**.

Using the Refine Option for Spectrum Enhancement

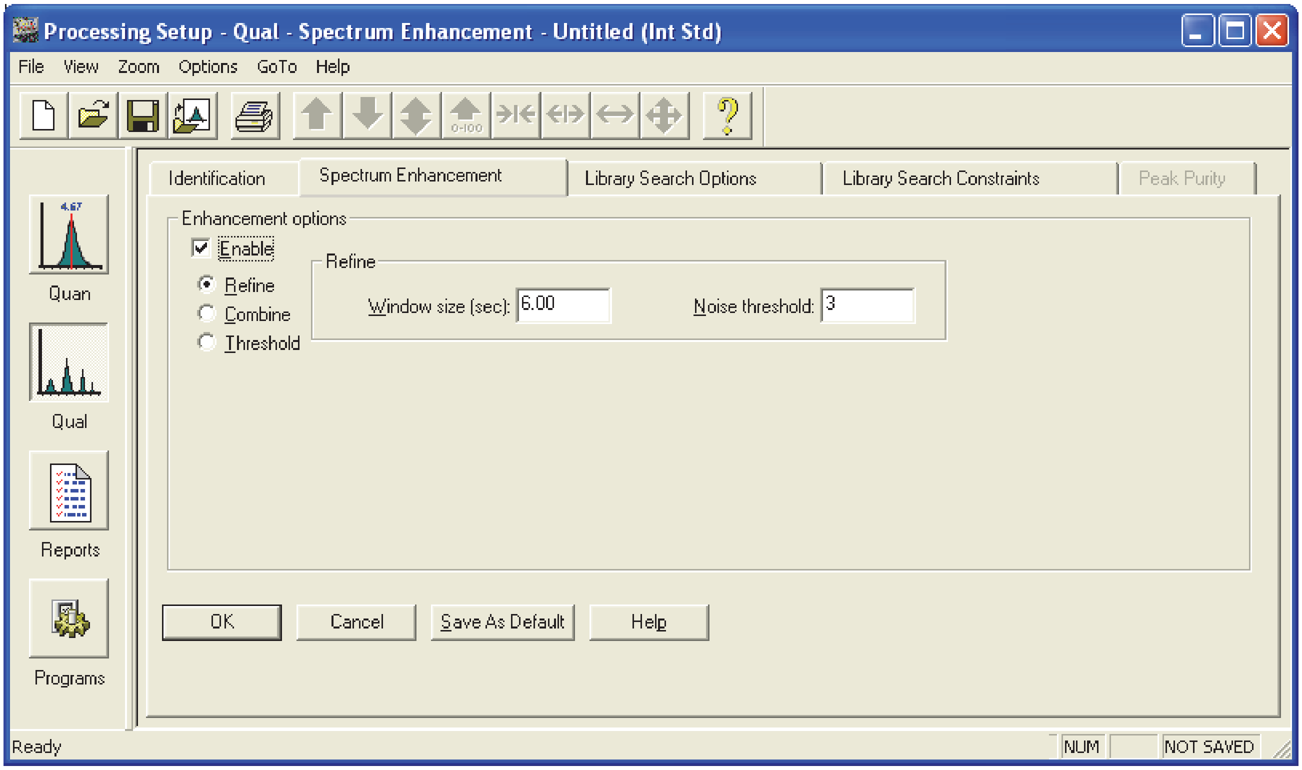
For information about the parameters in the Refine area on the Spectrum Enhancement page of the Processing Setup – Qual view, see “Spectrum Enhancement Page for Qual View” on page 322.

❖ To set up the Refine option parameters

1. From the Qual view of the Processing Setup window, click the **Spectrum Enhancement** tab.

   The Spectrum Enhancement Page opens. Figure 32 shows the parameters for the Refine option.

Figure 32. Spectrum Enhancement page of the Qual view



Enhancement options
☑ Enable
● Refine
○ Combine
○ Threshold

Refine
Window size (sec): 6.00
Noise threshold: 3

2. To make the spectrum enhancement options available, 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**.

Using the Threshold Option for Spectrum Enhancement

For information about the parameters in the Refine area on the Spectrum Enhancement page of the Qual view, see “Spectrum Enhancement Page for Qual View” on page 322.

❖ To set up the threshold option parameters for spectrum enhancement

1. From the Qual view of the Processing Setup window, click the **Spectrum Enhancement** tab.

   The Spectrum Enhancement page 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**.

Adding Report Templates to Processing Methods

Use the Reports view of the Processing Setup window to add template sample and summary reports to the processing method.

The following folder contains the report templates that are provided with the Xcalibur data system:

> *drive*:\Xcalibur\Templates folder

Use one or more of the sample templates to report the results for individual data files. Use one or more of the summary templates to report the results from multiple data files, such as the calibration results or a sequence summary.

For more information about the report templates provided with the Xcalibur data system, refer to the Sample XReport Templates appendix in the *XReport User Guide*s.

Follow these procedures to specify the appropriate reports for the processing method:

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

Setting Up the Report Parameters

For information about the parameters on the Reports view in the Processing Setup window, see “Reports View” on page 396.

❖ To set up the report parameters

1. From the Processing Setup window, doing one of the following:

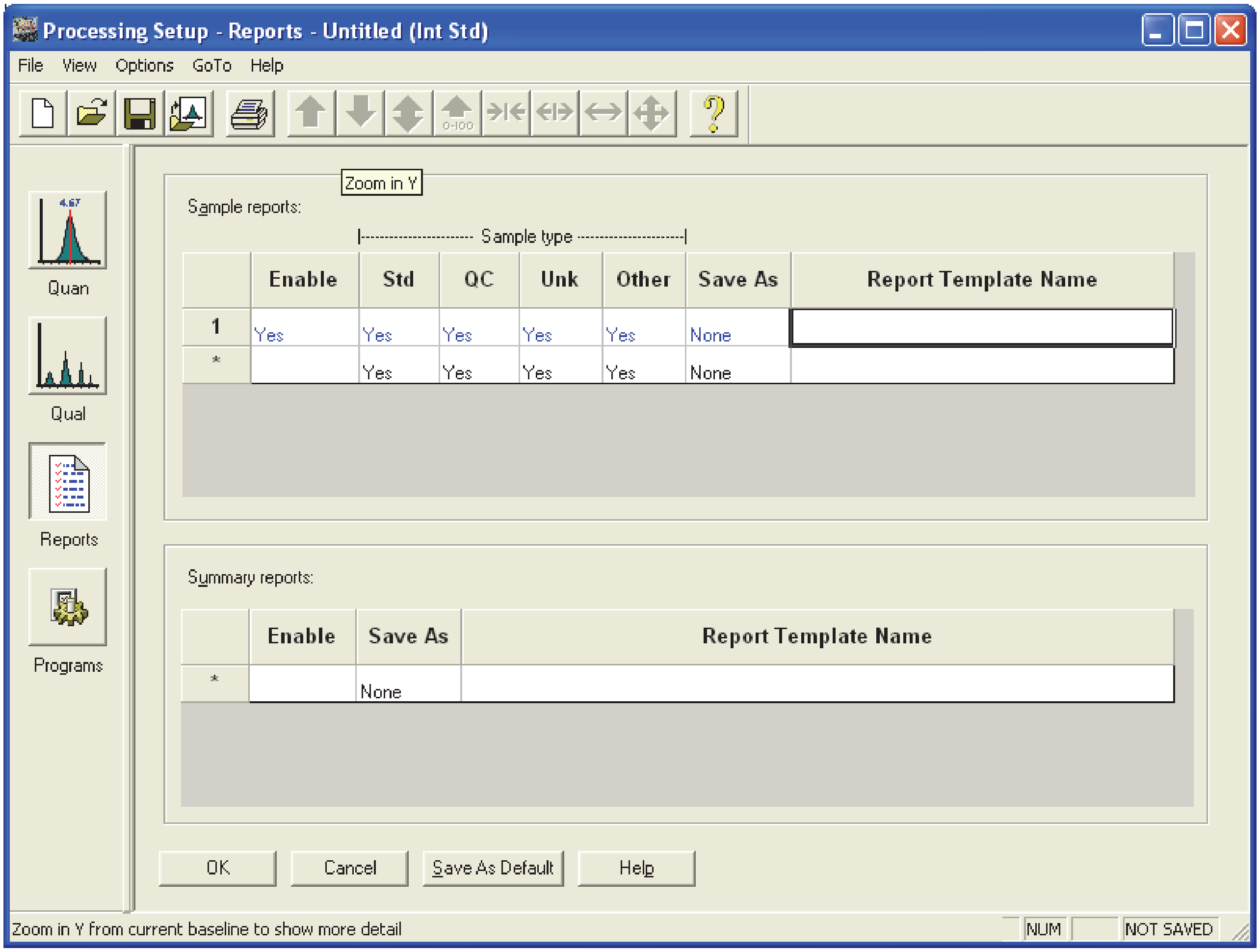
   - On the View bar, click the **Reports** icon, 📋.

   –or–

   - On the menu bar, choose **View** > **Reports**.

   The Reports View opens (Figure 33).

Figure 33. Reports view of the Processing Setup window



Processing Setup - Reports - Untitled (Int Std)

Sample reports:

		Sample type					
	Enable	Std	QC	Unk	Other	Save As	Report Template Name
1	Yes	Yes	Yes	Yes	Yes	None	
*		Yes	Yes	Yes	Yes	None	

Summary reports:

	Enable	Save As	Report Template Name
*		None	

Zoom in Y from current baseline to show more detail

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.

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

4. To select a sample or summary report, do the following:

   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.

5. To change the Sample Report options for different sample types, do the following:
    a. Click the appropriate cell under Std, QC, Unk, or Other.

       A check box appears.

    b. Select or clear the check box as required. Then, 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.

6. To change the export options for a sample or summary report, do the following:
    a. Click the appropriate cell in the Save As column.
    b. Select from the available export formats: **None**, **Text**, **Doc**, **HTML**, or **PDF**. Then, click outside the cell.

       The cell displays the selected export format.

7. 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.
8. 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.
9. 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

Use the Reports view to select a sample report to display the results for individual sample runs.

For information about the Reports view, see "Reports View" on page 396.

❖ To select a sample report template for the processing method

1. To open the Reports view, do one of the following:
    - Click the **Reports** icon, 📋, on the View bar.

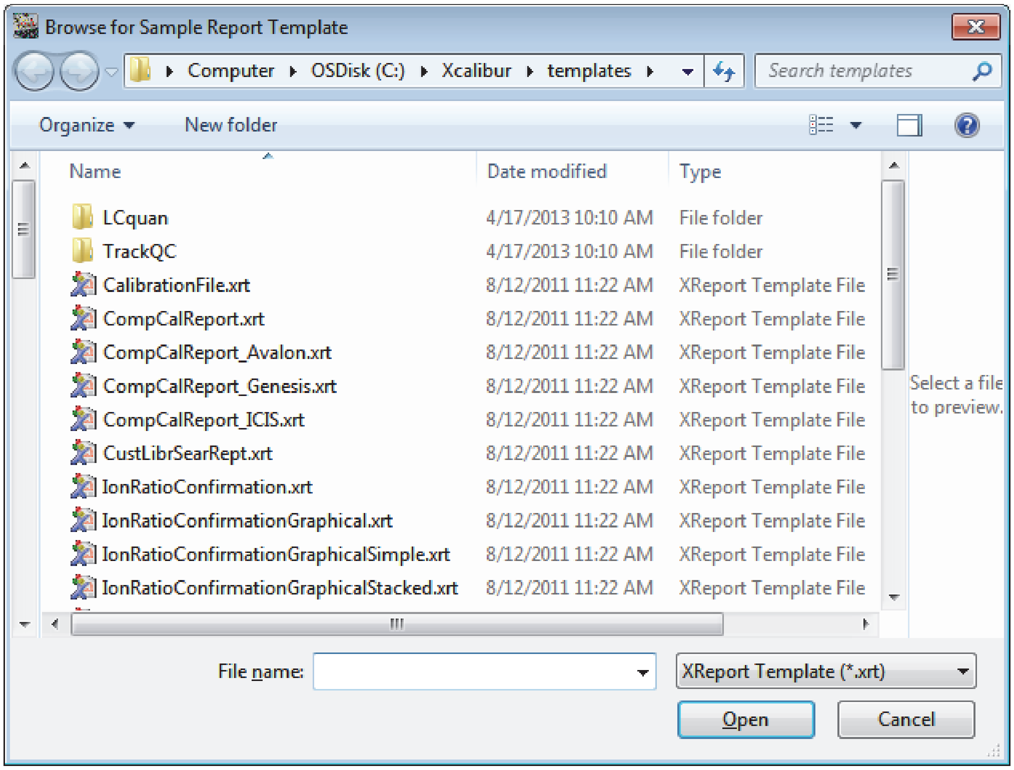
   –or–

    - Choose **View > Reports** from the menu bar.

2. In the Sample Reports area, double-click in the Report Template Name column.

   The Browse for Sample Report Template dialog box opens (Figure 34).

   Figure 34. Browse for Sample Report Template dialog box



Name	Date modified	Type
LCquan	4/17/2013 10:10 AM	File folder
TrackQC	4/17/2013 10:10 AM	File folder
CalibrationFile.xrt	8/12/2011 11:22 AM	XReport Template File
CompCalReport.xrt	8/12/2011 11:22 AM	XReport Template File
CompCalReport_Avalon.xrt	8/12/2011 11:22 AM	XReport Template File
CompCalReport_Genesis.xrt	8/12/2011 11:22 AM	XReport Template File
CompCalReport_ICIS.xrt	8/12/2011 11:22 AM	XReport Template File
CustLibrSearRept.xrt	8/12/2011 11:22 AM	XReport Template File
IonRatioConfirmation.xrt	8/12/2011 11:22 AM	XReport Template File
IonRatioConfirmationGraphical.xrt	8/12/2011 11:22 AM	XReport Template File
IonRatioConfirmationGraphicalSimple.xrt	8/12/2011 11:22 AM	XReport Template File
IonRatioConfirmationGraphicalStacked.xrt	8/12/2011 11:22 AM	XReport Template File

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

Use the Reports view to select a summary report to display the results of multiple data files, such as the calibration results or a sequence summary.

For information about the Reports view, see "Reports View" on page 396.

❖ To select a summary report template

1. To open the Reports view, do one of the following:

   - Click the **Reports** icon, , on the View bar.

   –or–

   - Choose **View > Reports** from the menu bar.

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**.

Printing a Processing Method Report

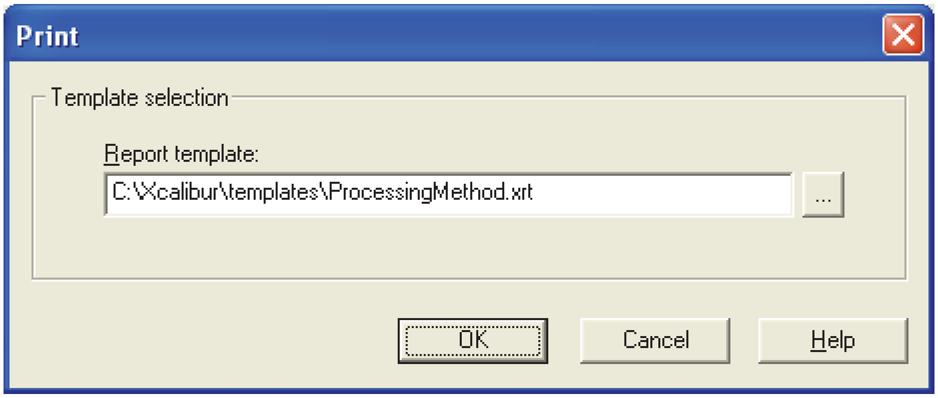
Follow this procedure to print a report of the processing method settings.

❖ To print a report for the current processing method

1. In the Processing Setup window, choose **File > Print** from the menu bar or click 🖨 in the toolbar.

   The Print Dialog Box opens (Figure 35).

   Figure 35. Print dialog box



C:\Xcalibur\templates\ProcessingMethod.xrt

2. To specify a template for the processing method report, do one of the following:

   - Type a file name and directory location in the Report Template box.

   –or–

   - Click the **Browse** icon, ..., and select a report template. If you have not created a template by using the Xreports program, browse to the following template: *drive*:\Xcalibur\templates\ProcessingMethod.xrt.

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

   The hourglass cursor indicates that the processing method is being printed.

Adding Programs or Macros to Processing Methods

Use the Programs page of the Processing Setup window to add programs and macros to processing methods.

The Xcalibur data system includes these predefined programs: Xconverter.exe, FileConverter.exe, and Excelexp.exe.

For information about Xconverter and Excelexp.exe, refer to the *Xcalibur Getting Started Guide*.

To add programs and macros to processing methods, see these topics:

- Selecting a Program or Macro
- Enabling and Setting Up a Program or Macro

Selecting a Program or Macro

❖ To select a program or macro

1. To open the Programs View from the Processing Setup window, do one of the following:
   - Click the **Programs** icon, ⚙, in the View bar.

   –or–

   - Choose **View > Programs**.
2. To select a program or macro for the current table row, do the following:
   a. Double-click in the Program or Macro Name column.

      The Browse for Program dialog box opens.

   b. Browse to the macro or program that you want to add.

      The program or macro name appears in the File Name box.

   c. Click **Open** to select the program and to close the dialog box.

Enabling and Setting Up a Program or Macro

You can add a program or macro to a stored processing method or a new processing method.

For more information, see "Programs View" on page 391.

❖ To enable a program or macro and to specify its processing parameters

1. If the Processing Setup window is not open, open it as follows from the Home Page window:
    - Click the **Processing Setup** icon, , on the Roadmap view.

    –or–

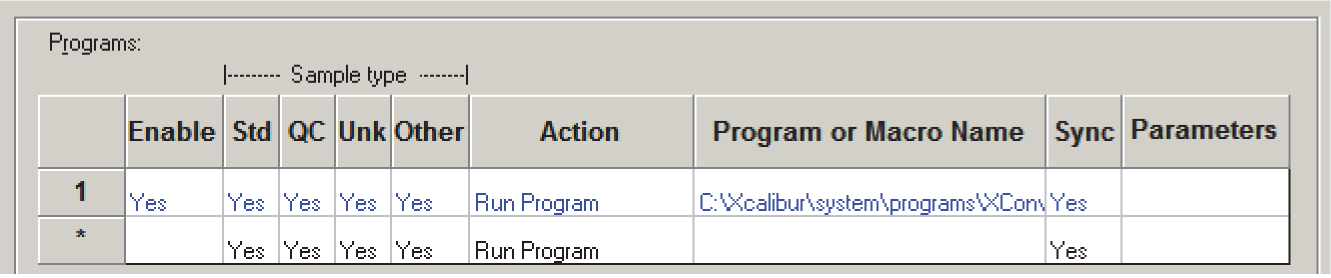
    - Choose **GoTo** > **Processing Setup** from the menu bar.
2. If the processing method that you want to modify is not open, open it as follows:
    a. Choose **File** > **Open**.
    b. Browse to your processing method and select it.
    c. Click **Open**.
3. Do one of the following:
    - Click the **Programs** icon, , in the View bar.

    –or–

    - Choose **View** > **Programs** from the menu bar.

    The Programs View opens (Figure 36).

Figure 36. Programs table



Programs:

|-------- Sample type -------|

	Enable	Std	QC	Unk	Other	Action	Program or Macro Name	Sync	Parameters
1	Yes	Yes	Yes	Yes	Yes	Run Program	C:\Xcalibur\system\programs\XCon	Yes	
*		Yes	Yes	Yes	Yes	Run Program		Yes	

4. To select a program or macro for the current table row, do the following:
    a. Double-click in the **Program** or **Macro Name** column.

    The Browse for Program dialog box opens.

    b. Browse to the macro or program that you want to add.

    The program or macro name appears in the File Name box.

    c. Click **Open** to select the program and to close the dialog box.

5. To enable a program or macro, do the following:
   a. Click the **Enable** column.

      A check box appears.

   b. Select the check box to enable the program or macro. Then, 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.

6. To select the sample types affected by the program or macro, select the check boxes in the appropriate Sample Type columns.

   By default, all of the sample types are selected and the table cell displays Yes. If you clear the check box for a sample type and then click outside the table cell, the cell becomes blank.

7. To select the action for a program, in the Action column, select **Run Program** for a program or **Run Excel Macro** for a macro. Then, click outside the cell.

   The action for the program appears in the cell.

8. To change the Sync setting for a program, do the following:
   a. Click the **Sync** column.

      A check box appears.

   b. Select or clear the check box as required. Then, click outside the cell.

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

9. To add command parameters for a program, select the corresponding cell in the Parameters column. Then, type the required commands.

10. To insert a row in the Programs table, double-click the row number where you want to insert the row, and then right-click any cell in the row and choose **Insert Row** from the shortcut menu.

11. To delete a row or rows in the Programs table, select the row or rows that you want to delete, and then choose **Delete Rows** from the shortcut menu.

12. To save the new settings, click **OK**.

13. To save the Programs table as the default table for new processing methods, click **Save As Default**.

4

Creating and Modifying Sequences

In the Sequence Setup view, you can create a new sequence semi-automatically or manually:

- To create a sequence file semi-automatically, use the New Sequence Template dialog box. You must also use the New Sequence Template dialog box to create a sequence with a bracket type other than the open bracket type.

  Only non-bracketed sequences can contain more than one processing method. To select more than one processing method for a sequence, create the sequence with the New Sequence Template dialog box and select the None option for the bracket type.

- To create a sequence manually, enter all the settings directly in the sequence table, import a CSV file to enter some of the required settings in the sequence table and then enter the remaining settings. or open and then modify an existing sequence.

Contents

- Opening the Sequence Setup View
- Creating a Sequence Semi-Automatically
- Creating a Sequence Manually
- Modifying Sequences
- Printing a Vial or Sequence List

❖ To create a new sequence

1. Open the Sequence Setup view as described in the next topic, "Opening the Sequence Setup View."
2. Enter most or all of the sequence information by following one of these procedures:
   - "Creating a Sequence Semi-Automatically" on page 69

   –or–

   - "Creating a Sequence Manually" on page 82

3. Modify the sequence as described in the next section “Modifying Sequences” on page 85.
4. Save the sequence.
5. Print a list of the vial positions or print a list of all the sequence columns as described in “Printing a Vial or Sequence List” on page 95.

Opening the Sequence Setup View

Use the Sequence Setup view to create, run, and batch reprocess single samples or sample sets. You can access the Sequence Setup view from the Xcalibur Home Page.

❖ To open the Sequence Setup view

From the Home Page window, do one of the following:

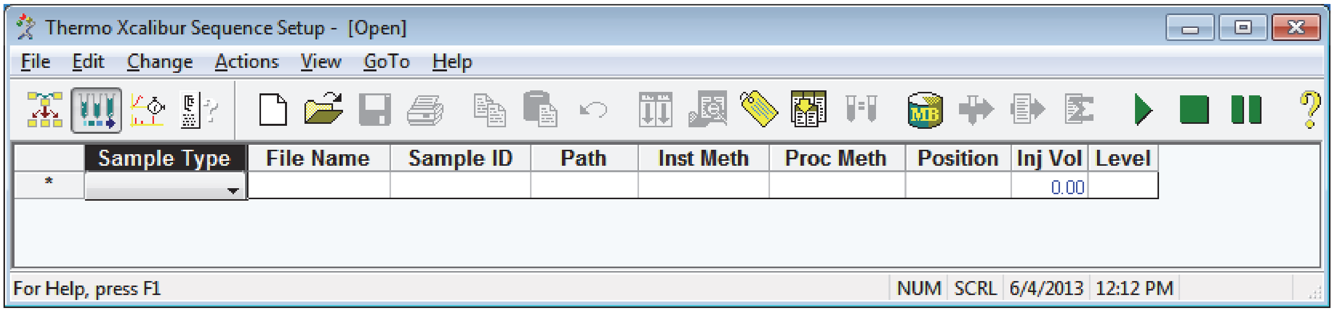
- Click the **Sequence View** icon, , in the Home Page window toolbar.

–or–

- Click the **Sequence Setup** icon, , in the Roadmap view.

Figure 37 shows the Sequence Setup view with a blank sequence table.

Figure 37. Sequence Setup view with a blank sequence table



	Sample Type	File Name	Sample ID	Path	Inst Meth	Proc Meth	Position	Inj Vol	Level
*								0.00	

To start a single run, you must create a sequence with at least one row and specify the file name and path where the raw data files are to be stored, the instrument method to be used to acquire the raw data, the position of the sample (vial or microwell in a microplate) in the autosampler, and the injection volume (unless you want the data system to use the injection volume value in the instrument method).

For most of the autosamplers that you can control from the Xcalibur data system, you can use the Change > Tray Type command to either view or view and change the tray type.

For information about creating and running sequences, see these topics:

- “Creating a Sequence Semi-Automatically,” on the next page
- “Creating a Sequence Manually” on page 82
- “Running a Single Sample or Multiple Samples” on page 101

Creating a Sequence Semi-Automatically

Use the New Sequence Template dialog box (see Figure 38 on page 70) to create a sequence semi-automatically, to set up sequence brackets, or both. This dialog box is especially useful when you are running large numbers of samples with bracketed calibration sets and QC samples.

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

- "Step 1: Opening the New Sequence Template Dialog Box," on this page
- "Step 2: Selecting the Bracket Type" on page 71
- "Step 3: Entering the Base File Name, Path, and Methods" on page 75
- "Step 4: Entering the Sample Settings" on page 77
- "Step 5: Saving the Changes to the New Sequence" on page 81

Step 1: Opening the New Sequence Template Dialog Box

For information about the parameters in the New Sequence Template dialog box, see "New Sequence Template Dialog Box" on page 230.

❖ To open the New Sequence Template dialog box

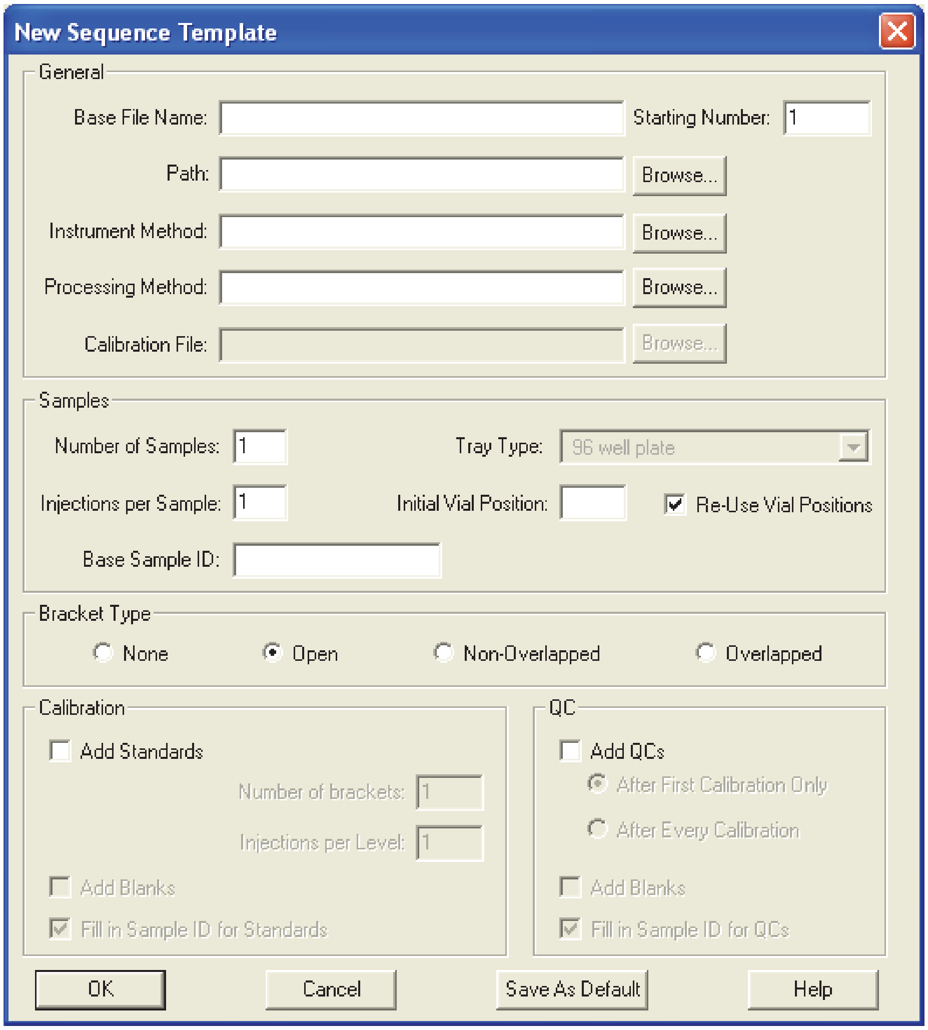
1. Open the Sequence Setup view (see "Opening the Sequence Setup View" on page 68).
2. Do one of the following:
    - In the Sequence Setup view, choose **File > New**.

   –or–

    - In the toolbar, click the **New Sequence** icon, 🗋.

   The New Sequence Template dialog box opens (Figure 38).

Figure 38. New Sequence Template dialog box



New Sequence Template

General

Base File Name:
Starting Number: 1
Path:
Instrument Method:
Processing Method:
Calibration File:

Samples

Number of Samples: 1
Tray Type: 96 well plate
Injections per Sample: 1
Initial Vial Position:
☑ Re-Use Vial Positions
Base Sample ID:

Bracket Type

○ None ● Open ○ Non-Overlapped ○ Overlapped

Calibration

☐ Add Standards
Number of brackets: 1
Injections per Level: 1
☐ Add Blanks
☑ Fill in Sample ID for Standards

QC

☐ Add QCs
● After First Calibration Only
○ After Every Calibration
☐ Add Blanks
☑ Fill in Sample ID for QCs

Step 2: Selecting the Bracket Type

For any sequence bracketing other than the Open bracket type, you must use the New Sequence Template dialog box to set up the sequence table. See the "New Sequence Template Dialog Box" on page 230 for more information about bracket types.

For information about opening the New Sequence Template dialog box, see "Step 1: Opening the New Sequence Template Dialog Box" on page 69.

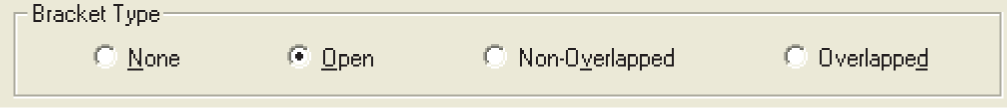
Follow the appropriate procedure for your analysis:

- To select the bracket type to be used for the current sequence
- To create an unbracketed sequence that uses a calibration file
- To create a sequence with more than one processing method
- To create a sequence with the Open bracket type
- To create a sequence with non-overlapping calibration standards
- To create a sequence with overlapping calibration standards

❖ To select 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. The default selection is the Open option (Figure 39).

Figure 39. Open option selected by default in the Bracket Type area



Bracket Type
○ None ● Open ○ Non-Overlapped ○ Overlapped

❖ To create an unbracketed sequence that uses a calibration file

1. In the Bracket Type area of the New Sequence Template dialog box, select the **None** option (Figure 40).

   Figure 40. None option selected to create an unbracketed sequence

   Bracket Type
   ● None ○ Open ○ Non-Overlapped ○ Overlapped

   The Calibration File box becomes available. When you add a calibration file to an unbracketed sequence, the data system stores the response data from the calibration standards in the calibration file.

2. In the Calibration File box, type the path and file name of a calibration file (.xcal file extension) or click **Browse** to select the directory and file name.

3. Enter the remaining parameter settings as described in these topics:
   - "Step 3: Entering the Base File Name, Path, and Methods" on page 75
   - "Step 4: Entering the Sample Settings" on page 77
4. Click **OK**.

   The sequence table appears in the Sequence Setup view. After you create an unbracketed sequence table, you can change the settings in all of the columns, and you can specify more than one processing method and more than one calibration file.

   You cannot change an unbracketed sequence to a bracketed sequence by editing the sequence table. For an unbracketed sequence, the Sample Type list contains only these selections: Unknown, QC, Std Clear, Std Update.

   If you do not want the data system to clear the response data from the calibration file before it processes the calibration set, change the sample type for the first calibration standard from Std Clear to Std Update.

❖ To create a sequence with more than one processing method

Note The following instructions apply to a qualitative analysis only. For instructions on setting up an unbracketed sequence for a quantitative analysis, see "To create an unbracketed sequence that uses a calibration file" on page 71.

1. In the Bracket Type area of the New Sequence Template dialog box, select the **None** option.

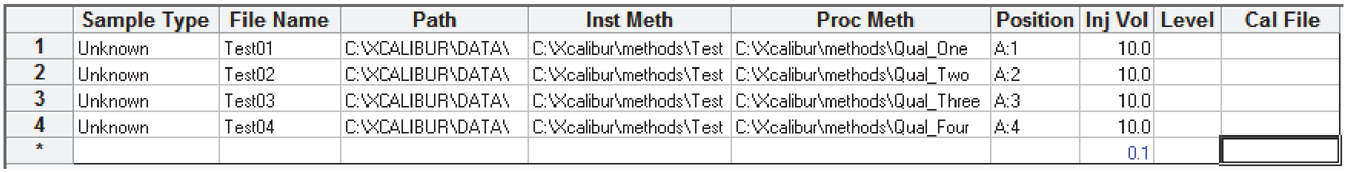
   The Calibration File box becomes available.

2. Enter the parameter settings in the General area. Select a qualitative processing method and leave the Calibration File box empty (see "Step 3: Entering the Base File Name, Path, and Methods" on page 75).
3. In the Sample area, enter the parameter settings ("Step 4: Entering the Sample Settings" on page 77).
4. In the Calibration area, leave the **Add Standards** check box clear.
5. In the QC area, leave the **Add QCs** check box clear.
6. Click **OK**.

   The data system automatically sets up the sequence table in the Sequence Setup view.

7. In the Processing Method column, select the processing method of interest for each sequence row (Figure 41).

Figure 41. An unbracketed sequence with multiple processing methods



	Sample Type	File Name	Path	Inst Meth	Proc Meth	Position	Inj Vol	Level	Cal File
1	Unknown	Test01	C:\XCALIBUR\DATA\	C:\Xcalibur\methods\Test	C:\Xcalibur\methods\Qual_One	A:1	10.0		
2	Unknown	Test02	C:\XCALIBUR\DATA\	C:\Xcalibur\methods\Test	C:\Xcalibur\methods\Qual_Two	A:2	10.0		
3	Unknown	Test03	C:\XCALIBUR\DATA\	C:\Xcalibur\methods\Test	C:\Xcalibur\methods\Qual_Three	A:3	10.0		
4	Unknown	Test04	C:\XCALIBUR\DATA\	C:\Xcalibur\methods\Test	C:\Xcalibur\methods\Qual_Four	A:4	10.0		
*							0.1		

❖ To create a sequence with the Open bracket type

1. Open the New Sequence Template dialog box (see “Step 1: Opening the New Sequence Template Dialog Box” on page 69).

   By default, the Open option is selected in the Bracket Type area (see Figure 39 on page 71).

   When you create a sequence with the Open bracket type, the data system injects the samples in the order listed in the sequence table. After acquiring all of the samples, the data system processes all of the calibration standards (Standard Bracket sample type) and produces one calibration curve per named component (analyte). Then, the data system reprocesses the entire sequence to determine the calculated amount of each analyte in the Unknown, Blank, QC, and calibration standard sample types.

   You can create a sequence with the Open bracket type semi-automatically by using the New Sequence Template dialog box or manually by making the appropriate selections and entries in the Sequence Setup view.

2. Make the appropriate entries and selections in the dialog box as described in these procedures.

   - “Step 3: Entering the Base File Name, Path, and Methods” on page 75
   - “Step 4: Entering the Sample Settings” on page 77

3. Click **OK**.

   The sequence table appears in the Sequence Setup view.

   You can modify the sequence table in the Sequence Setup view. For an open-bracketed sequence, these are the available sample types: Unknown, Blank, QC, and Std Bracket.

❖ To create a sequence with non-overlapping calibration standards

> **Note** When you create a sequence with the Non-Overlapped bracket type, the data system injects the samples in the order listed in the sequence table. After acquiring all of the samples, the data system processes the Start Bracket and End Bracket calibration standards in the first bracket and produces one calibration curve per named component (analyte). Then, the data system reprocesses the bracket to determine the measured amount of each analyte in the Unknown, Blank, QC, and calibration standard sample types. After processing the first bracket, the data system processes the second bracket, and so on.

1. In the Bracket Type area of the New Sequence Template dialog box, select the **Non-Overlapped** option.

2. Make the appropriate entries and selections in the dialog box as described in these procedures.

   - "Step 3: Entering the Base File Name, Path, and Methods," on the next page

   - "Step 4: Entering the Sample Settings" on page 77

3. Click **OK**.

   The data system automatically sets up the sequence table in the Sequence Setup view.

   You can modify the sequence in the Sequence Setup view. These are the available sample types: Unknown, QC, Blank, Start Bracket, End Bracket.

❖ To create a sequence with overlapping calibration standards

1. In the Bracket Type area of the New Sequence Template dialog box, select the **Overlapped** option.

   When you create a sequence with the Overlapped bracket type, the data system injects the samples in the order listed in the sequence table. After acquiring all of the samples, the data system processes the calibration standards in the first bracket and produces one calibration curve per named component (analyte). Then, the data system reprocesses the bracket to determine the measured amount of each analyte in the Unknown, Blank, QC, and calibration standard sample types. After processing the first bracket, the data system processes the second bracket, and so on.

2. When you open the processed sequence in the Quan Browser window, the overlapping standards appear in two brackets.

3. Make the appropriate entries and selections in the dialog box as described in these procedures.

   - "Step 3: Entering the Base File Name, Path, and Methods," on the next page

   - "Step 4: Entering the Sample Settings" on page 77

4. Click **OK**.

The data system automatically sets up the sequence table in the Sequence Setup view.

You can modify the sequence in the Sequence Setup view. These are the available sample types: Unknown, QC, Blank, Std Bracket.

Step 3: Entering the Base File Name, Path, and Methods

Use the General area of the New Sequence Template to specify the data file names and folder location, the instrument method for acquiring the raw data files, the processing method for processing the raw data and producing result files, and the calibration file for quantifying the samples in a non-bracketed sequence, if applicable.

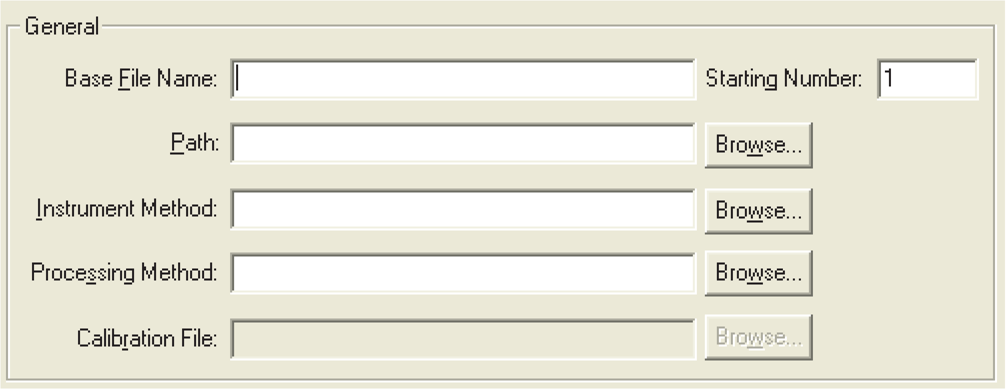
You can only select one instrument method and one processing method in the New Sequence Template dialog box. After the sequence table opens in the Sequence Setup view, you can select up to one instrument method per injection in the Inst Method column. For a bracketed sequence (Open, Overlapped, or Non-Overlapped bracket types), you can only select one processing method for the entire sequence.

If you want to use more than one processing method for the sample set, you must select the None option in the Bracket type area. The Calibration File box is only available when you select the None option for sequence bracketing. If you are performing a quantitative analysis, you must select the calibration file or files for the non-bracketed sequence before you submit the sequence for quantitative batch reprocessing.

❖ To specify the names and location of the data files and the instrument method for acquiring the data files

1. In the New Sequence Template dialog box, define the file parameters in the General area (Figure 42).

   Figure 42. General area of the New Sequence Template dialog box



Starting Number: 1

2. Type the base file name of the raw file in the Base File Name box.

   The data system uses this name for all of the raw files that it creates using the new sequence and appends a number to each data file. When the Starting Number is 1, the numbering starts at 01 and increments by 1 for each row. When the Starting Number is 10 or higher, the numbering starts with the starting number.

   If you do not specify a base file name, the data system assigns a default file name of 01 to the first sample (if the Starting Number is 1).

3. To change the starting number for the file name, type a number from **1** to **10 000** in the Starting Number box.

4. To indicate a location for the sample raw files, type a path location in the Path box or click **Browse** to select the directory where the data system stores the files.

5. 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 directory and file name.

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

   The New Sequence Template dialog box does not include a parameter setting for the number of calibration standards. When the data system creates the sequence table, it sets up the standard sample types on the basis of the following entries:

   - The number of calibration levels that are defined in the processing method
   - The bracket type and the number of samples selected in the New Sequence Template

   For example, if the processing method includes a calibration set of three defined standards, and you set up an open-bracket sequence with 12 samples, the data system creates a 15 row sequence with three calibration standards at the beginning of the sequence, followed by 12 samples.

   > **Note** For a quantitative analysis, the processing method includes the calibration information (named components, calibration levels and amounts, and curve type). The data system stores the response data from the calibration standards in the result files as you process or batch reprocess the sequence. For non-bracketed sequences, the data system stores this response data in a calibration file.

7. (Optional) If you are performing a quantitative analysis and you want to store the response data from the calibration standards in a calibration file, set up the processing information as follows:

   a. In the Processing Method box, select a processing method.

   b. In the Bracket Type area, select the **None** option (Figure 43).

Figure 43. None option selected in the Bracket Type area

Bracket Type

● None ○ Open ○ Non-Overlapped ○ Overlapped

The Calibration File box becomes available.

> **Note** You can acquire quantitative data without setting up the processing information. However, to process the data with a calibration file, you must set up the acquisition sequence or the processing sequence by selecting the None option in the New Sequence Template.

c. To select the calibration file (.xcal), do one of the following:

- In the Calibration File box, type the path and file name of a calibration file. Do not include the file extension (.xcal).

–or–

- Click **Browse** to select the directory and file name.

Step 4: Entering the Sample Settings

Use the Samples area of the New Sequence Template dialog box to specify the number of unknown samples in the sequence, the number of replicate injections per sample, the base sample ID, the tray type in use, the initial vial position for the sample runs, and whether you want the data system to reuse the same vial for replicate injections.

Use the Calibration area of the New Sequence Template dialog box to set up the calibration standards for a quantitative analysis. When you select the Add Standards check box in the Calibration area, the available parameters depend on the option selected in the Bracket Type area (see "Step 2: Selecting the Bracket Type" on page 71). To set up the calibration standards in the sequence table, you must select a processing method.

Use the QC area of the New Sequence Template dialog box to add quality control samples to the sequence.

> **Note** 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 sample type to use in a sequence.
>
> In the Sequence Setup view, the Level column displays the current calibration or QC level for the sequence row. This level is defined in the processing method listed in the Processing Method column.

To enter the information about the samples to be injected, follow these steps:

- "To specify the settings in the Samples area," on this page
- "To add calibration standards and blanks to the sequence" on page 79
- "To enter the quality control settings in the QC area" on page 80

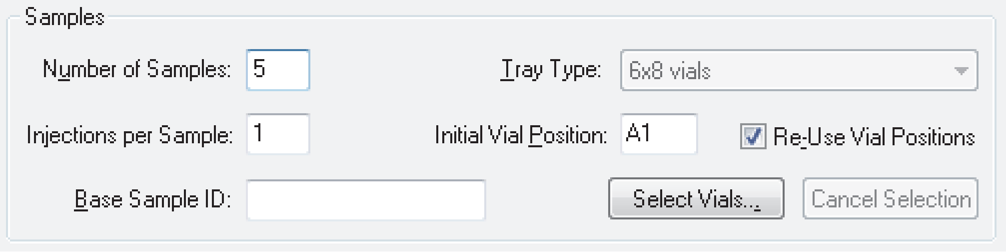
❖ To specify the settings in the Samples area

1. To specify the number of samples in the Samples area of the New Sequence Template dialog box, type the number of samples in the Number of Samples box (Figure 44).

   The default setting is 1.

   > **Tip** If the Select Vials button is available, you can also select the number of samples and the vial or microplate well positions of the samples by using an interactive plate graphic. However, this feature is not available for every autosampler controlled by the Xcalibur data system.

   Figure 44. Samples area of the New Sequence Template dialog box



Samples
Number of Samples: 5
Injections per Sample: 1
Base Sample ID:
Tray Type: 6x8 vials
Initial Vial Position: A1
☑ Re-Use Vial Positions

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.

   The default setting is 1. When you increase this value, the autosampler makes replicate injections from the same vial or well position.

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 (if available) from the Tray Type list.

   > **Tip** Depending on the autosampler, the Tray Type box is either a read-only display of the current tray type or a selectable list of the possible tray types.
   >
   > - If the Tray Type box is blank, you have not added an autosampler to the instrument configuration.
   > - If the configured tray type is unavailable, you cannot change the tray type from the Sequence Setup view. To change the tray type, you must modify the instrument configuration in the Foundation platform (see "Setting Up the Instrument Configuration in the Foundation Platform" on page 147).
   > - If the Tray Type list is available, you can select a different tray type. Or, you can change the tray type by choosing Change > Tray Name in the menu bar of the Sequence Setup view.

5. To specify the initial vial or microplate well position, type the first vial position or microplate well position in the Initial Vial Position box. Refer to the autosampler Help for the correct nomenclature.

6. Do one of the following:
   - Select the **Re-Use Vial Positions** check box if you want the autosampler to make replicate injections from the same microplate well or vial position.
   - Clear the **Re-Use Vial Positions** check box if you want the autosampler to make replicate injections from a separate microplate well or vial for each sample injection.

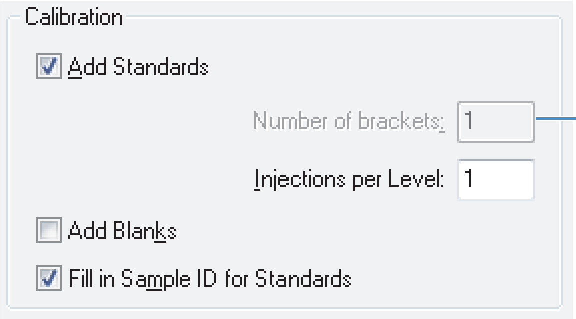
❖ To add calibration standards and blanks to the sequence

1. To add calibration standards to the sequence, do the following:

   a. Select the **Add Standards** check box.

   The calibration parameters that become available depend on the selected bracket type (Figure 45–Figure 47).

Figure 45. Calibration area for the Open bracket type



Calibration

☑ Add Standards

Number of brackets: 1

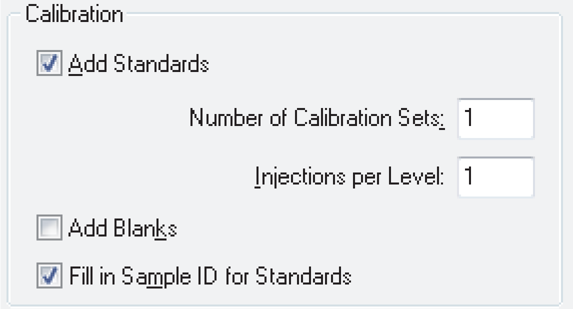
Injections per Level: 1

☐ Add Blanks

☑ Fill in Sample ID for Standards

The open bracket type is limited to one bracket.

Figure 46. Calibration area for the None bracket type



Calibration

☑ Add Standards

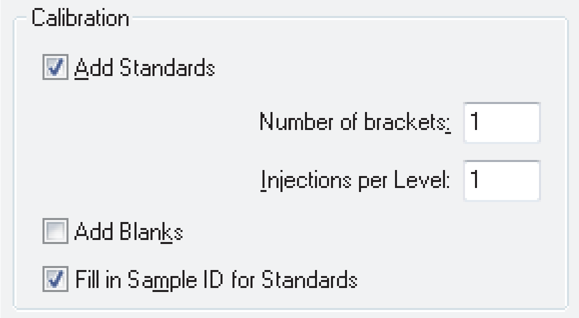
Number of Calibration Sets: 1

Injections per Level: 1

☐ Add Blanks

☑ Fill in Sample ID for Standards

Figure 47. Calibration area for the Non-Overlapped and Overlapped bracket types



Calibration

☑ Add Standards

Number of brackets: 1

Injections per Level: 1

☐ Add Blanks

☑ Fill in Sample ID for Standards

b. Depending on the bracket type, do one of the following:

   - For an open-bracket sequence, type a value for the number of injections per level in the Injections per Level box (Figure 45).
   - For an unbracketed sequence, type a value for the number of calibration sets in the Number of Calibration Sets box (Figure 46).
   - For a sequence with overlapping or non-overlapping brackets, type a value for the number of bracket sets in the Number of Brackets box (Figure 47).

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

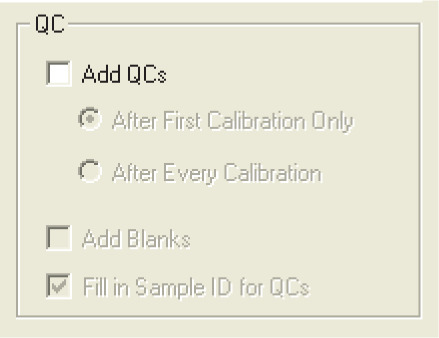
2. To add blank samples, select the **Add Blanks** check box.
3. (Optional) To have the data system enter the sample identification text in the Sample ID column for each calibration sample, select the **Fill In Sample ID for Standards** check box.

❖ To enter the quality control settings in the QC area

1. To add quality control samples to the sequence, do the following:

   a. Select the **Add QCs** check box (Figure 48).

   Figure 48. QC area of the New Sequence Template dialog box

   QC
   ☐ Add QCs
   ● After First Calibration Only
   ○ After Every Calibration
   ☐ Add Blanks
   ☑ Fill in Sample ID for QCs

   The After First Calibration Only and the After Every Calibration options become available.

   b. Select one of the following:

      - 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.

2. To add quality control blank samples, select the **Add Blanks** check box.
3. To have the data system enter the sample identification text in the Sample ID column for each QC sample, select the **Fill In Sample ID for QCs** check box.

Step 5: Saving the Changes to the New Sequence

Save the settings in the New Sequence Template dialog box, modify the sequence as desired, and then save the sequence. If you close the Home Page or start a sequence run directly after creating the sequence, the data system prompts you to save the changes.

❖ To save the settings and close the New Sequence Template dialog box

Click **OK**.

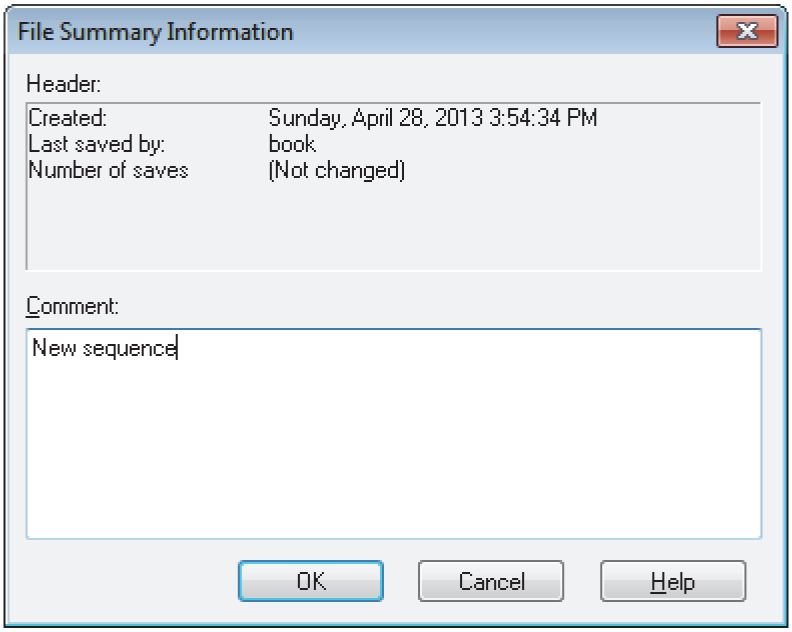
The settings are saved, and the New Sequence Template dialog box closes. The Sequence Setup view displays the default columns or the columns that you selected with the Column Arrangement dialog box (see "Column Arrangement Dialog Box" on page 223).

❖ To name the sequence and save it to a specific folder

1. From the menu bar, choose **File** > **Save As**.

   The File Summary Information dialog box appears (Figure 49).

   Figure 49. File Summary Information dialog box



Created: Sunday, April 28, 2013 3:54:34 PM
Last saved by: book
Number of saves (Not changed)

New sequence

2. In the Comment box, type an appropriate description. Then click **OK**.

   The Save As dialog box appears.

3. Browse to the folder where you want to save the sequence.
4. In the File Name box, type a file name.
5. Click **Save**.

Creating a Sequence Manually

For information about the sequence table parameters, see “Sequence Setup View” on page 199.

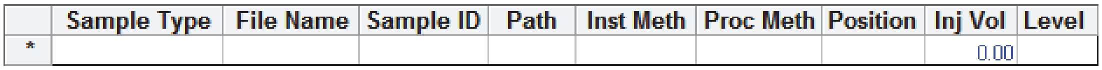
To create a new sequence manually, enter the appropriate information for each sample injection row by row into these columns: File Name, Sample ID, Path, Experiment Method, Processing Method, Position, Injection Volume, Level, Sample Weight, Sample Volume, ISTD Amount, and Dil Factor. To minimize the data entry process, the Sequence Setup view includes a fill down feature and a transfer row feature.

❖ To create a sequence manually

1. Open the Sequence Setup view (see “Opening the Sequence Setup View” on page 68).

   The sequence table is empty (Figure 50).

   Figure 50. Empty sequence table



	Sample Type	File Name	Sample ID	Path	Inst Meth	Proc Meth	Position	Inj Vol	Level
*								0.00	

2. To add or remove sequence columns and to change their arrangement, see “Adding, Removing, and Arranging the Sequence Columns” on page 88.

3. Follow the instructions in Table 3 for each sequence row.

> **Tip** To save time in duplicating column entries for sample rows, use the Fill Down command (see “Filling Down Sequence Parameters” on page 92).

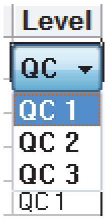
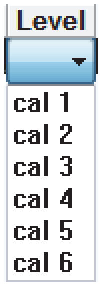
Table 3. Sequence column entries (Sheet 1 of 3)

Column	Entry
Sample Type	Double-click the column to open the Sample Type list and select one of the following sample types: **Unknown**, **Blank**, **QC**, or **Std Bracket**. When you create a sequence manually, you cannot specify a bracketing type, and the Std Update, Std Clear, Start Bracket, and End Bracket sample types are unavailable.
File Name	Type a file name for the data file.
Sample ID (Optional)	Type text to identify the sample. If you do not enter text in the Sample ID column, the data system automatically uses the vial position as the sample ID. If you enter text in the Sample ID column, the data system automatically appends the vial position to your text entry.

Table 3. Sequence column entries (Sheet 2 of 3)

Column	Entry
Path	Type a file location or double-click the column to open the Select Directory dialog box and select the path for the data file.
Inst Meth	Type the file location and name of the instrument method, or double-click the column to open the Select Instrument Method dialog box, where you can browse to and select the instrument method. Instrument methods have a .meth file extension. You can select a different instrument method for each injection. If you are creating a sequence to reprocess existing data files, you do not need to add an instrument method.
Proc Meth	Type the file location and name of the processing method, or double-click the column to open the Select Processing Method dialog box, where you can browse to and select the processing method. Processing methods have a .pmd file extension.You do not need to add a processing method to a sequence for data acquisition; however, the sequence must contain a processing method when you select one of these sample types: QC, Std Bracket, Std Clear, or Std Update.
Position	Type the appropriate alphanumeric text for the sample position. If you are using an autosampler, the notation for the position must correspond to the selected tray type. For information about the position notation for the autosampler's available tray types, refer to the Help for the autosampler.
Inj Vol	Type a value for the injection volume. The data system sends this value to the syringe pump or the autosampler. The injection volume displayed in the Inj Vol column matches the injection volume in your instrument 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.

Table 3. Sequence column entries (Sheet 3 of 3)

Column	Entry
Level   	To make the Level list available, select a processing method in the Processing Method column. Then, double-click the column to open the list. If the sample type is QC, Std Bracket, Std Clear, or Std Update, select a level from the Level list. The Level list contains the calibration standard or QC levels specified in the processing method.
Sample Wt (Optional)	If the sample type is QC, Std Bracket, Std Clear, or Std Update, specify a sample weight (amount). Type the sample weight (amount) of the target compound in the QC or Standard sample. The processing method defines the units.
ISTD Corr Amt (Optional)	Do the following to specify an internal standard bulk correction factor: • 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 (because of a preparation error), type the actual total amount or concentration of the internal standard in the sample in the ISTD Corr Amt box. The data system applies a bulk adjustment to the internal standard response factor. The units are defined in the processing method.
Dil Factor (Optional)	Type a value to specify the dilution factor for the sample.

4. To save the sequence, choose **File > Save As**.

   The File Summary Information dialog box opens.

5. Enter a description of the sequence and click **OK**.

   The Save As dialog box opens.

6. Do the following:

   a. In the File Name box, type a unique name for the sequence.

   b. In the Save In list, select the appropriate folder location for the sequence.

   c. Click **Save**.

Modifying Sequences

You can modify a sequence after you open it in the Sequence Setup view.

❖ To open an existing sequence

1. Open the Sequence Setup view from the Xcalibur Home Page window by clicking in the toolbar.

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

   The Open dialog box opens.

3. Browse to the appropriate folder location, select the sequence file of interest, and click **Open**.

   Sequence files have an .sld file extension.

To modify an existing sequence, follow these procedures:

- "Using the Edit Commands," on the next page
- "Adding, Removing, and Arranging the Sequence Columns" on page 88
- "Customizing the User Labels for a Sequence" on page 90
- "Going to a Sequence Row" on page 91
- "Filling Down Sequence Parameters" on page 92
- "Transferring Row Information" on page 94

Using the Edit Commands

The Sequence Editor Toolbar contains the following commands in the Edit category: Undo, Clear, Copy, Paste, Insert Row, Go to Row, and Fill Down. For information about the Go to Row command, see "Going to a Sequence Row" on page 91. For information about the Fill Down command, see "Filling Down Sequence Parameters" on page 92.

To edit a sequence table by using the Clear, Copy/Paste Cells, and Insert/Delete Rows commands, follow these procedures.

❖ To clear a table cell or row

1. Do one of the following:

   - Select a table cell by clicking it.

   - Select a table row by clicking the row number.

   –or–

   - Select a range of table rows by selecting the first row and dragging the cursor to the last row.

2. Choose **Edit > Clear**, or press **CTRL + X**.

   When you clear an entire sequence row, the data system clears all of the sequence table columns except for the Sample Type and Inj Vol columns. Instead of clearing these columns, the data system replaces the selection in the Sample Type column with the Unknown sample type and the volume in the Inj Vol column with 0.00.

❖ To copy a range of cells

1. Select the cells that you want to copy.
2. Right-click and select **Copy Cells** from the shortcut menu.
3. Select the cells where you want to paste the contents of the clipboard.
4. Right-click and select **Paste Cells** from the shortcut menu.

❖ To insert a row

1. Select the row directly below the line where you want to insert the row.
2. Choose **Edit > Insert Row**.

   The following message appears:

   > Insert above line *X*?

3. Do one of the following:

    - Click **Yes**.

      The data system inserts the new row above the selected row.

    –or–

    - Click **No** to cancel the Insert Row command.

❖ To delete a row or multiple rows

1. Do one of the following:

    - Click the row number of the row that you want to delete to select the entire row.

    –or–

    - Select a range of table rows by clicking the number of the first row that you want to delete and dragging the cursor to the number of the last row that you want to delete.

2. Choose the **Delete Row** command.

    The following message appears:

    Delete Rows *X* to *X*?

3. Do one of the following:

    - Click **Yes** to delete the rows.

    –or–

    - Click **No** to cancel the Delete Row command.

Adding, Removing, and Arranging the Sequence Columns

In the Sequence Setup view, you can add or remove columns and rearrange columns.

When you initially install the Xcalibur data system, the Sequence Setup view displays the following columns: Sample Type, File Name, Sample ID, Inst Meth, Proc Meth, Position, Inj Vol, and Level. To customize the Sequence Setup view, you can add the following columns: Comment, Dil Factor, ISTD Corr Amt, Sample Vol, Sample Wt, and five additional user-labeled columns.

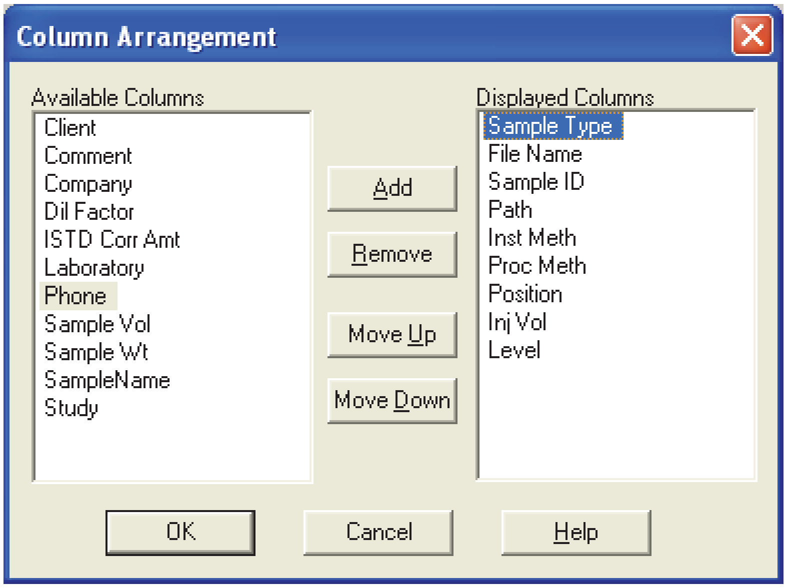
For information about the Column Arrangement dialog box, see "Column Arrangement Dialog Box" on page 223.

❖ To add or remove columns or change the column arrangement

1. In the Sequence Setup view, click in the toolbar or choose **Change > Column Arrangement**.

   The Column Arrangement Dialog Box opens (Figure 51). The sequence table 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.

   Figure 51. Column Arrangement dialog box



2. For each column that you want to add to the current sequence table, do the following:

   a. In the Available Columns list, select the column name.

   b. Click **Add**.

   The column name moves from the Available Columns list to the Displayed Columns list, and the new column appears in the sequence table.

3. For each column that you want to delete from the current sequence table, do the following:
    a. In the Displayed Columns list, select the column name.
    b. Click **Remove**.

    The column name moves from the Displayed Columns list to the Available Columns list, and the selected column disappears from the current sequence.

4. To change the position of a column, do the following:
    a. Select the column name in the Displayed Columns list.
    b. Do one of the following:
        - 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.

5. Click **OK** to close the Column Arrangement dialog box.

❖ To change the width of a column

1. move the cursor to the column headings row at the top of the sequence table and place the cursor at the right or left boundary of the column that is the incorrect width.

    The cursor changes to ↔.

2. Drag the column boundary to obtain the desired column width.

❖ To save the changes to the column arrangement

When you close the data system, the Home Page dialog box opens, prompting you to save your changes before you exit.

To save the changes to the Sequence Setup view, click **Yes**.

Customizing the User Labels for a Sequence

For information about the parameters for the User Labels dialog box, see "User Labels Dialog Box" on page 246. Figure 57 on page 96 shows the default headings in the print preview of a Sequence list. You can customize the heading labels for the following sequence table columns:

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

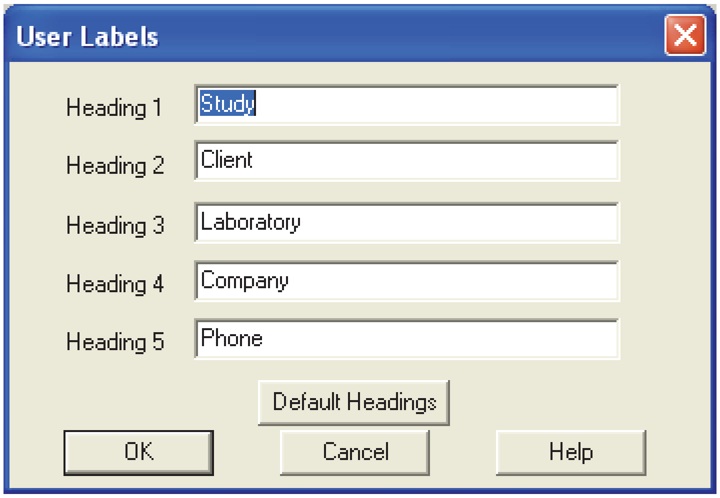
When you change the heading labels, the data system stores the custom heading labels in the current memory and in the sequence that you are creating or modifying. When you open an existing sequence, the data system displays the column heading labels stored with the sequence and loads these labels into the current memory.

❖ 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** from the menu bar.

   The User Labels dialog box opens (Figure 52).

   Figure 52. User Labels dialog box

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

2. For each column heading that you want to change, select the current heading name and type the new heading in the box. If you do not want to use a heading, select and delete the text and leave the box blank.

3. To reset the heading labels to their default settings, click **Default Headings**.

4. To save the new column heading labels and to close the User Labels dialog box, click **OK**.

Going to a Sequence Row

Use the Go To Line Number dialog box to select the sequence row that you want to edit. The sequence row number appears in the leftmost column of the sequence table.

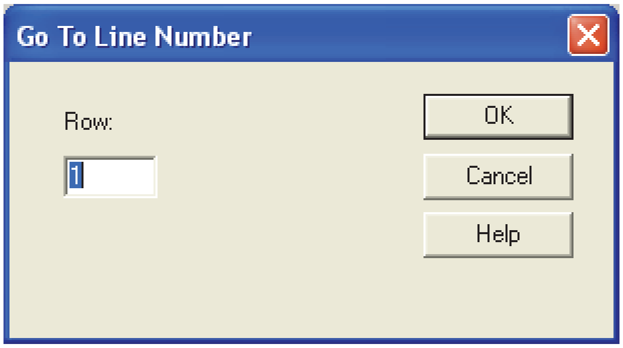
For more information, see "Go To Line Number Dialog Box" on page 228.

❖ To go to a specified row in the current sequence

1. In the menu bar of the Sequence Setup view, choose **Edit > Go To Row**.

   The Go To Line Number dialog box opens (Figure 53).

   Figure 53. Go to Line Number dialog box

   Row: 1

2. To specify a sequence row number, type a valid sequence row number in the Row box.
3. To go to the line number, click **OK**.

   The Go To Line Number dialog box closes, and the selected row appears near the top of the Sequence Setup view and is highlighted in blue.

Filling Down Sequence Parameters

Use the Fill Down dialog box to duplicate text entries or sequential numeric entries when you create or modify sequences. For information about the parameters in the Fill Down dialog box, see “Fill Down Dialog Box” on page 227.

> **Note** The Fill Down command is on the Edit menu, and the Fill Down icon is in the toolbar of the Sequence Setup view, but both the command and the icon are unavailable until you select at least two contiguous rows of a sequence table.

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

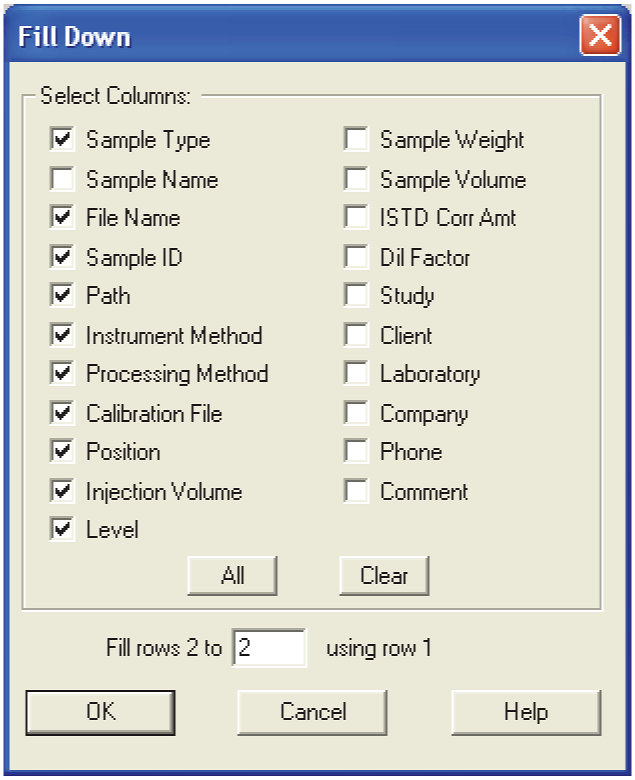
1. Starting with the row that you want to copy information from, select the columns that you want to copy data from, then drag the cursor downward through the contiguous row or rows that you want to copy information to.

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

2. Click ⇊ in the toolbar or choose **Edit > Fill Down**.

   The Fill Down dialog box opens (Figure 54). The check boxes for the columns that you selected are selected. The text at the bottom of the text box lists the starting row that is to be copied and the first and last rows to be filled.

   Figure 54. Fill Down dialog box



Select 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
☐ Study
☐ Client
☐ Laboratory
☐ Company
☐ Phone
☐ Comment

Fill rows 2 to 2 using row 1

The text at the bottom of the dialog box displays 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.

C is the row number of the last row selected.

You cannot change your selections for the first and second rows without first closing the Fill Down dialog box; however, you can edit C to change the row number of the last row to be filled.

3. To change the selection of the columns to be duplicated, do one of the following in the Fill Down dialog box:
   - Select the check boxes for the columns that you want to copy, and clear the check boxes for the columns that you do not want to copy.
   - To select all of the column check boxes, click **All**.
   - To clear all of the column check boxes, click **Clear**.
4. To fill the rows and close the dialog box, click **OK**.

Transferring Row Information

Use the Transfer Row Information dialog box to copy the row information for the first occurrence of a sample to other rows in the sequence with the same sample ID or position. The data system copies the information in all of the columns except File Name and Sample Type.

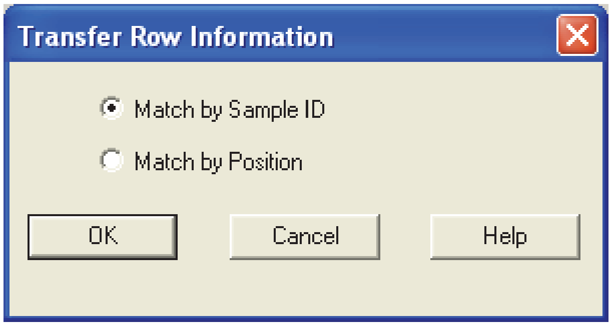
For information about the parameters in the Transferring Row Information dialog box, see "Transfer Row Information Dialog Box" on page 244.

❖ 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 (Figure 55).

   Figure 55. Transfer Row Information dialog box

   Transfer Row Information

   ● Match by Sample ID

   ○ Match by Position

2. Select one of these options:

   - Select the **Match by Sample ID** option to copy the row information from the first occurrence of a the same text in the Sample ID column to all sample rows that have the same text in the Sample ID column.

   - Select the **Match by Position** option to copy the row information from the first occurrence of a sample position (vial or microplate well position listed in the Position column of the sequence list) to all sample rows that have the same position.

3. 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.

4. To undo the copy operation, immediately choose **Edit > Undo** or click in the Sequence Editor toolbar.

Printing a Vial or Sequence List

For information about the parameters in the Print Selection dialog box, see "Print Selection Dialog Box" on page 237.

Follow these procedures:

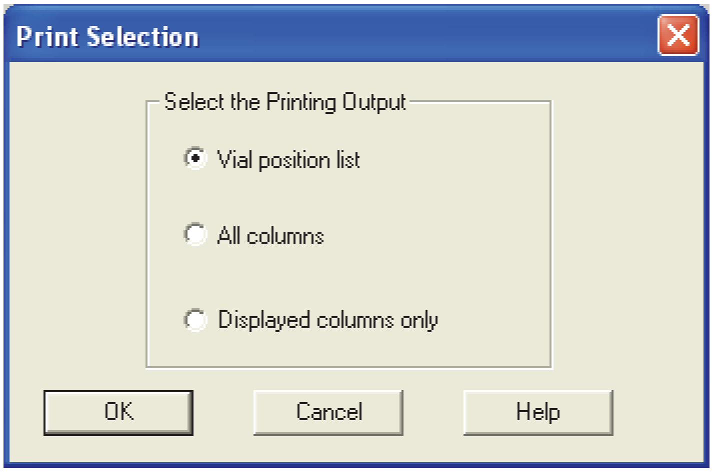
- "To preview a vial or sequence list," on this page
- "To print the vial or sequence list" on page 97

❖ To preview a vial or sequence list

1. To preview the vial or sequence list for the current sequence, choose **File > Print Preview** in the Sequence Setup view.

   The Print Selection dialog box opens (Figure 56).

   Figure 56. Print Selection dialog box



2. Do one of the following:
   - To preview the vial position list, select the **Vial Position List** option and click **OK**.

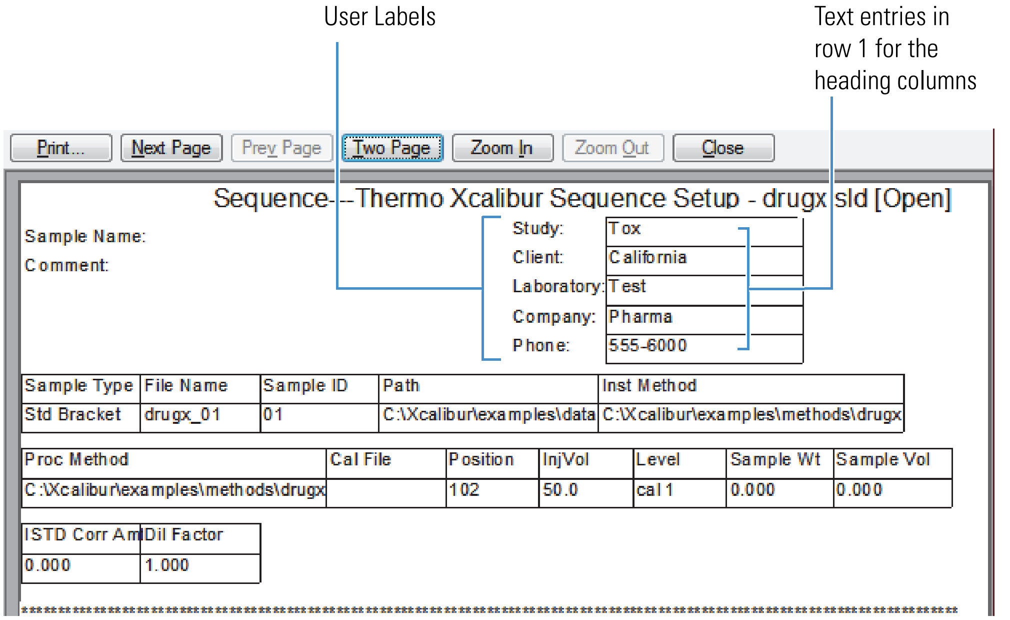
     The Vial list for the current sequence appears.
   - To preview all of the sequence columns, select the **All Columns** option and click **OK**.

     The Sequence list appears.
   - To preview the columns currently displayed in the Sequence Setup view, select the Displayed Columns Only option and click **OK**.

     The Sequence list appears.

In a Sequence list, the five headings that you can customize with the User Labels dialog box appear in the heading above each sequence row (Figure 57). The user-labeled column headings are the same for each sequence row, but the text entries associated with these headings can differ for each sequence row.

Figure 57. Sequence list with all of the columns displayed



User Labels

Text entries in row 1 for the heading columns

Sequence---Thermo Xcalibur Sequence Setup - drugx.sld [Open]

Sample Name:
Comment:

Study:	Tox
Client:	California
Laboratory:	Test
Company:	Pharma
Phone:	555-6000

Sample Type	File Name	Sample ID	Path	Inst Method
Std Bracket	drugx_01	01	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx

Proc Method	Cal File	Position	InjVol	Level	Sample Wt	Sample Vol
C:\Xcalibur\examples\methods\drugx		102	50.0	cal 1	0.000	0.000

ISTD Corr Am	Dil Factor
0.000	1.000

Tip The first page of the selected list appears 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.

3. To review the displayed list, do the following:
   - To move through the pages of the list, click **Next Page** or **Prev Page**.
   - To change the display, do the following:
     - Click **Two Page** to display two pages on the screen.
     - Click **Zoom In** to increase the magnification and **Zoom Out** to decrease the magnification.

❖ To print the vial or sequence list

1. To print the vial or sequence list for the current sequence, choose **File > Print** in the Sequence Setup view.

   The Print Selection dialog box opens.

2. Select the option for the list that you want to print.

   The Print dialog box opens.

3. Select print options under Print range and Copies, and choose **OK**.

   The application prints the selected list.

5

Running and Batch Reprocessing Sequences

This chapter describes how to run and batch reprocess sequences.

Whether you want to run a single sample or multiple samples, you must create a sequence. You can acquire raw data files without adding a processing method to a sequence, but you must add a processing method to a sequence to process or batch reprocess the raw data files.

When you add a processing method to a sequence before acquiring the data files and select one or more of the check boxes in the Processing Actions area of the Run Sequence dialog box, the data system processes the data files with the processing method as it acquires the data files. When you acquire data files using a sequence without a processing method, you can add a processing method to the sequence and batch reprocess the data files. With the exception of the audit trail, the processing results are the same, whether the data files are processed during data acquisition or reprocessed following data acquisition.

Contents

- Preparing to Run Samples from the Sequence Setup View
- Running a Single Sample or Multiple Samples
- Starting Each Run Manually
- Stopping the Current Sample Run or Pausing the Sequence Queue
- Viewing the Data As It Is Acquired
- Using the Acquisition Queue
- Batch Reprocessing a Sequence
- Managing the Xcalibur Processing Queue

Preparing to Run Samples from the Sequence Setup View

Before you run a single sample or a sample set from the Sequence Setup window, you must first create an instrument method and a sequence (list of samples to be injected).

An instrument method contains the settings for your chromatographic method and the data acquisition settings for the mass spectrometer. It also includes the tune method for the mass spectrometer.

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.

For more information, see the following:

- For information about creating instrument methods, see Chapter 2, "Creating Instrument Methods and Using the Direct Controls."
- For information about creating injection sequences, see Chapter 4, "Creating and Modifying Sequences."

❖ To open the sequence that you want to acquire from within the data system

1. Choose **Start > Programs** (or **All Programs) > Thermo Xcalibur > Xcalibur**.

   The Xcalibur data system opens to the Roadmap view of the Home Page window.

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

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

   –or–

   - In the menu bar, choose **View > Sequence Setup View**.

3. Open the sequence that you want to run as follows:

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

      The Open dialog box opens.

   b. Browse to the appropriate folder and select an appropriate sequence.

      The sequence file type has an .sld extension.

   c. Click **Open**.

      The sequence list appears in the Sequence Setup view.

❖ To open the saved sequence from its directory location

1. Using Windows™ Explorer, open the folder where the sequence of interest is stored.

2. Double-click the sequence file.

   The sequence list appears in the Sequence Setup view.

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

1. For a sample of type Std Update or QC, make sure that the sequence uses a processing method file with defined calibration and QC levels.
2. Double-click the Level box to open a list of levels from the processing method.
3. Select the correct level for the sample from the list of available levels.
4. Save the changes to the sequence.

Running a Single Sample or Multiple Samples

You must create a sequence table whether you are making a single injection from one sample vial, multiple injections from one sample vial, or multiple injections from multiple sample vials. Each row of the sequence table contains the information for one injection. If you are making multiple injections from the same sample vial, the sequence table contains one row for each injection, and each row lists the same sample position.

For data acquisition, each row of the sequence table must contain the following information: a data file name and location, an instrument method, a sample position, and an injection volume. The position nomenclature is specific to the instrument that you are using to make the injection. For an LC/MS system, an autosampler is typically used to make the injections and start the runs.

Note For information about the position nomenclature for your LC/MS system, refer to the *autosampler* Help in the *autosampler* view of the Instrument Setup window.

To make a single injection, you can create a one-row sequence table, or you can select a row in a multiple-row sequence table.

❖ To submit a single sample or a sequence for acquisition

1. Depending on whether you are making a single injection or multiple injections, do the following:
   - For a single injection, go to step 2.
   - For more than one injection, go to step 3.
2. To submit a single sample (one injection), do the following:
   a. In the sequence table, click the row number for the sample that you want to run.

      The data system highlights the entire row in blue.

b. Do one of the following:

- Choose **Actions > Run This Sample** from the menu bar.

–or –

- Click the **Run Sample** icon, , in the toolbar.

The Run Sequence Dialog Box and the Change Instruments In Use Dialog Box open.

c. Go to step 4.

3. To submit multiple contiguous samples or an entire sequence, do the following:

a. If you want to select a a subset of the samples in the sequence, double-click the row number of the first sample that you want to inject. Then drag the cursor to the row number of the last sample that you want to inject.

b. Do one of the following:

- Choose **Actions > Run Sequence** from the menu bar.

–or –

- Click the **Run Sequence** icon, , in the toolbar.

One of the following actions occurs:

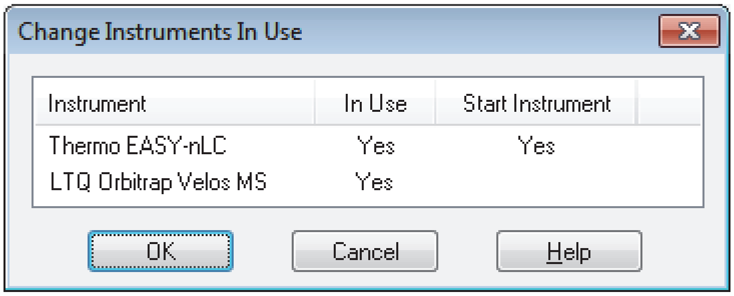
- If the data system detects a new instrument configuration, the Change Instruments In Use dialog box opens (Figure 58). Go to step 4.
- If the instrument configuration has not changed since the last sequence run, the Run Sequence dialog box opens (Figure 59). Go to step 5.

4. If the Change Instruments In Use dialog box opens, do the following:

a. Make sure that the appropriate instruments are listed as In Use.

Figure 58 shows the EASY-nLC nanoflow LC instrument and the LTQ Orbitrap Velos™ mass spectrometer as the instruments in use. The EASY-nLC, which includes an autosampler, is listed as the start instrument. When the EASY-nLC instrument makes an injection, it triggers the mass spectrometer to start data acquisition through a contact closure cable.

Figure 58. Change Instruments In Use dialog box with the autosampler listed as the start instrument



Instrument	In Use	Start Instrument
Thermo EASY-nLC	Yes	Yes
LTQ Orbitrap Velos MS	Yes	

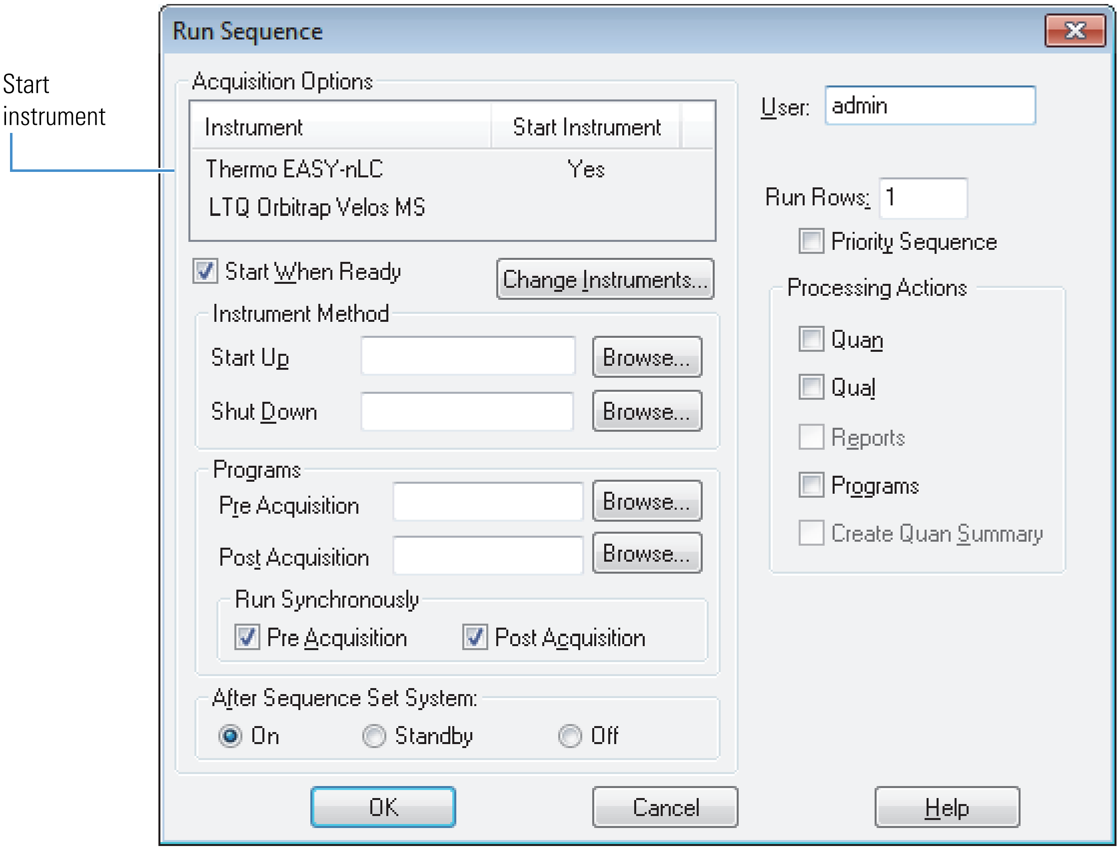
b. If the appropriate instrument is not listed as the Start Instrument, click its row in the Start Instrument column.

The blank cell now displays Yes.

c. Click **OK** to accept the new setting and close the dialog box.

The Run Sequence dialog box opens (Figure 59).

Figure 59. Run Sequence dialog box



Run Sequence

Acquisition Options

Instrument	Start Instrument
Thermo EASY-nLC	Yes
LTQ Orbitrap Velos MS	

☑ Start When Ready

Instrument Method
Start Up:
Shut Down:

Programs
Pre Acquisition:
Post Acquisition:

Run Synchronously
☑ Pre Acquisition ☑ Post Acquisition

After Sequence Set System:
● On ○ Standby ○ Off

User: admin

Run Rows: 1

☐ Priority Sequence

Processing Actions
☐ Quan
☐ Qual
☐ Reports
☐ Programs
☐ Create Quan Summary

5. Check whether the appropriate instrument is listed as the Start Instrument in the Acquisition Options area.

   The Start Instrument column displays Yes for the instrument that triggers data acquisition.

6. If the appropriate instrument is not listed as the Start Instrument, click **Change Instruments** to open the Change Instruments In Use dialog box. Follow the instructions in step 4 on page 102 to select the appropriate Start Instrument.

7. In the Run Rows box, check the sample row or sample range to be injected.

> **Note** If you do not select a sequence row for a single injection, the Xcalibur data system defaults to row 1. If you do not select the sequence rows for a sequence, the Xcalibur data system defaults to the entire range of sequence rows.

8. (Optional) Identify the operator, select startup and shutdown methods, and specify additional programs to be run as follows:

    a. In the User box, type up to 10 characters to maintain a record of the operator who started the run.

    b. In the Instrument Method area, specify a start-up method and a shut-down method.

    - In the Start Up box, specify the instrument method to be run immediately before the sequence starts.
    - In the Shut Down box, specify the instrument method to be run when the sequence is completed.

    c. In the Programs area, specify additional programs to be run.

    - In the Pre Acquisition box, specify the program to run before running the sequence.
    - In the Post Acquisition box, specify the program to run when the sequence is completed.
    - In the Run Synchronously area, specify whether to run the programs 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.

9. If you want the data system to start the sequence runs automatically when the instruments are ready, make sure that the Start When Ready check box is selected.

    By default, the Start When Ready check box is selected. This selection is appropriate for the typical instrument setup where the autosampler triggers the detector to start data acquisition when it makes an injection.

    If you clear this check box, you must click the **Start Analysis** icon, ▶, to start each run.

10. Specify the priority of the sequence.

    - 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.

11. In the After Sequence Set System area, select one of these options for the system status after the data system completes the sequence:

    - On option
    - Standby option
    - Off option

12. If your sequence includes a processing method, 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.

    > **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.

For information about stopping an active sequence, viewing the real-time acquisition of the chromatographic or spectral data, or managing the acquisition queue, see these topics:

- Stopping the Current Sample Run or Pausing the Sequence Queue
- Viewing the Data As It Is Acquired
- Using the Acquisition Queue

Stopping the Current Sample Run or Pausing the Sequence Queue

You can stop the current run or pause the sequence queue by using the Pause/Resume Sequence Queue and Stop Analysis icons on the Sequence Editor toolbar.

For information about deleting inactive samples and sequences from the acquisition queue, see “Using the Acquisition Queue” on page 113.

For information about the Start Analysis icon on the Sequence Editor toolbar, see “Starting Each Run Manually” on page 107.

❖ To stop the current run in an active sequence and go to the next sample

1. In the Sequence Editor toolbar, click the **Stop Analysis** icon, 🟩.

   The following actions occur:

   - The Pause/Resume Sequence Queue icon goes to the resume sequence queue state; that is, it appears depressed, ⏸.
   - The data system immediately stops the current run and acquires the raw data file.

2. To resume the sequence, click the **Pause/Resume Sequence Queue** icon, ⏸.

   The data system resumes the sequence at the next sample in the queue.

   Tip Click the **Stop Analysis** icon to prematurely terminate a run.

❖ To pause an active sequence

In the Sequence Editor toolbar, click the **Pause/ Resume Sequence Queue** icon, ⏸.

The following actions occur:

- The Pause/Resume Sequence Queue icon goes to the resume sequence queue state; that is, it appears depressed, ⏸.
- The data system continues to acquire data for the current sample until the run time specified in the instrument method expires. At the end of the run, the data system acquires the raw data file.

Tip Click the **Pause Analysis** icon to add additional time between the current run and the next run.

❖ To restart a paused sequence

Click the **Pause/Resume Sequence Queue** icon, which is currently in the resume sequence queue state; that is, it appears depressed, ⏸.

The data system resumes the sequence with the next sample in the queue.

Starting Each Run Manually

If you did not select the Start When Ready check box in the Run Sequence dialog box when you submitted the sequence to the acquisition queue, you must manually start each run when the instruments are ready.

❖ To start the run

Click the **Start Analysis** icon, ▶, on the Sequence Editor toolbar.

Viewing the Data As It Is Acquired

Use the Real Time Plot view to view data as it is being acquired.

In the Real Time Plot view, you use the Plot toolbar to lock and unlock the display and to zoom in or out on the chromatogram and spectrum views. For more information about this toolbar, see “Home Page – Plot Toolbar” on page 174.

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

1. Open the Real Time Plot view by doing one of the following from the Xcalibur Home Page:
   - Click the **Real Time Plot View** icon, , on the Home Page toolbar.

   –or–

   - Choose **View > Real Time Plot View** from the Home Page menu bar.
2. If the display is not already locked, click the **Lock Display** icon, 🔒, 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.

Icon	Menu command	Meaning
🔒	Lock Display	The display is unlocked, and you can review the data that has already been acquired for the current run on the screen, but you cannot view the real-time acquisition of data.
🔒	✓Lock Display	The display is locked, and you can view the real-time acquisition of data for the current run, but you cannot review the data.

These topics provide more information about viewing the data during data acquisition:

- Viewing Real-Time Data
- Monitoring a Chromatogram in Real Time
- Monitoring a Spectrum in Real Time
- Adding Plots to the Real-Time Plot Display

Viewing Real-Time Data

Use the Real Time Plot view to view data as it is being acquired.

❖ To view data as it is being acquired

1. Open the Real Time Plot view, if it is not already open (see "Viewing the Data As It Is Acquired" on page 107).
2. Unlock the display by clicking the **Lock Display** icon.

   After you unlock the display, data collection continues offscreen.
3. Pin the spectrum cell by clicking the pin icon, 📌, in the upper-right corner of the cell.

   The pin in the upper-right corner of the spectrum cell turns green. Cursor actions in other cells such as the chromatogram cell now affect the view displayed in the spectrum cell.
4. Click the peak of interest in the chromatogram cell.

   In the spectrum cell, a mass spectrum appears for the time-point that you clicked.
5. Click the **Lock Display** icon, 🔒, to resume monitoring real-time data acquisition.
6. 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.
7. 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 that you clicked.
8. Click the **Lock Display** icon, 🔒, 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.

❖ To view a chromatogram in locked and unlocked modes

1. Open the Real Time Plot view, if it is not already open (see "Viewing the Data As It Is Acquired" on page 107).
2. To unlock the display, do one of the following:
    - Choose **View > ✓Lock Display** from the menu bar.
    - Click the **Lock Display** icon, 🔒,

   –or–

    - Click the display.

   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 icon appears to be depressed.
3. 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.
4. 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**.

5. 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**.
6. To resume monitoring real-time data collection, do one of the following:
    - Click the **Lock Display** icon, 🔒.

    –or–

    - Choose **View > Lock Display** to lock the data display.

    The Real-Time Plot view 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 the locked and unlocked modes

1. Open the Real Time Plot view, if it is not already open (see "Viewing the Data As It Is Acquired" on page 107).
2. To unlock the display, do one of the following:
    - Choose **View >** ✓**Lock Display** from the menu bar.
    - Click the **Lock Display** icon, 🔒,

    –or–

    - Click the display.

    By unlocking the data from the instrument, you can 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.
3. To make the spectrum view the active and pinned view, click the pin icon, 📌, in the upper right corner of the cell.

    The pin icon appears pinned to the screen, 📌, to indicate that the spectrum cell is the active and pinned cell.

You can control a pinned cell with toolbar and menu commands. In addition, actions in other cells affect the spectra displayed in the pinned spectrum cell. For example, when you click a specific time point in the chromatogram cell, the spectrum for that time point appears in the spectrum cell.

4. Select the scan that 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**.
5. Select the *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**.
6. Select the *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**.
7. To resume monitoring real-time data collection, do one of the following:
    - Click the **Lock Display** icon, 🔒.

    –or–

    - Choose **View > Lock Display** to lock the data 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 Plots to the Real-Time Plot Display

You can add multiple plots to the chromatogram cell.

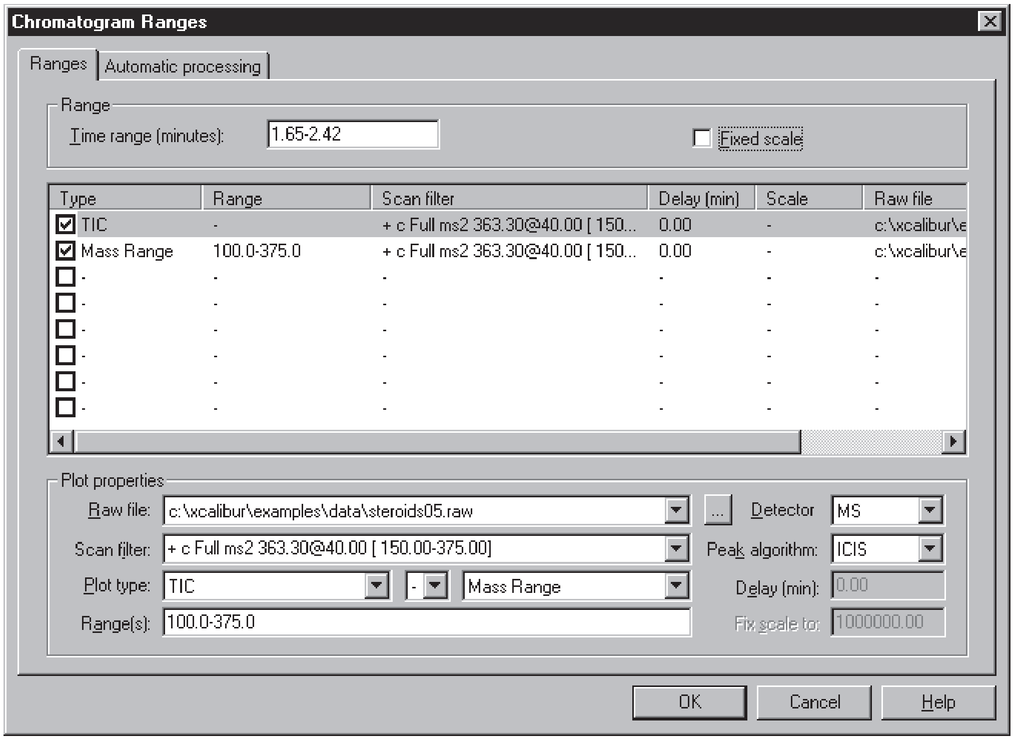
❖ To add multiple plots to the chromatogram cell

1. Open the Real Time Plot view, if it is not already open (see "Viewing the Data As It Is Acquired" on page 107).
2. Pin the chromatogram cell to make it the active and pinned cell.
3. From the menu bar of the Real Time Plot view, choose **View > Ranges**.

   The Chromatogram Ranges dialog box opens (Figure 60).

> **Note** Unlike the Qual Browser window, in the Home Page – Real Time Plot view, the chromatogram and spectrum views do not have shortcut menus.

Figure 60. Chromatogram Ranges dialog box



Range

Time range (minutes): 1.65-2.42

☐ Fixed scale

Type	Range	Scan filter	Delay (min)	Scale	Raw file
☑ TIC	-	+ c Full ms2 363.30@40.00 [150...	0.00	-	c:\xcalibur\e
☑ Mass Range	100.0-375.0	+ c Full ms2 363.30@40.00 [150...	0.00	-	c:\xcalibur\e
☐ -	-	-	-	-	-
☐ -	-	-	-	-	-
☐ -	-	-	-	-	-
☐ -	-	-	-	-	-
☐ -	-	-	-	-	-
☐ -	-	-	-	-	-

Plot properties

Raw file: c:\xcalibur\examples\data\steroids05.raw

Detector: MS

Scan filter: + c Full ms2 363.30@40.00 [150.00-375.00]

Peak algorithm: ICIS

Plot type: TIC - Mass Range

Delay (min): 0.00

Range(s): 100.0-375.0

Fix scale to: 1000000.00

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

Using the Acquisition Queue

The Acquisition Queue page of the Information view shows all the sequences and samples submitted for analysis (Figure 61). The file tree view shows two levels of detail: the sequence names and, within each branch, the sequence row number.

❖ To open the Acquisition Queue page

1. If the Information view is not open, open it by doing one of the following:
   - From the menu bar, choose **View > Info View**.

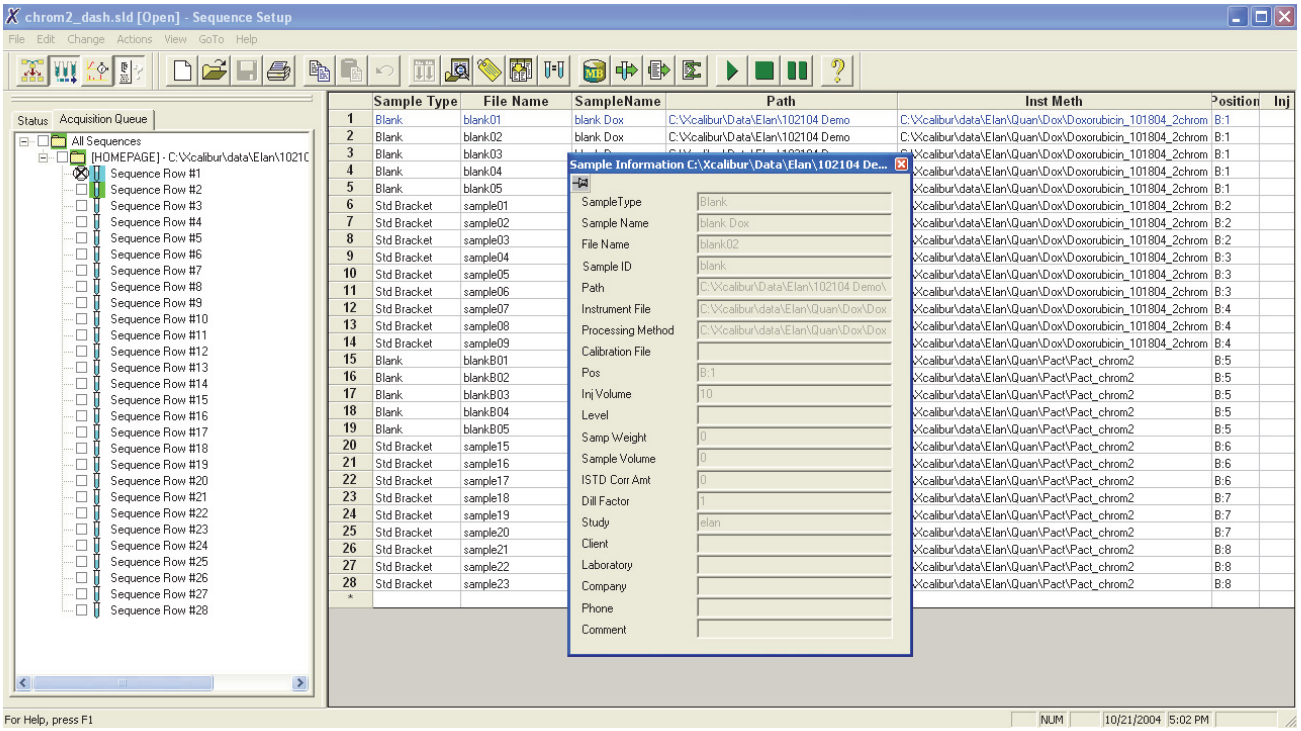
   –or–

   - In the toolbar, click the **Information View** icon, .
2. Click the **Acquisition Queue** tab.

Use the Acquisition Queue page to do the following:

- Delete sequences unless they are currently being run (active).
- 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 61. Acquisition Queue page with the Sample Information window displayed



- ☐ All Sequences
  - ☐ [HOMEPAGE] - C:\Xcalibur\data\Elan\1021C
    - ☒ Sequence Row #1
    - ☐ Sequence Row #2
    - ☐ Sequence Row #3
    - ☐ Sequence Row #4
    - ☐ Sequence Row #5
    - ☐ Sequence Row #6
    - ☐ Sequence Row #7
    - ☐ Sequence Row #8
    - ☐ Sequence Row #9
    - ☐ Sequence Row #10
    - ☐ Sequence Row #11
    - ☐ Sequence Row #12
    - ☐ Sequence Row #13
    - ☐ Sequence Row #14
    - ☐ Sequence Row #15
    - ☐ Sequence Row #16
    - ☐ Sequence Row #17
    - ☐ Sequence Row #18
    - ☐ Sequence Row #19
    - ☐ Sequence Row #20
    - ☐ Sequence Row #21
    - ☐ Sequence Row #22
    - ☐ Sequence Row #23
    - ☐ Sequence Row #24
    - ☐ Sequence Row #25
    - ☐ Sequence Row #26
    - ☐ Sequence Row #27
    - ☐ Sequence Row #28

	Sample Type	File Name	SampleName	Path	Inst Meth	Position	Inj
1	Blank	blank01	blank Dox	C:\Xcalibur\Data\Elan\102104 Demo	C:\Xcalibur\data\Elan\Quan\Dox\Doxorubicin_101804_2chrom	B:1	
2	Blank	blank02	blank Dox	C:\Xcalibur\Data\Elan\102104 Demo	C:\Xcalibur\data\Elan\Quan\Dox\Doxorubicin_101804_2chrom	B:1	
3	Blank	blank03			Xcalibur\data\Elan\Quan\Dox\Doxorubicin_101804_2chrom	B:1	
4	Blank	blank04			Xcalibur\data\Elan\Quan\Dox\Doxorubicin_101804_2chrom	B:1	
5	Blank	blank05			Xcalibur\data\Elan\Quan\Dox\Doxorubicin_101804_2chrom	B:1	
6	Std Bracket	sample01			Xcalibur\data\Elan\Quan\Dox\Doxorubicin_101804_2chrom	B:2	
7	Std Bracket	sample02			Xcalibur\data\Elan\Quan\Dox\Doxorubicin_101804_2chrom	B:2	
8	Std Bracket	sample03			Xcalibur\data\Elan\Quan\Dox\Doxorubicin_101804_2chrom	B:2	
9	Std Bracket	sample04			Xcalibur\data\Elan\Quan\Dox\Doxorubicin_101804_2chrom	B:3	
10	Std Bracket	sample05			Xcalibur\data\Elan\Quan\Dox\Doxorubicin_101804_2chrom	B:3	
11	Std Bracket	sample06			Xcalibur\data\Elan\Quan\Dox\Doxorubicin_101804_2chrom	B:3	
12	Std Bracket	sample07			Xcalibur\data\Elan\Quan\Dox\Doxorubicin_101804_2chrom	B:4	
13	Std Bracket	sample08			Xcalibur\data\Elan\Quan\Dox\Doxorubicin_101804_2chrom	B:4	
14	Std Bracket	sample09			Xcalibur\data\Elan\Quan\Dox\Doxorubicin_101804_2chrom	B:4	
15	Blank	blankB01			Xcalibur\data\Elan\Quan\Pact\Pact_chrom2	B:5	
16	Blank	blankB02			Xcalibur\data\Elan\Quan\Pact\Pact_chrom2	B:5	
17	Blank	blankB03			Xcalibur\data\Elan\Quan\Pact\Pact_chrom2	B:5	
18	Blank	blankB04			Xcalibur\data\Elan\Quan\Pact\Pact_chrom2	B:5	
19	Blank	blankB05			Xcalibur\data\Elan\Quan\Pact\Pact_chrom2	B:5	
20	Std Bracket	sample15			Xcalibur\data\Elan\Quan\Pact\Pact_chrom2	B:6	
21	Std Bracket	sample16			Xcalibur\data\Elan\Quan\Pact\Pact_chrom2	B:6	
22	Std Bracket	sample17			Xcalibur\data\Elan\Quan\Pact\Pact_chrom2	B:6	
23	Std Bracket	sample18			Xcalibur\data\Elan\Quan\Pact\Pact_chrom2	B:7	
24	Std Bracket	sample19			Xcalibur\data\Elan\Quan\Pact\Pact_chrom2	B:7	
25	Std Bracket	sample20			Xcalibur\data\Elan\Quan\Pact\Pact_chrom2	B:7	
26	Std Bracket	sample21			Xcalibur\data\Elan\Quan\Pact\Pact_chrom2	B:8	
27	Std Bracket	sample22			Xcalibur\data\Elan\Quan\Pact\Pact_chrom2	B:8	
28	Std Bracket	sample23			Xcalibur\data\Elan\Quan\Pact\Pact_chrom2	B:8	
*							

Sample Information C:\Xcalibur\Data\Elan\102104 De...

SampleType: Blank
Sample Name: blank Dox
File Name: blank02
Sample ID: blank
Path: C:\Xcalibur\Data\Elan\102104 Demo\
Instrument File: C:\Xcalibur\data\Elan\Quan\Dox\Dox
Processing Method: C:\Xcalibur\data\Elan\Quan\Dox\Dox
Calibration File:
Pos: B:1
Inj Volume: 10
Level:
Samp Weight: 0
Sample Volume: 0
ISTD Corr Amt: 0
Dill Factor: 1
Study: elan
Client:
Laboratory:
Company:
Phone:
Comment:

A check box appears to the left of the All Sequences folder, each queued sequence, and each sample. During a sequence run, the All Sequences folder, the folder for the active sequence, and the vial icon for the active sample have green backgrounds (Figure 62). The vial icon for a completed sample has a blue background and a large cross (☒) in its check box (Figure 63).

Figure 62. Acquisition queue with one queued sequence, a sample that is currently running, and two inactive samples

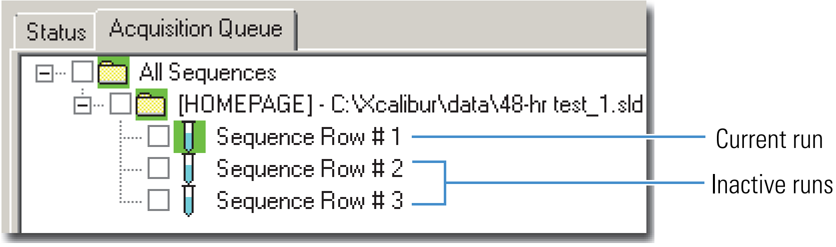
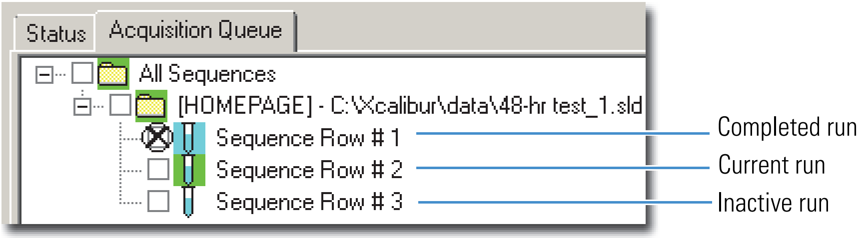


Figure 63. Acquisition queue with one queued sequence, a completed sample, a sample that is currently running, and one inactive sample



You can delete inactive samples and inactive sequences from the queue.

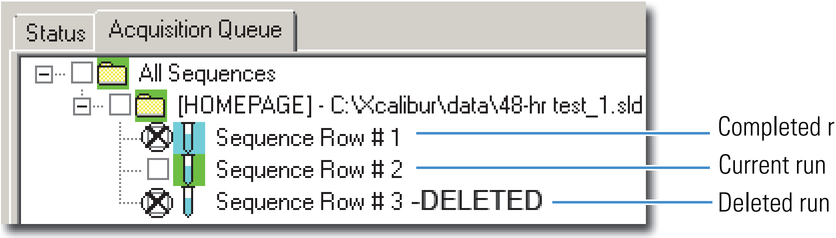
❖ To delete inactive samples from the queue

1. Select the check box to the left of the inactive samples that you want to delete.
2. Press the DELETE key.

   The data system identifies each deleted samples by a large cross in its check box (☒) and appends DELETED to the end of the sequence row.

   Figure 64 shows a sequence with one completed sample, one active sample, and one deleted sample. When the current run ends, the sequence will disappear from the queue.

Figure 64. Sequence with a deleted run

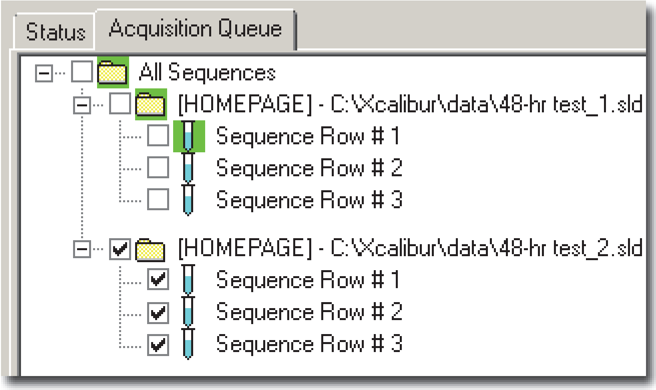


❖ To delete inactive sequences from the queue

1. Select the check box to the left of the inactive sequence or sequences that you want to delete.

   The data system automatically selects all of the sample check boxes in the selected sequence (Figure 65).

   Figure 65. Sequence queue with a sequence selected for deletion

   Sequence selected for deletion

2. Press the DELETE key.

   The deleted sequence disappears from the queue.

❖ To view the sample information for a sample in the acquisition queue

1. On the Acquisition Queue page of the Information view, do one of the following:
   - Right-click a sample to open a shortcut menu. Then, choose **Properties**.
   - Double-click a sample.

   The Sample Information dialog box opens. This dialog box shows the parameters for all of the sequence columns.

2. To keep the Sample Information dialog box open, click the pin icon.

❖ To close the sample information dialog box

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.

❖ To view the sequence information

1. On the Acquisition Queue page of the Information view, right-click a sequence and choose **Properties**.

   The Sample Information dialog box opens.

2. Pin the dialog box.

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

Batch Reprocessing a Sequence

The topics in this section describe how to batch reprocess a sequence:

- Adding the Quantitative Processing Information to a Sequence
- Reprocessing a Sample Batch
- Managing the Xcalibur Processing Queue

Adding the Quantitative Processing Information to a Sequence

If you acquired a sequence of raw data files for a sample set with unknowns, calibration standards, QC samples (optional), and blanks (optional), but you did not add a processing method to the sequence before acquiring the data files, follow this procedure to set up the sequence for quantitative batch reprocessing.

❖ To prepare an acquisition sequence for quantitative reprocessing

1. Open the acquisition sequence in the Sequence Setup view.
2. In the Processing Method column, double-click the first row.

   The Select Processing Method dialog box opens.
3. Select an appropriate processing method and click **Open**.

   The data system populates the Processing Method column with the selected processing method.
4. For each sequence row, click the **Sample Type** column to display the Sample Type list and select the appropriate sample type from the list.
5. Select the appropriate level for the calibration and QC standards as follows:
   - For each row that contains a calibration standard, click the **Levels** column and select the appropriate calibration level from the list.
   - For each row that contains a QC standard, click the **Levels** column and select the appropriate QC level from the list.
6. Save the modified sequence, and then batch reprocess the sequence as described in the next procedure, “Reprocessing a Sample Batch.”

Reprocessing a Sample Batch

Use the Batch Reprocess Setup dialog box to batch reprocess the data files in a sequence. For information about the parameters in the Batch Reprocess dialog box, see “Batch Reprocess Setup Dialog Box” on page 218.

❖ To batch reprocess the data files in a sequence

1. Open the sequence that contains the data files that you want to reprocess as follows:
   a. From the Sequence Setup view, choose **File > Open**.
   b. Browse to the sequence that you want to open and select it.
   c. Click **Open**.

      The sequence (list of data files and associated run parameters) appears in the Sequence Setup view.
2. If the sequence does not contain a processing method, add one as follows:
   a. Double-click any row in the Processing Method column.

      The Select Processing Method dialog box opens.

   b. Browse to and select an appropriate processing method.
   c. Click **Open** to select the method and to close the dialog box.

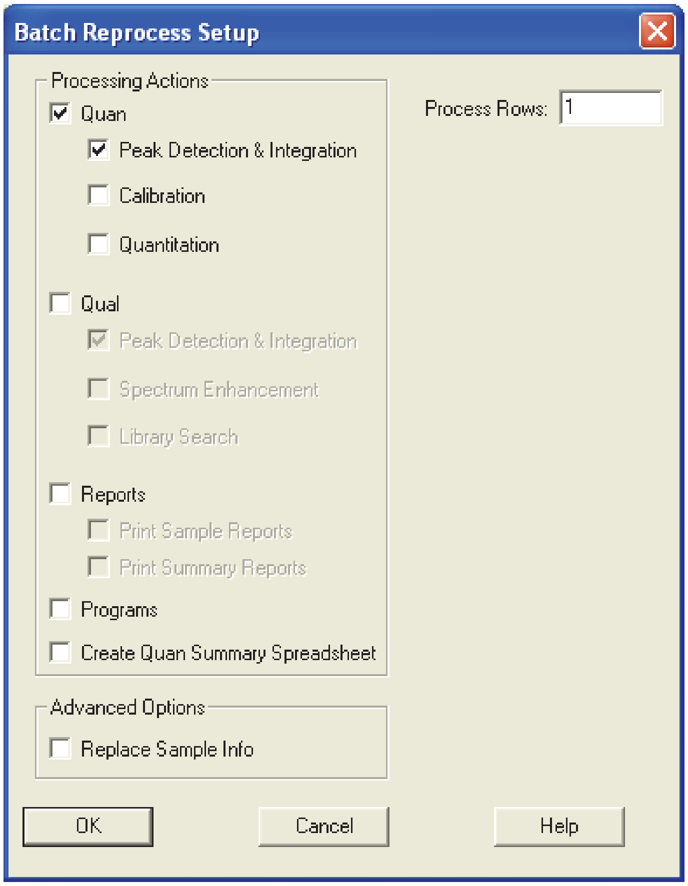
      All of the sequence rows become populated with the selected processing method.
3. To select the rows that you want to process, drag in the row number column to highlight the rows.
4. Do one of the following:
   - Click the **Batch Reprocess** icon, Σ, on the Sequence Editor toolbar.

   –or–

   - Choose **Actions > Batch Reprocess**.

   The Batch Reprocess Setup dialog box opens (Figure 66). The Process Rows box displays the sequence row or range of rows that you selected.

Figure 66. Batch Reprocess Setup dialog box



Batch Reprocess Setup

Processing Actions

☑ Quan
  ☑ Peak Detection & Integration
  ☐ Calibration
  ☐ Quantitation
☐ Qual
  ☑ Peak Detection & Integration
  ☐ Spectrum Enhancement
  ☐ Library Search
☐ Reports
  ☐ Print Sample Reports
  ☐ Print Summary Reports
☐ Programs
☐ Create Quan Summary Spreadsheet

Advanced Options

☐ Replace Sample Info

Process Rows: 1

5. To change the rows to be processed, type the first and last row to be processed in the Process Rows box.

   The format depends on the number of rows:

   - For one sample: *rownumber*
   - For multiple samples: *firstrownumber–lastrownumber*

6. In the Processing Actions area, select the processing actions for this set of data files as follows:

   - To enable the quantitative section of the processing method, select the **Quan** check box, and then select one or more of the following:
     - To apply the peak detection and integration parameters in the processing method, select the **Peak Detection and Integration** check box.
     - To create new calibration curves for each named component in the processing method, select the **Calibration** check box.
     - To quantitate all of the named components, select the **Calibration** and **Quantitation** check boxes.

- To enable the qualitative section of the processing method, select the **Qual** check box, and then select one or more of the following:
  - To apply the peak detection and integration settings for the unnamed peaks in the sample mixture, select the **Peak Detection and Integration** check box.

    For a qualitative analysis, the data system uses the peak detection and integration settings on a per-detector basis. For PDA data, the default peak detection algorithm is Avalon. For MS data, the default peak detection algorithm is ICIS.
  - To apply the spectrum enhancement settings of the processing method, select the **Spectrum Enhancement** check box.
  - To activate the library search settings of the processing method, select the **Library Search** check box.
- To print reports, select the **Reports** check box, and then select the report types:
  - To print a sample report for each injection, select the **Print Sample Reports** check box.
  - To print summary reports, select the **Print Summary Reports** check box.
  - To run the programs or macros that are enabled in the processing method, select the **Programs** check box.
  - To create a summary spreadsheet that opens in Microsoft™ Excel, select the **Create Quan Summary Spreadsheet** check box.

7. To replace information in the data file with information in the active sequence, select the **Replace Sample Info** check box in the Advanced Options area.
8. To save the settings and close the dialog box, click **OK**.

   The data systems begins the batch reprocessing of the selected sequence rows.

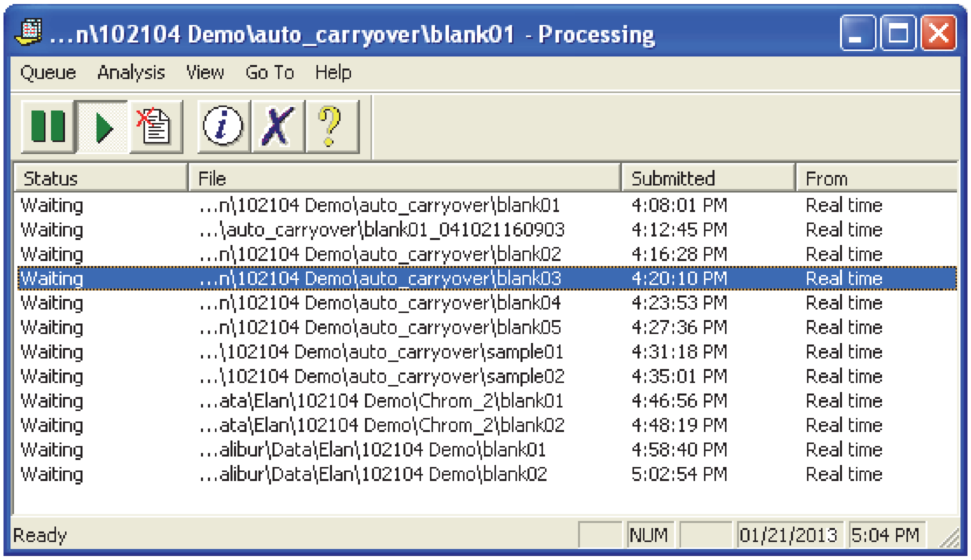
Managing the Xcalibur Processing Queue

The Queue Manager, shown in Figure 67, provides additional functions for managing queued processing sequences. 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.

❖ To manage the Xcalibur processing queue

1. From the Home Page window, choose **Tools > Queue Manager** (Figure 67).

Figure 67. Queue Manager window



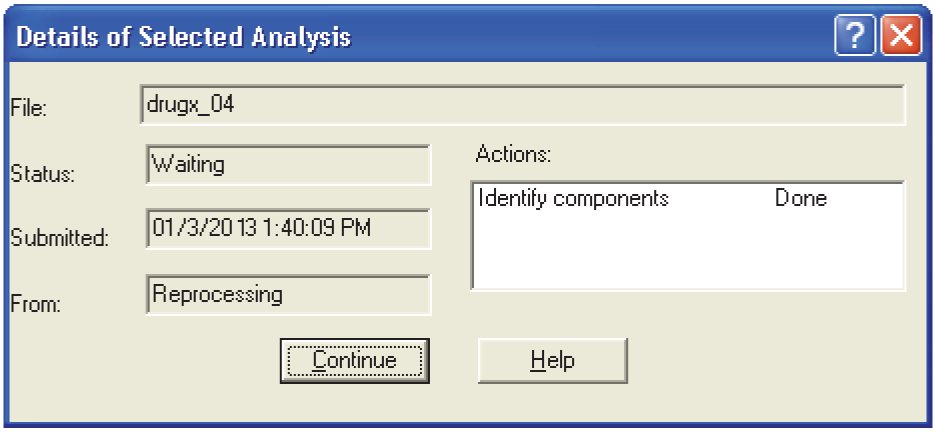
Status	File	Submitted	From
Waiting	...n\102104 Demo\auto_carryover\blank01	4:08:01 PM	Real time
Waiting	...\auto_carryover\blank01_041021160903	4:12:45 PM	Real time
Waiting	...n\102104 Demo\auto_carryover\blank02	4:16:28 PM	Real time
Waiting	...n\102104 Demo\auto_carryover\blank03	4:20:10 PM	Real time
Waiting	...n\102104 Demo\auto_carryover\blank04	4:23:53 PM	Real time
Waiting	...n\102104 Demo\auto_carryover\blank05	4:27:36 PM	Real time
Waiting	...\102104 Demo\auto_carryover\sample01	4:31:18 PM	Real time
Waiting	...\102104 Demo\auto_carryover\sample02	4:35:01 PM	Real time
Waiting	...ata\Elan\102104 Demo\Chrom_2\blank01	4:46:56 PM	Real time
Waiting	...ata\Elan\102104 Demo\Chrom_2\blank02	4:48:19 PM	Real time
Waiting	...alibur\Data\Elan\102104 Demo\blank01	4:58:40 PM	Real time
Waiting	...alibur\Data\Elan\102104 Demo\blank02	5:02:54 PM	Real time

Ready NUM 01/21/2013 5:04 PM

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**.

     The Details of Selected Analysis dialog box opens (Figure 68).
3. To close the Queue Manager window, press ALT+F4.

Figure 68. Details of Selected Analysis dialog box



Details of Selected Analysis

File: drugx_04

Status: Waiting

Submitted: 01/3/2013 1:40:09 PM

From: Reprocessing

Actions:

Identify components	Done

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.

6

Importing and Exporting Sequences

To import or export a sequence, follow these procedures:

Contents

- Changing the List Separator Character
- Checking Sequence Quality Before Importing
- Importing a Sequence
- Exporting a Sequence

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 the data system computer's operating system. The application generates an invalid file message if you try to import a file where the list separator character is different from 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 to a comma for the Windows 7 operating system

1. From the Windows taskbar, choose **Start > Settings > Control Panel**.

   The Control Panel window opens.

2. In the View By list, select **Small Icons** or **Large Icons**.

3. Click **Regional and Language Options**.

   The Region and Language dialog box opens to the Formats page.

4. Click **Additional Settings**.

   The Customize Formats dialog box opens to the Numbers page.

5. In the List Separator box, type a comma.
6. Click **Apply** to apply the new setting. Then click **OK** to close the Numbers page.
7. Click **OK** to close the Region and Language Options dialog box.
8. Close the Control Panel.

Checking Sequence Quality Before Importing

Before importing a .csv file, verify 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 .csv can be imported and converted to a sequence file

1. Create a comparison .csv file with the correct formatting by converting an example Xcalibur sequence file as follows:
   a. Open the Sequence Setup view.
   b. Choose **File > Open.**
   c. In the Look In box, browse to the [*drive*:]\Xcalibur\examples\methods folder and select **steroid.sld**.
   d. Click **Open**.
   e. To remove all but the first row of the sequence, click row number 2 and drag your cursor to the last row number. Then, press DELETE.

      The Delete Rows dialog box opens. If you are deleting rows 2 through 13 of the steroids sequence, the dialog displays this query: Delete Rows 2 to 13?

   f. Click **Yes**.
   g. Choose **File > Save As** and save the edited sequence file with a new name.
2. Export the single-row sequence to a .csv file as follows:
   a. Choose **File > Export Sequence**.

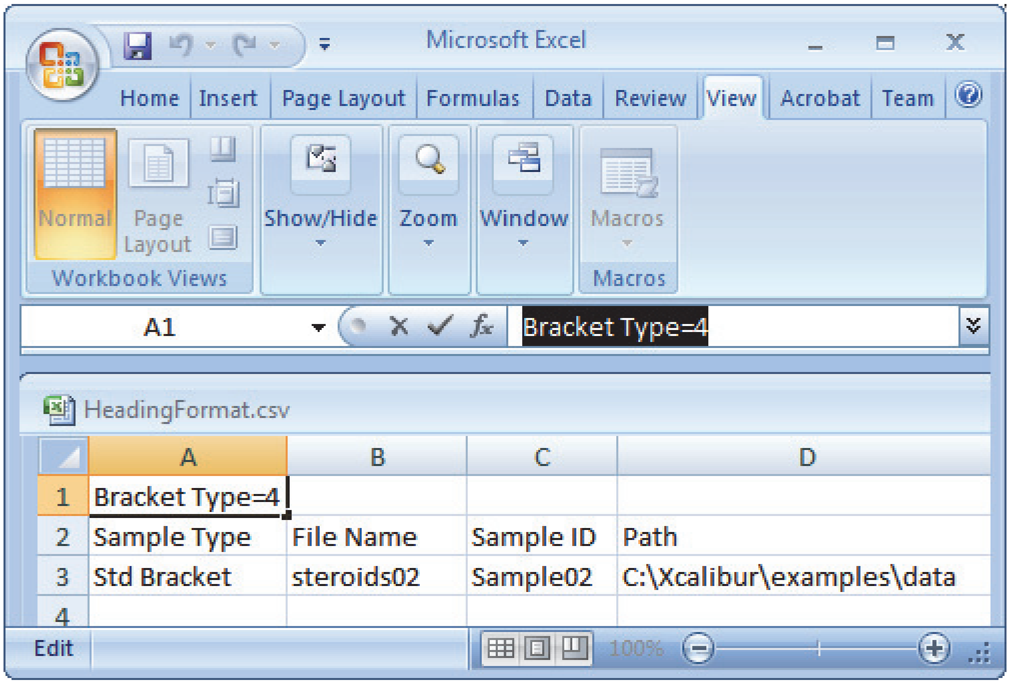
      The Export Sequence dialog box opens.

   b. Click **Browse** and select the folder where you want to store the .csv file.
   c. In the Export to File box, type a name for the .csv file.
   d. Click **OK**.

3. Open 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 (Figure 69).

Figure 69. Example .csv file



A1 Bracket Type=4

HeadingFormat.csv

	A	B	C	D
1	Bracket Type=4			
2	Sample Type	File Name	Sample ID	Path
3	Std Bracket	steroids02	Sample02	C:\Xcalibur\examples\data
4				

4. Import the .csv file sequence back into the Xcalibur data system to verify the import process.

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.

For information about the parameters in the Import Sequence dialog box, see "Import Sequence Dialog Box" on page 228.

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, see "Checking Sequence Quality Before Importing" on page 124.

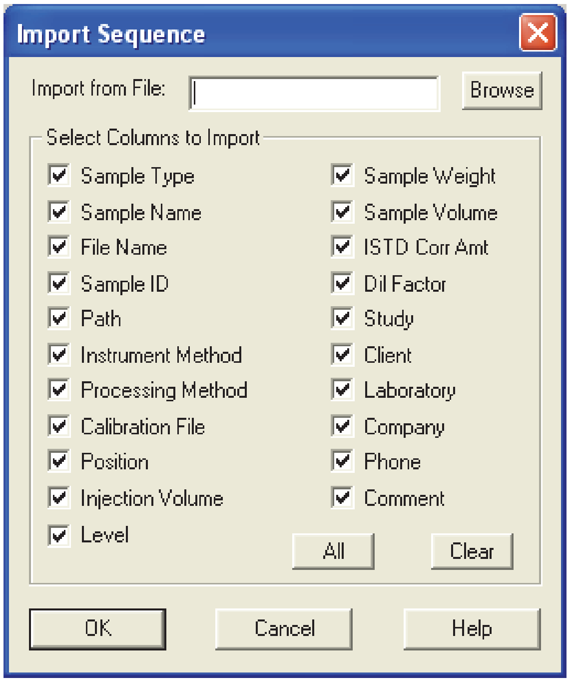
The imported sequence file must contain the same list separator character that is set in your computer control panel. To change the list separator column in your system, see "Changing the List Separator Character" on page 123.

❖ To import a sequence

1. Choose **File > Import Sequence** in the Sequence Setup view.

   The Import Sequence dialog box opens (Figure 70).

   Figure 70. Import Sequence dialog box



☑ 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
☑ Study
☑ Client
☑ Laboratory
☑ Company
☑ Phone
☑ Comment

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 data system assigns a .csv extension for you. If you enter an extension other than .csv, the following error message appears:

   > 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 that 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 imported file opens 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 123.

For information about the parameters in the Export Sequence dialog box, see "Export Sequence Dialog Box" on page 225.

❖ 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 that 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 check boxes.
   - Click **Clear** to clear all the column check boxes.
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 124.

7

Configuring and Managing the Data System

This chapter describes the data system configuration options, such as setting the font type and size for several of the views; the default directories for data files, methods, and report templates; and the default mass tolerance and mass precision values for processing. This chapter also describes how to use the File Converter utility to convert files from one format to another, how to check the disk space of the data system computer, and how to set up the instrument configuration in the Thermo Foundation platform.

For more information about setting up the instrument configuration, refer to the Thermo Foundation Help and the Help provided with each instrument device.

Contents

- Configuring the Xcalibur Data System
- Converting File Formats
- Checking Disk Space
- Confirming the Properties of Thermo Foundation Security Service
- Setting Up the Instrument Configuration in the Foundation Platform

Configuring the Xcalibur Data System

Use the Xcalibur Configuration dialog box to configure the data system. Use the pages in the dialog box to define the location of data, methods, and report templates on your data system computer; to edit customer information; to select the fonts that you want to use; and to select error handling options.

To configure the Xcalibur data system, follow these procedures:

- Opening the Xcalibur Configuration Dialog Box
- Selecting Default Folders
- Updating Customer Information
- Configuring Fonts
- Selecting a Default Peak Detection Algorithm
- Setting Up the Default Mass Options
- Selecting Default Labeling and Scaling Options
- Selecting Error Handling Options
- Defining the Dataset List

Opening the Xcalibur Configuration Dialog Box

❖ **To open the Xcalibur Configuration dialog box**

1. Choose **Start > Programs > Thermo Xcalibur > Xcalibur** from the taskbar.

   The Home Page window opens.

2. Choose **Tools > Configuration** from the Roadmap view of the Home Page window.

   The Xcalibur Configuration dialog box opens.

Selecting Default Folders

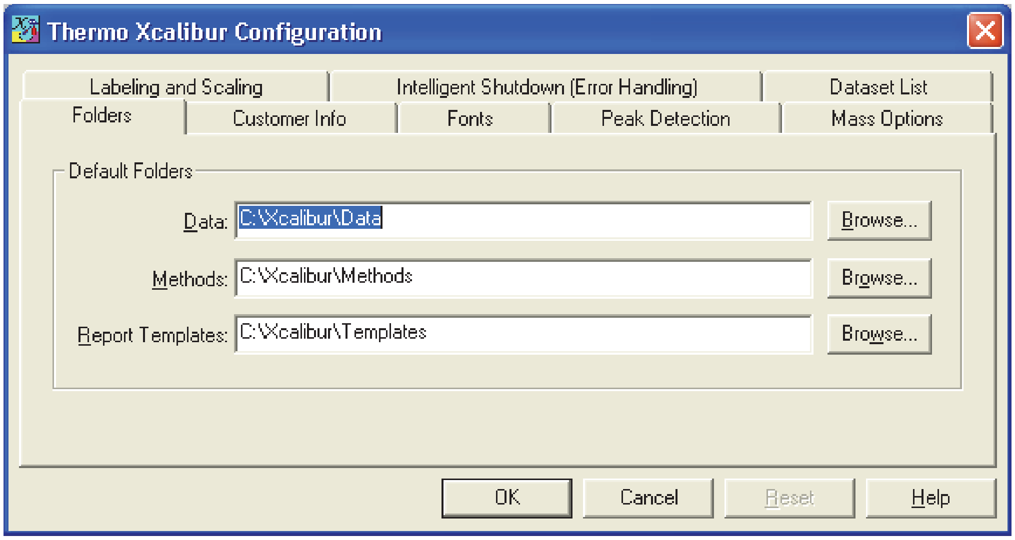
❖ **To select default file folders**

1. Open the Xcalibur Configuration dialog box as described in the previous topic, "Opening the Xcalibur Configuration Dialog Box."

2. Click the **Folders** tab.

   The Folders page of the Xcalibur Configuration dialog box opens (Figure 71).

Figure 71. Folders page



Data: C:\Xcalibur\Data

Methods: C:\Xcalibur\Methods

Report Templates: C:\Xcalibur\Templates

3. To specify the default folder for your Xcalibur data files, click **Browse** to the right of the Data box and select the folder.
4. To specify the default folder for your instrument methods, processing methods, and sequence files, click **Browse** to the right of the Methods box and select the folder.
5. To specify the default folder for your report templates, click **Browse** to the right of the Report Templates box and select the folder.
6. To save the settings, click **OK**.

Updating Customer Information

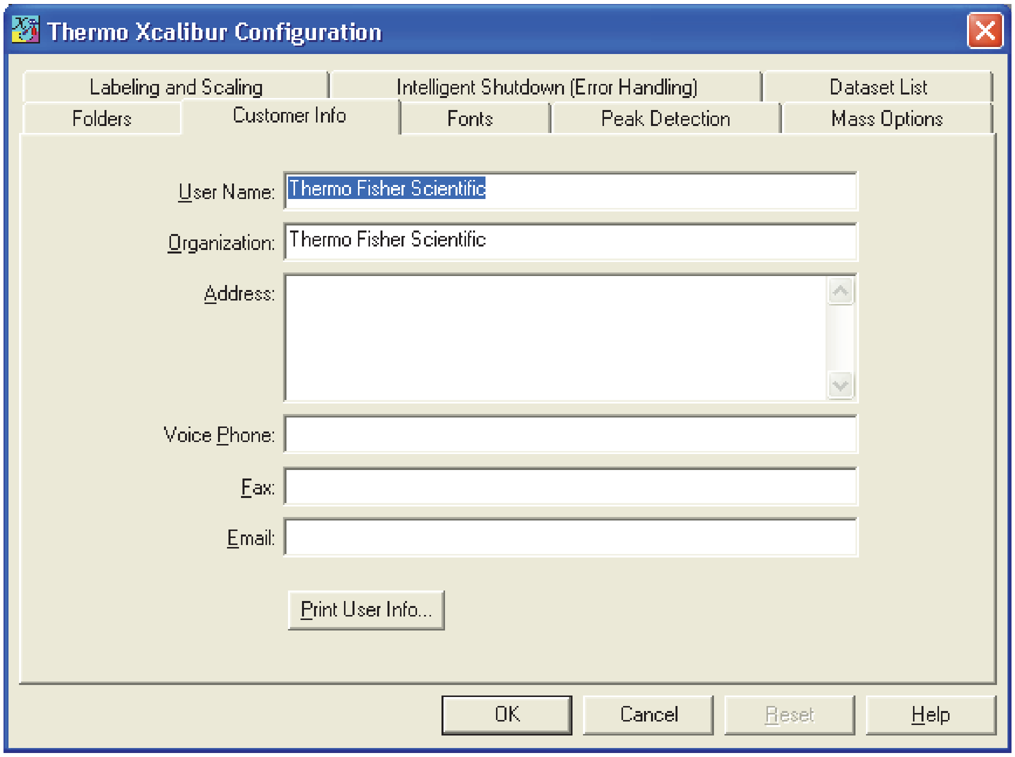
The Customer Info page of the Xcalibur Configuration dialog box displays the current licensing information for your Xcalibur MS detector. If this information is not already entered or it is incorrect, update the current entries.

❖ To update customer information

1. Open the Xcalibur Configuration dialog box as described in "Opening the Xcalibur Configuration Dialog Box" on page 130.
2. Click the **Customer Info** tab.

   The Customer Info page of the Xcalibur Configuration dialog box opens (Figure 72).

Figure 72. Customer Info page



User Name: Thermo Fisher Scientific

Organization: Thermo Fisher Scientific

3. If the information on the Customer Info page is incomplete or incorrect, type the new information.

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

Configuring Fonts

Grid plots in the Xcalibur data system use both a fixed-pitch font and a proportional font. The application default fixed-pitch font is Courier New with a minimum size of 7 points and a maximum size of 12 points. The Xcalibur default proportional font is Arial with a minimum size of 7 points and a maximum size of 12 points. To use other fonts, font styles, or font sizes, change the font settings.

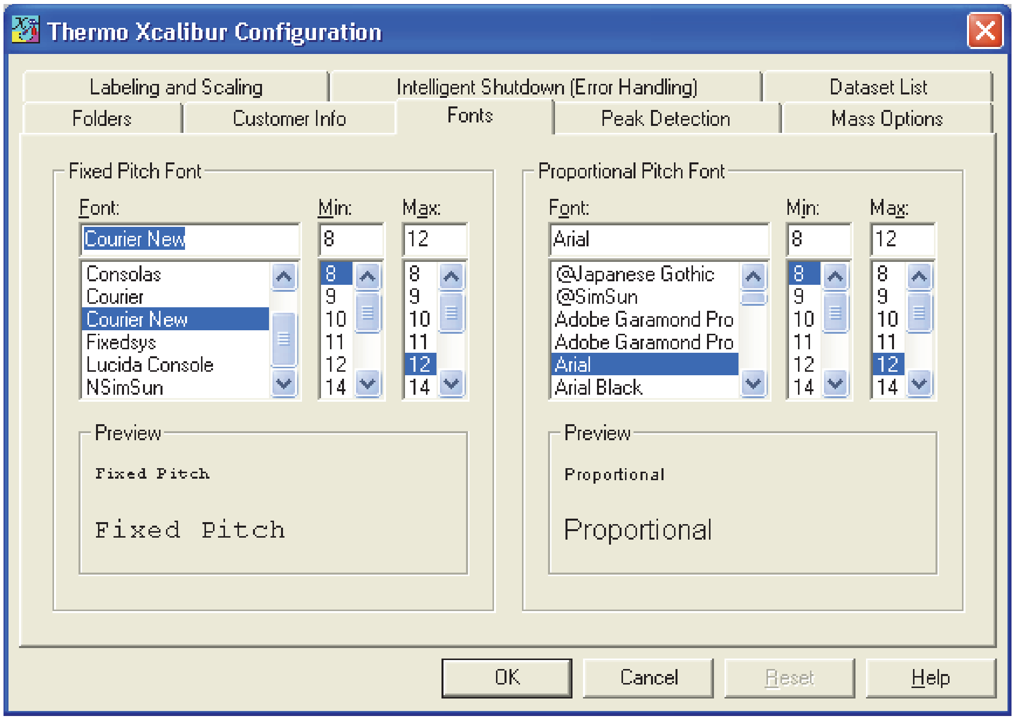
❖ To configure Xcalibur fonts

1. Open the Xcalibur Configuration dialog box as described in "Opening the Xcalibur Configuration Dialog Box" on page 130.

2. Click the **Fonts** tab.

   The Fonts page of the Xcalibur Configuration dialog box opens (Figure 73).

Figure 73. Fonts page



Fixed Pitch Font
Font: Courier New
Min: 8
Max: 12

Proportional Pitch Font
Font: Arial
Min: 8
Max: 12

3. To select a fixed-pitch font, do the following:
   a. Select a font name in the Fixed Pitch Font list.

      The selected font name is displayed at the top of the list.
   b. Enter the minimum size of the selected font in the Min list.
   c. Enter the maximum size of the selected font in the Max list.
   d. View the font sample, minimum size (top) and maximum size (bottom), in the Fixed Pitch Font Preview area.
4. To select a proportional font, do the following:
   a. Select a font name in the Proportional Pitch Font list.

      The selected font name is displayed at the top of the list.
   b. Enter the minimum size of the selected font in the Min list.
   c. Enter the maximum size of the selected font in the Max list.
   d. View the font sample, minimum size (top) and maximum size (bottom), in the Proportional Pitch Font Preview area.

Tip If the values in the spectrum list view appear in light gray when you work in the Qual Browser window, close the Qual Browser window and return to the Roadmap view of the Xcalibur Home Page. Choose **Tools > Configuration** to open the Xcalibur Configuration dialog box. Select the **Fonts** tab and set all font sizes to a minimum of 10 points.

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

Selecting a Default Peak Detection Algorithm

Use the Peak Detection page of the Xcalibur Configuration dialog box to view or change the default peak detection algorithms for all data types.

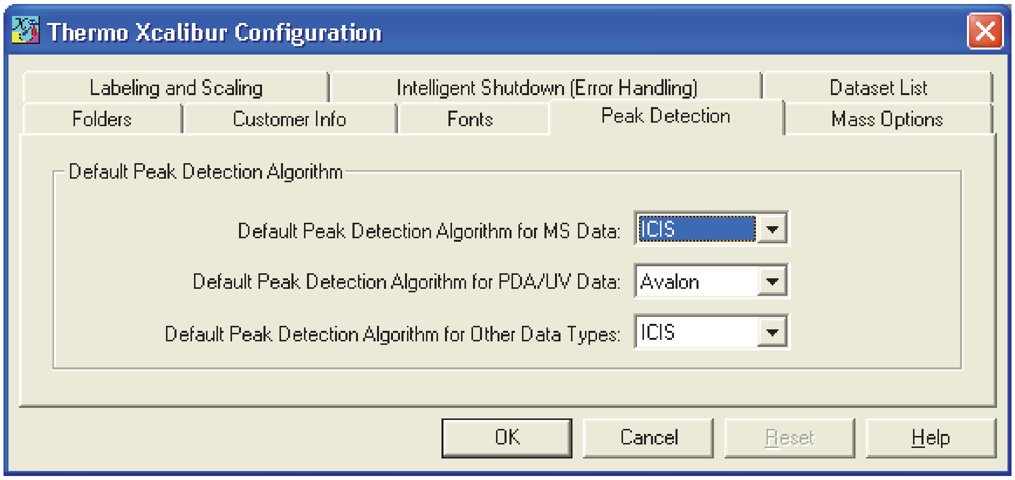
For more information, see "Peak Detection Page" on page 185.

❖ To specify peak detection parameters

1. Open the Xcalibur Configuration dialog box as described in "Opening the Xcalibur Configuration Dialog Box" on page 130.
2. Click the **Peak Detection** tab.

   The Peak Detection page of the Xcalibur Configuration dialog box opens (Figure 74).

   Figure 74. Peak Detection page



Default Peak Detection Algorithm for MS Data: ICIS
Default Peak Detection Algorithm for PDA/UV Data: Avalon
Default Peak Detection Algorithm for Other Data Types: ICIS

3. To select the Default Peak Detection Algorithm for MS Data, click an algorithm name from the corresponding list.
4. To select the Default Peak Detection Algorithm for PDA/UV Data, click an algorithm name from the corresponding list.
5. To select the Default Peak Detection Algorithm for Other Data Types, click an algorithm name from the corresponding list.
6. To save the settings, click **OK**.

Setting Up the Default Mass Options

Use the Mass Options page of the Xcalibur Configuration dialog box to set up the default mass tolerance, mass precision, and mass defect parameters that affect mass calculations and library searches.

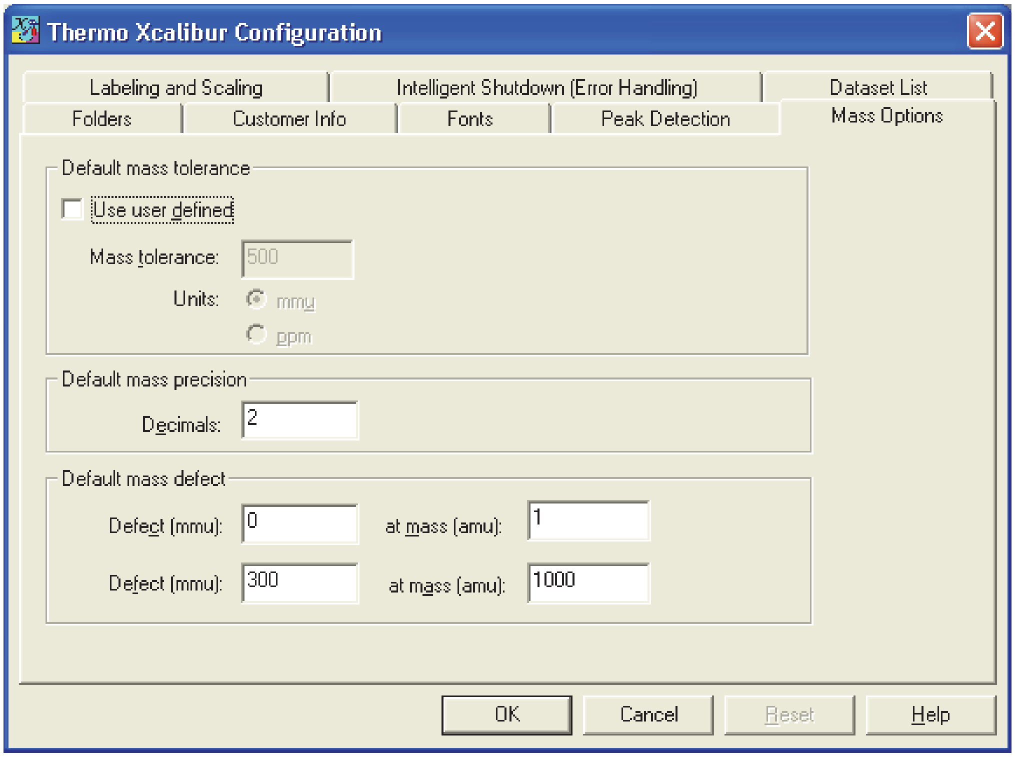
For more information, see “Mass Options Page” on page 184.

❖ To set up the mass options

1. Open the Xcalibur Configuration dialog box as described in “Opening the Xcalibur Configuration Dialog Box” on page 130.
2. Click the **Mass Options** tab.

   The Mass Options page of the Xcalibur Configuration dialog box opens (Figure 75).

Figure 75. Mass Options page



Default mass tolerance

☐ Use user defined

Mass tolerance: 500

Units: ● mmu ○ ppm

Default mass precision

Decimals: 2

Default mass defect

Defect (mmu): 0 at mass (amu): 1

Defect (mmu): 300 at mass (amu): 1000

3. Specify a default value for mass tolerance:
   a. Select the **Use User Defined** check box in the Default Mass Tolerance area.

      The Mass Tolerance box becomes available.
   b. Type a value from **0.1** to **50 000** in the Mass Tolerance box.
   c. Select either **mmu** (millimass units) or **ppm** (parts per million) from the Units options.

4. To specify a default value for mass precision, type a value from **0** to **5** in the Decimals box.
5. To specify the Default mass defects for lower values of mass, type a value from **–2500** to **2500** in the first Defect box. Then, type a mass value from **0** to **10 000** in the first At Mass box.

   For example, enter a value of **50** in the Defect box for a value of **200** in the At Mass box.
6. To specify the Default mass defects for higher values of mass, type a value from **–2500** to **2500** in the second Defect box. Then, type a mass value from **0** to **10 000** in the second At Mass box.

   For example, enter a value of **1000** in the Defect box for a value of **5000** in the At Mass box.
7. To save your settings, click **OK**.

Selecting Default Labeling and Scaling Options

Use the Labeling and Scaling page of the Xcalibur Configuration dialog box to view or change default parameter values for labels and scales of the *y* axes in the spectrum and chromatogram views.

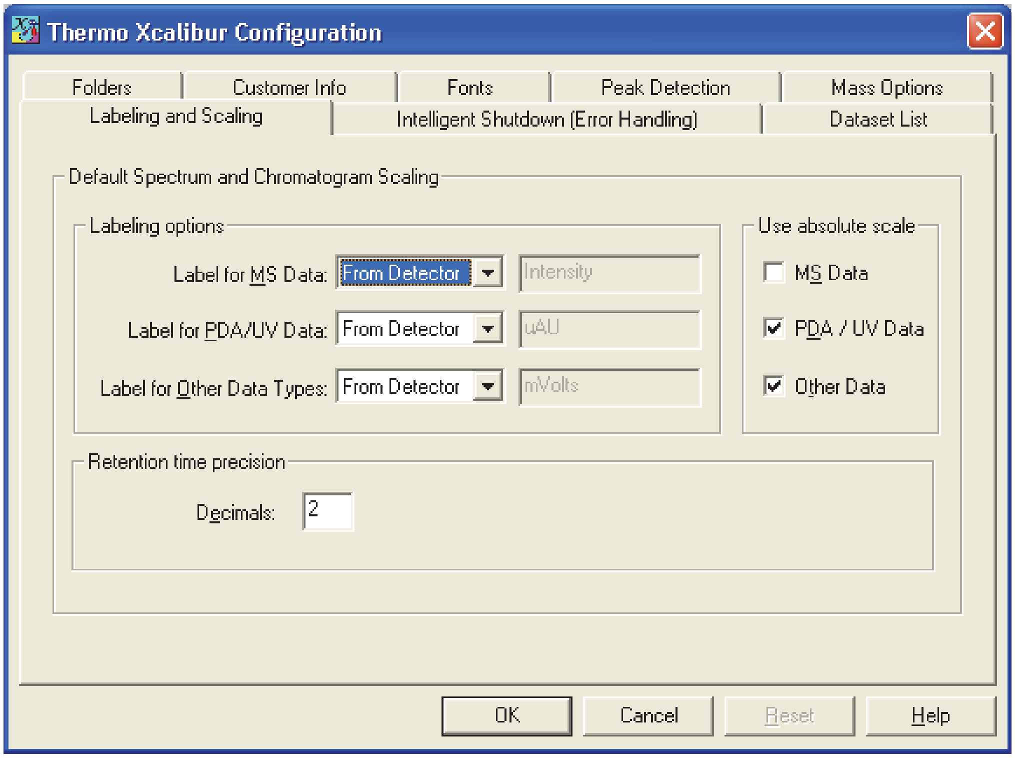
For more information, see "Labeling and Scaling Page" on page 183.

❖ To specify labeling and scaling parameters

1. Click the **Labeling and Scaling** tab.

   The Labeling and Scaling Page of the Xcalibur Configuration dialog box opens (Figure 76).

Figure 76. Labeling and Scaling page



Label for MS Data: From Detector Intensity

Label for PDA/UV Data: From Detector uAU

Label for Other Data Types: From Detector mVolts

☐ MS Data

☑ PDA / UV Data

☑ Other Data

Decimals: 2

2. In the Labeling Options area, to specify the Label for MS Data, select **From Detector** or **Custom** from the corresponding list.

   If you select **Custom**, type a label in the adjacent box.

3. To specify the Label for PDA/UV Data, select **From Detector** or **Custom** from the corresponding list.

   If you select **Custom**, type a label in the adjacent box.

4. To specify the Label for Other Data Types (other than MS and PDA/UV), select **From Detector** or **Custom** from the corresponding list.

   If you select **Custom**, type a label in the adjacent box.

5. In the Use Absolute Scale area, select the data types to display on the *y* axis.
6. In the Retention Time Precision area, type the number of decimal places to include when reporting retention times.
7. To save the settings, click **OK**.

Selecting Error Handling Options

Use the Intelligent Shutdown (Error Handling) page of the Xcalibur Configuration dialog box to define how the data system responds when an error occurs during data acquisition.

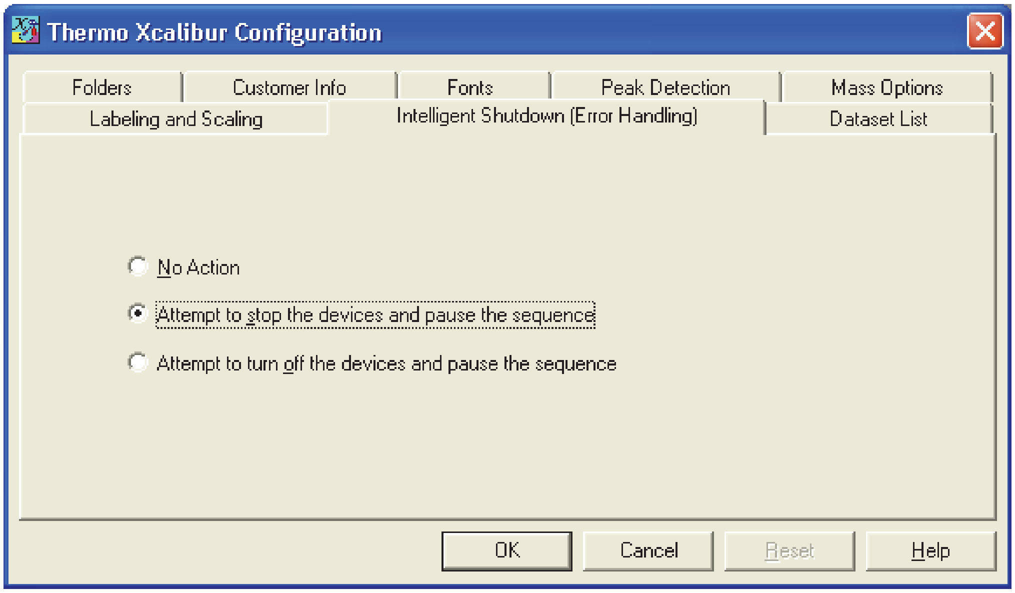
For more information, see "Intelligent Shutdown (Error Handling) Page" on page 182.

❖ To change the error handling option

1. Click the **Intelligent Shutdown** tab.

   The Intelligent Shutdown (Error Handling) page of the Xcalibur Configuration dialog box opens (Figure 77).

   Figure 77. Intelligent Shutdown (Error Handling page)



○ No Action

● Attempt to stop the devices and pause the sequence

○ Attempt to turn off the devices and pause the sequence

2. Select the error handling option, **Attempt to Stop the Devices and Pause the Sequence**.
3. To save the settings, click **OK**.

Defining the Dataset List

As the administrator, use the Dataset List page of the Xcalibur Configuration dialog box to define or edit the list of dataset names that the user can choose from when selecting a dataset.

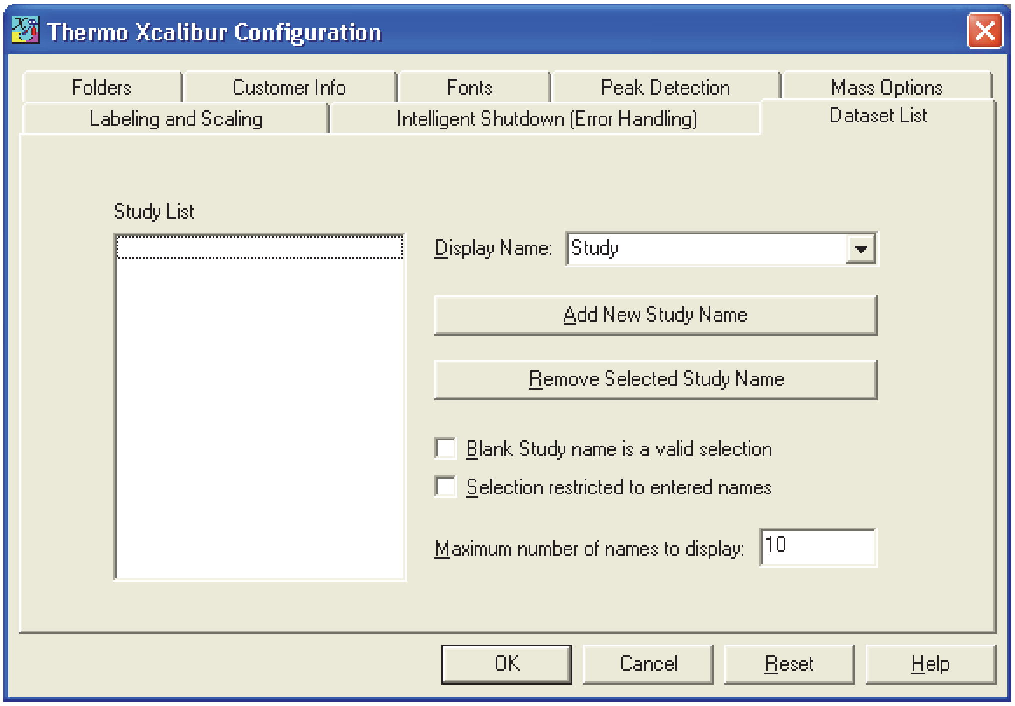
For more information, see "Dataset List Page" on page 178.

❖ To define the list of dataset names

1. In the Thermo Xcalibur Configuration dialog box, click the **Dataset List** tab.

   The Dataset List page of the Xcalibur Configuration dialog box opens (Figure 78).

   Figure 78. Dataset List page

   Display Name: Study

   ☐ Blank Study name is a valid selection

   ☐ Selection restricted to entered names

   Maximum number of names to display: 10

2. To specify the name for the data system to use for a dataset, either select a name from the Display Name list, or add a new name to the list.

3. To add new names to the Study List, do the following for each name that you want to add:

   a. Click **Add New Study Name**.

      The Create New Dataset Name dialog box opens.

   b. Type a name in the box and click **OK**.

      The new name appears in the Study List to the left.

Note If you change the display name to something besides Dataset, the data system renames the parameters on this page to reflect the change.

4. To delete a name from the list, select the name in the Study List and click **Remove Selected Study Name**.

5. To specify whether a blank study name is a valid selection, do the following:

   - Select the **Blank Dataset Name is a Valid Selection** check box to allow a user to select a blank name when asked to select a dataset in the Dataset Name Selector dialog box.

   - Clear this check box to require the user to select a valid dataset.

6. To specify whether the selection is restricted to the entered names, do the following:

   - Select the **Selection Restricted to Entered Names** check box to specify that only the names listed in the Study List appear in the Dataset Name Selector dialog box.

   - Clear this check box to specify that the names listed in the Study List as well as a those obtained from the database appear in the Dataset Name Selector dialog box.

7. To specify the maximum number of names to display in the Dataset Name Selector dialog box, type a number in the Maximum Number of Names to Display box.

8. To save the settings, click **OK**.

Converting File Formats

Use the Thermo File Converter application to convert data files from a format used in another data system to the Xcalibur .raw file type or to convert Xcalibur .raw files to other file types.

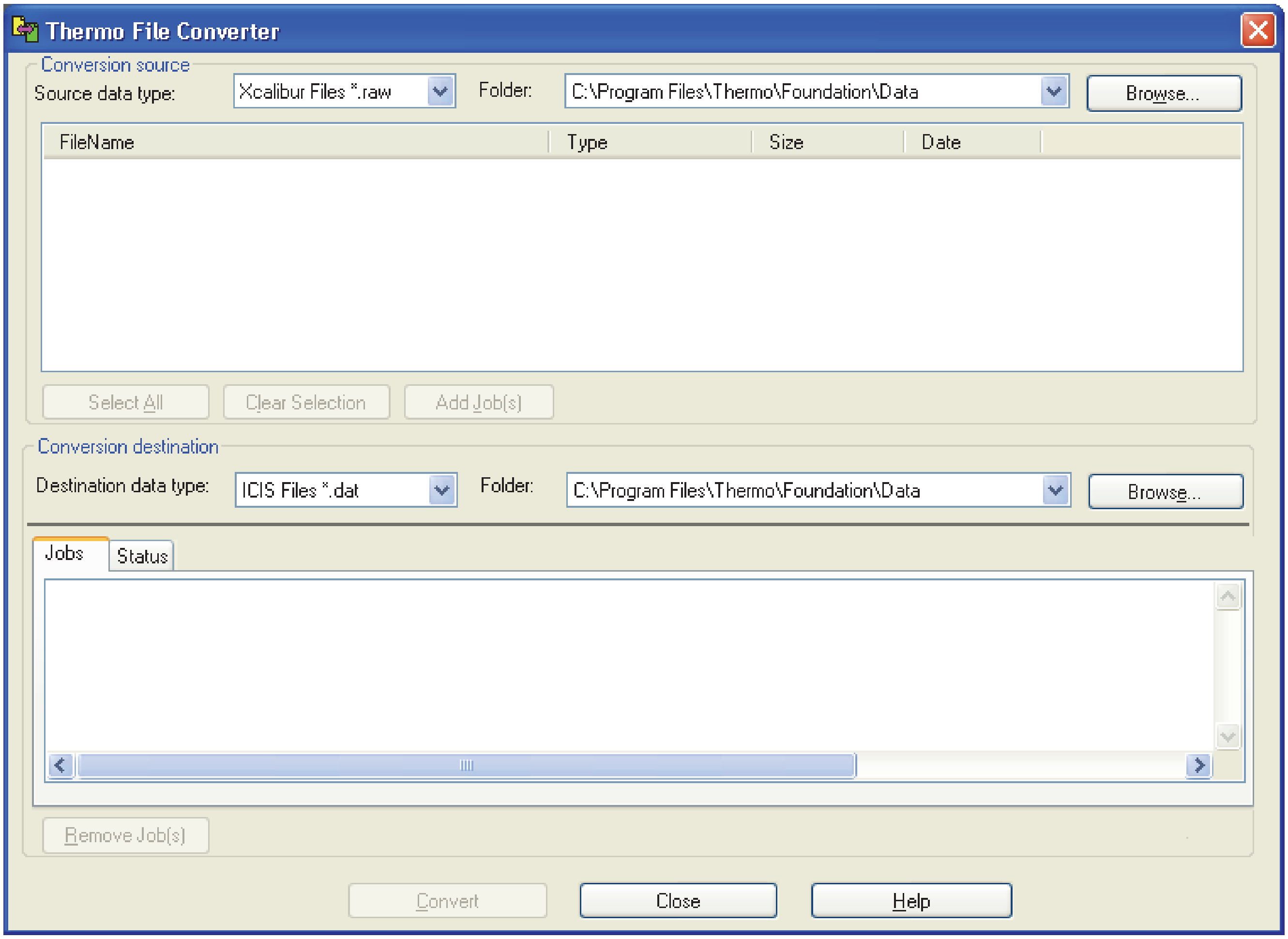
For more information, see “Thermo File Converter Application” on page 189.

❖ To convert data files from one file format to another with the Thermo File Converter application

1. Choose **Tools > File Converter** from the Roadmap view of the Home Page window.

   The Thermo File Converter Application opens (Figure 79).

Figure 79. Thermo File Converter dialog box



Source data type: Xcalibur Files *.raw
Folder: C:\Program Files\Thermo\Foundation\Data

Destination data type: ICIS Files *.dat
Folder: C:\Program Files\Thermo\Foundation\Data

2. To specify the source data type of the files you want to convert, select from the Source Data Type list in the Conversion Source area.

   The selections in the Source Data Type list are .raw, .dat, .ms, .cdf, and .spa. You can only batch process files with one source data type and one destination data type at a time. You can perform other data type conversions in separate batches.

3. To select the files to be converted, click **Browse** and select the folder that contains the files.

   The files appear in the Conversion Source list. The Xcalibur data system displays the File Name, Type, Size, and Date.

4. Create a list of files to convert using one of the following options:
   - To convert all of the files in the Conversion Source list, click **Select All**, and then click **Add Job(s)**.

     All of the files appear on the Jobs page in the Conversion Destination area at the bottom.
   - To convert a single file from the Conversion Source list, select the file and then click **Add Job(s)**.
   - To delete a file that appears in the Conversion Source list, select the file and then click **Clear Selection**.
5. To specify the destination data type of the files that you want to convert, select a destination from the Destination Data Type list in the Conversion Destination area.
6. To select a destination folder, click **Browse** to search for a folder to hold the converted files.

   The source files remain in their original directories.
7. To start the file conversion using batch processing of the files on the Jobs page, click **Convert**.

   You can monitor the conversion progress by clicking the Status tab in the Conversion Destination area.

   The application continues file conversion processing until all files are converted and stored in the specified destination folder.
8. To convert a different source data type, click **Clear Selection** to clear all files displayed in the Conversion Source list. Then repeat step 2 through step 7 for the other source data type.
9. To close the File Converter application, click **Close**.

Checking Disk Space

Use the Disk Space dialog box to determine how much available disk space you have on a disk drive.

❖ To open the Disk Space dialog box

Do one of the following:

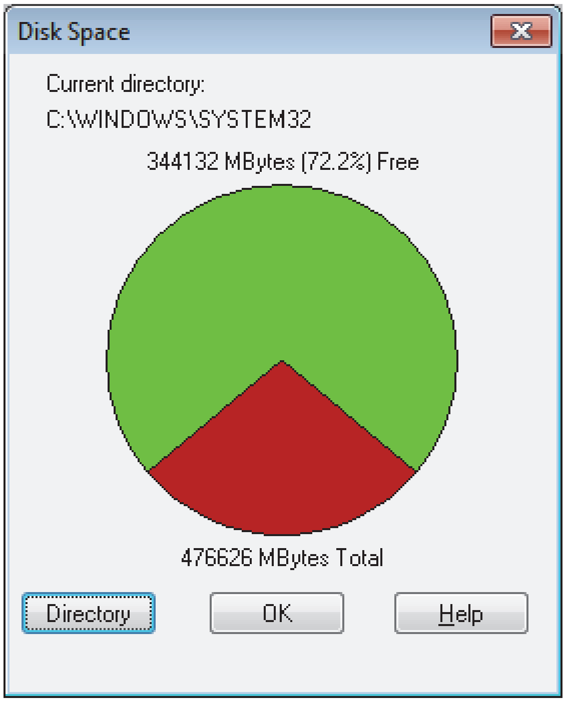
- From the Home Page menu, choose **Actions** > **Check Disk Space**.

–or–

- In the Sequence Editor toolbar, click the **Disk Space** icon, MB.

The Disk Space dialog box opens (Figure 80).

Figure 80. Disk Space dialog box



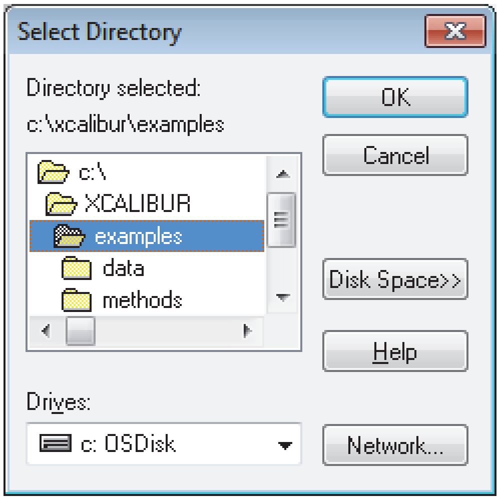
Current directory:
C:\WINDOWS\SYSTEM32
344132 MBytes (72.2%) Free
476626 MBytes Total

❖ To check the disk space for a particular directory

1. Click **Directory**.

   The Select Directory dialog box opens (Figure 81).

Figure 81. Select Directory dialog box



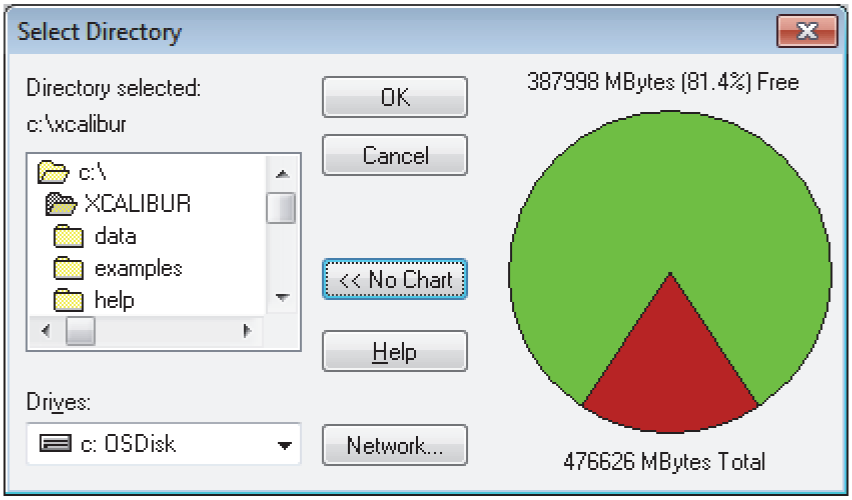
Directory selected:
c:\xcalibur\examples

Drives:
c: OSDisk

2. In the Drives list, select the drive of interest.
3. Click **Disk Space**.

   Information about the disk space appears on the right (Figure 82).

Figure 82. Select Directory dialog box with information about the disk space for drive C



Directory selected:
c:\xcalibur

Drives:
c: OSDisk

387998 MBytes (81.4%) Free

476626 MBytes Total

Confirming the Properties of Thermo Foundation Security Service

The authorization and auditing functions of an application such as the Xcalibur data system installed on the Thermo Foundation platform rely on two system services: the Thermo Foundation Security Service and the Thermo Foundation Database Service. These services are installed when you install the application software. They automatically start whenever a user restarts a workstation.

The main function of the Thermo Foundation Security Service, which is installed with the Xcalibur data system, is user authentication. If certain events require authentication, the Thermo Foundation Security Service verifies the user names and passwords entered.

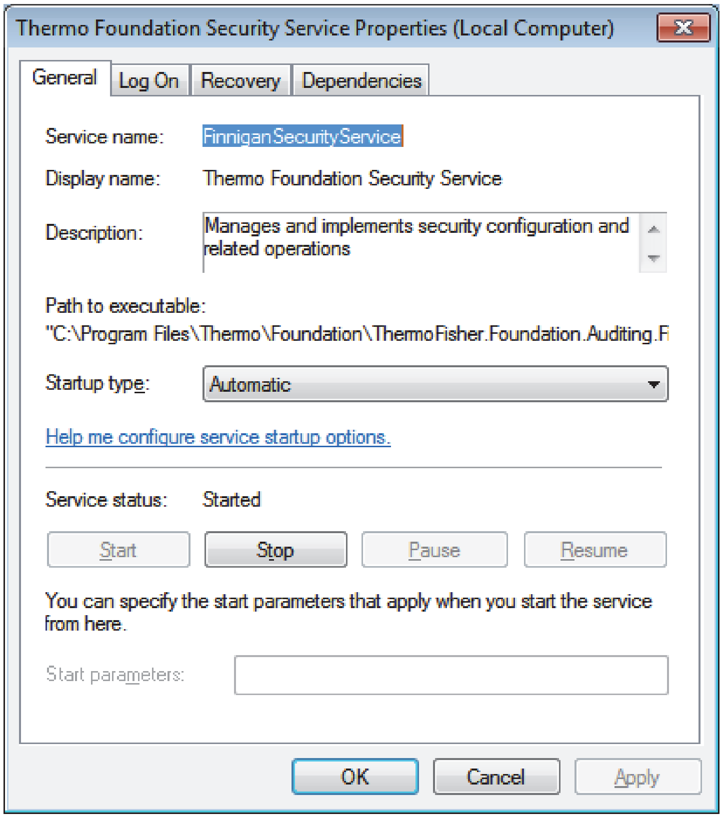
Note For information related to the Thermo Foundation Database Service, refer to the *Thermo Foundation Administrator Guide*.

❖ To confirm that the properties of the Thermo Foundation Security Service are set correctly

1. Open the Services window as follows:
   a. From the taskbar, choose **Start > Control Panel**.
   b. In the Adjust Your Computer Settings window, in the View By list, select **Category**. Then, choose **System and Security > Administrative Tools** and double-click **Services**.
2. Confirm the properties for the service as follows:
   a. Right-click **Thermo Foundation Security Service** and choose **Properties** from the shortcut menu.

   The Thermo Foundation Security Service Properties dialog box opens (Figure 83).

Figure 83. General page



Service name: FinniganSecurityService

Display name: Thermo Foundation Security Service

Description: Manages and implements security configuration and related operations

Path to executable:
"C:\Program Files\Thermo\Foundation\ThermoFisher.Foundation.Auditing.F

Startup type: Automatic

Service status: Started

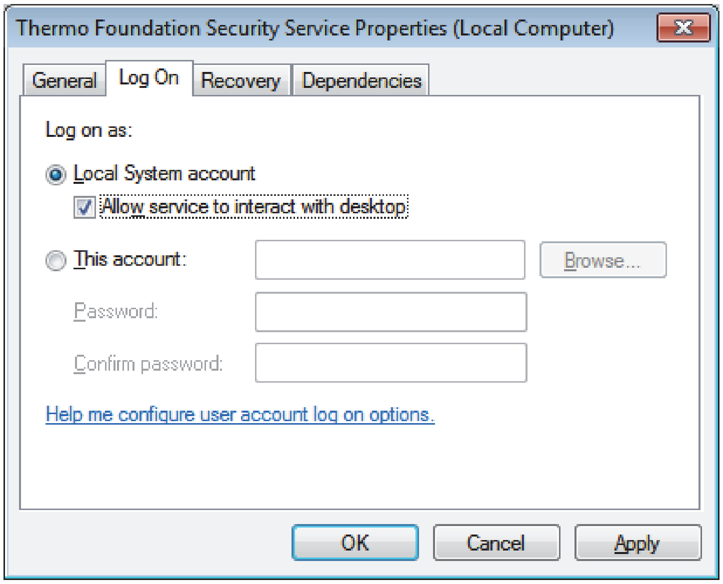
You can specify the start parameters that apply when you start the service from here.

b. On the General page, in the Startup Type list, select **Automatic**.

c. Confirm that Service Status reads **Started**.

d. Click the **Log On** tab to display the Log On page (Figure 84).

Figure 84. Log On page



Log on as:

● Local System account

☑ Allow service to interact with desktop

○ This account:

e. Under Log On As, select the **Local System Account** option.

f. Select the **Allow Service to Interact with Desktop** check box.

g. Click **OK** to close the dialog box.

Setting Up the Instrument Configuration in the Foundation Platform

To control your LC/MS or GC/MS system from the Xcalibur data system, you must first set up the instrument configuration in the Thermo Foundation™ platform. The instrument configuration includes the chromatography devices, the mass spectrometer, and the specific hardware options for these devices.

To set up the instrument configuration for your system, follow these procedures:

- Adding Devices to the Foundation Instrument Configuration
- Removing Devices from the Foundation Instrument Configuration

Adding Devices to the Foundation Instrument Configuration

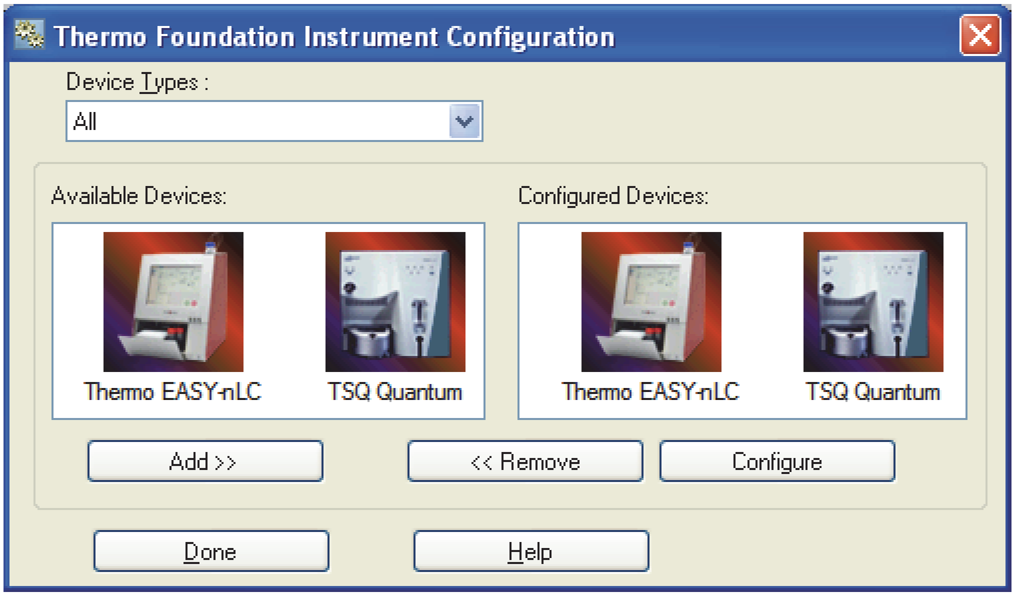
❖ To add hardware devices to the Foundation instrument configuration

1. Choose **Start > Programs** (or **All > Programs**) **> Thermo Foundation *x.x* > Instrument Configuration**, where *x.x* is the version.

> **Note** The data system computer must have compatible versions of the Foundation platform and the Xcalibur data system.

The Foundation Instrument Configuration dialog box opens (Figure 85).

Figure 85. Foundation Instrument Configuration window



2. To add devices to the instrument configuration, do the following for each device:

   a. In the Device Types list, select **All**.

      The Available Devices area lists the installed device drivers. If you do not see the device that you want to configure, you might need to install the device driver (instrument control software).

   b. In the Available Devices area, select the icon for the device you want to add.

      The device icon depresses to indicate that it is selected.

   c. To add the device to the Configured Devices area, click **Add**.

      A copy of the selected device icon appears in the Configured Devices area.

      Tip To copy a device icon to the Configured Devices area, you can also double-click the device icon in the Available Devices area.

3. To specify the configuration options for the devices in the Configured Devices area, do the following for each device:

   a. In the Configured Devices area, select the device icon for the device that you want to configure.

      The device icon depresses to indicate that it is selected.

   b. To configure the selected device, click **Configure**.

      The *DeviceName* Configuration dialog box opens (the device name corresponds to the selected device).

      Tip To open the *DeviceName* Configuration dialog box for a device, you can also double-click the device icon in the Configured Devices area.

   c. Enter the configuration information for the device.

      Tip For information about the configuration options for the current device, refer to the Help for the device.

   d. To save the settings and close the *DeviceName* Configuration dialog box, click **OK**.

      The Foundation Instrument Configuration dialog box reappears.

4. To save the instrument configuration settings and close the Foundation platform, click **Done**.

Removing Devices from the Foundation Instrument Configuration

❖ To remove hardware devices from the Foundation instrument configuration

1. Choose **Start > Programs > Thermo Foundation** ***x.x*** **> Instrument Configuration**, where *x.x* is the version.

   The Foundation Instrument Configuration window opens (see Figure 85 on page 147).

2. To remove a device from the instrument configuration, do the following:

   a. In the Configured Devices area, select the device icon that represents the device that you want to remove.

      The device icon depresses to indicate that it is selected.

   b. Click **Remove**.

   c. To save the settings and close the *DeviceName* Configuration dialog box, click **OK**.

      The Foundation Instrument Configuration window reappears.

3. To save the instrument configuration settings and close the window, click **Done**.

A

Home Page

This appendix describes the view, menus, toolbars, and dialog boxes that are available from the Home Page window. This appendix also describes the Queue Manager window.

Use the Home Page window to control or access all data system functions and features from three main views (Roadmap view, Sequence Setup view, and Real-Time Plot view). The visibility of some features is based on the instrument under data system control.

Note Before you can control an analytical instrument from the Xcalibur data system, you must first specify the instrument configuration in the Foundation platform.

Contents

- Home Page Views
- Home Page Menus
- Home Page Toolbars
- Home Page Dialog Boxes
- Queue Manager Window
- Thermo File Converter Application

Home Page Views

The Home Page window has these four views:

- "Information View," on the next page
- "Roadmap View" on page 156
- "Real Time Plot View" on page 157
- "Sequence Setup View" on page 199

The Information view has two tabbed pages and is located on the left side of the window. You can display it alongside any of the three main views.

Roadmap view

Use to access the other Xcalibur windows.

Sequence Setup view

Use to create, run, and batch reprocess sequences.

Real Time Plot view

Use to view real-time data acquisition.

You can access the Instrument Setup, Processing Setup, Qual Browser, Quan Browser, and Library Browser windows from the Home Page window:

Use the Instrument Setup window to create instrument methods and to access the direct controls for the configured instrument devices.

For more information, see Chapter 2, "Creating Instrument Methods and Using the Direct Controls," and Appendix B, "Instrument Setup."

Use the Processing Setup window to create processing methods.

For more information, see Chapter 3, "Creating Processing Methods," and Appendix D, "Processing Setup."

Use the Qual Browser window to review qualitative data.

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

Use the Quan Browser window to review quantitative data.

Refer to the *Xcalibur Quan Browser Reviewing Quantification Data User Guide*.

Use the Library Browser window to create custom user libraries of spectral data and to run library searches.

Refer to the *Xcalibur Library Browser Creating and Searching Libraries User Guide*.

Information View

The Information view consists of these two pages:

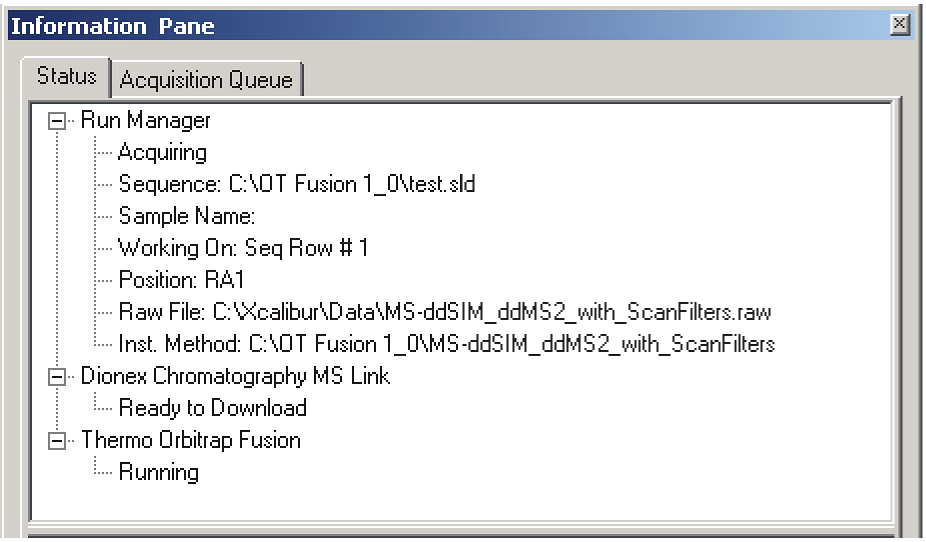
- Status Page – Information View
- Acquisition Queue Page – Information View

Note The Information view is normally displayed on the left side of the Home Page window. If this view is not displayed, the view has been turned off.

Status Page – Information View

Figure 86 shows the Status page of the Information view.

Figure 86. Status page of the Information view



Run Manager
- Acquiring
- Sequence: C:\OT Fusion 1_0\test.sld
- Sample Name:
- Working On: Seq Row # 1
- Position: RA1
- Raw File: C:\Xcalibur\Data\MS-ddSIM_ddMS2_with_ScanFilters.raw
- Inst. Method: C:\OT Fusion 1_0\MS-ddSIM_ddMS2_with_ScanFilters

Dionex Chromatography MS Link
- Ready to Download

Thermo Orbitrap Fusion
- Running

The Status page of the Information view provides the following overall summary of the Xcalibur data system status. Table 4 describes the status readouts under Run Manager.

Table 4. Run Manager and Instrument areas on the Status page (Sheet 1 of 2)

Readback	Description
Run Manager	
Check Devices	Displays the instrument status as Ready to Download, Devices Are Getting Ready, or Acquiring
Sequence	Displays the name of the current sequence. If you pause the sequence, this status readout displays PAUSED.
Sample Name	Displays the current sample name. The SampleName column is an optional column in the sequence table that contains the user-specified sample name for a sample

Table 4. Run Manager and Instrument areas on the Status page (Sheet 2 of 2)

Readback	**Description**
Working On	Displays the current sequence row.
Position	Displays the current vial or microwell position when the autosampler is the start instrument. Refer to the documentation provided with the autosampler for information about the vial notation.
Raw File	Displays the current raw data file name.
Inst. Method	Displays the current instrument method.
Instruments	
The readback status of each Xcalibur-configured instrument appears on the Status page. When you click the *Instrument Name* on the Status page, the Xcalibur data system displays current readings for the instrument on tabbed pages below the Run Manager pane. The information displayed reflects the parameters that you set for the instrument in the Instrument Setup window. Right-click any of the instruments to display a shortcut menu, where you can switch your instrument to On, Off, or Standby mode.	

Acquisition Queue Page – Information View

The Acquisition Queue page of the Information view displays all of the sequences that have been submitted to the current Xcalibur acquisition queue. The processing sequence proceeds from the top sequence to the bottom sequence and from the top sequence row to the bottom sequence row for each sequence. The data system places a large “X” to the left of each completed sequence row as it acquires the samples.

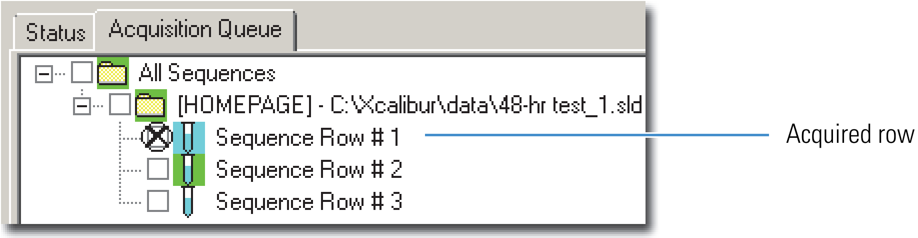
The All Sequences folder lists the queued sequences. The folder beneath the All Sequences folder in the directory tree lists the current acquisition sequence. The data system lists the sequence rows shown in the Sequence folder by their directory paths and file name, for example: C:\methods\Test.sld.

The submitted sequences are organized in a tree view control that displays the directories as an indented outline. Click the + button to expand the directory, or click the – button to collapse the directory. Each row of the tree view control contains a check box to indicate the status:

- As the data system acquires a sequence or sequence row, a large “X” appears in the check box.
- If you select a sequence or sequence row, a small check appears in the check box.
- f you delete the selected sequence or sequence row, and the word DELETED appears to the right of the sequence or sequence row.

Figure 87 shows an acquisition queue with one acquired sample.

Figure 87. Acquisition sequence



❖ To remove a selected list or sequence row from the acquisition queue

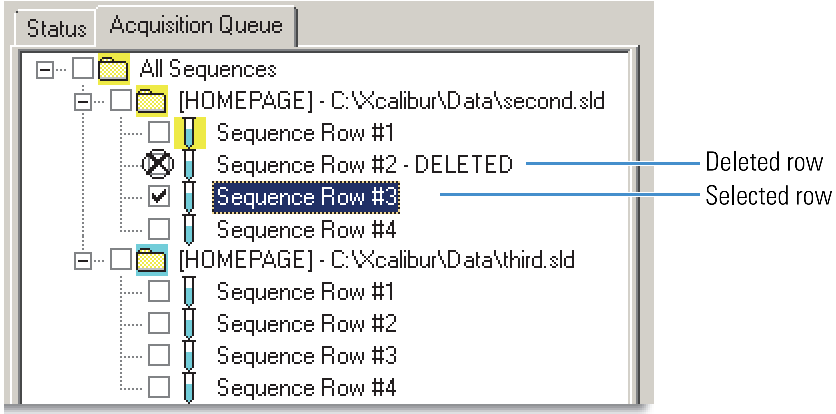
1. Click the sequence or sequence row to select it.

   A small "✓" appears in the check box to the left of the sequence or sequence row.

2. To delete the selected sequence or sequence row, press the DELETE key.

   A large "X" appears in the check box to the left and the text DELETED appears to the right of the deleted sequence or sequence row.

   Figure 88. Acquisition queue with two sequences



Roadmap View

Use the Roadmap view of the Home Page window to branch out to other parts of the Xcalibur data system and to select other views.

From the Roadmap view, click any of the workspace icons to open the view or window for that application.

You can also display shortcut menus by right-clicking the workspace icons.

Shortcut Menus

Table 5 lists the shortcut menu commands that you can access by right-clicking the icons on the Roadmap view.

An asterisk indicates a command that is available when you open the Xcalibur data system from the computer that is connected to the acquisition instrument.

Table 5. Shortcut menus for the icons on the Roadmap view of the Home Page window (Sheet 1 of 2)

Shortcut Command	Description
Instrument Setup icon	
GoTo	Opens the Instrument Setup window, where you can create instrument methods and access the direct controls for each instrument device.
Open Last Used Instrument Method*	Opens the Instrument Setup window and populates the parameter settings with those from the last active instrument method.
Sequence Setup icon	
GoTo	Opens the Sequence Setup view of the Home Page window.
Processing Setup icon	
GoTo	Opens the Processing Setup window, where you can create processing methods.
Qual Browser icon	
GoTo	Opens the Qual Browser window, where you can review qualitative data.
Open Last Acquired Raw File*	Opens the last acquired raw file in the Qual Browser window.
Open Sequence in Progress*	Opens the sequence currently being acquired in the Qual Browser window.
Open Last Sequence Completed*	Opens the last sequence acquired in the Qual Browser window.
Open Last Reprocessed Sequence	Opens the last sequence that you batch reprocessed in the Sequence Setup view.
Quan Browser icon	
GoTo	Opens the Quan Browser window.
Open Last Sequence Completed*	Opens the last processed sequence in the Quan Browser window.

Table 5. Shortcut menus for the icons on the Roadmap view of the Home Page window (Sheet 2 of 2)

Shortcut Command	Description
Library Browser icon	
GoTo	Opens the Library Browser window, where you can create and search mass spectral libraries.

Menu Bar

For information about the Roadmap view menu bar, see these topics:

- "File Menu – Roadmap and Real Time Plot Views" on page 159
- "View Menu – Roadmap and Sequence Setup Views" on page 163
- "GoTo Menu – Home Page" on page 164
- "Actions Menu – Roadmap and Real Time Plot Views" on page 165
- "Help Menu – Home Page" on page 170

Toolbars

For information about the Roadmap view toolbars, see "Home Page Toolbars" on page 170.

Real Time Plot View

While your instrument is acquiring sample data, you can watch the real-time updates of status, spectra, and chromatograms in the Home Page – Real Time Plot view. You can display the chromatograms as UV analog traces, total ion current [TIC] chromatograms, mass range chromatograms, or base peak chromatograms.

The Real Time Plot view is the area located in the workspace, where the Xcalibur data system displays real-time spectra and chromatograms. You can change the display of raw files using commands from the menu bar or the toolbar. To control the way information appears in the Real Time Plot view, use the Plot toolbar.

The cell grid in the Real Time Plot view differs from the cell grid in the Qual Browser window.

- The spectrum and chromatogram views in the Real Time Plot view do not have shortcut menus.
- The number of cells displayed depends on the instrument method. For a mass spectrometer, the Real Time Plot view contains at least one spectrum cell and one chromatogram cell. The view can contain additional cells to display other signals, for example, the analog signal from a UV/Vis detector or the pressure trace from an analytical pump.

For more information about viewing the raw data as it is acquired and working with the Plot toolbar, see "Viewing the Data As It Is Acquired" on page 107.

Menu Bar

For information about the Real Time Plot view menu bar, see these topics:

- "File Menu – Roadmap and Real Time Plot Views," on the next page
- "View Menu – Real Time Plot View" on page 160
- "GoTo Menu – Home Page" on page 164
- "Actions Menu – Roadmap and Real Time Plot Views" on page 165
- "Help Menu – Home Page" on page 170

Toolbars

For information about the Real Time Plot view toolbars, see "Home Page Toolbars" on page 170.

Home Page Menus

The Xcalibur Home page has the following menus. The menus and menu commands change, depending on whether you display the Roadmap view, Sequence Setup view, or Real Time Plot view.

- "File Menu – Roadmap and Real Time Plot Views" on page 159
- "View Menu – Home Page" on page 159
- "GoTo Menu – Home Page" on page 164
- "Actions Menu – Roadmap and Real Time Plot Views" on page 165
- "Tools Menu – Roadmap View" on page 169
- "Help Menu – Home Page" on page 170

For information about the File, Edit, Change, Actions, and Help menus for the Sequence Setup view, see "Sequence Setup Menus" on page 206.

File Menu – Roadmap and Real Time Plot Views

The commands in the File menu of the Home Page window change depending on which views are displayed.

This topic describes the File menu for the Roadmap and Real Time Plot views. For information about the File menu for the Sequence Setup view, see “File Menu – Sequence Setup View” on page 206.

Table 6 lists the File menu commands for the Roadmap and Real Time Plot views of the Home Page window.

Table 6. File menu – Roadmap and Real Time Plot view commands

Command	Description
Change *Study* Name	Opens the *Study* Name Selector dialog box, where you can select a study name from the list of predefined names or create a new name. The name 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, Change Dataset Name, or Change *Custom* Name, where *Custom* is a user-specified name.
Exit	Closes the Home Page window. The Home Page window must be open to operate the Xcalibur data system and to communicate with Xcalibur components.

View Menu – Home Page

The menu commands in the View menu depend on the view displayed.

- View Menu – Real Time Plot View
- View Menu – Roadmap and Sequence Setup Views

View Menu – Real Time Plot View

Table 7 lists the View menu commands for the Real Time Plot view of the Home Page window.

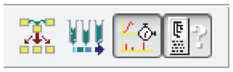
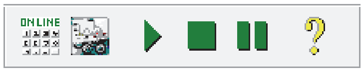
Table 7. View menu – Real Time Plot commands (Sheet 1 of 3)

Icon	Command	Description
Controls		
🔒	Lock Display	Unlocks the data from the instrument. With the data unlocked, you can use the Home Page window toolbar buttons or menu commands to review previously acquired data.When the display is in unlocked mode, the Xcalibur data system continues to gather and save all data. In unlocked mode, the lock icon in the toolbar appears pushed out, and the Lock Display command has no check mark. To relock the data to the instrument, choose **Options > Lock Display**. When the data system begins to analyze a sample, the chromatogram and spectrum displays in the Home Page window are real time, and the data is locked to the instrument. In locked mode, the lock icon in the toolbar appears to be depressed, and the Lock Display command has a check mark. You can click 🔒 in the Home Page window toolbar to lock the data to and unlock the data from the instrument. To unlock the data from the instrument, you can also click the chromatogram or spectrum views.
–	Reset Display	Resets the display parameters to the settings defined in the current instrument method. The Status page of the Info view lists the current instrument method during data acquisition (see "Status Page – Information View" on page 153). For a mass spectrometer, the current instrument method contains chromatogram and spectrum display parameters for the Home Page window. When the data system begins to analyze a sample, it resets the Home Page window according to the current instrument method. While a sample is running, you can change the display parameters by using the Home Page window menu commands.
–	Ranges	Opens the Ranges dialog box, where you can set up the mass range, time, average scan, filter, and background subtraction for the spectrum that is displayed in the Real Time Plot view.
Zoom		
Use the View > Zoom menu commands to zoom in or out of the display by a factor of two, to normalize the display, or to view the entire *x*-axis range.		
⇧	Zoom In Y	Zooms in on the *y* axis by a factor of two from the current baseline. For example, you can change the *y*-axis range from 0–100 to 0–50.

Table 7. View menu – Real Time Plot commands (Sheet 2 of 3)

Icon	Command	Description
⇩	Zoom Out Y	Zooms out on the *y* axis by a factor of two. For example, you can change the *y*-axis range from 0–25 to 0–50.
⇕	Normalize	Normalizes the intensity scale of the data display to a fixed range on the *y* axis, from 0–25% to 0–100%.
→|←	Zoom In X	Zooms in on the *x* axis by a factor of two. For example, you can change the *x*-axis range from 0–20 to 5–15.
←|→	Zoom Out X	Zooms out on the *x* axis by a factor of two from the center. For example, you can change the *x*-axis range from 7.5–12.5 to 5–15.
↔	Display All	Displays the entire range 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 minutes.
Pan		
The Pan menu contains these commands: Next Scan and Previous Scan.		
	Next Scan	Displays the next mass scan with its scan number.
	Previous Scan	Displays the previous mass scan with its scan number.
Display Options		
Opens the Display Options dialog box, where you can select the style, color, label (chromatogram and spectrum only), axis, normalization, and smooth (chromatogram only) options for your chromatogram, spectrum, or other configured instrument signal (for example, a pressure trace).		
	Roadmap View	Opens the Roadmap view of the Xcalibur Home Page window. This view displays a schematic representation of the Xcalibur data system windows and their relationships.
	Sequence Setup View	Opens both the Sequence Setup view and the Sequence Editor toolbar. Use the Sequence Setup view to create, edit, save, open, run, or batch reprocess sequences.
	Real Time Plot View	Opens both the Real Time Plot view and the Plot toolbar. Use the Real Time Plot view to view chromatogram and spectrum data for the current sample. Use the Plot toolbar to do the following: • Start, pause, or resume analyses • Zoom in or out on the *x* or *y* axis • Normalize • Show the next scan • Show the previous scan
	Info View	Opens the Info view if it is hidden, or closes the Info view if it is open. Use the Info view to monitor the run status, the instrument status, and the acquisition queue.

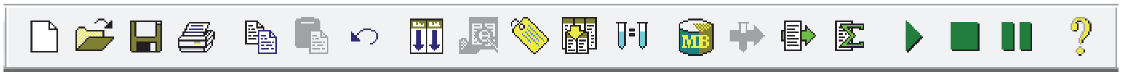
Table 7. View menu – Real Time Plot commands (Sheet 3 of 3)

Icon	Command	Description
–	View Toolbar	Opens or hides the View toolbar. The View toolbar contains the Roadmap view, Sequence Setup view, Real Time Plot view, and Information View icons.
		
–	Roadmap Toolbar	Opens the Roadmap toolbar. Use these toolbar icons to open the Instrument Setup or Processing Setup window, start or stop an analysis, or pause or resume a sample sequence.
		
–	Sequence Editor Toolbar	Opens the Sequence Editor toolbar. In the Real Time Plot view, use the Check Disk Space icon to open the Disk Space dialog box and check the disk space.
–	Plot Toolbar	Use the Plot toolbar to do the following: • Start, pause, or resume analyses • Zoom in or out on the *x* or *y* axis • Normalize • Show the next scan • Show the previous scan
–	Show Large Toolbar	View all of the Home Page window toolbars as 32-bit (height) large toolbars or 24-bit (height) small toolbars. Click the command to switch between large and small toolbars.
–	Customize Toolbars	Opens the Customize Toolbar dialog box, which you can use to add command icons to and delete command icons from the Home Page toolbars.

View Menu – Roadmap and Sequence Setup Views

Table 8 lists the View menu commands for the Roadmap and Sequence Setup views of the Home Page window.

Table 8. View menu – Roadmap and Sequence Setup commands

Icon	Command	Description
	Roadmap View	Opens the Roadmap view of the Xcalibur Home Page window. This view displays a schematic representation of the Xcalibur data system windows and their relationships.
	Sequence Setup View	Opens both the Sequence Setup view and the Sequence Editor toolbar. Use the Sequence Setup view to create, edit, save, open, run, or batch reprocess sequences.
	Real Time Plot View	Opens both the Real Time Plot view and the Plot toolbar. Use the Real Time Plot view to view chromatogram and spectrum data for the current sample.
	Info View	Opens the Info view if it is hidden, or closes the Info view if it is open. Use the Info view to monitor the run status, the instrument status, and the acquisition queue.
–	View Toolbar	Select the Roadmap view, Sequence view, Real Time Plot view, or Information View with a single click from the View toolbar at any time.
–	Roadmap Toolbar	Open the Instrument Setup window, open the Processing Setup window, start or stop an analysis, or pause or resume a sample sequence.
–	Sequence Editor Toolbar	Opens the Sequence Editor toolbar. In the Real Time Plot view, use the Check Disk Space icon to open the Disk Space dialog box and check the disk space. In the Sequence Setup view, use the icons on this toolbar to check the disk space, edit sequences, and start sequence runs. Also use the buttons on this for file management.
		
–	Plot Toolbar	In the Sequence Setup view, use the Plot toolbar to start, pause, or resume analyses.
–	Show Large Toolbar	Use to switch between large and small toolbars. View all of the Home Page window toolbars as 32-bit (height) large toolbars or 24-bit (height) small toolbars.
–	Customize Toolbars	Opens the Customize Toolbar dialog box, which you can use to add command icons to and delete command icons from the Home Page toolbars.

GoTo Menu – Home Page

Table 9 lists the GoTo menu commands that are available for the Home Page window.

Table 9. GoTo menu commands

Icon	Command	Description
	GoTo > Instrument Setup	Opens the Instrument Setup window. For information about the Instrument Setup window, see “Instrument Setup” on page 193.
	GoTo > Processing Setup	Opens the Processing Setup window. For information about the Processing Setup window, see “Processing Setup” on page 247.
–	GoTo > Qual Browser	Opens the Qual Browser window. For information about the Qual Browser window, refer to the *Xcalibur Qual Browser Reviewing Qualitative Data User Guide*.
–	GoTo > Quan Browser	Opens the Quan Browser window. For information about the Quan Browser window, refer to the *Xcalibur Quan Browser Reviewing Quantification Data User Guide*.
–	GoTo > Library Browser	Opens the Library Search window. For information about the Library Search window, refer to the *Xcalibur Library Browser Creating and Searching Libraries User Guide*.

Actions Menu – Roadmap and Real Time Plot Views

The Actions menu commands in the Home Page window change depending on whether the Roadmap or Real Time Plot view is displayed or the Sequence Setup view is displayed. This topic describes the Actions menu for the Roadmap and Real Time Plot views. For information about the Actions menu for the Sequence Setup view, see "Actions Menu – Sequence Setup View" on page 210.

Table 10 lists the Action menu commands for the Roadmap and Real Time Plot views of the Home Page window.

Table 10. Actions menu – Roadmap and Real Time Plot commands (Sheet 1 of 4)

Icon	Command	Description
MB	Check Disk Space	Opens the Disk Space dialog box, where you can determine how much available disk space you have on your disk drive or drives. For more information, see "Checking Disk Space" on page 143.
▶	Start Analysis	Starts the sequence run manually. By default, the Start When Ready check box is selected. If you want to make automated injections with the autosampler set up as the start instrument, do not clear this check box. For information about connecting the contact closure signal between the mass spectrometer and the autosampler, see the Getting Connected Guide for your mass spectrometer. For information about specifying the start instrument, see "Running a Single Sample or Multiple Samples" on page 101. When you clear the Start When Ready check box in the Start Options area of the Run Sequence dialog box, you must do one of the following to start each sample run: • Choose **Actions > Start Analysis** in the menu bar. –or– • Click the **Start Analysis** icon, ▶, in the toolbar. Before you send the Start Analysis command, make sure that the data system is in the Ready state. For more information, see "Starting Each Run Manually" on page 107.

Table 10. Actions menu – Roadmap and Real Time Plot commands (Sheet 2 of 4)

Icon	Command	Description
🟩	Stop Analysis	Stops the current sample run. When you choose Stop Analysis, the following actions occur: • The Pause/Resume Sequence Queue icon goes to the resume sequence queue state; that is, it appears depressed, ⏸. • The data system immediately stops the current run and acquires the raw data file. • On the Info view – Status page, the Sequence readback under Run Manager displays PAUSED. To resume the sequence, click the **Pause/Resume Sequence Queue** icon, ⏸. The data system resumes the sequence at the next sample in the queue. For more information, see "Stopping the Current Sample Run or Pausing the Sequence Queue" on page 106.
⏸	Pause Analysis	Pauses the current sequence after the current sample run ends. When you choose Pause Analysis, the following actions occur: • A check appears to the left of the Pause Analysis command. • The Pause/Resume Sequence Queue icon goes to the resume sequence queue state; that is, it appears depressed, ⏸. • The data system continues to acquire data for the current sample until the run time specified in the instrument method expires. At the end of the run, the data system acquires the raw data file. • At the end of the current run, the data system enters the Paused state as indicated by the PAUSED text for the Sequence readback under Run Manager on the Information view – Status page. ❖ **To restart a paused sequence** Choose ✓ **Pause Analysis**. The data system resumes the sequence with the next sample in the queue.
–	Devices On	Places the system in the On state when the current sequence is completed. In this state, all power and flows are maintained at operational levels. Set the Xcalibur data system in the On state to run another sequence without waiting. This option has the same effect as choosing the On option in the After Sequence Set System area in the Run Sequence dialog box in the Sequence Setup view.

Table 10. Actions menu – Roadmap and Real Time Plot commands (Sheet 3 of 4)

Icon	Command	Description
–	Devices Standby	Places the system in the Standby state when the current sequence is completed. Set the Xcalibur data system in 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 the Standby option in the After Sequence Set System area in the Run Sequence dialog box.
–	Devices Off	Places the system in the Off state when the current sequence is completed. The Off state indicates that all power to the instrument that can be controlled by the data system is turned off. This action includes power to all heaters and most subassemblies, but in some cases it might not include all subassemblies. This option has the same effect as choosing the Off option in the After Sequence Set System area in the Run Sequence dialog box. **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 maintenance manual.

Table 10. Actions menu – Roadmap and Real Time Plot commands (Sheet 4 of 4)

Icon	Command	Description
–	Automatic Devices On	Sets the Xcalibur data system to automatically turn on all devices controlled by the application before starting a data acquisition. If this command has a check mark to its left, the data system automatically turns on all devices that are in the Off or Standby state. If this command does not have a check mark to its left, the data system posts the following message if you have one or more devices in a Standby or Off state: One or more devices to be used by this sequence are not On. The sequence will not start until all the requested devices are ready. Do you want all the devices to be switched 'On'? Press 'Yes' to switch devices On, or 'No' to continue with devices in the 'Off' or in 'Standby' state. If you select 'No' you will need to select the Devices On command from the Actions menu before the sequence will proceed.
–	Reinstate Warnings	Restores the display of messages that you have turned off by selecting the Don't Ask Again check box. Periodically, the data system displays a message or dialog box that includes the following: ☐ Don't ask again. If you select this option when you see it, the data system does not display this message again until you turn warnings back on using the Reinstate Warnings command. To turn off warnings, select this check box: ☑ Don't ask again

Tools Menu – Roadmap View

The Tools menu is available only in the Roadmap view of the Home Page window. Table 11 describes the Tools menu commands.

Table 11. Tools menu commands

Icon	Command	Description
–	Configuration	Opens the Thermo Xcalibur Configuration dialog box, where you can define the Xcalibur default folders, enter customer information, and change Xcalibur fixed-pitch and proportional-pitch fonts. For more information, see "Xcalibur Configuration Dialog Box" on page 177.
	Queue Manager	Opens the Thermo Xcalibur Queue Manager window, where you can monitor the processing status. For more information, see "Queue Manager Window" on page 188.
	File Converter	Opens the Thermo File Converter application, where you can convert files from one file type to another file type. For more information, see "Thermo File Converter Application" on page 189.
–	Library Manager	Opens the Thermo Library Manager application, where you manage can NIST libraries used with NIST searching software and convert libraries between the ICIS/GCQ/ITS 40, MassLab, NIST, and ANDI-MS formats. For more information, refer to the *Xcalibur Searching and Creating Libraries User Guide*.
–	Add Tools	Opens the Add Programs to Tool Menu dialog box, where you can add to or remove programs from the Home Page window menu bar. The data system displays the added programs as menu commands when you choose the Tools menu from the Home Page window. For example, you can add menu commands to open Metabolite ID and Windows™ Explorer™ to Tools menu. For more information, see "Add Tool Dialog Box" on page 403.

Help Menu – Home Page

Table 12 lists the Help menu commands on the Home Page window.

Table 12. Help menu commands

Command	**Description**
Home Page Help	Opens the Xcalibur Help and displays the Help topic for the Home Page window.
View Help	Opens the Xcalibur Help and displays the Help topic for the current Roadmap, Sequence Setup, or Real Time Plot view.
Xcalibur Help	Opens the Xcalibur Help to the Welcome page.
Glossary	Opens the glossary.
How To Use Online Help	Opens the Xcalibur Help to the Help topic that describes how to use the Help viewer.
About Home Page	Opens the About Home Page dialog box, which displays the installed version number of the Xcalibur data system and the product copyright notice. Clicking Version Info opens the Version Info page, where you can view the version information for the layered applications and the instrument drivers.

Home Page Toolbars

For information about the Home Page toolbars, see these topics:

- "Home Page – View Toolbar," on the next page
- "Home Page – Roadmap Toolbar" on page 172
- "Home Page – Plot Toolbar" on page 174

For information about the Sequence Editor toolbar, see "Sequence Editor Toolbar" on page 214.

Home Page – View Toolbar

Table 13 lists the icons in the View toolbar of the Home Page window.

Table 13. View toolbar icons

Icon	Command	Description
	Roadmap View	Opens the Roadmap view on the right side of the Home Page window. The Roadmap view displays a schematic representation of all Xcalibur windows and their relationships. Clicking a graphical icons opens its respective window. In addition, each icon has a shortcut menu. For more information about the Roadmap view, see "Roadmap View" on page 156.
	Sequence Setup View	Opens the Sequence Setup view on the right side of the Home Page window. Use the Sequence Setup view to create, edit, save, or open a sample sequence. For more information about the Sequence Setup view, see Appendix C, "Sequence Setup."
	Real Time Plot View	Opens the Real Time Plot view, where you can view the chromatogram and spectrum data for the current sample. Use the Plot toolbar to start, pause, or resume analyses, zoom in or out on the *x* or *y* axis, normalize, show the next scan, or show the previous scan. For more information about the Real Time Plot view, see "Real Time Plot View" on page 157 and "Viewing the Data As It Is Acquired" on page 107.
	Information View	Opens the Information view on the left side of the Home Page window. Use the Information view to monitor the Run Manager status, the instrument statuses, and the acquisition queue. The Information view has two tabbed pages and is located on the left side of the window. Clicking this icon displays the Information View if it is hidden or hides the Information View if it is displayed. For more information about the Information view, see "Information View" on page 153.

Home Page – Roadmap Toolbar

Table 14 lists the buttons in the Roadmap toolbar of the Home Page window.

Table 14. Roadmap toolbar buttons (Sheet 1 of 2)

Icon	Command	Description
ON LINE	Instrument Setup	Opens the Instrument Setup window, where you can create instrument methods and access the direct controls for the instrument devices.
	Processing Setup	Opens the Processing Setup window, where you can create or modify a processing method.
▶	Start Analysis	Starts the sequence run manually. By default, the Start When Ready check box is selected. If you want to make automated injections with the autosampler set up as the start instrument, do not clear this check box. For information about connecting the contact closure signal between the mass spectrometer and the autosampler, see the Getting Connected Guide for your mass spectrometer. For information about specifying the start instrument, see “Running a Single Sample or Multiple Samples” on page 101. When you clear the Start When Ready check box in the Start Options area of the Run Sequence dialog box, you must do one of the following to start each sample run: • Choose **Actions > Start Analysis** in the menu bar. –or– • Click the **Start Analysis** icon, ▶, in the toolbar. Before you send the Start Analysis command, make sure that the data system is in the Ready state. For more information, see “Starting Each Run Manually” on page 107.

Table 14. Roadmap toolbar buttons (Sheet 2 of 2)

Icon	Command	Description
🟩	Stop Analysis	Stops the current sample run. When you choose Stop Analysis, the following actions occur: • The Pause/Resume Sequence Queue icon goes to the resume sequence queue state; that is, it appears depressed, ⏸. • The data system immediately stops the current run and acquires the raw data file. • On the Info view – Status page, the Sequence readback under Run Manager displays PAUSED. To resume the sequence, click the **Pause/Resume Sequence Queue** icon, ⏸. The data system resumes the sequence at the next sample in the queue. For more information, see "Stopping the Current Sample Run or Pausing the Sequence Queue" on page 106.
	Pause/Resume Sequence Queue	The Pause/Resume Sequence Queue icon has two states: • In the pause sequence queue state, the icon appears raised, ⏸. • In the resume sequence queue state, the icon appears depressed, ⏸. When you click ⏸, the following events occur: • The Pause/Resume Sequence Queue icon goes to the resume sequence queue state; that is, it appears depressed, ⏸. • The data system continues to acquire data for the current sample until the run time specified in the instrument method expires. Then it acquires the raw data file. • On the Info view – Status page, the Sequence readback displays PAUSED in flashing red text. When you click ⏸, the following events occur: • The Pause/Resume Sequence Queue icon goes to the pause sequence queue state; that is, it appears raised, ⏸. • When the current run finishes, sample processing continues with the next sample in the sample queue. You can review the sample queue at any time on the Acquisition Queue page of the Home Page – Information view.
⏸	Pause sequence queue	
⏸	Resume sequence queue	
?	Xcalibur Help	Displays the contents window for Xcalibur Help.

Home Page – Plot Toolbar

Table 15 lists the buttons in the Plot toolbar of the Home Page window.

Table 15. Plot toolbar buttons (Sheet 1 of 3)

Icon	Command	Description
▶	Start Analysis	Starts the sequence run manually. By default, the Start When Ready check box is selected. If you want to make automated injections with the autosampler set up as the start instrument, do not clear this check box. For information about connecting the contact closure signal between the mass spectrometer and the autosampler, see the Getting Connected Guide for your mass spectrometer. For information about specifying the start instrument, see “Running a Single Sample or Multiple Samples” on page 101. When you clear the Start When Ready check box in the Start Options area of the Run Sequence dialog box, you must do one of the following to start each sample run: • Choose **Actions > Start Analysis** in the menu bar. –or– • Click the **Start Analysis** icon, ▶, in the toolbar. Before you send the Start Analysis command, make sure that the data system is in the Ready state. For more information, see “Starting Each Run Manually” on page 107.
■	Stop Analysis	Stops the current sample run. When you choose Stop Analysis, the following actions occur: • The Pause/Resume Sequence Queue icon goes to the resume sequence queue state; that is, it appears depressed, ⏸. • The data system immediately stops the current run and acquires the raw data file. • On the Info view – Status page, the Sequence readback under Run Manager displays PAUSED. To resume the sequence, click the **Pause/Resume Sequence Queue** icon, ⏸. The data system resumes the sequence at the next sample in the queue. For more information, see “Stopping the Current Sample Run or Pausing the Sequence Queue” on page 106.

Table 15. Plot toolbar buttons (Sheet 2 of 3)

Icon	Command	Description
⏸	Pause/Resume Sequence Queue Pause sequence queue Resume sequence queue	The Pause/Resume Sequence Queue icon has two states: • In the pause sequence queue state, the icon appears raised, ⏸. • In the resume sequence queue state, the icon appears depressed, ⏸. When you click ⏸, the following events occur: • The Pause/Resume Sequence Queue icon goes to the resume sequence queue state; that is, it appears depressed, ⏸. • The data system continues to acquire data for the current sample until the run time specified in the instrument method expires. Then it acquires the raw data file. • On the Info view – Status page, the Sequence readback displays PAUSED in flashing red text. When you click ⏸, the following events occur: • The Pause/Resume Sequence Queue icon goes to the pause sequence queue state; that is, it appears raised, ⏸. • When the current run finishes, sample processing continues with the next sample in the sample queue. You can review the sample queue at any time on the Acquisition Queue page of the Home Page – Information view.
⇧	Zoom In Y	Zooms in on the *y* axis by a factor of two from the current baseline. For example, you can change the *y*-axis range from 0–100 to 0–50.
⇩	Zoom Out Y	Zooms out on the *y* axis by a factor of two. For example, you can change the *y*-axis range from 0–25 to 0–50.
⇳	Normalize	Normalizes the intensity scale of the data display to a fixed range on the *y* axis, from 0–25% to 0–100%.
▸|◂	Zoom In X	Zooms in on the *x* axis by a factor of two. For example, you can change the *x*-axis range from 0–20 to 5–15.
◂|▸	Zoom Out X	Zooms out on the *x* axis by a factor of two from the center. For example, you can change the *x*-axis range from 7.5–12.5 to 5–15.
◂|▸	Display All	Displays the entire range 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 minutes.
↶📊	Show Previous Scan	Displays the previous mass scan with its scan number. This icon is available when the spectrum view is active.
📊↷	Show Next Scan	Displays the next mass scan with its scan number. This icon is available when the spectrum view is active.

Table 15. Plot toolbar buttons (Sheet 3 of 3)

Icon	Command	Description
🔒	Lock Display	Unlocks the data from the instrument so that you can use the toolbar icons or menu commands to review the data. When the display is in unlocked mode, the data system continues to gather and save all data. In unlocked mode, the lock icon in the toolbar appears raised. When the data system begins to analyze a sample, the chromatogram and spectrum displays in the Home Page window are real time and the data is locked to the instrument. In locked mode, the lock icon in the toolbar appears to be depressed, 🔒. To relock the data to the instrument, click 🔒 in the Plot toolbar.
?	Help	When the Roadmap view is open, clicking ? opens the Xcalibur Help to the Roadmap View topic.

Home Page Dialog Boxes

You can access the following dialog boxes from the Tools menu on the Roadmap view of the Xcalibur Home Page window.

- "Xcalibur Configuration Dialog Box," on the next page
- "Thermo File Converter Application" on page 189

Note For information about the Library Manager application, see "Library Manager Application" on page 97.

You can access these dialog boxes from the Real-Time Plot view of the Xcalibur Home Page window or from the Qual Browser window:

- "Chromatogram Ranges Dialog Box for the Real Time Plot" on page 186
- "Spectrum Ranges Dialog Box for the Real-Time Plot" on page 186

From the Queue Manager window, you can access the "Details of Selected Analysis Dialog Box" on page 187.

Note For information about checking the disk space, see "Checking Disk Space" on page 143.

Xcalibur Configuration Dialog Box

Use the pages of the Xcalibur Configuration dialog box to define the location of data, methods, and report templates on your data system computer; to edit customer information; to select the fonts that you want to use; and to select error-handling options.

These topics describe the parameters on the pages of the Xcalibur Configuration dialog box:

- Customer Info Page
- Dataset List Page
- Folders Page
- Fonts Page
- Intelligent Shutdown (Error Handling) Page
- Labeling and Scaling Page
- Mass Options Page
- Peak Detection Page

For information about how to use these pages, see "Configuring the Xcalibur Data System" on page 130.

Customer Info Page

Use the Customer Information page of the Xcalibur Configuration dialog box to confirm and update the following Xcalibur software license information.

For more information, see "Updating Customer Information" on page 131.

Table 16 describes the parameters on the Customer Info page of the Xcalibur Configuration dialog box.

Table 16. Xcalibur software license parameters (Sheet 1 of 2)

Parameter	Description
User Name	Specifies the name assigned to the Xcalibur license agreement. To change the user name, log on to your computer as an administrator.
Organization	Specifies the organization assigned to the Xcalibur license agreement. To change the organization, log on to your computer as an administrator.
Address	Specifies the address assigned to the Xcalibur license agreement. Commas separate the sections of the address, for example: city, state, and country.
Voice Phone	Specifies the voice telephone number assigned to the Xcalibur license agreement.
Fax	Specifies the fax telephone number assigned to the Xcalibur license agreement.

Table 16. Xcalibur software license parameters (Sheet 2 of 2)

Parameter	Description
Email	Specifies the e-mail address assigned to the Xcalibur license agreement.
Print User Info	Prints a report that lists the current user name, organization, address 1, address 2, voice phone number, and fax telephone number.

Dataset List Page

Use the Dataset List page of the Xcalibur Configuration dialog box to define or edit the list of dataset names available when the user chooses a dataset. Only the administrator can access this feature.

For more information, see "Defining the Dataset List" on page 139.

Note The names of several parameters on this page change when you select a new Display Name. The default Display Name is Dataset. When you change the Display Name, the following four parameters are renamed: Dataset List, Add New Dataset Name, Remove Selected Dataset Name, and Blank Dataset Name Is a Valid Selection. For example, if you change the Display Name from Dataset to Study, the parameter Dataset List changes to Study List.

Table 17 describes the parameters on the Dataset List page of the Xcalibur Configuration dialog box.

Table 17. Dataset List page parameters (Sheet 1 of 2)

Parameter	Description
Dataset List	Lists the dataset names that are stored in the registry. To add a new dataset name to the list, click **Add New Dataset Name**.
Display Name	Specifies the name that the data system uses for a dataset. You can type a new name, or you can select a new name from the list. The options are Dataset, Study, and Job. When you change the Display Name, the parameters on this page and elsewhere are renamed to reflect the change. For example, if you change the Display Name from Dataset to Study, the Dataset List parameter changes to Study List.
Add New Dataset Name	Opens the Create a New Dataset Name dialog box, where you can type a new dataset name. The data system adds the new dataset name to the Dataset List and the registry.
Remove Selected Dataset Name	Removes the currently selected name from the Dataset List and from the registry but action does not remove the name from the database if the name has already been used.
Blank Dataset Name Is a Valid Selection	When you select this check box, you can select a blank name for a dataset. When you clear this check box, you must select a valid dataset.

Table 17. Dataset List page parameters (Sheet 2 of 2)

Parameter	Description
Selection Restricted to Entered Names	When you select this check box, the Dataset Name Selector dialog box lists only the names in the Dataset List. Clear to show the names listed in the Dataset List as well as a those obtained from the database in the Dataset Name Selector dialog box.
Maximum Number of Names to Display	Specifies the maximum number of dataset names that are shown in the Dataset Name Selector dialog box. In the Dataset Name Selector dialog box, the dataset names from the Dataset List are shown first. Then, if allowed, the most recent dataset names stored in the database are used to fill the list until the maximum number of entries is shown.

Folders Page

Use the Folders page of the Xcalibur Configuration dialog box to specify the default location of your Xcalibur data, methods, and report templates.

For more information, see "Selecting Default Folders" on page 130.

Table 18 describes the parameters on the Folders page of the Xcalibur Configuration dialog box.

Table 18. Folders page parameters

Parameter	Description
Default Folders	
Data	Specifies the current default path to the folder that contains your Xcalibur data. To change the path, click **Browse** and select the folder where you want to store your data. When you click **OK**, the data system changes the default path in the Data box to the new path.
Methods	Specifies the current default path to the folder that contains your Xcalibur methods. To change the path, click **Browse** and select the folder where you want to store your. When you click **OK**, the data system changes the default path in the Methods box to the new path.
Report Templates	Specifies the current default path to the folder that contains your Xcalibur report templates. To change the path, click **Browse** and select the folder where you want to store your report templates. When you click **OK**, the data system changes the default path in the Report Templates box to the new path.

Fonts Page

Use the Fonts page of the Xcalibur Configuration dialog box to change the appearance of fonts in the data system.

For more information, see "Configuring Fonts" on page 132.

> **Note** If the data system displays the elemental composition values in light gray, close Qual Browser and choose **Xcalibur Roadmap** > **Tools** > **Configuration** to display the Configuration page. Select the **Fonts** tab and set all font sizes to a minimum of 10 points.

Table 19 describes the parameters on the Fonts page of the Xcalibur Configuration dialog box.

Table 19. Fonts page parameters (Sheet 1 of 2)

Parameter	Description
Fixed Pitch Font	
Font	Specifies the fixed pitch (non-proportional) font that the Xcalibur data system currently uses; the name appears in the topmost Font box. The default fixed-pitch font is Courier New. The Fixed Pitch Font list displays all of the fixed-pitch fonts that are currently available on your data system. Fixed-pitch fonts have characters whose width is constant. To change the font, select a font in the Font list. The data system displays the selected font in the topmost box and displays an example in the associated Preview area. When you click OK, the Xcalibur data system implements this font throughout all Xcalibur programs wherever fixed-pitch fonts are used.
Min	Specifies the minimum fixed-pitch font size that the data system currently uses; the number appears in the topmost Min box. The default minimum fixed-pitch font size is 7 points. To change this value, select another font size in the list. The data system displays the selected font size in the topmost box and displays both the current font and the selected font size in the top row of the associated Preview area.
Max	Specifies the maximum fixed-pitch font size that the data system currently uses; the number appears in the topmost Max box. The default maximum fixed-pitch font size is 12 points. To change this value, select another font size in the list. The data system displays the selected font size in the topmost box and displays both the current font and the selected font size in the bottom row of the associated Preview area.
Fixed Pitch Font Preview	
Preview	View the following examples: • Example text with fixed-pitch font at minimum size. • Example text with fixed-pitch font at maximum size.

Table 19. Fonts page parameters (Sheet 2 of 2)

Parameter	Description
Proportional Pitch Font	
Font	Specifies the proportional-pitch font that the data system currently uses; the name appears in the topmost Font box. The default proportional-pitch font for the data system is Arial. The Proportional Pitch Font list displays all of the proportional-pitch fonts that are currently available on your data system. Proportional pitch fonts have characters that vary in width. For example, the widest character is **W**. To change the font, select a font in the Font list. The application displays the selected font in the topmost box and displays an example in the associated Preview area. When you click OK, the data system implements this font throughout all Xcalibur programs wherever proportional-pitch fonts are used.
Min	Specifies the minimum proportional-pitch font size that the data system currently uses; the number appears in the topmost Min box. The default minimum proportional-pitch font size is 7 points. To change this value, select another font size in the list. The application displays the selected font size in the topmost box and displays both the current font and the selected font size in the top row of the associated Preview area.
Max	Specifies the maximum proportional-pitch font size that the data system currently uses; the number appears in the topmost Max box. The default maximum proportional-pitch font size is 12 points. To change this value, select another font size in the list. The application displays the selected font size in the topmost box and displays both the current font and the selected font size in the bottom row of the associated Preview area.
Proportional Pitch Font Preview	
Preview	Displays the following examples: • Example text with proportional-pitch font at minimum size. • Example text with proportional-pitch font at maximum size.

Intelligent Shutdown (Error Handling) Page

Use the Intelligent Shutdown page of the Xcalibur Configuration dialog box to specify the response that the Xcalibur data system makes when an error occurs during data acquisition.

For more information, see "Selecting Error Handling Options" on page 138.

Table 20 describes the parameters on the Intelligent Shutdown page of the Xcalibur Configuration dialog box.

Table 20. Intelligent Shutdown page parameters

Parameter	Description
No Action	Directs the data system to take no action and try to continue to the next sample when an error occurs during data acquisition.
Attempt to Stop the Devices and Pause the Sequence	Directs the data system to send a Stop command to all devices and pause the acquisition sequence before the next injection when an error occurs during data acquisition.
Attempt to Turn Off the Devices and Pause the Sequence	Directs the data system to send a Turn Off Device command to all devices and pause the acquisition sequence before the next injection when an error occurs during data acquisition.

Labeling and Scaling Page

Use the Labeling and Scaling page of the Xcalibur Configuration dialog box to enter default values for labels and scales used to display data in the chromatogram and spectrum views.

For more information, see "Selecting Default Labeling and Scaling Options" on page 137.

Table 21 describes the parameters on the Labeling and Scaling page of the Xcalibur Configuration dialog box.

Table 21. Labeling and Scaling page parameters (Sheet 1 of 2)

Parameter	Description
Default Spectrum and Chromatogram Scaling	
Labeling Options	
Select default values for labeling and scaling in the displays of spectrum and chromatogram data. The values you specify as defaults are applied throughout the Xcalibur data system only if no other value is available in the currently open method or raw file. In Processing Setup and Quan Browser, for example, the data system uses the default values for labeling and scaling when you change the value for Detector Type. In Qual Browser, however, the data system uses the default values when you display a new spectrum, chromatogram, or map plot, or if the layout file (.lyt) in Qual Browser is unavailable.	
Label for MS Data	Specifies the default source of labels for the *y* axis of MS data. Specify either custom (user-defined) labels or labels from the detector. If you select custom labels, use the adjacent box to specify the label; for example, specify Intensity as a label.
Label for PDA/UV Data	Specifies the default source of labels for the *y* axis of PDA/UV data. Specify either custom (user-defined) labels or labels from the detector. If you select custom labels, use the adjacent box to specify the label. For example, specify µAU as a label.
Label for Other Data Types	Specifies the default source of labels for the *y* axis of data types other than MS and PDA/UV. Specify either custom (user-defined) labels or labels from the detector. If you select custom labels, use the adjacent box to specify the label. For example, specify mVolts as a label.
Use Absolute Scale	
Selecting these check boxes specifies absolute scaling as the default for displays of spectrum and chromatogram data. The values you select are applied throughout the data system only if no other value is available in the currently open method or raw file.	
MS Data	When you select this check box, the default (global) settings use absolute scaling with MS data.
PDA/UV Data	When you select this check box, the default (global) settings use absolute scaling with PDA/UV data.

Table 21. Labeling and Scaling page parameters (Sheet 2 of 2)

Parameter	Description
Other Data	When you select this check box, the default (global) settings for data types other than MS and PDA/UV use absolute scaling.
Retention Time Precision	
Decimals	Specifies the number of decimal places to include when reporting retention times. The value can be from 1 to 5.

Mass Options Page

Use the Mass Options page of the Xcalibur Configuration dialog box to select default values for Mass Tolerance, Mass Units, and Mass Precision. If you select the check box labeled Use User Defined, you can specify the default values for the parameters in the Default Mass Tolerance area. The data system uses these defaults throughout to acquire and display your data. If you do not select the Use User Defined check box, the application uses the values for mass options that are stored in the open raw file in the data system.

For more information, see "Setting Up the Default Mass Options" on page 135.

(Use the Masses dialog boxes in the Processing Setup, Qual Browser, and Quan Browser windows to change the default settings for tolerance and precision in those windows.)

Table 22 describes the parameters on the Mass Options page of the Xcalibur Configuration dialog box.

Table 22. Mass Options page parameter (Sheet 1 of 2)

Parameter	Description
Default Mass Tolerance	
Use User Defined	Makes the user-defined default settings for mass tolerance and mass units available.
Mass Tolerance	Specifies the user-defined default setting for mass tolerance. To activate the user-defined settings, select the **Use User Defined** check box. Then, type a value from **0.1** to **50000**. The data system uses the default mass tolerance value only when you create a new method. It does not modify any existing methods (for example, processing methods or Qual Browser layout files). Qual Browser does not use the default mass tolerance value unless you delete the default layout file. The data system then creates a new default layout file with this mass tolerance value.
Units	Specifies the default units that are used in processing mass spectral data. To make the user-defined settings available, select the **Use User Defined** check box. Then, select either the **mmu** option or the **ppm** option.

Table 22. Mass Options page parameter (Sheet 2 of 2)

Parameter	Description
Default Mass Precision	
Decimals	Specifies the default number of decimal places (places after the decimal point) that the data system uses to process mass spectral data. Specify from **0** to **5** decimal places. The number of decimal places applies throughout the data system. The data system uses the default mass precision value only when you create a new method. It does not modify any existing methods (for example, processing methods or Qual Browser layout files). Qual Browser does not use the default mass precision value unless you delete the default layout file. The application then creates a new default layout file with this mass precision value.
Default Mass Defect	
Specifies the parameters used in library searches so that you can 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 the mass defect to larger molecules because, in general, they are composed of more atoms than smaller molecules; larger molecules need a larger correction factor to approximate the linear function that the data system uses to calculate masses. The values that you specify for the default mass defect are applied throughout the data system if no other value is available in the currently open method or raw file.	
Defect (mmu)	Specifies default values (in millimass units) for the mass defect. 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 (amu)	Specifies the default 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.

Peak Detection Page

Use the Peak Detection page of the Xcalibur Configuration dialog box to select which peak detection algorithm to use as the default for different data types. All new processing setup methods are created using the currently selected Xcalibur default peak detection algorithm. You can return to the Peak Detection page at any time to change the Xcalibur default peak detection algorithm. Specify a default algorithm to use for different data types in the Default Peak Detection Algorithm area.

For more information, see "Selecting a Default Peak Detection Algorithm" on page 134.

Table 23 describes the parameters on the Peak Detection page of the Xcalibur Configuration dialog box.

Table 23. Peak Detection page parameters

Parameter	Description
Default Peak Detection Algorithm	
Default Peak Detection Algorithm for MS Data	Specifies the default peak detection algorithm for MS data. Selections: ICIS, Genesis, or Avalon
Default Peak Detection Algorithm for PDA/UV Data	Specifies the default peak detection algorithm for PDA/UV data. Selections: ICIS, Genesis, or Avalon
Default Peak Detection Algorithm for Other Data Types (Data types other than MS and PDA/UV)	Specifies the default peak detection algorithm for data types other than MS, PDA, or UV data. Selections: ICIS, Genesis, or Avalon

Chromatogram Ranges Dialog Box for the Real Time Plot

Use the Chromatogram Ranges dialog box to view and edit the mass range, time range, and other properties of a chromatogram plot:

- In Qual Browser, for all plots in the active chromatogram view
- On the Home Page, for the active chromatogram plot in Real Time Plot mode

You can also apply automatic processing options such as smoothing and background subtraction.

For more information about the Chromatogram Ranges dialog box, refer to the *Xcalibur Qual Browser User Guide*.

Spectrum Ranges Dialog Box for the Real-Time Plot

Use the Spectrum Ranges dialog box to view and edit the mass range, time, and other properties of a spectrum plot:

- In Qual Browser, for all plots in the active spectrum view
- On the Home Page, for the active spectrum plot in Real Time Plot mode

You can also apply automatic processing options such as smoothing and background subtraction.

For more information about the Spectrum Ranges dialog box, refer to the *Xcalibur Qual Browser Reviewing Qualitative Data User Guide*.

Details of Selected Analysis Dialog Box

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

For more information, see "Managing the Xcalibur Processing Queue" on page 120.

Table 24 describes the parameters in the Details of Selected Analysis dialog box.

Table 24. Details of Selected Analysis dialog box parameters

Parameter	Description
File (read-only)	Displays the file name you have selected from the 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 (read-only)	Displays the Xcalibur processing status of the file listed in the File box. For example, this box might display Creating Summary.
Submitted (read-only)	Displays the date as Month/Day/Year and time in hours:minutes:seconds that the file listed in the File box was submitted for processing. For example, this box might display 02/22/99 16:24:15.
From (read-only)	Displays the source of the batch processing task submission. For example, this box might display Reprocessing.
Actions (read-only)	Displays the current Xcalibur actions and their status. For example, the box might display Create Summary, In Progress.
Continue	Closes the Details of Selected Analysis dialog box and returns the focus to the Processing Queue Manager window, where you can select another file to review in the Details of Selected Analysis dialog box or monitor the processing queue.

Queue Manager Window

Use the Queue Manager window to control the Xcalibur processing queue. Each time you select Processing options in the Run Sequence or Batch Reprocess dialog box in the Sequence Setup view, a queue service starts in the background. When the Run Manager program finishes an analysis, it sends the data to the queue for processing. Sequences are submitted using a first-in first-out queue priority. You can pause processing, resume processing, purge the queue, and obtain information about processing.

For more information, see "Managing the Xcalibur Processing Queue" on page 120.

Table 25 describes the parameters in the Queue Manager window.

Table 25. Processing Queue Manager window parameters (Sheet 1 of 2)

Icon	Command	Description
Queue		
⏸	Pause	Pauses all processing operations temporarily and places the Xcalibur processing in Standby mode.
▶	Resume	Resumes processing.
–	Purge Queue	Removes all processing requests from the Processing Queue Manager. You can use this command during troubleshooting to clear the application of all processing tasks.
–	Exit	Closes the Processing Queue Manager window.
Analysis		
✗	Remove From Queue	Removes all selected processing requests from the Processing Queue Manager. You can use this command during troubleshooting to clear the application of all processing tasks.
i	Details	Opens the Details of Selected Analysis Dialog Box so that you can view additional information about a selected processing task.
View		
–	Toolbar	Displays or hides the toolbar.
–	Status Bar	Displays or hides the status bar. The status bar is a horizontal box at the bottom of the Processing Queue Manager window.
–	Refresh	Updates the Xcalibur processing queue with the most current information.
GoTo		
X	Xcalibur Home Page	Returns you to the Roadmap view of the Home Page window.

Table 25. Processing Queue Manager window parameters (Sheet 2 of 2)

Icon	Command	Description
Help		
?	Queue Manager Help	Opens Help for the Queue Manager.
–	Xcalibur Help	Opens the Xcalibur Help to the Welcome topic.
–	Glossary	Opens the glossary.
–	How To Use Help	Opens the Help topic that describes how to use the Help viewer.
–	About Queue Manager	Opens the About Queue Manager dialog box. This dialog box displays the installed version number of the Queue Manager program and the Thermo Fisher Scientific copyright notice.

Thermo File Converter Application

Use the Thermo File Converter application to convert one data file type to another data file type.

For more information, see "Converting File Formats" on page 140.

Note

- The Xcalibur data system does not currently support all interconversion combinations and posts a message whenever you request an unsupported conversion.
- Not all formats have the same data fields. The data system can only convert matching data fields and does not typically convert instrument method information.
- You can also convert files by running XConvert.exe when processing or batch reprocessing data files in the Sequence Setup view. For more information, see "XConvert.exe" on page 415.

The Xcalibur data system provides file interconversions for the following file types.

Table 26. File interconversions for data file types

File type	File extension
Xcalibur	*.raw
ICIS	*.dat
GCQ	*.ms
Magnum	*.ms
ANDI	*.cdf
AutoMass	*.spa

Table 26. File interconversions for data file types

File type	File extension
MassLab2	*.raw
LaserMAT	*.*

❖ To convert a file

1. Select the source and destination directories and the conversion type in the Thermo File Converter window.
2. Click **Convert**.

   The application automatically performs the file conversion and creates a new file. The Status page displays the conversion status of each job.

Table 27 describes the parameters in the Thermo File Converter window.

Table 27. Thermo File Converter window parameters (Sheet 1 of 3)

Parameter	Description
Conversion Source	
Source Data Type	Specifies the data type of the file that you want to convert into another data type. All of the files in the Folder list in the Conversion Source area are displayed in the Conversion Source table. You can select the following data types from the Source Data Type list for conversion into another data type: • Xcalibur Files (*.raw) • ICIS Files (*.dat) • GCQ Files (*.ms) • Magnum Files (*.ms) • ANDI Files (*.cdf) • Automass Files (*.spa) • Mass Lab 2 Files (*.raw) • Lasermat Files (*.*) The source data type is selected from the Destination Data Type list.
Folder	Specifies the path to the source file that you want to convert to another data type. The list contains all the paths that you have recently selected. Click **Browse** in the Conversion Source area to select another path to source files.
Browse	Select the folder that contains the files that you want to convert to another data type and click **OK**. The data system displays the path to the folder in the Folder list and the previous path remains in the folder list. If the selected folder has no file of the type specified in the Source Data Type list, no entries appear in the Conversion Source table.

Table 27. Thermo File Converter window parameters (Sheet 2 of 3)

Parameter	Description
Conversion Source table	Displays the file name, type, size, and date of the files located in the directory specified in the Folder list and of the type of file specified in the Source Data Type list.
Select All	Selects all of the files that appear in the Conversion Source table. The data system highlights all of the files.
Clear Selection	Deselects the currently selected files. This button is only active when you select one or more files in the Conversion Source table.
Add Job(s)	Add the specified conversion job to the Jobs page of the Conversion Destination area. Each file conversion is considered a separate job. The following is an example of a job displayed on the Jobs page for the conversion of an Xcalibur file of type .raw to an ANDI file of type .cdf: C:\Xcalibur\examples\data\drugx_06.raw C:\Xcalibur\examples\data\drugx_06.cdf The Add Job(s) button is only active when you select one or more files on the Jobs page. You can only add a job if you have selected a valid data type in the Destination Data Type list and have selected a valid destination from the Folder list in the Conversion Destination area.
Conversion Destination	
Destination Data Type	Specifies the data type that you want the source data files converted to. You can select the following data types from the Destination Data Type list: • ICIS Files (*.dat) • ANDI Files (*.cdf) • Text Files (*.txt) The data system selects the data type that a source data type file can be converted from in the Source Data Type list.
Folder	Specifies the destination folder for the converted files. The list contains all the paths that you have recently selected. To select another destination folder, click **Browse** in the Conversion Destination area and select an appropriate folder.
Browse	Select the folder to hold your converted files and click **OK**. The data system displays the path to the folder, and the previous path remains in the Folder list.

Table 27. Thermo File Converter window parameters (Sheet 3 of 3)

Parameter	Description
Jobs page	Displays the jobs that have been selected for conversion. The job display format is as follows: C:\Xcalibur\examples\data\drugx_06.raw C:\Xcalibur\examples\data\drugx_06.cdf To remove a job before running the conversion, select the job and click **Remove Job(s)**.
Remove Job(s)	Removes jobs that are selected for removal from the Jobs page. You must remove a job before converting it.
Status page	This page in the Conversion Destination area displays the status of jobs that have been converted. The format is as follows: Successfully converted C:\Xcalibur\examples\data\drugx_06.raw to C:\Xcalibur\examples\data\drugx_06.cdf This page also displays the status of unsuccessful conversions.
Other Buttons	
Convert	Starts the conversion of all jobs displayed on the Jobs page in the Conversion Destination area. The data system stores the converted files in the displayed folder. The status of all converted files appears on the Status page. This page in the Conversion Destination area displays the status of jobs that have been converted. The format is as follows: Successfully converted C:\Xcalibur\examples\data\drugx_06.raw to C:\Xcalibur\examples\data\drugx_06.cdf This page also displays the status of unsuccessful conversions.

Instrument Setup

This appendix provides reference information about the Instrument Setup window, where you create instrument methods and access the instrument menus.

Contents

- Instrument Setup Window
- Instrument Setup Window View Bar
- Instrument Setup Window Menus
- Instrument Setup Window Toolbar

For information about creating instrument methods, see "Creating an Instrument Method" on page 13.

Instrument Setup Window

After selecting which instruments you want the Xcalibur data system to control using the Instrument Configuration application of the Foundation platform, use the Instrument Setup window to prepare the instrument for daily use and to create instrument methods.

The Instrument Setup window displays the icons of all of the Xcalibur instruments that you selected using the Instrument Configuration application. (See the View bar on the left side of the window.) If you have configured more instruments than can be displayed on your screen, a vertical scroll bar appears in the View bar so that you can access all the instruments.

The Instrument Setup window contains an instrument view for each configured instrument of the mass spectrometry system. Selecting an instrument icon on the View bar opens the view for that instrument. Each instrument view contains one or more pages of parameters that are required to control the instrument during a sample run.

In the Instrument Setup window, you can create new instrument methods, modify existing instrument methods, and save instrument method files. You can import previously acquired data files to help you set up time segments and scan events based upon the data acquired.

You can also enter a method summary that appears in the Open dialog box and on all method printouts. All changes are audited by logon ID and user self-identification so that you can describe why you changed a method.

> **Note** Before you use the Instrument Setup window, use the Instrument Configuration program to select the instruments for your experiment.

Instrument Setup Window View Bar

The View bar is a vertical bar on the left of the Instrument Setup window. It contains an icon for each of the instruments that you have selected using the Instrument Configuration window in the Foundation platform.

Instrument Setup Window Menus

Instrument Setup window contains the following menus: File, *Instrument Name*, and Help.

For information about these menus, see these topics:

- File Menu – Instrument Setup
- Instrument Menu – Instrument Setup
- Help Menu – Instrument Setup

File Menu – Instrument Setup

Table 28 lists the File menu commands for the Instrument Setup window and their descriptions.

Table 28. File menu commands (Sheet 1 of 2)

Command	Description
New	Resets the instrument method parameters to their default settings. The title bar displays the name Untitled for the instrument method.
Open	Opens the Open dialog box, where you can select an existing instrument method file.
Save	Opens the File Save – Audit Trail dialog box if the file has been saved before so that you can enter audit information about the active file.
Save As	Opens the File Summary Information dialog box where you can add a comment, as well as view header information about the active file. When you click OK, the data system opens the File Save – Audit Trail Dialog Box so you can enter audit information about the active file. When you click Continue, the data system saves the file.

Table 28. File menu commands (Sheet 2 of 2)

Command	Description
Summary Information	Opens the File Summary Information dialog box, where you can add a comment, as well as view header information about the active file.
Change Dataset Name	Opens the *Dataset* Name Selector dialog box, where you can 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	Opens the Thermo Foundation Audit Viewer, where you can view all auditable events and changes made to data files in the current application.
Print	Opens the Print dialog box, where you can select the printer and the page range to print for the instrument method.
Print Preview	Opens the print preview window, where you can view the page setup before printing the instrument method.
Print Setup	Opens Print Setup dialog box, where you can select the following printing options: printer, form, orientation, and one- or two-sided printing.
Most Recently Used Files	Displays the paths and names of the last four files used. These file name are located above the Exit command. Both open and closed files are displayed. Click a displayed file to load it. If the selected file was closed, the data system opens it.
Exit	Closes the active window. If you exit before clicking OK from an active dialog box, the data system asks if you want to save your changes.

Instrument Menu – Instrument Setup

The Xcalibur data system groups commands that deal with instrument-specific controls in the *Instrument Name* menu. You can activate device commands from either the mouse or keyboard.

Note To change the displayed instrument view, click the icon for the instrument of interest on the View bar. Each instrument-specific menu contains instrument-specific menu commands.

When you choose Help > *Instrument Name* Help, the Help system for the specific instrument device opens.

Help Menu – Instrument Setup

Table 29 lists the Help menu commands for the Instrument Setup window and their descriptions.

Table 29. Help menu commands

Command	Description
Instrument Name Help	Opens the Help for the selected instrument. For the device drivers provided on the LC Devices DVD, this Help describes the instrument configuration, instrument method, and direct control parameters for the specific device. For autosamplers, the Help describes the sample position notation for sequences. For Thermo Scientific mass spectrometers, this Help describes the instrument configuration and instrument method parameters for the mass spectrometer.
Instrument Setup Help	Opens the general Instrument Setup window Help topic. For information about a specific device, see the *Instrument Name* Help.
Help On Current Item	Opens the Help topic for the Instrument Setup page that is currently displayed.
Instrument Name Contents and Index	Opens the Help for the selected instrument.
Xcalibur Help	Open Xcalibur Help.
Glossary	Opens the glossary.
How To Use Help	Opens the Help topic that describes how to use the Help viewer.
About Instrument Setup	Displays the Thermo Fisher Scientific copyright notice and installed version numbers of the following: • Layered applications • Foundation platform • Xcalibur data system • Device drivers

Instrument Setup Window Toolbar

Table 30 lists the items and their descriptions on the Instrument Setup window toolbar.

Table 30. Toolbar for the Instrument Setup window

Button	Description
New	Resets the instrument method parameters to their default settings. The title bar displays the name Untitled for the instrument method.
Open	Opens the Open dialog box, where you can select an existing instrument method file.
Save	If you have already saved the instrument method, clicking the Save icon saves the instrument method. If your method has not been saved before, clicking Save opens the Save As dialog box. Select the name and location for your instrument method. When you click Save, the File Summary Information dialog box opens. Enter header information for your instrument method. When you click OK, the File Save – Audit Trail Dialog Box opens. Enter audit information about the active file and click **Continue** to save the file.
Print	Prints the parameter settings in your instrument method.
Home Page	Opens the Home Page window – Roadmap view.
Help	Opens the Help topic for the Instrument Setup page that is currently displayed.

C

Sequence Setup

Use the Sequence Setup view of the Home Page window to set up a sequence table for acquiring, processing, or acquiring and processing a sample set containing unknown samples, calibration standard samples, quality control samples, and blank samples.

Contents

- Sequence Setup View
- Sequence Setup Menus
- Sequence Editor Toolbar
- Sequence Setup View Dialog Boxes

For information about creating and modifying sequences, see Chapter 4, “Creating and Modifying Sequences.” For information about running and batch reprocessing sequences, see Chapter 5, “Running and Batch Reprocessing Sequences.”

Sequence Setup View

Clicking the Sequence Setup icon on the Roadmap view or the Sequence View icon on the Home Page View toolbar, or choosing View > Sequence Setup view from the Home Page window menu opens the sequence table and the Sequence Editor toolbar.

Each sample injection to be acquired or raw data file to be reprocessed is defined by the settings of its sequence row as described in Table 31.

You can enter the sample information into each row manually or you can use the New Sequence Template dialog box to enter the sample information semi-automatically. For more information about creating and modifying sequences, see Chapter 4, “Creating and Modifying Sequences.”

Tip For a quantitative analysis, the Xcalibur data system organizes the sample data into brackets. Each bracket contains two sample categories. The calibration standards make up one category. The other sample types including unknowns, blanks, and QC samples make up the other category.

The Xcalibur data system provides four options for sequence bracketing: None, Open, Overlapped, and Non-Overlapped. Only the None option for sequence bracketing allows the use of more than one processing method per sequence. Because the sequence table editor allows only Open sequence bracketing, you must use the New Sequence Template dialog box to set up the other bracketing options.

Table 31 describes the columns in the Sequence Setup table.

Table 31. Sequence table parameters (Sheet 1 of 6)

Parameter	Description
Sample Type	Specifies the type of sample described by the sequence row. The sample type defines how the data system processes the sample data. These sample types are available for all bracket types: Unknown, Blank, and QC. The available standard sample types depend on the bracket type and include the following: Std Clear, Std Update, Start Bracket., and End Bracket.
Unknown	An Unknown is a sample with an unknown amount of the analyte or analytes
Blank	A Blank is a sample matrix or solvent blank.
QC	A QC is a quality control sample that contains known amounts of the analyte or analytes in a sample matrix or solvent blank.
Std Clear	Standard Clear is available with the None bracketing option. When the data system processes a Std Clear sample, it clears the data for all of the calibration levels in the calibration file and populates the associated calibration level with data from the current data file. A calibration file can contain data for multiple named components (analytes) and multiple calibration levels.
Std Update	Standard Update is available with the None bracketing option. When the data system processes a Std Update sample, it updates the associated calibration level with additional data from the current data file.
Start Bracket	Start Bracket is available only with the Overlapping and Non-Overlapping bracketing options. The Start Bracket sample type defines the beginning of the current bracket. When the data system encounters the Start Bracket sample type during post-acquisition processing, it clears the calibration data for the associated calibration level.

Table 31. Sequence table parameters (Sheet 2 of 6)

Parameter	Description
End Bracket	End Bracket is available with the Non-Overlapping bracketing option. The End Bracket sample type defines the end of the current bracket. With the Non-Overlapping bracketing option, each bracket must begin with the Start Bracket sample type for each calibration level and end with the End Bracket sample type for each calibration level. During post-acquisition processing, the data system processes the standard sample types first and then calculates the calibration curve for each target component (analyte) by using the information from the Start Bracket and End Bracket sample types for the current bracket. After the data system calculates the calibration for each analyte, it processes all of the sample types in the current bracket. **Tip** To select the sample type for a sequence row, click the Sample Type column, and then click the down arrow that appears to display the list of sample types. For more information about sample types and sequence bracketing, see "Step 2: Selecting the Bracket Type" on page 71.
File Name	Specifies the name of the file that contains the sample data. The File Name is a combination of the Base File Name prefix and a sequential sequence number. • If you use the New Sequence Template dialog box to create a sequence, you define the base file name in the Base File Name box and the starting number for the sequence in the Starting Number box. • If you use the default Starting Number of 1, the suffix for the first sample is 01, the suffix for the second sample is 02, and so on. • If you change the Starting Number to a value of 10 or higher, the suffix for the first sample is the Starting Number, and subsequent rows in the sequence are incremented by 1. For example, if the Starting Number is 10, the suffix for the first sample is 10, the suffix for the second sample is 11, and so on.
Sample ID	Specifies identifying text for each sample. To change the current ID, type a new alphanumeric value in the Sample ID box. The sample ID value does not have to be a unique identifier. If you use the New Sequence Template dialog box 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. If the instrument configuration includes an autosampler, the data system uses the sample vial or microwell position as the suffix for each sample. For information about the position notation, refer to the Help for your autosampler.

Table 31. Sequence table parameters (Sheet 3 of 6)

Parameter	Description
Path	Specifies the path to the raw file or files that the Xcalibur data system creates for the sample data. The data system 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 data system enters the path in the Path box. You can also type the path in the Path box.
Instrument Method	Specifies the path and file name of the instrument method to be used to control the instruments of the mass spectrometry system during a sample run. 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. You can select up to one instrument method per injection.
Processing Method	Specifies the path and file name of the processing method to be used to process the samples. 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 data system 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. With the Open, Overlapping, and Non-Overlapping bracketing options, you can select only one processing method for the entire sequence. When you create the sequence manually, the data system defines the bracketing option as Open.
Calibration File	Specifies the calibration file to be used for an unbracketed sequence (None bracket type). To quantitatively process an unbracketed sequence, you must specify a calibration file. 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 data system 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.

Table 31. Sequence table parameters (Sheet 4 of 6)

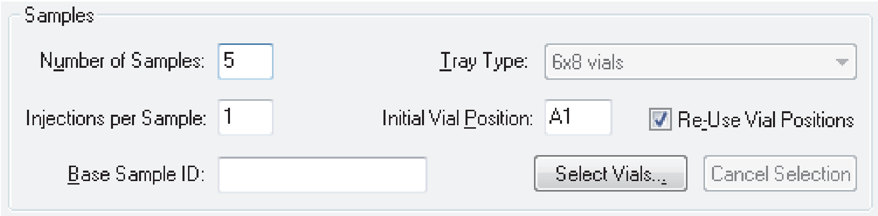
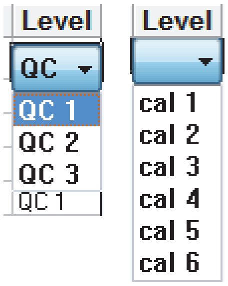
Parameter	Description
Position	Specifies the vial or microwell position in the autosampler. To change the position, type a value in the Position box. For information about the tray, microwell plate, and vial notation, refer to the Help for your autosampler. If you use the New Sequence Template dialog box to create your sequence, you can use the following parameters in the Samples area to set up the vial positions: • Type the initial vial position in the Initial Vial Position box. • If the Select Vials button is available, you can click it to open a graphical representation of the autosampler tray that you can use to select the vial positions. • Select the Re-Use Vial Positions check box to set up the sequence to makes replicate injections from the same vial position.  Samples Number of Samples: 5 Tray Type: 6x8 vials Injections per Sample: 1 Initial Vial Position: A1 ☑ Re-Use Vial Positions Base Sample ID:
Injection Volume	Specifies 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 instrument method. 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.
Level	Specifies the calibration level for a standard sample type or the quality control level for a QC sample.  To specify the calibration level for a standard or QC sample type, you must first add a processing method to the sequence. After you add a processing method to the sequence, the level list appears when you double-click the Level column for a standard or QC sample type.

Table 31. Sequence table parameters (Sheet 5 of 6)

Parameter	Description
Sample Weight	Specifies the amount of a component that has been placed in the sample. The processing method specifies the unit for this sample weight. The unit is included in Xcalibur reports. The data system does not convert units. To change the sample weight, type the weight in the Sample Weight box.
Sample Volume	Specifies the volume of a component that has been placed in the sample. The processing method specifies the unit for this volume. The unit is only included in Xcalibur reports. The data system does not convert units. To change the sample volume, type the sample volume in the Sample Volume box.
ISTD Correction Amount	Specifies 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, you can apply a bulk adjustment factor 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.
Dilution Factor	Specifies the dilution factor that was used to prepare the sample. The valid range is 0.000 to 10 000.000. The data system interprets a value of 0.000 as no dilution. If for example, you type a value of 2 in the Dil Factor column for the Unknown sample types, the data system multiplies the calculated amount by a factor of 2. To change the dilution factor, type a value in the Dil Factor box.
Comment	Use this box to add comments about the sample.

Table 31. Sequence table parameters (Sheet 6 of 6)

Parameter	Description
Sample Name	Specifies the sample name for the sample.
Heading 1 [*Study*] Heading 2 [*Client*] Heading 3 [*Laboratory*] Heading 4 [*Company*] Heading 5 [*Phone*]	Use these columns to convey additional information about the sample to others or as a reminder to yourself. For information about changing the column heading labels, see "Customizing the User Labels for a Sequence" on page 90.

Sequence Setup Menus

The menu bar of the Sequence Setup view contains the following menus from left to right: File, Edit, Change, Actions, View, GoTo, and Help. This section describes the following menus:

"File Menu – Sequence Setup View," on this page

"Edit Menu – Sequence Setup View" on page 208

"Change Menu – Sequence Setup View" on page 209

"Actions Menu – Sequence Setup View" on page 210

For information about the View, GoTo, and Help menus, see "Home Page Menus" on page 158.

File Menu – Sequence Setup View

Table 31 lists the File menu commands for the Sequence Setup view of the Home Page window.

Table 32. File menu – Sequence Setup commands (Sheet 1 of 2)

Icon or button	**Command**	**Description**
🗋	New	Opens the New Sequence Template dialog box that you use to create a new sequence.
📂	Open	Opens the Open dialog box that you use to open an existing sequence file.
💾	Save	Opens the File Summary Information dialog box, where you can enter an auditable comment about the sequence. After you save the comment by clicking OK, the Save As dialog box opens.
–	Save As	Opens the File Summary Information dialog box, where you can enter an auditable comment about the sequence. After you save the comment by clicking OK, the Save As dialog box opens.
–	Summary Information	Opens the File Summary Information dialog box, where you can view, change, or delete the comment about the current file.
–	Import Sequence	Opens the Import Sequence dialog box that you can use to locate (drive and directory) and import one or more columns of a stored sequence. For more information, see "Import Sequence Dialog Box" on page 228.
–	Export Sequence	Opens the Export Sequence dialog box that you can use to export one or more columns of the current sequence to a new location and with a new name. For more information, see "Export Sequence Dialog Box" on page 225.

Table 32. File menu – Sequence Setup commands (Sheet 2 of 2)

Icon or button	Command	Description
–	Change Dataset Name	Opens the *Dataset* Name Selector dialog box. Use this dialog box to select a dataset name 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 or Change Study Name. For more information, see "Study Name Selector Dialog Box" on page 404.
–	View Audit Trail	Opens the Thermo Foundation Audit Viewer, where you can view all auditable events and changes made to data files in the current application.
🖨	Print	Opens the Print Selection dialog box that you can use to print a sequentially numbered vial position list from the current sequence, selected rows in a sequence, or currently displayed columns of the current sequence.
–	Print Preview	Opens the Print Selection dialog box. After you click OK to close the Print Selection dialog box, the data system displays a preview of the text to be printed.
–	Page Setup	Opens the Page Setup dialog box, where you can select the following printing options: paper, orientation, margins, and printer.
–	*Recently Used Files*	View the paths and names of the four most recently used files. These are located above the Exit command. The Xcalibur data system displays both open and closed files. Click a displayed file to load it. If the selected file was closed, the data system opens it.
–	Exit	Closes the active window. If you exit before clicking **OK** from an active dialog box, the data system prompts you to save your changes.

Edit Menu – Sequence Setup View

The Edit menu is available only in the Sequence Setup view of the Home Page window. Table 33 describes the Edit menu commands.

Table 33. Edit menu commands

Button or icon	Command	Description
↶	Undo	Cancels your previous action.
–	Clear	Removes the text in selected sequence table cells or entire sequence rows. The data system clears the text from the selected boxes. When you clear and entire row, the data system replaces the previously selected sample type in the Sample Type column with the Unknown sample type. For more information, see “Using the Edit Commands” on page 86.
⎘	Copy	Copies the selected rows or columns from the sequence to the clipboard.
📋	Paste	Pastes copied sequence rows or columns from the clipboard to the sequence table.
–	Insert Row	Inserts a row above the selected row. For more information, see “Using the Edit Commands” on page 86.
–	Delete Row	Deletes one or more adjacent rows from the sequence. For more information, see “Using the Edit Commands” on page 86.
–	Go To Row	Opens the Go to Row dialog box. Use this dialog box to move the cursor in the current sequence to a specified row number. This action is extremely useful when you are reviewing or modifying a long sequence. For more information, see “Go To Line Number Dialog Box” on page 228 and “Going to a Sequence Row” on page 91.
⇊	Fill Down	Copies information from a sample row to a series of rows and avoid repetitive cut-and-paste operations. For more information, see “Fill Down Dialog Box” on page 227 and “Filling Down Sequence Parameters” on page 92.
🔍	Browse File Name	Depending on the selected file type, this command does the following: • When you select a cell in the File Name column, this command opens the Select Data File dialog box, where you can browse to and select a data file. • When you select a cell in the Inst Meth column, this command opens the Select Instrument Method dialog box, where you can browse to and select an instrument method. • When you select a cell in the Proc Meth column, this command opens the Select Processing Method dialog box, where you can browse to and select a processing method.

Change Menu – Sequence Setup View

Table 34 describes the Change menu commands that are available in the Sequence Setup view of the Home Page window. This menu is not available from the other Home Page views.

Table 34. Change menu commands

Icon	Command	Description
	User Labels	Opens the User Labels dialog box, where you can change the column headings of five columns in the Sequence Setup view. The default headings are Study, Client, Laboratory, Company, and Phone. For more information, see "User Labels Dialog Box" on page 246.
–	Tray Name	Opens the Tray Selection dialog box, where you can select the autosampler tray type for the current sequence. This dialog box is not available for all autosamplers. For more information, see "Tray Selection Dialog Box" on page 245.
	Column Arrangement	Opens the Column Arrangement dialog box, where you can select the columns that you want to display for the current sequence. For more information, see "Column Arrangement Dialog Box" on page 223.
	Transfer Row Info	Opens the Transfer Row Info dialog box. Use this 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. For more information, see "Transfer Row Information Dialog Box" on page 244.

Actions Menu – Sequence Setup View

Table 35 describes the Actions menu commands for the Sequence Setup view of the Home Page window.

Table 35. Actions menu – Sequence Setup commands (Sheet 1 of 4)

Icon	Command	Description
MB	Check Disk Space	Opens the Disk Space dialog box, where you can determine how much available disk space you have on a disk drive.
⇨	Run This Sample	Opens the Run Sequence dialog box with a selection of one sequence row in the Run Rows box. Use the Run Sequence dialog box to set up the run parameters.
⇨	Run Sequence	Opens the Run Sequence dialog box with a selection all the sequence rows. Use the Run Sequence dialog box to set up the run parameters.
Σ	Batch Reprocess	Opens the Batch Reprocess dialog box, where you can set up the reprocessing options for the current sequence and start the batch reprocessing process.
–	Open [Method] File	Opens either an instrument method or a processing method selected from the sequence table in the Sequence Setup view. • When you select an instrument method in the Inst Meth column of the sequence and then select this command, the data system opens the Instrument Setup window and displays the selected file so that you can edit the parameters. • When you select a processing method in the Proc Meth column of the sequence and then select this command, the data system opens the Processing Setup window and displays the selected file so that you can edit the parameters. This command is only active when you select an instrument method or a processing method.

Table 35. Actions menu – Sequence Setup commands (Sheet 2 of 4)

Icon	Command	Description
▶	Start Analysis	Starts the sequence run manually. By default, the Start When Ready check box is selected. If you want to make automated injections with an autosampler, do not clear this check box. For information about connecting the contact closure signal between the mass spectrometer and the autosampler, see the *Getting Connected Guide* for your mass spectrometer. For information about specifying the start instrument, see "Running a Single Sample or Multiple Samples" on page 101. When you clear the Start When Ready check box in the Start Options area of the Run Sequence dialog box, you must do one of the following to start each sample run: • Choose **Actions > Start Analysis** in the menu bar. –or– • Click the **Start Analysis** icon, ▶, in the toolbar. Before you send the Start Analysis command, make sure that the data system is in the Ready state. For more information, see "Starting Each Run Manually" on page 107.
■	Stop Analysis	Stops the current sample run. When you choose Stop Analysis, the following actions occur: • The Pause/Resume Sequence Queue icon goes to the resume sequence queue state; that is, it appears depressed, ⏸. • The data system immediately stops the current run and acquires the raw data file. • On the Info view – Status page, the Sequence readback under Run Manager displays PAUSED. To resume the sequence, click the **Pause/Resume Sequence Queue** icon, ⏸. The data system resumes the sequence at the next sample in the queue. For more information, see "Stopping the Current Sample Run or Pausing the Sequence Queue" on page 106.

Table 35. Actions menu – Sequence Setup commands (Sheet 3 of 4)

Icon	Command	Description
⏸	Pause Analysis	Pauses the current sequence after the current sample run ends. When you choose Pause Analysis, the following actions occur: • A check appears to the left of the Pause Analysis command. • The Pause/Resume Sequence Queue icon goes to the resume sequence queue state; that is, it appears depressed, ⏸. • The data system continues to acquire data for the current sample until the run time specified in the instrument method expires. At the end of the run, the data system acquires the raw data file. • At the end of the current run, the data system enters the Paused state as indicated by the PAUSED text for the Sequence readback under Run Manager on the Information view – Status page. ❖ **To restart a paused sequence** Choose ✓ **Pause Analysis**. The data system resumes the sequence with the next sample in the queue.
–	Devices On	Places the system in the On state when the current sequence is completed. In this state, all power and flows are maintained at operational levels. Set the data system in the On state to run another sequence without waiting. This option has the same effect as choosing the On option in the After Sequence Set System area in the Run Sequence dialog box in the Sequence Setup view.
–	Devices Standby	Places the system in the Standby state when the current sequence is completed. Set the data system in 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 the Standby option in the After Sequence Set System area in the Run Sequence dialog box.

Table 35. Actions menu – Sequence Setup commands (Sheet 4 of 4)

Icon	Command	Description
–	Devices Off	Places the system in the Off state when the current sequence is completed. The Off state indicates that all power to the instrument that can be controlled by the data system is turned off. This action includes power to all heaters and most subassemblies, but in some cases it might not include all subassemblies. This option has the same effect as choosing the Off option in the After Sequence Set System area in the Run Sequence dialog box. **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 maintenance manual.
–	Automatic Devices On	Sets the Xcalibur data system to automatically turn on all devices controlled by the data system before starting a data acquisition. If this command has a check mark to its left, the data system automatically turns on all devices that are in the Off or Standby state. If this command does not have a check mark to its left, the Xcalibur data system posts the following message if you have one or more devices in a Standby or Off state: One or more devices to be used by this sequence are not ‘On’. The sequence will not start until all the requested devices are ready. Do you want all the devices to be switched ‘On’? Press ‘Yes’ to switch devices On, or ‘No’ to continue with devices in the ‘Off’ or in ‘Standby’ state. If you select ‘No’ you will need to select the Devices On command from the Actions menu before the sequence will proceed.
–	Reinstate Warnings	Restores the display of messages that you have turned off by selecting the **Don’t Ask Again** check box. Periodically, the data system displays a message or dialog box that includes the following: ☐ Don’t ask again. If you select this option when you see it, the data system does not display this message again until you turn warnings back on using the Reinstate Warnings command. To turn off warnings, select this check box: ☑ Don’t ask again

Sequence Editor Toolbar

Table 36 lists the buttons in the Sequence Editor toolbar of the Home Page window.

Table 36. Sequence Editor toolbar buttons (Sheet 1 of 4)

Icon or Button	Command	Description
🗋	New Sequence	Opens the New Sequence Template dialog box that you can use to create a new sequence.
📂	Open	Opens the Open dialog box that you use to open an existing sequence file.
💾	Save	Opens the File Summary Information dialog box, where you can enter an auditable comment about the sequence. After you save the comment by clicking OK, the Save As dialog box opens.
🖨	Print	Opens the Print Selection dialog box that you can use to print a sequentially numbered vial position list from the current sequence, selected rows in a sequence, or currently displayed columns of the current sequence.
⎘	Copy	Copies selected rows or columns from the sequence to the clipboard.
📋	Paste	Pastes copied sequence rows or columns from the clipboard to the screen.
↶	Undo	Cancels your previous action.
⇊	Fill Down	Copies information from a sample row to a series of rows to avoid repetitive cut-and-paste operations. For more information, see "Fill Down Dialog Box" on page 227 and "Filling Down Sequence Parameters" on page 92.
🔍	Browse File Name	Depending on the selected file type, this command does the following: • When you select a cell in the File Name column, this command opens the Select Data File dialog box, where you can browse to and select a data file. • When you select a cell in the Inst Meth column, this command opens the Select Instrument Method dialog box, where you can browse to and select an instrument method. • When you select a cell in the Proc Meth column, this command opens the Select Processing Method dialog box, where you can browse to and select a processing method.

Table 36. Sequence Editor toolbar buttons (Sheet 2 of 4)

Icon or Button	Command	Description
	User Labels	Opens the User Labels dialog box, where you can change the column headings of five columns in the Sequence Setup view. The default headings are Study, Client, Laboratory, Company, and Phone. For more information, see "User Labels Dialog Box" on page 246.
	Column Arrangement	Opens the Column Arrangement dialog box, where you can select the columns that you want to display for the current sequence. For more information, see "Column Arrangement Dialog Box" on page 223.
	Transfer Row Info	Opens the Transfer Row Info dialog box. Use this 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. For more information, see "Transfer Row Information Dialog Box" on page 244.
MB	Disk Space	Opens the Disk Space dialog box, where you can determine how much available disk space you have on your disk drive or drives.
	Run Sample	Opens the Run Sequence dialog box. If you do not select a sequence row before clicking this icon, the Run Rows box lists row 1. If you select a sequence row before clicking this icon, the Run Rows box lists the selected row number.
	Run Sequence	Opens the Run Sequence dialog box. If you do not select a range of sequence rows, the Run Rows box lists the entire sequence range. If you select a range of rows, the Run Rows box lists the selected range.
	Batch Reprocess	Opens the Batch Reprocess Setup dialog box. If you do not select a range of sequence rows before clicking this icon, the Process Rows box lists the entire sequence range.

Table 36. Sequence Editor toolbar buttons (Sheet 3 of 4)

Icon or Button	Command	Description
▶	Start Analysis	Starts the sequence run manually. By default, the Start When Ready check box is selected. If you want to make automated injections with an autosampler, do not clear this check box. For information about connecting the contact closure signal between the mass spectrometer and the autosampler, see the *Getting Connected Guide* for your mass spectrometer. For information about specifying the start instrument, see "Running a Single Sample or Multiple Samples" on page 101. When you clear the Start When Ready check box in the Start Options area of the Run Sequence dialog box, you must do one of the following to start each sample run: • Choose **Actions > Start Analysis** in the menu bar. –or– • Click the **Start Analysis** icon, ▶, in the toolbar. Before you send the Start Analysis command, make sure that the data system is in the Ready state. For more information, see "Starting Each Run Manually" on page 107.
■	Stop Analysis	Stops the current sample run. When you click the Stop Analysis icon, the following actions occur: • The Pause/Resume Sequence Queue icon goes to the resume sequence queue state; that is, it appears depressed, ⏸. • The data system immediately stops the current run and acquires the raw data file. • On the Info view – Status page, the Sequence readback under Run Manager displays PAUSED. To resume the sequence, click the **Pause/Resume Sequence Queue** icon, ⏸. The data system resumes the sequence at the next sample in the queue. For more information, see "Stopping the Current Sample Run or Pausing the Sequence Queue" on page 106.

Table 36. Sequence Editor toolbar buttons (Sheet 4 of 4)

Icon or Button	Command	Description
⏸	Pause/Resume Sequence Queue	Pauses the current sequence after the current sample run ends. When you click the Pause/Resume Sequence Queue icon, the following actions occur: • A check appears to the left of the Pause Analysis command. • The Pause/Resume Sequence Queue icon goes to the resume sequence queue state; that is, it appears depressed, ⏸. • The data system continues to acquire data for the current sample until the run time specified in the instrument method expires. At the end of the run, the data system acquires the raw data file. • At the end of the current run, the data system enters the Paused state as indicated by the PAUSED text for the Sequence readback under Run Manager on the Information view – Status page. ❖ **To restart a paused sequence** Click ⏸. The data system resumes the sequence with the next sample in the queue. You can review the sample list queue at any time using the Acquisition Queue page of the Home Page Information view.
?	Help	Opens Xcalibur Help and displays the contents window for the Sequence Setup view.

Sequence Setup View Dialog Boxes

You can open these dialog boxes in the Sequence Setup view. This list is in alphabetical order.

- 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
- Print Selection 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 the Batch Reprocess Setup 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 in the processing method. Whether you are processing or reprocessing the data, the results are the same. This user 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 data system posts a message describing the problem.

For information about using the Batch Reprocess Setup dialog box, see “Batch Reprocessing a Sequence” on page 116.

This table describes the parameters in the Batch Reprocess Setup dialog box.

Table 37. Batch Reprocess Setup dialog box (Sheet 1 of 2)

Parameter	Description
Process Rows	
Process Rows	Specifies 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, type10–22.
Processing Actions	
Quan	Selecting this check box enables these check boxes for quantitative processing: Peak Detection & Integration, Calibration, and Quantitation processing.
Peak Detection & Integration (Quan)	Selecting this check box turns on peak detection and integration processing for the samples selected from the current sequence and displayed in the Process Rows box. Define the peak detection and integration parameters in the quantitative section of the processing method. The sequence must include a valid processing method and valid raw data files.
Calibration (Quan)	Selecting this check box turns on calibration processing for the samples selected from the current sequence and displayed in the Process Rows box. The processing method defines the calibration settings. To update the calibration during batch reprocessing, the selected sequence rows must include a valid processing method, valid raw data files, and the appropriate calibration level selections in the Level column of the sequence table.
Quantitation (Quan)	Selecting this check box turns on quantitation processing for the samples selected from the current sequence and displayed in the Process Rows box. The processing method defines the quantitative processing parameters. For quantitative processing, the selected sequence rows must include a valid processing method and valid raw data files.
Qual	Selecting this check box makes the following check boxes available for qualitative processing: Peak Detection & Integration, Spectrum Enhancement, and Library Search.
Peak Detection & Integration (Qual)	Selecting this check box turns on peak detection and integration for the samples selected from the current sequence and displayed in the Process Rows box. Define these parameters in the qualitative section of the processing method. For qualitative processing, the selected sequence rows must include a valid processing method and valid raw data files.

Table 37. Batch Reprocess Setup dialog box (Sheet 2 of 2)

Parameter	Description
Spectrum Enhancement (Qual)	Selecting this check box turns on spectrum enhancement processing for the samples selected from the current sequence and displayed in the Process Rows box. Set up spectrum enhancement in the processing method by defining the parameters on the Spectrum Enhancement Page for Qual View in the Processing Setup window. To perform spectrum enhancement, the selected sequence rows must include a valid processing method and valid raw data files.
Library Search (Qual)	Selecting this check box turns on library searches for the samples selected from the current sequence and displayed in the Process Rows box. Set up library searches in the processing method by defining the library search parameters on the Library Search Constraints Page for Qual View in the Processing Setup window. To run library searches, the selected sequence rows must include a valid processing method and valid raw data files.
Reports	Selecting this check box makes these check boxes available: Print Sample Reports and Print Summary Reports.
Print Sample Reports	Selecting this check box turns on printing for sample reports. Set up sample reports in the processing method by defining the sample report parameters in the Reports view of the Processing Setup window. To print sample reports, the selected sequence rows must include a valid processing method and valid raw data files.
Print Summary Reports	Selecting this check box turns on printing for summary reports. Set up summary reports in the processing method by defining the summary report parameters in the Reports view of the Processing Setup window. To print summary reports, the selected sequence rows must include a valid processing method and valid raw data files.
Programs	Selecting this check box turns on the Programs that the processing method specifies. Running programs requires a valid processing method.
Create Quan Summary Spreadsheet	When you select this check box, the data system creates a spreadsheet that you can open in Excel after batch reprocessing is complete.
Advanced Options	
Replace Sample Info	Selecting this check box removes sequence data in the raw data files and replaces it with the active sequence data To use the data in the current raw file, make sure the check box is clear.

Change Instruments In Use Dialog Box

Use the Change Instruments In Use dialog box to select the instruments that you are using to run the current sequence and the start instrument that triggers data acquisition for each run. If you change the Foundation instrument configuration after running the previous sequence, this dialog box automatically appears.

For more information about using the Change Instruments In Use dialog box, see "Running a Single Sample or Multiple Samples" on page 101.

❖ To add an instrument to 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 *x.x* > 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.

❖ To select the start instrument

1. In the row of the instrument that you want to use as the start instrument, click the Start Instrument column to change the blank entry to Yes.
2. Click **OK** to accept the changes and close the dialog box.

This table describes the columns in the Change Instruments in Use dialog box.

Table 38. Change Instruments In Use dialog box parameters

Parameter	Description
Instrument	Displays the list of instruments that have been configured for operation as Xcalibur devices. To change the entries in the Instrument column, you must use the Instrument Configuration window.
In Use	Specifies whether the instrument is in use for this sequence run. The rows in this list display either Yes (in use) or a blank entry (not in use). When you configure an instrument using the Instrument Configuration window, its default status is Yes. If you do not want to use the instrument for the current sequence run, 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.
Start Instrument	Specifies the Start Instrument. 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 the Column Arrangement dialog box to select which columns to display and the position or order of the columns in the current sequence.

This table describes the parameters in the Column Arrangement dialog box. For information about using the Column Arrangement dialog box, see "Adding, Removing, and Arranging the Sequence Columns" on page 88.

This table describes the parameters in the Column Arrangement dialog box.

Table 39. Column Arrangement dialog box parameters (Sheet 1 of 2)

Parameter	Description
Available Columns	Displays the columns that do not currently appear in the Sequence Setup view but that you can add. 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 up the User Labels column heading, use the User Labels Dialog Box.
Displayed Columns	Displays the columns that currently appear in the Sequence Setup View. The left-to-right order of the columns for a particular sequence corresponds to the top-to-bottom order in the Displayed Columns list.

Table 39. Column Arrangement dialog box parameters (Sheet 2 of 2)

Parameter	Description
Buttons	
Add	To add a column to the sequence, select the column in the Available Columns list box. Click **Add** to move the column name to the Displayed Columns list. The Sequence Setup view displays the columns listed in the Displayed Columns list.
Remove	To remove a sequence column from the current display, select the column from the Displayed Columns list. Click **Remove** to move the column name to the Available Columns list.
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 data system 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 data system 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 the United States is the comma. In this case, the data system 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 data system 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 check boxes so that you can include any, all, or none of the sequence columns.

For more information about using the Export Sequence dialog box, see "Exporting a Sequence" on page 127.

This table describes the parameters in the Export Sequence dialog box.

Table 40. Export Sequence dialog box parameters

Parameter	Description
Export to File	Specifies the destination path and file name for the exported file. The data system saves the file with a .csv extension.
Select Columns to Export	This area contains check boxes that correspond to columns in the Sequence Setup View. 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 the Fill Down dialog box to fill selected rows of selected columns with duplicate text entries or appropriately sequenced number entries. 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 that you select.

For information about using the Fill Down dialog box, see "Filling Down Sequence Parameters" on page 92.

> **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 Fill Down command on the Edit menu and the Fill Down icon in the toolbar become available.

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

This table describes the parameters in the Fill Down dialog box.

Table 41. Fill Down dialog box parameters

Parameter	Description
Select Columns	This area lists the sequence columns. When you make a selection in the sequence table and click the Fill Down icon in the toolbar or choose Edit > Fill Down from the menu bar, the Fill Down dialog box opens with the check boxes for the corresponding column selected. You can change the selection by selecting or clearing the check boxes.
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.

This table describes the parameters in the Go To Line Number dialog box.

Table 42. Go To Line Number dialog box parameters

Parameter	Description
Row	Type the row number 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 data system moves the focus to the selected 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 data system 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.

Each country has a default list separator. For example, the default list separator for the United States is the comma. In this case, the data system 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 check boxes so that you can include any, all, or none 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.

For information about checking the list separator, see "Changing the List Separator Character" on page 123. For more information about using the Import Sequence dialog box, see "Importing a Sequence" on page 125.

This table describes the parameters in the Import Sequence dialog box.

Table 43. Import Sequence dialog box parameters

Parameter	Description
Import From File	Specifies 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 Setup View. 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.

For information about using the New Sequence Template dialog box to create a sequence semi-automatically, see "Creating a Sequence Semi-Automatically" on page 69.

This table describes the parameters in the New Sequence Template dialog box.

Table 44. New Sequence Template dialog box parameters (Sheet 1 of 8)

Parameter	Description
General	
Base File Name	Specifies the base file name that the data system 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 data system to add as a suffix to the name you entered into the Base File Name box. The file name of the raw data files consists of the base file name and the starting number suffix. 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	Specifies the path to the raw data files. 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 data system enters the path in the Path box. You can also type the path in the Path box.
Instrument Method	Specifies the path and instrument method for the samples in the 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.meth. 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.

Table 44. New Sequence Template dialog box parameters (Sheet 2 of 8)

Parameter	Description
Processing Method	Specifies the path and processing method for the samples in the 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 data system 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.
Calibration File	Specifies 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 want to 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** 1. Click **Browse** located to the right of the Calibration File box. The Select Calibration File dialog box opens. 2. From this dialog box, browse to the calibration file. 3. 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 data system includes this path and calibration file name in the Cal File column of the sequence. ❖ **To display the calibration file column** 1. Choose **Change > Column Arrangement**. 2. In the Available Columns list, select **Cal File**. Then click **Add**. 3. Click **OK** to close the dialog box. ❖ **To create a new calibration file** Type the path and calibration file name that you want the data system to create during batch processing. Do not include the .xcal file extension.

Table 44. New Sequence Template dialog box parameters (Sheet 3 of 8)

Parameter	Description
Samples	
Number of Samples	Specifies the number of Unknown samples for the data system 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 two calibration sets and five samples, The data system orders the new sequence as follows: • Calibration Standard Samples (Set 1) • Unknowns (3 Samples) • Calibration Standard Samples (Set 2) • Unknowns (2 Samples)
Tray Type	Specifies 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 data system displays your new selection in the Tray Type list.
Injections Per Sample	Specifies the number of replicate injections per sample position.
Initial Vial Position	Specifies the first vial position in the new sequence. The vial or microwell plate notation depends on the configured autosampler. The default position is the first position for the configured vial tray or microwell plate. To start at another position, do one of the following: • Type the position in the Initial Vial Position box. • Interactively select the position as follows (not available for some autosamplers): a. Click **Select Vials** to open the Vial Selection dialog box. b. Select the initial vial position by clicking the graphic. c. Click **OK** to close the dialog box and accept the new position. d. Click **Cancel** to make the Number of Samples box available.
Re-Use Vial Numbers	Specifies whether to reuse the 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 data system creates a sequence in which each sample is drawn from a different vial.

Table 44. New Sequence Template dialog box parameters (Sheet 4 of 8)

Parameter	Description
Base Sample ID	Specifies the prefix for the sample identification. Type an alphanumeric prefix in the Base Sample ID box that the data system applies to each sample in the new sequence. If the instrument configuration includes an autosampler, the data system appends the row position to the sample ID prefix and starts sample ID numbering at the initial vial position. For example, if you type Assay in the Base Sample ID box, and the initial vial position for the sequence is A:1, the data system numbers the first five samples as follows: • AssayA:1 • AssayA:2 • AssayA:3 • AssayA:4 • AssayA:5
Bracket Type	
None	If you select this option, the data system creates a sequence with 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 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

Table 44. New Sequence Template dialog box parameters (Sheet 5 of 8)

Parameter	Description
Open	If you select this option, the data system creates a sequence with 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	If you select this option, the data system creates a sequence with 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 44. New Sequence Template dialog box parameters (Sheet 6 of 8)

Parameter	Description
Overlapped	If you select this option, the data system creates a sequence with 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	Selecting this check box makes the parameters in the Calibration area available and the data system adds calibration standards to the sequence table. When you select this check box, you must also select a processing method that contains defined calibration levels. If you select the Add Standards check box without selecting a valid processing method for the sequence, the data system displays a warning message when you click OK to close the dialog box and creates a sequence with only Unknown sample types.

Table 44. New Sequence Template dialog box parameters (Sheet 7 of 8)

Parameter	**Description**
Number of Calibration Sets	This box is available when you select the None option in the Bracket Type area. Type the number of calibration sets that you want in your new sequence. The valid range of values is 1 to 10.
Number of brackets	This box is available when you select the Non-Overlapped option or the Overlapped option in the Bracket Type area. Enter the number of brackets that you want in your new sequence. The valid range of values is 1 to 10.
Injections Per Level	Specifies the number of replicate calibration standard samples that are to be run at each defined calibration level. The data system groups replicate calibration samples in the new sequence. The valid range of values is 1 to 10.
Add Blanks	Selecting this check box 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	If you select this check box, the data system populates the Sample ID column in the new sequence for each standard sample type. If you type a name in the Base Sample ID box in the Samples area, the data system uses the name as the prefix and the vial position as the suffix to provide a sample ID for the standard samples. If you leave the Sample ID box empty, the data system uses the vial position to provide a sample ID for the standard samples. If you clear this check box, the data system leaves the Sample ID column empty for standard sample types. By default, the Fill In Sample ID for Standards check box is selected.
QC	
Add QCs	Selecting this check box makes the parameters in the QC area available, and the data system adds QC samples to the sequence table. When you select this check box, you must also select a processing method that contains defined QC levels. If you select the Add QCs check box without selecting a valid processing method for the sequence, the data system displays a warning message when you click OK to close the dialog box and creates a sequence without QC levels.
After First Calibration Only	When you select this option, the data system adds 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 available if you select the Add QCs check box.
After Every Calibration	When you select this option, the data system adds a quality control sample after every calibration sample set in the new sequence. This option is available if you select the Add QCs check box.

Table 44. New Sequence Template dialog box parameters (Sheet 8 of 8)

Parameter	Description
Add Blanks	Selecting this check box adds 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	If you select this check box, the data system populates the Sample ID column in the new sequence for each QC sample type. If you type a name in the Base Sample ID box in the Samples area, the data system uses the name as the prefix and the vial position as the suffix to provide a sample ID for the QC samples. If you leave the Sample ID box empty, the data system uses the vial position to provide a sample ID for the QC sample types. If you clear this check box, the data system leaves the Sample ID column empty for QC sample types. By default, the Fill In Sample ID for QCs check box is selected.

Print Selection Dialog Box

Use the Print Selection dialog box to print a vial or sequence list. For information about using the Print Selection dialog box, see "Printing a Vial or Sequence List" on page 95.

This table describes the parameters in the Print Selection dialog box.

Table 45. Print Selection dialog box parameters

Parameter	Description
Select the Printing Output	
Vial Position List	Select this option to print a sequentially numbered vial position list from the active sequence. The vial position list summarizes the sequence settings for each vial. A vial position list is useful when you are setting up the autosampler tray vial sequence.
All Columns	Select this option to print selected rows in a sequence.
Displayed Columns Only	Select this option to print the currently displayed columns of the active sequence. To change the sequence columns displayed, choose **Change > Column Arrangement**.

Run Sequence Dialog Box

Use the Run Sequence dialog box to select acquisition options and processing action options for 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, 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. The second time, select samples 5 through 10.

For more information about using the Run Sequence dialog box, see "Running a Single Sample or Multiple Samples" on page 101. For information about modifying the instrument configuration, see "Setting Up the Instrument Configuration in the Foundation Platform" on page 147.

This table describes the parameters in the Run Sequence dialog box.

Table 46. Run Sequence dialog box parameters (Sheet 1 of 6)

Parameter	Description
Acquisition Options	
Instrument	Displays the instruments that you configured for operation as Xcalibur devices in the Instrument Configuration window of the Foundation platform.
Start Instrument (read-only)	A Yes in this column specifies that the instrument starts the run. For an LC/MS system, the Start Instrument is typically the autosampler because the autosampler triggers data acquisition when it injects the sample into the chromatograph. You can change the start instrument and the instruments in use by opening the Change Instruments In Use Dialog box (see "Change Instruments In Use Dialog Box" on page 221).
Start When Ready	Determines whether the Xcalibur data system automatically starts a sequence run when the instruments are in the Ready state. By default, this check box is selected. Clear this check box if you want to start the sequence run manually. When the Start When Ready check box is selected, the data system places the sequence in the processing queue as soon as you click OK and starts each sequence run when the instruments are in the Ready state. If you clear the Start When Ready check box, the data system waits until you do one of the following to start each sequence run: • Click the Start Analysis icon, ▶. –or– • Choose Actions > Start Analysis.
Change Instruments	Opens the Change Instruments In Use dialog box, where you can change the status of the instruments in use or select a different start instrument.

Table 46. Run Sequence dialog box parameters (Sheet 2 of 6)

Parameter	Description
Instrument Method	
Start Up/Browse	Specifies the instrument (.meth) file that runs before the sequence run starts.
Shut Down/Browse	Specifies the instrument (.meth) file that runs after the sequence run finishes.
Programs	
Pre Acquisition/ Browse	Specifies the executable (.exe or .bat program) that runs before data acquisition.
Post Acquisition/ Browse	Specifies the .exe or .bat program that runs after data acquisition.
Run Synchronously	Run Pre Acquisition and Post Acquisition programs either synchronously (in series) or asynchronously (in parallel) with data acquisition. To run programs synchronously, the Run Manager waits until they can be run before acquisition, after acquisition, or both. 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 46. Run Sequence dialog box parameters (Sheet 3 of 6)

Parameter	Description
Pre Acquisition/ Post Acquisition	Runs 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 data system can run the Pre Acquisition program before 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 data system displays the new program or macro name. You can also type the command line. 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 46. Run Sequence dialog box parameters (Sheet 4 of 6)

Parameter	Description
Pre Acquisition/ Post Acquisition (continued)	You can run the XConvert.exe program during a sequence run. To convert the current file (myfile.raw) from the Xcalibur (.raw) file format to the ANDI (.cdf) file format and copy it to the current default data directory, use the following command line: `XConvert /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. For more examples, see Appendix F, "Executable Programs and Command Line Arguments." 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	
The On option is the default selection in this area.	
On	Select the On option 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	Select the Standby option to place 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.

Table 46. Run Sequence dialog box parameters (Sheet 5 of 6)

Parameter	Description
Off	Select the Off option to place 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 power shutoff 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.
User	By default, this box lists the name of the data system computer user. You can type a name in this box with up to 24 alphanumeric characters to identify the operator who submitted the sequence.
Run Rows	Specifies the currently selected sequence rows. You can also enter a different row or a new range in the box. The range can only include contiguous sample rows. To enter a range, type the first row number, a hyphen, and the last row number, *firstrow-lastrow.*
Priority Sequence	If you select this check box, the data system processes 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 data system 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	Selecting this check box makes the quantitative processing actions that the processing method defines available. Define the quantitative processing actions for a processing method in the Quan view of the Processing Setup window (see "Setting Up the Quantitative Processing Parameters" on page 21).
Qual	Selecting this check box makes the qualitative processing actions that the processing method defines available. Define the qualitative processing actions for a processing method in the Qual view of the Processing Setup window (see "Setting Up the Qualitative Processing Parameters" on page 50).
Reports	Selecting this check box makes the report actions that the processing method defines available. Define the reporting options for a processing method in the Reports view of the Processing Setup window (see "Adding Report Templates to Processing Methods" on page 59).

Table 46. Run Sequence dialog box parameters (Sheet 6 of 6)

Parameter	Description
Programs	Selecting this check box launches software programs that the processing method defines for the samples selected from the current sequence and displayed in the Process Rows box. Define the programs for a processing method in the Programs view of the Processing Setup window (see "Adding Programs or Macros to Processing Methods" on page 64). Enabling programs requires a valid processing method and a valid raw file.
Create Quan Summary	Creates a summary of the quantitation data. Select the Create Quan Summary check box to print a summary.

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 47 describes the parameters in the Transfer Row Information dialog box.

Table 47. 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 Tray Selection list 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, this dialog box is not available; 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, the following message appears:

> Invalid autosampler vial position. A valid example vial position would be [ ].
>
> The format inserted in the [ ] above corresponds to the currently configured autosampler.

Table 48 describes the parameters in the Tray Selections dialog box.

Table 48. 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 data system displays the selected tray in the list box.

User Labels Dialog Box

Use the User Labels dialog box to define the column headings for the user-specific information in the sequence table. These column headings are stored with the sequence. In addition to the sequence table, these column headings 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 do not want to use a heading, delete the text and leave the box blank. When all of the heading captions are correct, click **OK**.

For more information about using the User Labels dialog box, see "Customizing the User Labels for a Sequence" on page 90.

D

Processing Setup

This appendix describes the Processing Setup window, the views in the Processing Setup window, and the dialog boxes that you can access from the Processing Setup window.

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

In the Sequence Setup view, when you run or batch reprocess a sequence that contains a processing method, the data system uses the processing method to initiate processing for qualitative and quantitative data, to create reports, and to run additional programs or macros, such as shutdown procedures.

Contents

- Processing Setup Window
- Processing Setup Dialog Boxes
- Processing Setup Views

For information about creating processing methods, see Chapter 3, “Creating Processing Methods.”

Processing Setup Window

The Processing Setup window consists of a view bar, title bar, menu bar, toolbar, workspace, status bar, and access to Help. The workspace contains one of four views. You can access each view by clicking its button on the View bar or by choosing the view from the View menu (see Figure 8 on page 16).

The Qual and Quan views contain chromatogram and spectrum views. In addition, these three buttons appear at the bottom of the Reports and Programs views and above the spectrum and chromatogram views in the Qual and Quan Views: OK, Cancel, and Save As Default.

For more information about the elements of the Processing Setup window, see these topics:

- Processing Setup Title Bar
- Processing Setup Toolbar
- Processing Setup View Bar
- Processing Setup Menus
- Chromatogram and Spectrum Views in the Qual and Quan Views
- OK, Cancel, and Save As Default Buttons

For information about the views, see "Processing Setup Views" on page 294.

Processing Setup Title Bar

Figure 8 on page 16 shows the Processing Setup window.

The title bar components are as follows:

- The Processing Setup – *View* – *Page* – Study: *Name* – *Untitled*
- The active view (Quan, Qual, Reports, or Programs)
- The active page (for example, Identification)
- The active study (for example, Study:*Name*)

> **Note** On the Dataset List page of the Thermo Xcalibur Configuration dialog box, you can select the term to be used for datasets. The selections are Study, Job, and Dataset. You can also include a blank name as a dataset option.

- 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 Toolbar
- Reports and Programs Views Toolbar

Qual and Quan Views Toolbar

Table 49 lists the toolbar buttons that are available for the Qual and Quan views of the Processing Setup window.

Table 49. Qual and Quan views (Sheet 1 of 2)

Icon or Button		Description
🗋	New	Sets the processing method parameters to the default values and displays Untitled for the processing method name in the title bar.
📂	Open	Opens the Open dialog box, where you can browse to and select an existing processing method.
💾	Save	Opens the Save As dialog box, where you can enter a name for the processing method and save it.
📈	Open Raw File	Opens the Open Raw File dialog box, where you can browse to and select an existing raw data (.raw) file.
🖨	Print	Opens the Print dialog box, where you can browse to and select a report template for the processing method and submit the report to the default printer. For more information, see "Print Dialog Box" on page 288.
⇩	Zoom Out Y	Zooms out on the *y* axis by a factor of two to show more data. For example, you can change the *y*-axis range from 0–25 to 0–50.
⇧	Zoom In Y	Zooms in on the *y* axis by a factor of two 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	Determines the minimum and maximum signal in the chromatogram and then normalizes the data over the full range of the *y* axis. This option is suggested for PDA and UV data.
⇧ 0-100	Normalize	Normalizes 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	Zooms in on the *x* axis by a factor of two to show more detail. For example, you can change the *x*-axis range from 0–20 to 5–15.
←|→	Zoom Out X	Zooms out on the *x* axis by a factor of two from the center to show more data, for example, you can change the *x*-axis range from 7–12.5 to 5–15.

Table 49. Qual and Quan views (Sheet 2 of 2)

Icon or Button		Description
↔	Display All Data	Displays the entire *x*-axis range or all text in a report. For example, you can change the *x*-axis range from 7.5–12.5 to 0–20 minutes, if the run time for the data file is 20 minutes.
✥	Reset Scaling to Full Scale	Resets the chromatogram and spectrum scaling to the default values.
?	Product Help	Opens the Processing Setup window Help topic.

Reports and Programs Views Toolbar

Table 50 lists the toolbar buttons that are available for the Reports and Program views of the Processing Setup window

Table 50. Reports and Programs views

Icon or Button		Description
🗋	New	Sets the processing method parameters to the default values and displays Untitled for the processing method name in the title bar.
📂	Open	Opens the Open dialog box, where you can browse to and select an existing processing method.
💾	Save	Opens the Save As dialog box, where you can enter a name for the processing method and save it.
	Open Raw File	Opens the Open Raw File dialog box, where you can browse to and select an existing raw data file .raw.
🖨	Print	Opens the Print dialog box, where you can browse to and select a report template for the processing method and submit the report to the default printer. For more information, see "Print Dialog Box" on page 288.
?	Product Help	Opens the Processing Setup window Help topic.

Processing Setup View Bar

From the View bar, located to the left side of the Processing Setup window, click one of the four buttons to do the following.

Opens the Quan view, where you can set up the parameters for a quantitative analysis. For information about the Quan view, see "Quan View" on page 342.

Opens the Qual view, where you can set up the processing parameters for a qualitative analysis. For information about the Qual view, see "Qual View" on page 295.

Opens the Reports view, where you can set up reports for the processing method. For information about the Reports view, see "Reports View" on page 396.

Opens the Programs view, where you can add programs and macros to the processing method. For information about the Programs view, see "Programs View" on page 391.

Processing Setup Menus

The menus in the Processing Setup window are as follows from left to right:

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

File Menu – Processing Setup

Table 51 describes the commands in the File menu of the Processing Setup window. The equivalent toolbar button appears below the command.

Table 51. Processing Setup window – File menu (Sheet 1 of 2)

Icon or Button	Command	Description
🗋	New	Sets the processing method parameters to the default values and displays Untitled for the processing method name in the title bar.
📂	Open	Opens the Open dialog box, where you can browse to and select an existing processing method.
💾	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	Opens the Open Raw File dialog box, where you can open an existing raw data (.raw) file.
–	Summary Information	Opens the File Summary Information dialog box, where you can read the summary information about the active file or edit the text in the Comment box.
–	Change Dataset Name	Opens the *Study* Name Selector dialog box, where you can select a dataset from a predefined list of names or create a new *Study* name. The text of this menu item might be different if the administrator chooses to use another name for a dataset. For example, this menu item might be *Change Job Name*. For more information, see "Study Name Selector Dialog Box" on page 404.
–	Audit Trail	Opens the Thermo Foundation Audit Viewer, where you can view all auditable events and changes made to data files in the current view.
–	Import Method	Opens the Open Result File dialog box, where you can locate (drive and directory) and open a result file that contains the processing method of interest.
–	Print Setup	Opens the Print Setup dialog box, where you can select the following printing options: printer, form, orientation, and one- or two-sided printing.

Table 51. Processing Setup window – File menu (Sheet 2 of 2)

Icon or Button	Command	Description
🖨	Print	Opens the Print dialog box, where you can select a report template for printing the processing method, and then submit the report to the default printer or the printer that you selected in the Print Setup dialog box. For more information, see "Print Dialog Box" on page 288.
–	A list of the most recently used files	Displays the paths and names of the four most recently used files. These are located above the Exit command. You can select a processing method from this list.
–	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 – Processing Setup

Table 52 describes the GoTo menu of the Processing Setup window.

Table 52. Processing Setup window – Go To menu

Command	Description
Instrument Setup	Opens the Instrument Setup window, where you can create instrument methods and access the direct controls, if available, for the chromatography system and the mass spectrometer. The direct controls for the chromatography system are also available from the Tune window for the mass spectrometer. For information about the Instrument Setup window, see Chapter 2, "Creating Instrument Methods and Using the Direct Controls," and Appendix D, "Processing Setup."
Quan Browser	Opens the Quan Browser window, where you can open, review, and rework a sequence of processed files (.sld), a result file (.rst), or a Quanbrowser file (xqn). For information about the Quan Browser window, refer to the *Xcalibur Quan Browser User Guide*.
Qual Browser	Opens the Qual Browser window, where you can review raw data files and result data files containing spectra and chromatograms. For information about the Qual Browser window, refer to the *Xcalibur Qual Browser User Guide*.
Library Browser	Opens the Library Browser window, where you can work with reference spectra, spectra exported from Qual Browser, or spectra appended to libraries during qualitative processing. For information about the Library Browser window, refer to the *Xcalibur Creating and Searching Libraries User Guide*.
Xcalibur Home Page	Opens 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. Use the Home Page window to access all Xcalibur functions and features.

Help Menu – Processing Setup

Table 53 describes the Help menu of the Processing Setup window.

Table 53. Processing Setup window – Help menu

Command	Description
Processing Setup Help	Opens the Xcalibur Help topic for the Processing Setup window.
View Help	Opens the Xcalibur Help topic for the current view.
Help On Current Item	Opens the Xcalibur Help topic for the currently view or dialog box.
Xcalibur Help	Opens the Xcalibur Help to the Welcome topic.
Glossary	View the glossary.
How To Use Help	Opens the Xcalibur Help to the Using This Help topic, which provides instructions on how to use the Contents, Index, and Search pages of the Help.
About Processing Setup	Opens the version information. Click **Version** to open the Version Info dialog box and view the version information for the Xcalibur data system, the Foundation platform, and the configured instruments.

Options Menu – Processing Setup

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

These tables describe the Options menus:

- Options menu for the Quan view
- Options menu for the Qual view
- Options menu for the Reports and Programs views

Table 54 describes the Options menu for the Quan view.

Table 54. Options menu for the Quan view (Sheet 1 of 2)

Command	Description
Identification	Opens the Identification Options dialog box, where you set up the void time and baseline parameters for peak identification purposes (see "Identification Options Dialog Box" on page 286).
Masses	Opens the Masses dialog box, where you set up the default settings for mass tolerance and mass precision (see "Masses Dialog Box" on page 287). This is the same dialog box for the Quan Browser window and the Quan and Qual views of the Processing Setup window.
Standard Dilution	Opens the Standard Dilution dialog box, where you can set up the calibration-level information for target components (see "Standard Dilution Dialog Box" on page 292). This command appears in the menu only if you have defined at least one target compound on the Calibration page and the Levels page is open.
Chromatography By	Opens the Chromatography By dialog box, where you can select the appropriate chromatography mode: GC or LC. See "Default Chromatography Options Dialog Box" on page 275.
Spectrum	Opens the Spectrum Options dialog box, where you can specify a low-intensity cutoff percentage for peak detection purposes (see "Spectrum Options Dialog Box" on page 291). 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.

Table 54. Options menu for the Quan view (Sheet 2 of 2)

Command	**Description**
Calibration Options	Opens the Calibration Options dialog box, where you can select internal or external calibration for the current processing method (see "Calibration Options Dialog Box" on page 270).
Delete *Component*	Removes the selected component from the processing method. The data system removes the component from the Components pane.
Display	Opens the Display Options dialog box for the selected view. Use this dialog box to change the style, color, labels, axes, and normalization of the chromatogram and spectrum views. For information about the Display Options dialog box, refer to the Help or the *Xcalibur Qual Browser User Guide*.
Settings	Opens the Settings dialog box (see "Settings Dialog Box" on page 290). By default, the application loads the most recently used method into the Processing Setup window 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 views 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 55 describes the Options menu for the Qual view.

Table 55. Options menu for the Qual view

Command	Description
Identification	Opens the Identification Options dialog box, where you set up the void time and baseline parameters for peak identification purposes (see "Identification Options Dialog Box" on page 286).
Masses	Opens the Masses dialog box, where you set up the default settings for mass tolerance and mass precision (see "Masses Dialog Box" on page 287). This is the same dialog box for the Quan Browser window and the Quan and Qual views of the Processing Setup window.
Display	Opens the Display Options dialog box for the selected view. Use this dialog box to change the style, color, labels, axes, and normalization of the chromatogram and spectrum views.
Settings	Opens the Settings dialog box ("Settings Dialog Box" on page 290). By default, the data system loads the most recently used method into the Processing Setup window 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 views at startup.
Enable Warnings	Turns 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 56 describes the Options menu for the Reports and Programs views.

Table 56. Options menu for the Reports and Programs views

Command	Description
Settings	Opens the Settings dialog box ("Settings Dialog Box" on page 290). By default, the data system loads the most recently used method into the Processing Setup window 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 views at startup.
Enable Warnings	Turns 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 – Processing Setup

Table 57 describes the View menu commands.

Table 57. Processing Setup window – View menu

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

Zoom Menu – Processing Setup

Table 58 describes the Zoom menu commands.

Table 58. Processing Setup window – Zoom menu

Icon	Command	Description
⇧	Zoom In Y	Zooms in on the *y* axis by a factor of two from the current baseline to show more detail. For example, you can change the *y*-axis range from 0–100 to 0–50.
⇩	Zoom Out Y	Zooms out on the *y* axis by a factor of two to show more data. For example, you can change the *y*-axis range from 0–25 to 0–50.
⇧ 0-100	Normalize	Normalizes 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	Zooms in on the *x* axis by a factor of two to show more detail. For example, you can change the *x*-axis range from 0–20 to 5–15.
←|→	Zoom Out X	Zooms out on the *x* axis by a factor of two from the center to show more data. For example, you can change the *x*-axis range from 7.5–12.5 to 5–15.
↔	Display All	Displays the entire *x*-axis range 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	Resets the scaling to the full scale display.

Chromatogram and Spectrum Views in the Qual and Quan Views

The chromatogram and spectrum views display the chromatogram and spectrum from the currently opened raw file. Initially, the data system displays the spectrum corresponding to the apex scan of the first detected peak. If no peak has been detected in the chromatogram view, the spectrum for the first scan in the raw file appears.

When you change a parameter such as the Detector Type, Filter, and Trace in the Qual and Quan views, click **OK** to change the chromatogram displayed in the chromatogram view.

These views are available on the following pages:

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

You can use the chromatogram and spectrum views to assess the effects of the processing method settings and to automate data entry for some of the processing method parameters. For example, you can use the chromatogram view to set the expected retention time and retention time window on the Identification page of the Qual or Quan views. You can use the spectrum view in the Qual view to set Mass Ranges on the Identification page and the parameters in the Combine area on the Spectrum Enhancement page.

To rescale the chromatogram displayed in the chromatogram view, use the following:

- Toolbar buttons
- Zoom menu commands
- The cursor

> **Note** The cursor action is always applied to the pinned cell. Within an active cell, cursor actions rescale the chromatogram shown in the view.

OK, Cancel, and Save As Default Buttons

The Processing Setup window has OK, Cancel, and Save As Default buttons that are located above the chromatogram and spectrum views in the Qual and Quan views and at the bottom of the view in the Reports and Programs views.

These buttons 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.

  > **Tip** When you change a parameter such as the Detector type, Filter, and Trace in the Qual and Quan views, click **OK** to change the chromatogram displayed in the chromatogram view.

- To undo all changes made to the page and revert to the previously applied values, click **Cancel**.

- To validate and save the settings on the current page as default settings, click **Save As Default**.

  The data system uses these settings for all new processing methods. The data system writes over the previous default values and cannot recover them.

These actions do not affect the saved version of the processing method. You can only modify the saved version by choosing File > Save.

The data system 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.

Processing Setup Dialog Boxes

You can open the following dialog boxes from the Processing Setup window. These dialog boxes are listed in alphabetical order.

- "Apply Changes? Dialog Box," on the next page
- "Avalon Event List Dialog Box" on page 265
- "Calibration and Quantitation Flags Dialog Box" on page 269
- "Calibration Options Dialog Box" on page 270
- "Chromatography Options Dialog Box" on page 271
- "Correction for Isotope Contribution Dialog Box" on page 271
- "Data Flags Dialog Box" on page 274
- "Default Chromatography Options Dialog Box" on page 275
- "Display Options Dialog Box" on page 275
- "Genesis Advanced Detection Options Dialog Box" on page 281
- "Genesis Advanced Chromatogram Options Dialog Box" on page 276
- "ICIS Advanced Parameters Dialog Box" on page 284
- "Identification Options Dialog Box" on page 286
- "Masses Dialog Box" on page 287
- "Print Dialog Box" on page 288
- "Search List Dialog Box" on page 289
- "Settings Dialog Box" on page 290
- "Spectrum Options Dialog Box" on page 291
- "Standard Dilution Dialog Box" on page 292

Apply Changes? Dialog Box

The Apply Changes? dialog box opens in the Processing Setup window when you make 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 the 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 59 describes the parameters in the Apply Changes? dialog box.

Table 59. Apply Changes? dialog box parameters (Sheet 1 of 2)

Parameter	Description
Don't Tell Me About This Again	Selecting this check box suppresses 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 the validation is successful, and continues with your selected action. If the 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 59. Apply Changes? dialog box parameters (Sheet 2 of 2)

Parameter	Description
Buttons	
Yes	Applies changes to a Processing Setup page before proceeding with your selected action. When you click Yes, 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, the data system does the following in the future: • Does not display the Apply Changes? dialog box. • Applies changes automatically. • If a validation error occurs, the data system stops your intended action and returns you to the Processing Setup window. If the validation is successful, the data system applies the changes and proceeds with your selected action.
No	Discards unapplied changes to a Processing Setup page before proceeding with your selected action. The data system discards all changes, as though you pressed Cancel on the page. Then it continues with your selected action. If you also select the Don't Tell Me About This Again check box, the data system does the following in the future: • 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, the data system discards them.

Avalon Event List Dialog Box

Use the Avalon Event List dialog box to specify advanced component detection criteria in the Quan or Qual views of the Processing Setup window.

> **Tip** On the Detection page of the Quan view or the Identification page of the Qual view, automatically calculate values for the Initial Value events before you modify the timed events in the Avalon Event List dialog box. See "Avalon Identification Page for Qual View" on page 299 or "Avalon Detection Page for Quan View" on page 351.

❖ To change an existing event in the event list

1. Select the row that you want to change.

   The time, integration event, and value for the selected event appear in the Time (Min), Event, and Value boxes below the table.

2. In the Time (Min) box, type a time for the event to begin. If you type a new time for an initial value event, a new event appears in the list.

   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.

3. In the Value box, type a new value for the event.

   The valid range is specific to each event.

4. Click **Change** to automatically update the Event list, both here and on the Detection page of the Quan view or the Identification page of the Qual view, and automatically update the chromatogram display.

❖ To add an event to the event list

1. Type a time in the Time (Min) box.
2. Select an event from the list.
3. Type a value in the Value box.

   The valid range is specific to each event.

4. Click **Add**.

❖ To delete an event from the event list

1. Select the row you want to delete.

   The time, integration event, and value for the selected event appear in the boxes below the table.

2. Click **Delete**.

Table 60 describes the parameters in the Avalon Event List dialog box.

Table 60. Avalon Event List dialog box parameters (Sheet 1 of 3)

Parameter	Description
Integration Events	
Initial value events: Start/End Threshold, Bunch Factor, Area Threshold, P-P Resolution, Negative Peaks, Tension, and Tangent Skim. The Threshold and Bunch Factor parameters are the most important ones in controlling peak detection.	
Start/End Threshold	This integration event is directly related to the root-mean-square (RMS) noise in the chromatogram. It specifies the start and end thresholds, the fundamental control used for peak detection.
Bunch Factor	Specifies 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. Range: 1.000–999.000; however, for best results, use an integer between 1 and 6. A bunch factor larger than 6 groups peaks into clusters.
Area Threshold	Controls the area cutoff. The 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 baseline drop is specified as a percent of peak height overlap. Range: 0.010–99.990
Negative Peaks	Controls the integration of negative chromatographic peaks. Selecting On turns this integration event on at the specified time. Selecting Off turns this integration event off at the specified time.
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. Range: 0.000–999.990

Table 60. Avalon Event List dialog box parameters (Sheet 2 of 3)

Parameter	Description
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. You can also identify which peak in the cluster is the parent. The data system 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. Range: 0.000–1.000
Additional timed events	
Shoulders On	Turns on the detection of shoulders.
Shoulders Off	Turns off the detection of shoulders.
Force Cluster On	Turns on the grouping of peaks into a single peak.
Force Cluster Off	Turns off the grouping of peaks into a single peak.
Disable Cluster On	Turns on the grouping effect in the specified time range.
Disable Cluster Off	Turns off the grouping effect in the specified time range.
Event List Entry	
Time	The time entry for events that are listed as Initial Value cannot be changed. Use this box to enter a time value for an event.
Event	Contains a list of integration events. Select an integration event from this list.
Value	Use this box to enter a value for an event.
Buttons	
Add	Adds 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	Removes a highlighted event from the Event list. You cannot delete initial values.

Table 60. Avalon Event List dialog box parameters (Sheet 3 of 3)

Parameter	Description
Change	Updates a highlighted timed event 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	Closes 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 result files, in printed reports, and in Quan Browser.

For information about setting up the flags in the processing method, see "Setting Up the Calibration and Quantitation Flags" on page 42.

Table 61 describes the parameters in the Calibration and Quantitation Flags dialog box.

Table 61. Calibration and Quantitation Flags dialog box parameters

Parameter	Description
Calibration Flag	
R-Squared	Specifies a flag threshold for the goodness of fit of the calibration curve. The data system calculates a coefficient of determination (R-squared) whenever it computes a calibration curve. If the value is less than the R-squared threshold, the data system sets the R-squared flag in the result file to True; otherwise, it is set to False.
Quantitation Flags	
Detection Limit	Specifies 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 result file to True; otherwise, it is set to False.
Linearity Limit	Specifies 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 result file to True; otherwise, it is set to False.
Quantitation Limit	Specifies 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 result file to True; otherwise, it is set to False.
Carry Over Limit	Specifies 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 result 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 Processing Setup – Quan View – Calibration page. The default calibration mode is Internal Standard.

For information about using the Calibration Options dialog box, see "Changing the Calibration Mode" on page 23. For more information about the Quan view – Calibration page, see "Calibration Page for Quan View" on page 378 and "Setting Up the Calibration Parameters" on page 39.

Table 62 describes the parameters in the Calibration Options dialog box.

Table 62. Calibration Options dialog box parameters

Parameter	Description
Calibration By	
Internal Standard	When you select this option, the data system uses the internal standard calibration technique and displays the ISTD options on the Calibration Page for Quan View.
External Standard	When you select this option, the data system uses the external standard calibration technique and hides the ISTD options on the Calibration Page for Quan View.
%RSD Calculation Method	
Use Calculated Amounts	When you select this option, the data system computes the standard deviation on the basis of the calculated amounts for each standard. This is the behavior of previous Xcalibur versions.
Use Response Values	When you select this option, the data system uses 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 for the processing method.

You can access this dialog box from the Processing Setup window by choosing Options > Chromatography from the menu bar.

For information about using the Chromatography Options dialog box, see "Changing the Chromatography Mode" on page 22.

Your choice affects the options available on the Detection page of the Quan view in the Processing Setup window. 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 data system fails to determine the type of instrument, the system displays the Default Chromatography Options Dialog Box.

Table 63 describes the parameters in the Chromatography Options dialog box.

Table 63. Chromatography Options dialog box parameters

Parameter	Description
Chromatography By	
GC	Specifies the gas chromatography mode. Select the GC (gas chromatography) option to make the Spectrum Option available on the Detection page in Quan view.
LC	Specifies the liquid chromatography mode. Select the LC option for liquid 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.

You can access this dialog box from the Calibration page of the Quan view in the Processing Setup window by clicking Isotope%.

For information about using the Correction for Isotope Contribution dialog box, see "Correcting for Calibration Impurities" on page 44.

Table 64 describes the parameters in the Correction for Isotope Contribution dialog box.

Table 64. Correction for Isotope Contribution dialog box parameters (Sheet 1 of 2)

Parameter	Description
Contribution of ISTD to Target Compound (%)	Specifies the following 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 x value 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 the next parameter, Contribution of Target Compound to Internal Standard box, for a complete description of the y variable.

Table 64. Correction for Isotope Contribution dialog box parameters (Sheet 2 of 2)

Parameter	Description
Contribution of Target Compound to ISTD (%)	Specifies the following 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 y value 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 [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 data system at the retention time for TM [pure]. This amount consists of TM [corr] + ISTD [impurity]. See the previous row, Contribution of Internal Standard to Target Compound box, for a complete description of the x variable.

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 result file. If you set a value to 0.0, the flag is always reported as False.

You can access this dialog box from the Detection page of the Processing Setup – Quan view by clicking Flags.

For information about using the Data Flags dialog box, see "Setting Up the Detection Data Flags in Quan View" on page 38.

Table 65 describes the parameters in the Data Flags dialog box

Table 65. Data Flags dialog box parameters

Parameter	Description
Area Threshold	Specifies a value for the Area Threshold Data Flag. This value 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	Specifies a value for the Height Threshold Data Flag. This value 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 Options Dialog Box

The first time that you run Processing Setup, the data system 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 Options dialog box opens where you can set the default chromatography detection mode. Your choice affects the parameters available on the Detection page of the Quan view:

- 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 by using the Chromatography Options Dialog Box.

Table 66 describes the parameters in the Default Chromatography Options dialog box.

Table 66. Default Chromatography Options dialog box parameters

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

Display Options Dialog Box

In the Qual and Quan views of the Processing Setup window, use the pages of the Display Options dialog box to select Style, Color, Labels, Axis, Band Width, Normalization, and Composition settings. The available parameters on these pages depend on whether the view in the active cell is a chromatogram or spectrum.

For information about the Display Options dialog box, refer to the Help or the *Xcalibur Qual Browser User Guide*.

Genesis Advanced Chromatogram Options Dialog Box

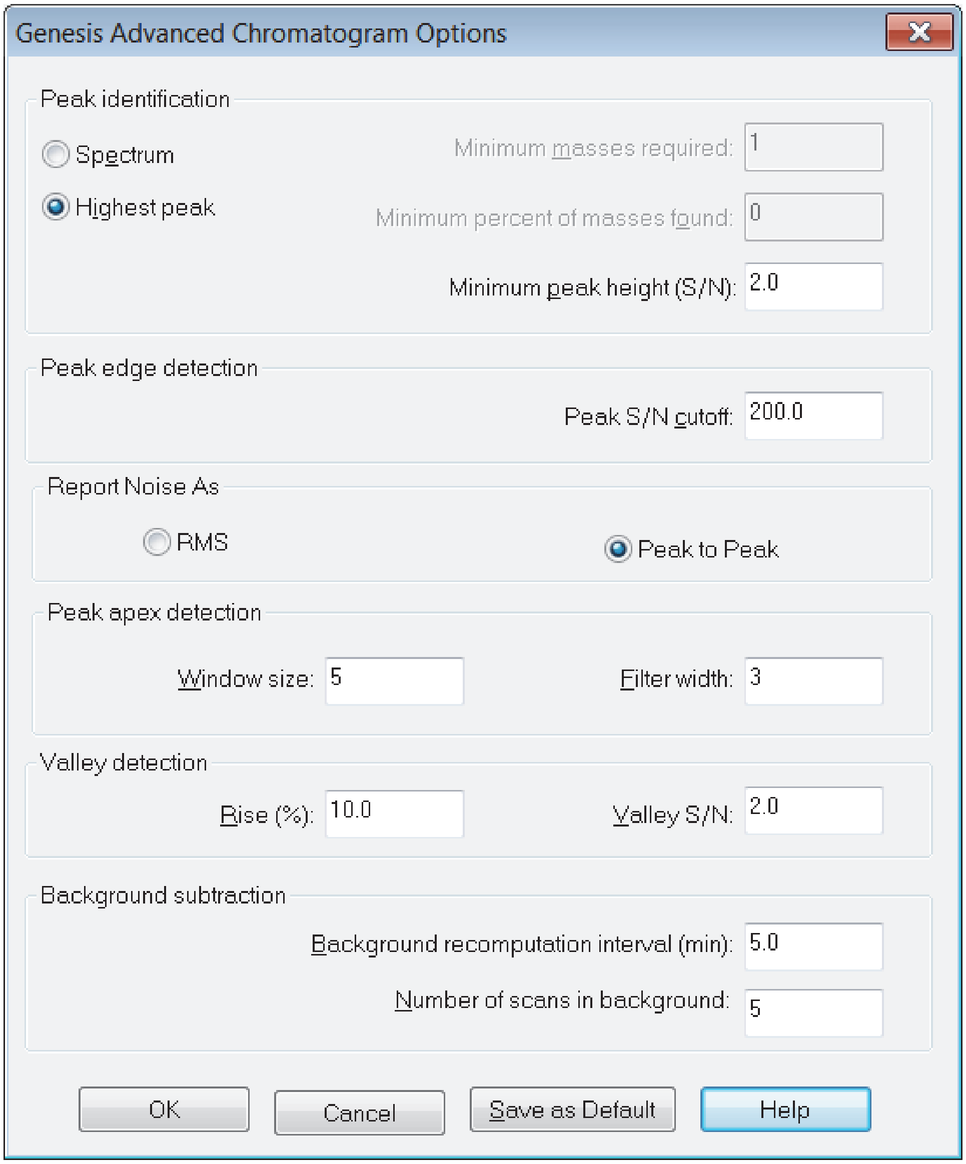
Use the Genesis Advanced Chromatogram Options dialog box to specify advanced criteria to detect your chromatographic peak. You can use these additional criteria if the standard detection criteria do not provide the desired results.

❖ To open the Genesis Advanced Chromatogram Options dialog box

On the Processing Setup – Qual view – Identification page, select **Genesis** in the Peak Detect list. Then, click **Advanced**.

The Genesis Advanced Chromatogram Options dialog box opens (Figure 89).

Figure 89. Genesis Advanced Chromatogram Options dialog box



○ Spectrum
● Highest peak
Minimum masses required: 1
Minimum percent of masses found: 0
Minimum peak height (S/N): 2.0
Peak S/N cutoff: 200.0
○ RMS
● Peak to Peak
Window size: 5
Filter width: 3
Rise (%): 10.0
Valley S/N: 2.0
Background recomputation interval (min): 5.0
Number of scans in background: 5

Table 67 describes the parameters in the Genesis Advanced Chromatogram Options dialog box.

Table 67. Genesis Advanced Chromatogram Options dialog box parameters (Sheet 1 of 4)

Parameter	Description
Peak Identification	
Spectrum	Select this option to identify peaks 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* value 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. When you select this option, the Minimum Masses Required and the Minimum Percent of Masses Found parameters become available. 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	Select this option to identify the highest peaks within the retention time window that are above the minimum peak height. This option uses the Minimum Peak Height (S/N) parameter.
Minimum Masses Required	Specifies the minimum number of masses that are simultaneously reaching a maximum intensity as a criterion for peak detection. The valid range is 1 to 999. This parameter becomes available when you select the Spectrum option. To change the minimum number, type the new number in the Minimum Mass Required box.

Table 67. Genesis Advanced Chromatogram Options dialog box parameters (Sheet 2 of 4)

Parameter	Description
Minimum Percent of Masses Found	Specifies the minimum percent of masses that are simultaneously reaching a maximum intensity as a criterion for peak detection. For example, if you set this value at 25% and only 10% of the mass spectral peaks being monitored reach a maximum intensity during the elution of a chromatographic peak, the data system rejects the peak. The valid range is 0 to 100 percent. This parameter becomes available when you select the Spectrum option. To change the minimum percent of masses found, type the new percentage value in the Minimum Percent of Masses Found box.
Minimum Peak Height (S/N)	Specifies the minimum peak height (signal-to-noise) for peak detection. The data system ignores all chromatogram peaks that have signal-to-noise values that are less than the Minimum Peak Height (S/N) value. To enter a minimum peak height, type the value in the Minimum Peak Height (S/N) box. The valid range is 1.0 to 999.0.
Peak Edge Detection	
Set a chromatogram peak detection criterion 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	Specifies the signal-to-noise ratio below which the data system defines the peak edge. For example, if the signal-to-noise ratio 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 signal-to-noise ratio 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	Specifies that the data system calculate noise as RMS.
Peak To Peak	Specifies that the data system calculate noise as peak-to-peak.

Table 67. Genesis Advanced Chromatogram Options dialog box parameters (Sheet 3 of 4)

Parameter	Description
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 peak identification conditions are met, the data system examines the region around this possible peak apex to determine whether the other peak identification criteria are satisfied. The data system 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	Specifies 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	Specifies 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.
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 (%)	Specifies 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	Specifies 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.

Table 67. Genesis Advanced Chromatogram Options dialog box parameters (Sheet 4 of 4)

Parameter	Description
Background Subtraction	
Minimizes the contaminating effect of background on the peak identification process. When you select background subtraction, the data system does the following: 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 recalculation compensates for the possibility that the composition of the background might change over the course of a run.	
Background Recomputation Interval (min)	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.
Number of Scans in Background	Specifies 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 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.

❖ To open the Genesis Advanced Detection Options dialog box

1. On the Identification page of the Processing Setup – Quan view, select **Genesis** in the Peak Detect list.
2. On the Detection page of the Processing Setup – Quan view, click **Advanced**.

Table 68 describes the parameters in the Genesis Advanced Detection Options dialog box.

Table 68. Genesis Advanced Detection Options dialog box parameters (Sheet 1 of 3)

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	Specifies the signal-to-noise ratio below which the data system defines the peak edge. For example, if the signal-to-noise ratio 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 signal-to-noise ratio reaches a value less than 200. The valid range is 50.0 to 10 000.0. To change the cutoff value, type the new value in the Peak S/N Cutoff box. When you click OK, the data system applies the new peak detection parameter.
Report Noise As	
RMS	Select this option to calculate noise as RMS.
Peak To Peak	Select this option to calculate noise as peak-to-peak.

Table 68. Genesis Advanced Detection Options dialog box parameters (Sheet 2 of 3)

Parameter	Description
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 (%)	Specifies 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 integration parameter 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 setting.
Valley S/N	Specifies the signal-to-noise criterion that the data system uses for valley detection. The valid range is 1.0 to 100.0. To change the valley signal-to-noise criterion, type the new value in the Valley S/N box. When you click OK, the data system applies the new peak detection setting.

Table 68. Genesis Advanced Detection Options dialog box parameters (Sheet 3 of 3)

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	Specifies 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.

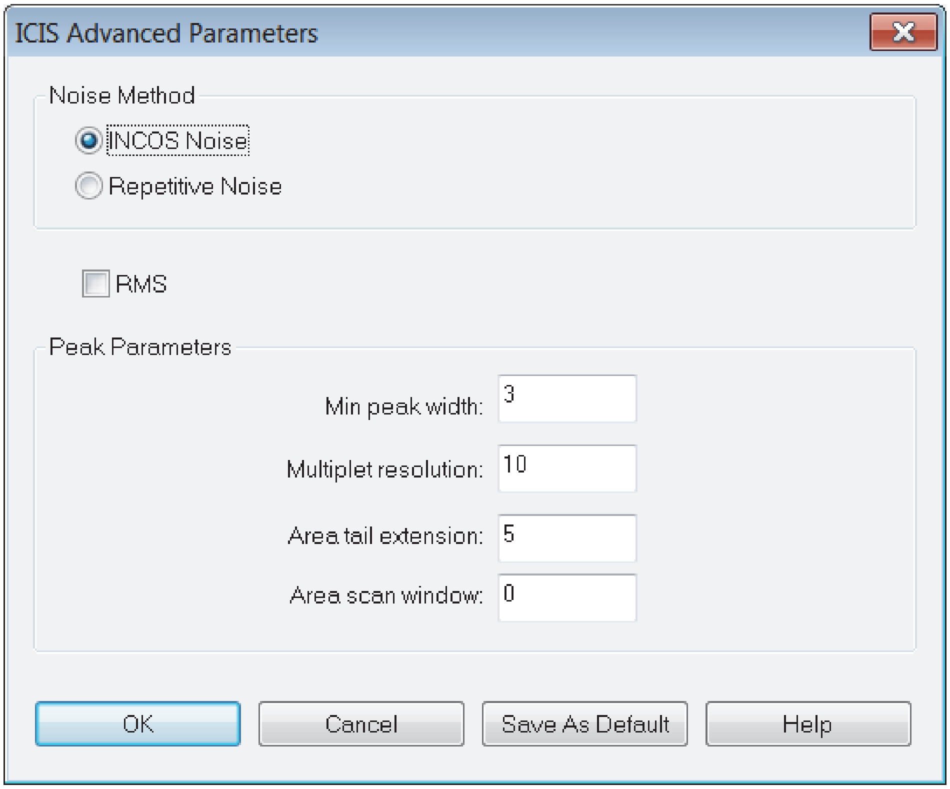
❖ To open the ICIS Advanced Parameters dialog box

From the Processing Setup window, do one of the following:

- From the Quan View of the Processing Setup window, click the **Detection** tab to display the Detection Page for Quan View and click **Advanced**.
- From the Qual View of the Processing Setup window, click the **Identification** tab to display the Identification Page for Qual View and click **Advanced**.

The ICIS Advanced Parameters dialog box opens (Figure 90).

Figure 90. ICIS Advanced Parameters dialog box



ICIS Advanced Parameters

Noise Method

● INCOS Noise

○ Repetitive Noise

☐ RMS

Peak Parameters

Min peak width: 3

Multiplet resolution: 10

Area tail extension: 5

Area scan window: 0

Table 69 describes the parameters in the ICIS Advanced Parameters dialog box.

Table 69. ICIS Advanced Parameters dialog box parameters

Parameter	Description
Noise Method	
INCOS Noise	Selecting this option specifies the use of a a single-pass algorithm to determine the noise level. The ICIS peak detection algorithm uses this value.
Repetitive Noise	Selecting this option specifies the use of 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	When this check box is selected, the data system calculates 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 criterion determines if two peaks are resolved. Type an integer in this box. 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	Type 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.

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.

You can access this dialog box by choosing Options > Identification from the Qual or Quan view of the Processing Setup window.

For information about using this dialog box, see "Setting Up the Void Time and Baseline Identification Options" on page 19.

Table 70 describes the parameters in the Identification Options dialog box.

Table 70. 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 data system subtracts this time from the elution time for all remaining peaks to estimate the correct relative retention time.
Baseline	
Baseline and Noise Window	Specifies 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, the data system cannot calculate the baseline for a peak correctly because the baseline is 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	Specifies a value that controls how the data system draws the baseline in the noise data. The higher the baseline noise tolerance value, the higher the baseline it draws through the noise data. The valid range is 0.0 to 100.0.
Minimum Number of Scans in Baseline	Specifies 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.

Masses Dialog Box

In the Quan and Qual views of the Processing Setup window and in the Quan Browser window, use this dialog box to specify tolerance and precision settings for the mass data displayed in the chromatogram, spectrum, map, and ion map plots.

Specify the default values for tolerance and precision on the Mass Options page of the Xcalibur Configuration dialog box.

Table 71 describes the parameters in the Masses dialog box.

Table 71. Masses dialog box parameters

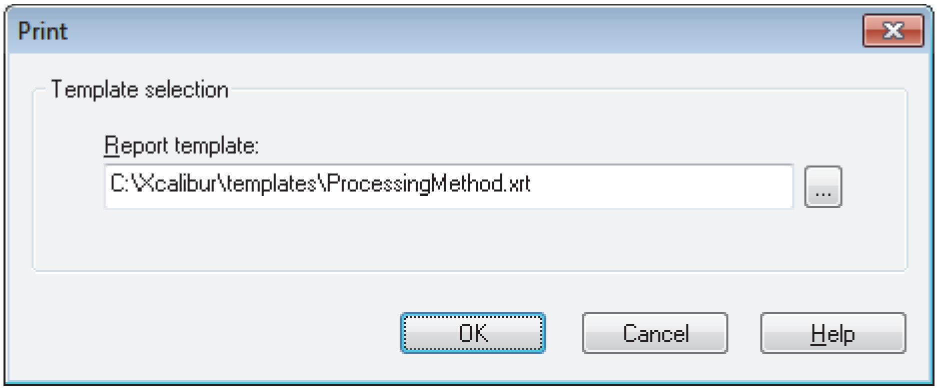
Parameter	Description
Mass tolerance	
Mass tolerance	Specifies the value for mass tolerance. Type a value in the range of 0.1 to 50 000, and select the units to apply to the value. The data system uses the tolerance value to create the mass range limit.
Units	Specifies the units of measurement in which the data system processes your data. Select **mmu** (millimass units) or **ppm** (parts per million).
Mass precision	
Decimals	Specifies the number of decimal places (mass precision) that the data system uses to display mass values. You can specify from 0 to 5 decimal places. The number of decimal places applies to the mass data in a window.

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 (Figure 91).

You can access this dialog box by choosing File > Print from the Processing Setup window menu bar.

Figure 91. Processing Setup Print dialog box



C:\Xcalibur\templates\ProcessingMethod.xrt

Note The 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 is the time of the print job, not the time that the method was created.

Table 72 describes the parameters in the Print dialog box.

Table 72. Print dialog box parameter

Parameter	Description
Report Template	This box displays the path name 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.

❖ To open the Search List dialog box

From the Processing Setup – Qual view – Library Search Options page, click **Search List**.

The Search List dialog box opens (Figure 92).

Figure 92. Search List dialog box

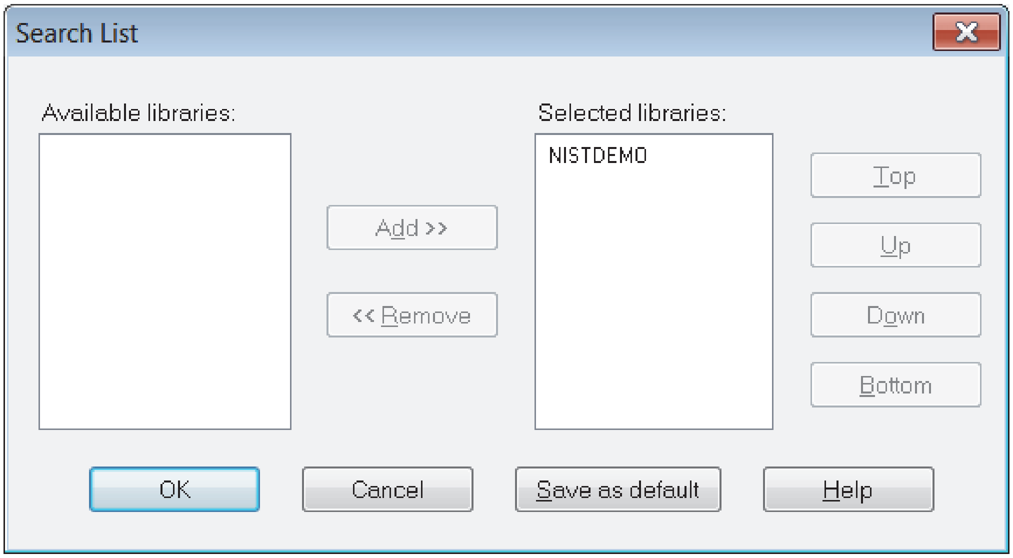


Table 73 describes the parameters in the Search List dialog box.

Table 73. Search List dialog box parameters (Sheet 1 of 2)

Parameter	Description
Available Libraries	Displays the libraries that are currently excluded from searching during processing. The data system regenerates this list when you open the dialog box.
Selected Libraries	Displays the libraries that are currently included in searches during processing. The order of the libraries defines the order in which they are searched by the data system. The data system 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 data system checks the Selected Libraries list and displays a warning dialog box if any of these are not available on your system.

Table 73. Search List dialog box parameters (Sheet 2 of 2)

Parameter	Description
Buttons	
Add	Moves a library from the Available Libraries list box to the Selected Libraries list box.
Remove	Moves a library from the Selected Libraries list box to the Available Libraries list box.
Top	Moves a library in the Selected Libraries list box to the top of the list (first in the search order).
Up	Moves a library in the Selected Libraries list box up one position (earlier in the search order).
Down	Moves a library in the Selected Libraries list box down one position (later in the search order).
Bottom	Moves 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 the Processing Setup window. 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 data system to open a raw file in the Chromatogram and Spectrum views when you open a processing method.

You can access this dialog box by choosing Options > Settings from the menu bar of the Processing Setup window.

For information about using the Settings dialog box, see "Setting Up the Startup Options" on page 17.

Table 74 describes the parameters in the Settings dialog box.

Table 74. Settings dialog box parameters (Sheet 1 of 2)

Parameter	Description
Startup Mode	
Specifies whether the Processing Setup window opens with a new method or with the most recently used method.	
Load Last Processing Method	Selecting this option specifies that the data system loads the most recently used method when you start a Processing Setup session.
Create New Processing Method	Selecting this option specifies that the data system starts a new method when you begin a Processing Setup session.

Table 74. Settings dialog box parameters (Sheet 2 of 2)

Parameter	Description
Auto-Open Raw File	
Specifies whether 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	When you select this option, the data system automatically opens the raw file associated with the processing method. The data system populates the chromatogram and spectrum cells with the raw file associated with the processing method when it was last saved.
Off	When you select this option, no raw file opens when you open a processing method. To open a raw file, you must use the Open Raw File command.

Spectrum Options Dialog Box

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

For information about using the Spectrum Options dialog box, see "Setting Up the Spectrum Options for Chromatography by GC" on page 34.

Table 75 describes the parameters in the Spectrum Options dialog box.

Table 75. Spectrum Options dialog box parameter

Parameter	Description
Low Intensity Cutoff (%)	Specifies 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 option 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.

When you are working on the Levels page of the Processing Setup – Quan view, you can access this dialog box by choosing Options > Standard Dilutions from the menu bar.

For information about using the Standard Dilution dialog box, see "Using the Standard Dilutions Dialog Box to Set Up the Calibration Levels" on page 46.

Table 76 describes the parameters in the Standard Dilution dialog box.

Table 76. Standard Dilution dialog box parameters (Sheet 1 of 2)

Parameter	Description
Target Compound Components (read-only)	This parameter displays the total number of target compound components defined in the processing method, including ISTD and non-ISTD component types.
Selected Components (read-only)	This parameter displays the selected number of non-ISTD components for standard dilution.
Base Amounts	
Component (read-only)	This column displays the names of the target components listed in the Components pane of the Processing Setup – Quan view.
Amount	Specifies the base amount (for example, the stock concentration) for each target compound. To enter a base amount, type the value in the Amount box. You must provide a value for each listed Component for the data system to be able to calculate the amounts for each calibration level.

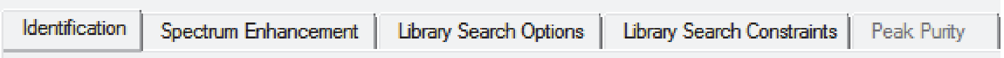
Table 76. Standard Dilution dialog box parameters (Sheet 2 of 2)

Parameter	Description
Dilution Factors	
Cal Level	Specifies the names of the calibration levels. The data system 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 data system highlights the row. Press DELETE. The data system transfers these Cal Level values to the Cal Level column of the Calibration Levels table on the Levels page for each component.
Dilution	Specifies the stock dilution factor 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 data system repeats this procedure for all calibration levels and all components.

Processing Setup Views

These topics describe the Processing Setup views.

- "Qual View," on the next page

  - "Identification Page for Qual View" on page 295
  - "Spectrum Enhancement Page for Qual View" on page 322
  - "Library Search Options Page for Qual View" on page 326
  - "Library Search Constraints Page for Qual View" on page 331
  - "Peak Purity Page for Qual View" on page 340
- "Quan View" on page 342

  - "Identification Page for Quan View" on page 343
  - "Detection Page for Quan View" on page 351
  - "Calibration Page for Quan View" on page 378
  - "Levels Page for Quan View" on page 383
  - "System Suitability Page for Quan View" on page 385
  - "Peak Purity Page for Quan View" on page 389
- "Programs View" on page 391
- "Reports View" on page 396

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.

These topics describe the Qual view pages:

- "Identification Page for Qual View," on this page
  - "Avalon Identification Page for Qual View" on page 299
  - "ICIS Identification Page for Qual View" on page 306
  - "Genesis Identification Page for Qual View" on page 314
- "Spectrum Enhancement Page for Qual View" on page 322
- "Library Search Options Page for Qual View" on page 326
- "Library Search Constraints Page for Qual View" on page 331
- "Peak Purity Page for Qual View" on page 340

For information about the OK, Cancel and Save as Default buttons, see "OK, Cancel, and Save As Default Buttons" on page 261. For information about the chromatogram and spectrum views, see "Chromatogram and Spectrum Views in the Qual and Quan Views" on page 260.

Identification Page for Qual View

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

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

For information about using this page, see "Setting Up the Qual View Identification Parameters" on page 50.

For parameter descriptions, see these topics:

- "Avalon Identification Page for Qual View" on page 299
- "ICIS Identification Page for Qual View" on page 306
- "Genesis Identification Page for Qual View" on page 314

For information about the valid trace combinations, see these topics:

- Valid MS Trace Combinations
- Valid Analog Trace Combinations
- Valid A/D Card Trace Combinations
- Valid PDA Trace Combinations
- Valid UV Trace Combinations

Valid MS Trace Combinations

Table 77 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 77. 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

Table 78 shows the valid trace combinations available in the Trace lists. The Mass Range/Wavelength Range control is unavailable.

Table 78. Valid Analog trace combinations parameters

Trace 1	Operator	Trace 2	Resulting controls
Analog n (1 ≤ n ≤ 4)	[blank]	[unavailable]	None
Analog n (1 ≤ n ≤ 4)	–	Analog m (1 ≤ m ≤ 4, m /= n)	None
Analog n (1 ≤ n ≤ 4)	+	Analog m (1 ≤ m ≤ 4, m /= n)	None

Valid A/D Card Trace Combinations

Table 79 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 79. Valid A/D Card trace combinations parameters

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

Valid PDA Trace Combinations

Table 80 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 80. 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

Table 81 lists the valid trace combinations available in the Trace lists for UV detectors. The Mass Range/Wavelength Range control is unavailable.

Table 81. 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

Avalon Identification Page for Qual View

Use the Avalon Identification page for the Qual view of the Processing Setup window 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.

> **Note** Use the Avalon integration algorithm for chromatograms acquired with a PDA or UV detector.

For more information, see "Setting Up the Qual View Identification Parameters" on page 50.

Table 82 describes the parameters on the Qual view – Avalon Identification page.

Table 82. Avalon Identification page for Qual view parameters (Sheet 1 of 7)

Parameter	Description
Detector	
Type	Specifies the type of detector used to acquire the data: • MS (mass spectrometer) • Analog (analog detector) • A/D Card (analog-to-digital converter) • PDA (photodiode array detector) • UV (UV or UV-Vis detector)
Peak Detect	Specifies the peak detection algorithm for the Qual view: Genesis, ICIS, or Avalon.
Delay	Specifies the delay time, in minutes, required to synchronize analog or digital data with MS scans. The Delay value compensates for any difference (negative or positive) in the sample arrival time at the UV and MS detectors. The valid range is –5.0 to +5.0 minutes.

Table 82. Avalon Identification page for Qual view parameters (Sheet 2 of 7)

Parameter	Description
Filter	Specifies the scan filter to be applied. Use a scan filter to specify that processing is to be applied to a subset of the scans in a raw file. The Filter list contains the scan filters for the current 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. 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 For more information, refer to the *Xcalibur Qual Browser User Guide* for information about scan formats.
Trace	From the three Trace lists, specify the type of chromatogram that you want to use for data processing as follows: 1. From the first list, select a basic chromatogram type, for example, TIC. 2. From the second list, select a logical operator: + or –. Your selection of an operator makes the third list available. 3. In the third list, 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. The valid trace types depend on the detector type.
MS detector	For MS scans, valid trace types are TIC, Mass Range, and Base Peak. For more information, see “Valid MS Trace Combinations” on page 296.

Table 82. Avalon Identification page for Qual view parameters (Sheet 3 of 7)

Parameter	Description
Analog detector	For Analog data, the data system supports up to four channels (labeled Analog 1–4). For more information, see "Valid Analog Trace Combinations" on page 297.
A/D card	For data from an A/D Card, the data system supports four channels (labeled A/D Card Ch 1–4). For more information, see "Valid A/D Card Trace Combinations" on page 297.
PDA detector	For PDA data, valid trace types are Wavelength Range, Total Scan, or Spectrum Maximum. For more information, see "Valid PDA Trace Combinations" on page 298.
UV detector	For UV detector data, the data system supports four channels (labeled Channel A–D). For more information, see "Valid UV Trace Combinations" on page 298.
Mass	Specifies the mass range for the Mass Range trace type. The data system 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 of *m/z* values from 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" on page 123.
Mass 1	Specifies the mass range for the first trace type. The data system 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 of *m/z* values from 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" on page 123.

Table 82. Avalon Identification page for Qual view parameters (Sheet 4 of 7)

Parameter	Description
[Mass] 2	Specifies the mass range for the second trace type. The data system 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 of *m/z* values from 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" on page 123.
BP	Specifies the mass value for the base peak. The data system 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	Specifies the mass range for the second Mass Range trace type. The data system 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 of *m/z* values from 123 through 456, type **123–456.**
Wavelength	Specifies 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 of *m/z* values from 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" on page 123.

Table 82. Avalon Identification page for Qual view parameters (Sheet 5 of 7)

Parameter	Description
Wavelength 1	Specifies the wavelength or wavelength range for the first trace type. The data system 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 of *m/z* values from 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" on page 123.
[Wavelength] 2	Specifies the wavelength or wavelength range for the second trace type. The data system 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 of *m/z* values from 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" on page 123.
Selected Retention Time Window	
Use the Ranges box to define the detection window for qualitative processing.	
Range (min)	Enter a time span to limit qualitative processing. A qualitative processing method processes a peak only if its apex retention time lies in the specified 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.

Table 82. Avalon Identification page for Qual view parameters (Sheet 6 of 7)

Parameter	Description
Avalon Peak Integration	
Specifies 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	Specifies the degree of data smoothing to be performed on the active component peak before 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 before integration, type a value in the Smoothing Points box. See also the "Avalon Detection Page for Quan View" on page 351.
Event List	
❖ **To modify the event list** Click **Advanced** to open the Avalon Event List dialog box. For information about using the Avalon Event List dialog box to edit the Event list, see "Avalon Event List Dialog Box" on page 265.	
Event List	The table contains a minimum of seven 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 detect peaks, Avalon uses the settings for initial value events and user-defined timed events that are in the Event list.
Time	This column contains either the term *initial value* or a time value, in minutes. You cannot change the time value for an initial value
Event	This column displays the integration events.
Value	This column displays the values associated with initial value events and timed events. The range of allowed values is specific to each event.

Table 82. Avalon Identification page for Qual view parameters (Sheet 7 of 7)

Parameter	Description
Auto Calculate Initial Events	This button is available when a raw file is open in the Processing Setup window. When you click this button, the data system automatically determines the best value for each of the seven initial value events on the basis of the data in the current raw file and then displays these values in the Value column of the event list. The data system does not estimate values for timed events; that is, events that have a time value in the Time column. It determines initial values for these events only: Start Threshold, End Threshold, Area Threshold, P-P [Resolution] Threshold, Bunch Factor, Negative Peaks, and Tension.
Limit Peaks	
Select Top Peaks	
Enable	Selecting this check box limits peak detection to a specified number that is based on either peak area or peak height.
Select by Area	Selecting the Select by Area option restricts detection to the most significant peaks on the basis of area rather than height.
Select by Height	Selecting the Select by Height option restricts detection to the most significant peaks on the basis of height rather than area.
Num to Select	Specifies the maximum number of peaks to be detected. The data system selects the largest peaks on the basis of intensity (height) or area.
Rel Peak Height Threshold	
Enable	Selecting this check box limits 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	Specifies a percentage threshold to limit the number of peaks submitted for further processing. The data system discards any detected peaks with an intensity less than the threshold percentage of the most intense peak.
Buttons	
Save As Default	Validates and saves the settings on the current page as default settings. The data system uses these settings for all new processing methods. The software writes over the previous default values and cannot recover them.
Advanced	Opens the Avalon Event List dialog box, where you can edit the list of peak integration events.

ICIS Identification Page for Qual View

Use the ICIS Identification page for the Qual View of the Processing Setup window 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.

For more information, see "Setting Up the Qual View Identification Parameters" on page 50.

Table 83 describes the parameters on the Qual view – ICIS Identification page.

Table 83. ICIS Identification page for Qual view parameters (Sheet 1 of 8)

Parameter	Description
Detector	
Type	Specifies 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	Specifies the peak detection algorithm.
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.

Table 83. ICIS Identification page for Qual view parameters (Sheet 2 of 8)

Parameter	Description
Filter	Specifies the current scan filter for the active raw data (.raw) file. You can use a scan filter to apply processing 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 data system 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
Trace	Specifies the type of chromatogram you want to use for data processing. From the three Trace lists, you can select: 1. From the first list, a basic chromatogram type, for example, TIC. 2. From the second list, a logical operator: + or – . Your selection of an operator activates the third list. 3. In the third list, 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. The valid trace types depend on the detector type.
MS detector	For MS scans, valid trace types are TIC, Mass Range, and Base Peak. For more information, see "Valid MS Trace Combinations" on page 296.

Table 83. ICIS Identification page for Qual view parameters (Sheet 3 of 8)

Parameter	Description
Analog detector	For Analog data, the data system supports up to four channels (labeled Analog 1–4). For more information, see "Valid Analog Trace Combinations" on page 297.
A/D card	For data from an A/D Card, the data system supports four channels (labeled A/D Card Ch 1–4). For more information, see "Valid A/D Card Trace Combinations" on page 297.
PDA detector	For PDA data, valid trace types are Wavelength Range, Total Scan, or Spectrum Maximum. For more information, see "Valid PDA Trace Combinations" on page 298.
UV detector	For UV detector data, the data system supports four channels (labeled Channel A–D). For more information, see "Valid UV Trace Combinations" on page 298.
Mass *(m/z)*	Specifies the mass range for the Mass Range trace type. The data system 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 of *m/z* values from 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" on page 123.
Mass 1 *(m/z)*	Specifies the mass range for the first trace type. The data system 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 of *m/z* values from 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" on page 123.

Table 83. ICIS Identification page for Qual view parameters (Sheet 4 of 8)

Parameter	Description
[Mass] 2 (*m/z*)	Specifies the mass range for the second trace type. The data system 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 of *m/z* values from 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" on page 123.
BP	Specifies the mass value for the base peak. The data system 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	Specifies the mass range for the second trace type, Mass Range. The data system 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 of *m/z* values from 123 through 456, type **123–456**.
Wavelength (nm)	Specifies 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 of *m/z* values from 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" on page 123.

Table 83. ICIS Identification page for Qual view parameters (Sheet 5 of 8)

Parameter	Description
Wavelength 1 (nm)	Specifies the wavelength or wavelength range for the first trace type. The data system 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 of *m/z* values from 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" on page 123.
[Wavelength] 2 (nm)	Specifies the wavelength or wavelength range for the second trace type. The data system 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 of *m/z* values from 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" on page 123.
Selected Retention Time Window	
Range	Enter a time span to limit qualitative processing. The qualitative processing method 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.

Table 83. ICIS Identification page for Qual view parameters (Sheet 6 of 8)

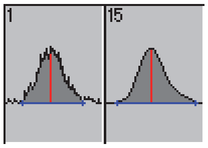
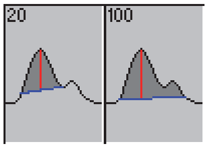
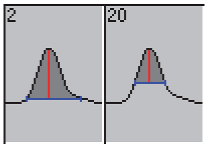
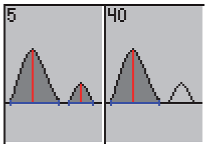
Parameter	Description
ICIS Peak Integration	
Smoothing Points 	Specifies the number of points in the moving average used to smooth the data. Default: 1 Range: 1–15 The ICIS peak detection algorithm uses this value.
Baseline Window 	Specifies the number of scans to review for a local minima. Default: 40 Range: 1–500 The ICIS peak detection algorithm uses this value.
Area Noise Factor 	Specifies the noise-level multiplier used to determine the peak edges after the data system determines the start and end points of a possible peak for the selected component. As you increase this value, the integrated peak area decreases. Default: 5 Range: 1–500 The ICIS peak detection algorithm uses this value.
Peak Noise Factor 	Specifies the noise-level multiplier used to determine the potential peak signal threshold. Default: 10 Range: 1–1000 The ICIS peak detection algorithm uses this value.
Constrain Peak Width	Select this check box to constrain the integrated area of a component peak by specifying a peak height threshold and a tailing factor. When you select the Constrain Peak Width check box, the Peak Height (%) and Tailing Factor boxes become available.

Table 83. ICIS Identification page for Qual view parameters (Sheet 7 of 8)

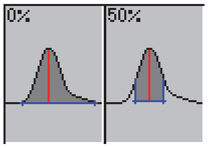
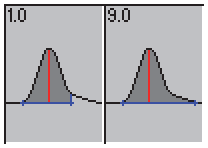
Parameter	Description
Peak Height (%) 	Specifies the percent of the total peak height (100%) that a signal must be above the baseline the data system turns integration on or off. To enter a value for this parameter, select the Constrain Peak Width check box. Then type a value in the Peak Height (%) box. Range: 0.0–100.0.
Tailing Factor 	Specifies 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 edge of a constrained peak. To enter a value for this parameter, select the Constrain Peak Width check box. Then type a value in the Tailing Factor box. Range: 0.5–9.0
Min (graphical representation)	Displays a representative drawing of the minimum value for the selected parameter. The location of the cursor defines the selected parameter. For example, if you click the Smoothing Points box, the graphic shows the typical result obtained with the minimum number of smoothing points: a peak with reduced noise. The number in the upper left corner of the graphic is a representative low value for the active parameter. It is not necessarily the minimum value for the parameter.
Max (graphical representation)	Displays a representative drawing of maximum value for the selected parameter. The location of the cursor defines the selected 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. It is not necessarily the maximum value for the parameter.

Table 83. ICIS Identification page for Qual view parameters (Sheet 8 of 8)

Parameter	Description
Limit Peaks	
Select Top Peaks	
Enable	Selecting this check box limits peak detection to a specified number on the basis of either peak area or peak height.
Select by Area	Select the Area option to restrict detection to the most significant peaks on the basis of area rather than height.
Select by Height	Select the Height option to restrict detection to the most significant peaks on the basis of height rather than area.
Num to Select	Enter the maximum number of peaks to be detected. The data system selects the largest peaks on the basis of intensity (height) or area.
Rel Peak Height Threshold	
Enable	Selecting this check box limits 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 data system discards any detected peaks with an intensity less than the threshold percentage of the most intense peak.
Buttons	
Save As Default	Validates and saves the settings on the current page as default settings. The data system uses these settings for all new processing methods. The software writes over the previous default values and cannot recover them.
Advanced	Opens 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 of the Qual view of the Processing Setup window 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.

For more information, see "Setting Up the Qual View Identification Parameters" on page 50.

Table 84 describes the parameters on the Genesis Identification page of the Qual view.

Table 84. Genesis Identification page for Qual view parameters (Sheet 1 of 8)

Parameter	Description
Detector	
Type	Specifies 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	Specifies the peak detection algorithms.
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 84. Genesis Identification page for Qual view parameters (Sheet 2 of 8)

Parameter	Description
Filter	Specifies the current scan filter for the active raw data (.raw) file. You can use a scan filter to apply processing 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 data system 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
Trace	Specifies the type of chromatogram you want to use for data processing. From the three Trace lists, you can select: 1. From the first list, a basic chromatogram type, for example, TIC. 2. From the second list, a logical operator: + or – . Your selection of an operator activates the third list. 3. In the third list, 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. The valid trace types depend on the detector type.
MS detector	For MS scans, valid trace types are TIC, Mass Range, and Base Peak. For more information, see “Valid MS Trace Combinations” on page 296.

Table 84. Genesis Identification page for Qual view parameters (Sheet 3 of 8)

Parameter	Description
Analog detector	For Analog data, the data system supports up to four channels (labeled Analog 1–4). For more information, see "Valid Analog Trace Combinations" on page 297.
A/D card	For data from an A/D Card, the data system supports four channels (labeled A/D Card Ch 1–4). For more information, see "Valid A/D Card Trace Combinations" on page 297.
PDA detector	For PDA data, valid trace types are Wavelength Range, Total Scan, or Spectrum Maximum. For more information, see "Valid PDA Trace Combinations" on page 298.
UV detector	For UV detector data, the data system supports four channels (labeled Channel A–D). For more information, see "Valid UV Trace Combinations" on page 298.
Mass	Specifies the mass range for the Mass Range trace type. The data system 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" on page 123.
Mass 1	Specifies the mass range for the first trace type. The data system 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" on page 123.

Table 84. Genesis Identification page for Qual view parameters (Sheet 4 of 8)

Parameter	Description
[Mass] 2	Specifies the mass range for the second trace type. The data system 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” on page 123.
BP	Specifies the mass value for the base peak. The data system 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	Specifies the mass range for the second trace type, Mass Range. The data system 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 of *m/z* values from 123 through 456, type **123–456**.
Wavelength	Specifies the wavelength range for the Wavelength Range or Spectrum Maximum trace type. The data system 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 of *m/z* values from 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” on page 123.

Table 84. Genesis Identification page for Qual view parameters (Sheet 5 of 8)

Parameter	Description
Wavelength 1	Specifies the wavelength or wavelength range for the first trace type. The data system 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 of *m/z* values from 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" on page 123.
[Wavelength] 2	Specifies the wavelength or wavelength range for the second trace type. The data system 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 of *m/z* values from 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" on page 123.
Selected Retention Time Window	
Range	Specifies a retention time window to limit qualitative processing. The qualitative section of a processing method 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.

Table 84. Genesis Identification page for Qual view parameters (Sheet 6 of 8)

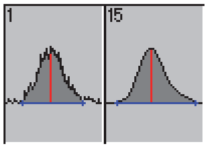
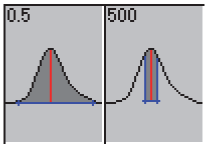
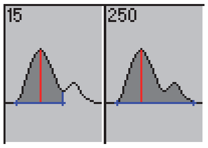
Parameter	Description
Genesis Peak Integration	
Smoothing Points 	Specifies the degree of data smoothing to be performed on the active chromatogram before peak detection and integration. To change this value, type a value in the Smoothing Points box. Default: 1 Range: Odd integers from 1 (no smoothing) through 15 (maximum smoothing)
S/N Threshold 	Specifies the signal-to-noise threshold for peak integration. The data system only integrates peaks with a signal-to-noise value that is greater than this value. To change this value, type a value in the S/N Threshold box. Default: 0.5 Range: 0.0–999.0
Enable Valley Detection	Selecting this check box turns on the valley detection integration algorithm and activates the Expected Width parameter. This integration algorithm 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.
Expected Width (sec) 	Specifies the expected peak width, in seconds, for valley detection. This parameter controls the minimum peak width for a peak when the valley detection algorithm is turned on. Selecting the Enable Valley Detection check box makes this box available. When valley detection is turned on, the data system ignores a valley (local minima) that is within the following window: peak apex ± expected width/2 When the data system finds a valley outside the expected peak width window, it terminates the peak at that point. The data system always terminates a peak when the signal reaches the baseline, independent of the value set for the expected peak width. To enter a value for this parameter, select the Enable Valley Detection check box. Then type a value in the Expected Width box. Range: 0.0–999.0

Table 84. Genesis Identification page for Qual view parameters (Sheet 7 of 8)

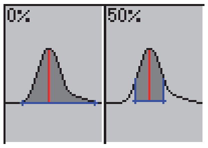
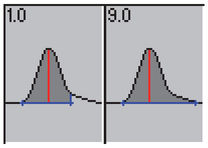
Parameter	Description
Constrain Peak Width	Selecting this check box turns on the constrain peak width integration algorithm and activates the Peak Height (%) and Tailing Factor boxes.
Peak Height (%) 	Specifies the percent of the total peak height (100%) that determine the start and end points for the peak. To integrate the area under a peak, the data system drops a vertical line to the baseline at these points. The integrated area of a peak is constrained to the peak width between these points. To enter a value for this parameter, select the Constrain Peak Width check box. Then type a value in the Peak Height (%) box. Range: 0.0–100.0
Tailing Factor 	Controls how the data system integrates the tail of a peak. The tailing factor is the maximum ratio of the trailing edge to the leading edge of a constrained peak. To enter a value for this parameter, select the Constrain Peak Width check box. Then type a value in the Tailing Factor box. Range: 0.5–9.0
Min (graphical representation)	Displays a representative drawing of the minimum value for the selected parameter. The location of the cursor defines the selected parameter. For example, if you click the Smoothing Points box, the graphic shows the typical result obtained with the minimum number of smoothing points: a peak with reduced noise. The number in the upper left corner of the graphic is a representative low value for the active parameter. It is not necessarily the minimum value for the parameter.
Max (graphical representation)	Displays a representative drawing of maximum value for the selected parameter. The location of the cursor defines the selected 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. It is not necessarily the maximum value for the parameter.

Table 84. Genesis Identification page for Qual view parameters (Sheet 8 of 8)

Parameter	Description
Limit Peaks	
Select Top Peaks	
Enable	Select this check box to activate the parameters in the Select Top Peaks area. These parameters limit peak detection to a specified number of peaks on the basis of either peak area or peak height.
Select by Area	Select the Area option to restrict detection to the most significant peaks on the basis of area rather than height.
Select by Height	Select the Height option to restrict detection to the most significant peaks on the basis of height rather than area.
Num to Select	Type the maximum number of peaks to be detected. The data system selects the largest peaks on the basis of intensity (height) or area.
Rel Peak Height Threshold	
Enable	Select this check box to activate the % of Highest Peak parameter. This parameter limits 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	Specifies a percentage threshold that limits the number of peaks submitted for further processing. The data system discards any detected peaks with an intensity less than the threshold percentage of the most intense peak.
Buttons	
Save As Default	Validates and saves the settings on the current page as default settings. The data system uses these settings for all new processing methods. The data system writes over the previous default values and cannot recover them.
Advanced	Opens Genesis Advanced Chromatogram Options dialog box, where you can set advanced peak identification and detection parameters. The Genesis peak detection algorithm uses these parameters. For more information, see “Genesis Advanced Chromatogram Options Dialog Box” on page 276.

Spectrum Enhancement Page for Qual View

Use the Spectrum Enhancement page for the Qual view of the Processing Setup window to select the algorithm to be used to remove the background noise from the spectrum of interest.

When you select the Enable check box, these three options become available:

- 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

Select the Refine option to remove the contribution of background ions from the spectrum of interest. The Refine algorithm determines which ions in the selected spectrum are part of the background noise and removes them to produce a “refined” spectrum.

For more information, see “Using the Refine Option for Spectrum Enhancement” on page 57.

Refine requires two parameters that you can set and test interactively: Window Size (sec) and Noise Threshold. Using these settings, the Refine algorithm does the following:

1. Discards masses without a peak maximum within ±1 scan of the defined chromatogram peak apex.
2. Searches for a minimum intensity in the user-specified window on either side of the peak apex. These points define the peak start and peak end.
3. Measures the background noise level in the mass chromatogram using scans at and beyond the peak start and peak end, and then estimates the contribution of noise to the peak apex scan through extrapolation.
4. Adjusts the mass intensity of the apex scan by subtracting the estimated noise contribution.
5. Uses the user-specified noise threshold to determine whether the adjusted intensity is significant in comparison to the background noise. If the ion meets the following condition, the data system discards the *m/z* value for the ion from the final spectrum.

   Adjusted Intensity < Noise Threshold × Background Noise

Table 85 describes the parameters for the Refine option on the Spectrum Enhancement page of the Processing Setup – Qual view.

Table 85. Refine option parameters

Parameter	Description
Enhancement Options	
Refine	
Window Size	Specifies a time window for the Refine option. 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	Specifies 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, the data system discards ions from the enhanced spectrum unless their intensities are twice the measured background noise.
Button	
Save As Default	Validates and saves the settings on the current page as default settings. The data system uses these settings for all new processing methods. The data system writes over the previous default values and cannot recover them.

Combine Option in the Spectrum Enhancement Page for Qual View

Select the Combine option to use the Combine algorithm to remove the background noise from the spectra or spectrum of interest.

For more information, see "Using the Combine Option for Spectrum Enhancement" on page 55.

The Combine algorithm produces a single enhanced spectrum for each detected peak as follows:

- Averages all the scans across each peak top region
- Subtracts the background contribution (averaged from a number of scans and scaled appropriately) determined from the baseline regions on either side of each peak.

The Combine algorithm requires six parameters that you can set and test interactively. The data system applies the algorithm to all detected chromatogram peaks in the time range that is specified in the Selected Retention Time Window area on the Qual view – Identification page. 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 the Combine parameters, you might find it helpful to display scan numbers in the chromatogram cell.

❖ To display the scan number label in the chromatogram view

1. Open a raw file of interest by choosing **File > Open Raw File** from the menu bar.
2. Pin the chromatogram view.
3. Right-click the chromatogram view and choose **Display Options** from the shortcut menu.

   The Display Options dialog box opens.
4. Click the **Labels** tab to display the Labels page.
5. In the Label With area, select the **Scan Number** check box.

Table 86 describes the parameters for the Combine option on the Spectrum Enhancement page of the Processing Setup – Qual view.

Table 86. Combine option parameters (Sheet 1 of 2)

Parameter	Description
Background Subtraction Left Region	
Region Width (points)	Specifies 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.

Table 86. Combine option parameters (Sheet 2 of 2)

Parameter	Description
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 data system uses these settings for all new processing methods. The software writes over the previous default values and cannot recover them.

Threshold Option in the Spectrum Enhancement Page for Qual View

Select the Threshold option to use the Threshold algorithm to remove the background noise from the spectrum of interest.

For more information, see "Using the Threshold Option for Spectrum Enhancement" on page 58.

The Threshold algorithm limits the number of ions in the final spectrum before 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 87 describes the parameters for the Threshold option on the Spectrum Enhancement page of the Processing Setup – Qual view.

Table 87. Threshold option on the Spectrum Enhancement page for Qual view parameters (Sheet 1 of 2)

Parameter	Description
Enhancement Options	
Threshold	
Cutoff Threshold (%)	Enter a limiting intensity value as a percentage of the most intense mass. The data system produces an enhanced spectrum by discarding any ions with an intensity below the specified threshold.

Table 87. Threshold option on the Spectrum Enhancement page for Qual view parameters (Sheet 2 of 2)

Parameter	**Description**
Button	
Save As Default	Validate and save the settings on the current page as default settings. The data system 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

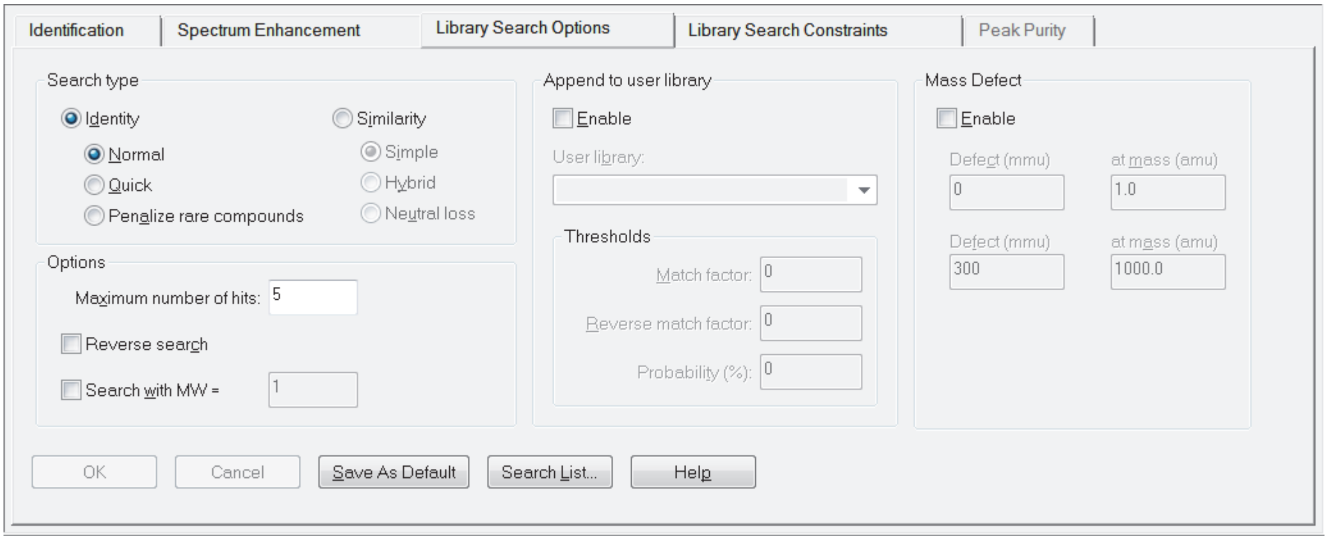
The Library Search Options page in the Processing Setup – Qual view consists of the parameters to define a comparison search of your compound to published compound data or a defined user library. It consists of three main areas: Search Type, Options, and Append to User Library.

Use the Library Search Options page to set up the library search criteria for the processing method.

For more information about running an automated library search, refer to the *Xcalibur Creating and Searching Libraries User Guide*.

Figure 93 shows the Library Search Options page.

Figure 93. Library Search Options page



Search type
● Identity
● Normal
○ Quick
○ Penalize rare compounds
○ Similarity
● Simple
○ Hybrid
○ Neutral loss

Options
Maximum number of hits: 5
☐ Reverse search
☐ Search with MW = 1

Append to user library
☐ Enable
User library:
Thresholds
Match factor: 0
Reverse match factor: 0
Probability (%): 0

Mass Defect
☐ Enable
Defect (mmu) 0 at mass (amu) 1.0
Defect (mmu) 300 at mass (amu) 1000.0

Table 88 describes the parameters on the Library Search Options page.

Table 88. Library Search Options page for Qual view parameters (Sheet 1 of 5)

Parameter	Description
Search Type	
Identity	Selecting this option makes the Normal, Quick, and Penalize Rare Compounds options available. Select this option to apply an identity search algorithm for library matching of spectra.
Normal	Select this option to 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	Select this option to 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	Select this option to 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 found in a limited number of these databases. When you select the Penalize Rare Compounds option, matching compounds (hits) that are found in few databases or only in 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	Selecting this option makes the Simple, Hybrid, and Neutral Loss options available. Select this option to apply a Similarity search algorithm for library matching of spectra.

Table 88. Library Search Options page for Qual view parameters (Sheet 2 of 5)

Parameter	Description
Simple	Selecting this option applies 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.
Hybrid	Selecting this option applies 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	Selecting this option applies 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 data system 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	Specifies the maximum number of search results to be returned by a library search and reported in the result file. The data system 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.

Table 88. Library Search Options page for Qual view parameters (Sheet 3 of 5)

Parameter	Description
Search with MW =	Select this check box to 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	Select this check box to 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	Specifies the name of the user library to be used to store spectra. To select a user library, click the arrow to display the list of Xcalibur user libraries. Select a user library in the list.
Thresholds	
Match Factor	Specifies a forward match factor threshold for spectra subject to the Append to User Library option. The data system 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 data system records the search result list in the result 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.

Table 88. Library Search Options page for Qual view parameters (Sheet 4 of 5)

Parameter	Description
Reverse Match Factor	Specifies a Reverse Match Factor threshold for spectra subject to the Append to User Library option. The data system 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 data system records the search result list in the result 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.
Probability	Specifies a Probability threshold for spectra subject to the Append to User Library option. The data system 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 data system records the search result list in the result 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 limits of probability are 0 to 100.
Mass Defect	
Enable	Selecting this check box makes the mass defect boxes available. Select this check box to include mass defect values for library searches in a processing method.
Defect	Specifies 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 a larger value for higher mass ranges in the second box.

Table 88. Library Search Options page for Qual view parameters (Sheet 5 of 5)

Parameter	Description
At Mass	Specifies 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	Validates and saves the settings on the current page as default settings. The data system uses these settings for all new processing methods. The software writes over the previous default values and cannot recover them.
Search List	Opens the Search List dialog box (see "Search List Dialog Box" on page 289).

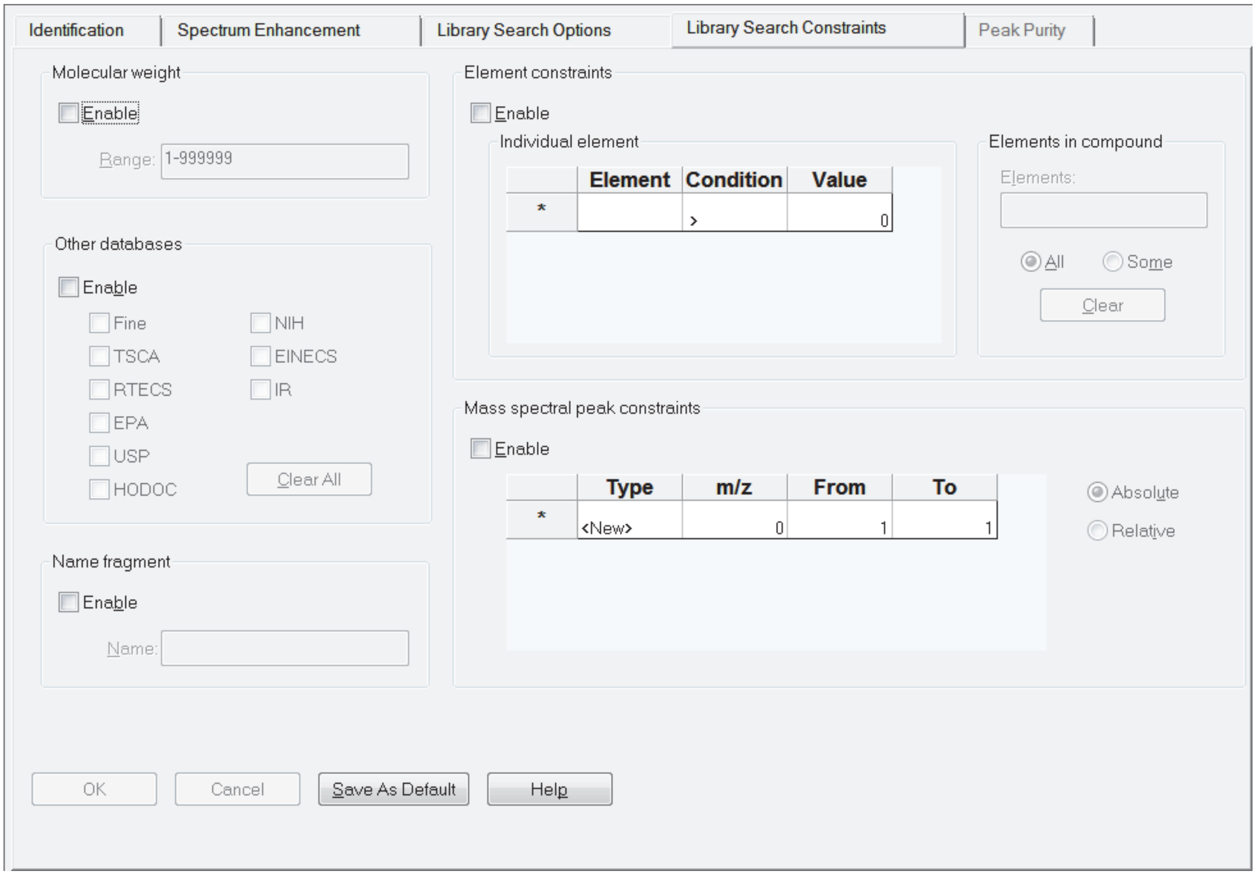
Library Search Constraints Page for Qual View

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.

For more information about running an automated library search, refer to the *Xcalibur Creating and Searching Libraries User Guide*.

Figure 94 shows the Library Search Constraints page.

Figure 94. Library Search Constraints page



Range: 1-999999

Name:

Elements:

	Element	Condition	Value
*		>	0

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

Table 89 describes the parameters on the Library Search Constraints page.

Table 89. Library Search Constraints page for Qual view parameters (Sheet 1 of 7)

Parameter	Description
Molecular Weight	
Enable	Selecting this check box limits 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	Selecting this check box limits 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 data system reports search results featured in one or more of the selected databases. (A search result does not have to be found in all the selected databases.)
Fine	Select this check box to report search results from reference compounds or spectra also found in the commercially available Fine Chemical Index.
TSCA	Select this check box to report search results from reference compounds or spectra also found in the Toxic Substances Control Act Inventory (TSCA).
RTECS	Select this check box to report search results from reference compounds or spectra also to be found in the Registry of Toxic Effects of Chemical Substances (RTECS).
EPA	Select this check box to report search results from reference compounds or spectra also found in the Environmental Protection Agency (EPA) Environmental Monitoring Methods Index.
USP	Select this check box to report search results from reference compounds or spectra also found in the US Pharmacopoeia (USP)/U.S.A.N.
HODOC	Select this check box to report search results from reference compounds or spectra also found in the CRC Handbook of Data of Organic Compounds (HODOC).
NIH	Select this check box to report search results from reference compounds or spectra also to be found in the NIH-NCI Inventory File.

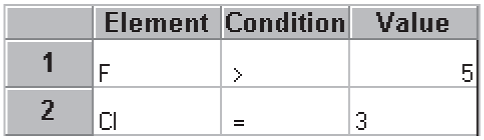
Table 89. Library Search Constraints page for Qual view parameters (Sheet 2 of 7)

Parameter	Description
EINECS	Select this check box to report search results from reference compounds or spectra also found in the European Index of Commercial Chemical Substances (EINECS).
IR	Select this check box to report search results from reference compounds or spectra also found in the NIST/EPA Gas Phase IR Database.
Clear All	Clear all the check boxes in the Other Databases area.
Name Fragment	
Enable	Selecting this check box limits the library search results to compounds with a specific name or name fragment.
Name	Enter a text string of up to 39 characters to represent a fragment of a compound name, for example, “cyclo.” During the library search, the data system filters search results and only returns those containing the specified text in their names. The entry is case insensitive: “CYCLO” returns compounds containing the fragments “cyclo,” “Cyclo,” and “CYCLO.”
Element Constraints	
Enable	Selecting this check box limits 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.

Table 89. Library Search Constraints page for Qual view parameters (Sheet 3 of 7)

<table>
<tr><th>Parameter</th><th>Description</th></tr>
<tr><td>Individual Element</td><td></td></tr>
<tr><td>Individual Element table</td><td>Use this table to set up the criteria for 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.


<table>
<tr><th></th><th>Element</th><th>Condition</th><th>Value</th></tr>
<tr><td>1</td><td>F</td><td>></td><td>5</td></tr>
<tr><td>2</td><td>Cl</td><td>=</td><td>3</td></tr>
</table>
In the example shown here, the data system would only return search results for compounds that contain

More than five fluorine atoms, and
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.</td></tr>
<tr><td>[Row Number]</td><td>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.</td></tr>
<tr><td>Element</td><td>Enter the IUPAC-approved abbreviation for the element that 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, type the required abbreviation. For example, to apply carbon as an element limit, type C. The data system adds a new row to the table for further entries.</td></tr>
</table>

Table 89. Library Search Constraints page for Qual view parameters (Sheet 4 of 7)

Parameter	Description
Condition	Enter a condition for an element limit. The data system uses this value together with the Condition list and Value box in the same row of the Individual Element table. Valid conditions are as follows: • < (less than) • > (greater than) • = (equals) To enter an element limit condition, double-click the box to open the list. Then select the required condition.
Value	Enter a numerical value for an element limit. This value 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 for library compounds to satisfy the limit. To enter an element limit value, type the required number. The valid range is 0 to 99.
Elements in Compound	
Elements	Specifies the elements that must be present in returned search results. To enter an element list, type the IUPAC-approved abbreviation for each element. Separate each element in the list (of up to 30 characters) by a comma.
All	Selecting this option specifies that the data system return 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	Selecting this option specifies that the data system return 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, and HCHO but not CH2Cl2. Compare with the All option.
Clear	Deletes the text in the Elements box.

Table 89. Library Search Constraints page for Qual view parameters (Sheet 5 of 7)

Parameter	Description
Mass Spectral Peak Constraints	
Enable	Selecting this check box makes the mass spectral peak constraints table available. Use this table to 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, *m/z*, From, and To.	
Type	Specifies the type of ion. The available selections are as follows: Normal, Loss, Rank, or Maxmass.
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 the following: • A fragment ion at an *m/z* value 15 less than the molecular ion • An abundance in the range specified in the From and To columns
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 that meets these conditions: • At the specified *m/z* value • Ranked between the range specified in the From and To columns If you specify the same number in both fields, the designated ion must have that rank in the retrieved spectrum.

Table 89. Library Search Constraints page for Qual view parameters (Sheet 6 of 7)

Parameter	Description
Maxmass	Maxmass sets a limit on the *m/z* value of the most significant high-mass ion. Library search results must feature the following: • An ion at the specified *m/z* value • No significantly larger masses at higher *m/z* values • An abundance in the range specified in the From and To columns
m/z	Enter the *m/z* value of the mass spectral peak to be constrained in a Normal, Rank, or Maxmass type limit. The data system 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 column to enter the value of a neutral loss. The data system 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 column 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. You can specify the same number in both From and To boxes. In this case, the data system discards a library search result unless the designated mass spectral peak is present in exactly the specified abundance or rank in the retrieved spectrum.
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. You can specify the same number in both From and To boxes. In this case, the data system discards a library search result unless the designated mass spectral peak is present in exactly the specified abundance or rank in the retrieved spectrum.
[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 89. Library Search Constraints page for Qual view parameters (Sheet 7 of 7)

Parameter	Description
Absolute	Specifies 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 data system 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 data system 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	Specifies 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 this example, library search results must contain the following: • 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	Validates and saves the settings on the current page as default settings. The data system uses these settings for all new processing methods. The software writes over the previous default values and cannot recover them.

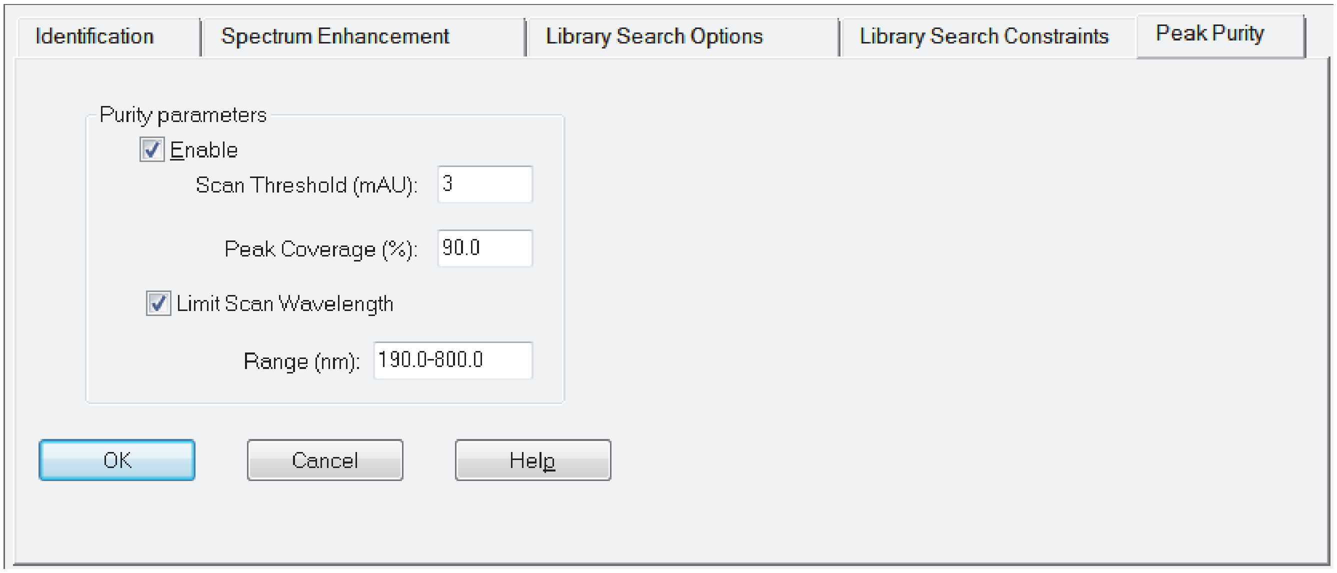
Peak Purity Page for Qual View

Use the Peak Purity page of the 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.

For PDA data, the data system can calculate the spectral purity of your chromatographic peaks by comparing the similarity of the spectra across the peak to a spectrum from the peak apex. The calculation is affected by the integration of the scan chromatogram and by the scan threshold, peak coverage, and scan wavelengths that you set on the Peak Purity page.

Figure 95 shows the Peak Purity page for the Qual view.

Figure 95. Peak Purity page in the Qual view



Purity parameters

☑ Enable

Scan Threshold (mAU): 3

Peak Coverage (%): 90.0

☑ Limit Scan Wavelength

Range (nm): 190.0-800.0

Table 90 describes the parameters on the Peak Purity page.

Table 90. Peak Purity page for Qual view parameters

Parameter	Description
Purity Parameters	
Enable	Selecting this check box activates the peak purity parameters.
Scan Threshold (mAU)	Specifies a minimum value of intensity for wavelength scans in milliabsorbance units (mAU). A peak purity calculation 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 specified Scan Threshold (mAU) value is reached. Default: 3 mAU Range: 0 to 1000 mAU (or 1 AU) In a sample with high background or noise, start with a value of 40 mAU for the scan threshold.
Peak Coverage (%)	Specifies a maximum percent value for the width of the integrated peak. A peak purity calculation 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 specified Peak Coverage (%) value is reached. Use peak coverage for symmetrical peaks. Default: 95% of the integrated peak Range: 0–100
Limit Scan Wavelength	Select this check box to limit the scan wavelength range for a peak purity calculation. Selecting this check box activates the Range (nm) box.
[Wavelength] Range	Specifies a range of UV-Vis scans (in nanometers). A peak purity calculation 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. Select the Limit Scan Wavelength check box to activate this box. The default wavelength range is the full width of the scan.

Quan View

Use the Quan view of the Processing Setup window to set up a quantitative processing method. 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.

Note Use the New Sequence Template dialog box of the Home Page – Sequence Setup view to generate a sequence semi-automatically, on the basis of a processing method. When you use the New Sequence Template dialog box to set up a sequence, you can also set up the None, Overlapped, and Non-Overlapped bracket types.

The Quan view consists of a menu bar, a toolbar, and five or six pages. The first five pages are available for all detector types. The Peak Purity page is available for the PDA (photo diode array) detector type only. The chromatogram and spectrum views appear at the bottom of the Identification, Detection, and Peak Purity pages. The following buttons, which are part of the Processing Setup window, appear in every Quan view page: OK, Cancel, and Save As Default.

For information about the OK, Cancel, and Save As Default buttons, see "OK, Cancel, and Save As Default Buttons" on page 261. For information about the chromatogram and spectrum views, see "Chromatogram and Spectrum Views in the Qual and Quan Views" on page 260.

These topics describe the Quan view pages:

- "Identification Page for Quan View," on the next page
- "Detection Page for Quan View" on page 351
    - "Avalon Detection Page for Quan View" on page 351
    - "Genesis Detection Page for Quan View" on page 359
    - "ICIS Detection Page for Quan View" on page 369
- "Levels Page for Quan View" on page 383
- "System Suitability Page for Quan View" on page 385
- "Peak Purity Page for Quan View" on page 389

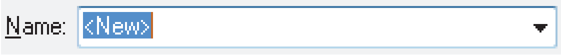
Identification Page for Quan View

Use the Identification page to name components and specify retention time, detector type, and peak identification, detection, and integration criteria for each named component.

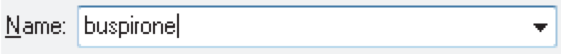
To set up the parameters on the Identification page, follow these procedures:

❖ To add analytes (components) to the components list in the Components pane

1. For each component that you want to add to the components list, select the <New> entry in the Name list, and then type the name of the new component.



Name: <New>



Name: buspirone

2. Press **ENTER** or click **OK** to add the new component.

   The new component appears in the Components pane.

❖ To delete a component in the components list

1. In the list in the Components pane, select the name of the component that you want to delete.
2. From the menu bar, choose **Options > Delete *component name***.

   A confirmation message appears.

3. Click **OK** to complete the deletion and close the message box. Or, click **Cancel** to close the message box without deleting the selected component.

❖ To select the detector type

In the Detector Type list, select the detector type used to acquire the trace.

❖ To select a peak detection algorithm

1. Select the component of interest in the Components pane.
2. In the Peak Detect list, select an algorithm.
3. Click **OK**.

   The default parameters for the selected peak detection algorithm appear on the Identification and Detection pages.

❖ To select a scan filter in the Filter list

In the Filter list, select a scan filter from the list of filters used to acquired the mass spectral data.

The selected scan filter appears in the Filter box.

❖ To apply a scan filter that is not listed in the Filter list

Do one of the following:

- Select a new filter from the list and edit the scan filter.

–or –

- Type a new scan filter into the box using the appropriate scan filter format (refer to the *Xcalibur Qual Browser User Guide.*)

❖ To specify the trace (chromatogram) to be processed

1. In the first list, select a basic chromatogram type, for example, TIC.
2. In the second list, select a logical operator: + or –.

   The third list becomes available.

3. In the third list, 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.

Table 91 describes the parameters on the Quan view – Identification page. For information about using the Quan view – Identification page, see "Setting Up the Quan View Identification Parameters" on page 24.

Table 91. Identification page for Quan view parameters (Sheet 1 of 7)

Parameter	Description
Name	Displays a list of component names for the active processing method. For a new processing method, this list displays only <New>. Use this list to add new components to the processing method. See "To add analytes (components) to the components list in the Components pane" on page 343. To display the identification settings for a component in the list, click the name of the component in the Components pane on the right side of the page.
Detector Type	Specifies the detector type: • MS (mass spectrometer) • Analog • A/D Card (analog-to-digital converter) • PDA (photodiode array detector) • UV (ultraviolet or ultraviolet-visible detector)

Table 91. Identification page for Quan view parameters (Sheet 2 of 7)

Parameter	Description
Peak Detect	Specifies the peak detection algorithm for the component selected in the Components pane: • Genesis—for Xcalibur 1.0 data files • ICIS—for mass spectrum traces • Avalon—for UV-Vis and analog traces The default parameters for the selected peak detection algorithm appear on the Identification and Detection pages.
Filter	Lists the scan filters for the current raw file .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 select a scan filter from the list of filters used to acquire the raw file, select one of the scan filters in the Filter list. The selected scan filter appears in the Filter box. You can also apply a scan filter that is not listed in Filter box by typing a new scan filter in the Filter box. The scan filter must follow the format described in the *Xcalibur Qual Browser User Guide*.
Trace	From the three Trace lists, specify the type of chromatogram that you want to use for data processing. See "To select a scan filter in the Filter list" on page 343 and "To apply a scan filter that is not listed in the Filter list" on page 344. 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. The valid trace types depend on the detector type.
MS detector	For MS scans, valid trace types are TIC, Mass Range, and Base Peak. For more information, see "Valid MS Trace Combinations" on page 296.
Analog detector	For Analog data, the data system supports up to four channels (labeled Analog 1–4). For more information, see "Valid Analog Trace Combinations" on page 297.
A/D card	For data from an A/D Card, the data system supports four channels (labeled A/D Card Ch 1–4). For more information, see "Valid A/D Card Trace Combinations" on page 297.

Table 91. Identification page for Quan view parameters (Sheet 3 of 7)

Parameter	Description
PDA detector	For PDA data, valid trace types are Wavelength Range, Total Scan, or Spectrum Maximum. For more information, see "Valid PDA Trace Combinations" on page 298.
UV detector	For UV detector data, the data system supports four channels (labeled Channel A–D). For more information, see "Valid UV Trace Combinations" on page 298.
For MS detector type:	
Mass (*m/z*)	Specifies the mass range for the Mass Range trace type. This box becomes available 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 (see "Changing the List Separator Character" on page 123).
Mass1	Specifies the mass range for the first trace type. This box becomes available 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 "Printing a Vial or Sequence List" on page 95.

Table 91. Identification page for Quan view parameters (Sheet 4 of 7)

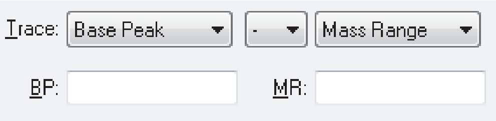
Parameter	Description
[Mass] 2	Specifies the mass range for the second trace type. This box becomes available when you select a Mass Range ± Mass Range trace combination for an MS detector type. To change the range or to add a new range, type the range in the box. The format is *LowMass–HighMass*. For 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 (see "Changing the List Separator Character" on page 123).
BP	Specifies the range in which to search for the highest peak. This box appears when you select a Base Peak trace for an MS detector type.  Trace: Base Peak - Mass Range BP: MR: 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	Specifies the mass range for the second Mass Range trace type. This box appears 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 91. Identification page for Quan view parameters (Sheet 5 of 7)

Parameter	Description
For PDA detector type:	
Wavelength	Specifies the wavelength range for the Wavelength Range or Spectrum Maximum trace type. This box appears 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 (see “Changing the List Separator Character” on page 123).
Wavelength 1	Specifies the wavelength or wavelength range for the first trace type. This box appears 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 (see “Changing the List Separator Character” on page 123).

Table 91. Identification page for Quan view parameters (Sheet 6 of 7)

Parameter	Description
[Wavelength] 2	Specifies the wavelength or wavelength range for the second trace type. This box appears 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 (see "Changing the List Separator Character" on page 123).
Keys	Specifies user 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 (min)	Specifies the expected retention time for the selected component. The valid range depends on the configured hardware. For GC/MS and LC/MS systems, the valid range is 0 to 999 minutes. To change the time or to enter a new time, type the number of minutes in the Expected (retention time) box.
Window (sec)	Specifies the retention time window for 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 selected component to adjust the expected retention time of another component. To use the selected 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 components that you select as RT Reference components appear in the Adjust Using list.
View Width	Specifies 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.

Table 91. Identification page for Quan view parameters (Sheet 7 of 7)

Parameter	**Description**
Adjust Using check box	Select whether to adjust the expected retention time (RT) of the selected component (selected in the Components pane and displayed in the Name box) using the actual retention time of a RT Reference component, such as an internal standard. The Adjust Using list to the right of this check box contains a list of components that you have set up as RT Reference components. There must be at least one RT Reference component in the processing method for this check box to be available.
Adjust Using list	Specifies the RT Reference component that the data system uses to adjust the expected retention time of the selected component. 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, select a component in the Adjust Using list. The data system uses the actual retention time of the RT Reference component to correct the retention time of the selected 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	
List of components in the Components pane	Lists all of the component names that are defined for the active processing method. This list is located in the Components pane on the right side of the window.
Buttons	
Save as Default	Validates and saves the settings on the current page as default settings. The data system 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 data system 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.

Detection Page for Quan View

Use the Detection page of the Processing Setup – Quan view to specify peak integration and detection criteria.

On the basis of your selected default peak detection algorithm or your selection in the Peak Detect list on the Identification page for the selected component, the data system displays the corresponding version of this page:

- "Avalon Detection Page for Quan View," on this page
- "Genesis Detection Page for Quan View" on page 359
- "ICIS Detection Page for Quan View" on page 369

For information about using the Quan view – Detection page, see "Setting Up the Quan View Integration and Detection Parameters" on page 26.

Avalon Detection Page for Quan View

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

After selecting Avalon as the peak detection algorithm on the Identification page of the Quan view, this page appears when you open the Detection page of the Quan view.

> **Note** Click **Advanced** to open the Avalon Event List dialog box where you can change parameters in the Event list.

These topics describe the parameters on the Avalon Detection page for the Processing Setup – Quan view:

- "Quan View – Avalon Detection Page Buttons," on the next page
- "Avalon Peak Integration Parameters" on page 352
- "Avalon Peak Detection Parameters – LC Mode" on page 354
- "Avalon Peak Detection Parameters – GC Mode" on page 354

For information about changing the chromatography mode, see "Chromatography Options Dialog Box" on page 271.

Quan View – Avalon Detection Page Buttons

Table 92 describes the buttons at the bottom of the Quan view – Detection page.

Table 92. Buttons at the bottom of the Quan view – Detection page for the Avalon algorithm

Parameter	Description
Save As Default	Validates and saves the settings on the current page as default settings. The data system uses these settings for all new processing methods. This option guarantees that the settings for the components are consistent and valid. These default settings are then used for all new components. The data system writes over the previous default values and cannot recover them.
Advanced	For the Avalon peak detection algorithm, this button opens the Avalon Event List dialog box, where you can modify the integration events list that is displayed on the Detection page. For information about the Avalon Event List dialog box, see "Avalon Event List Dialog Box" on page 265.
Flags	Opens the Data Flags dialog box, where you can set peak area and peak height threshold values. The data system reports these data flags in result files, printed reports, and Quan Browser. For information about the Data Flags dialog box, see "Data Flags Dialog Box" on page 274.

Avalon Peak Integration Parameters

Table 93 describes the parameters in the Avalon Peak Integration area of the Quan view –Detection page.

Table 93. Avalon peak Integration parameters (Sheet 1 of 2)

Parameter	Description
Avalon Peak Integration	
Specifies the peak integration settings. Use the Auto Calculate Initial Events feature to determine optimal values for the seven initial value (time = 0.0) integration events that are required by the Avalon integration algorithm. You can change the value of an initial value (time = 0.0) integration event, but you cannot delete it.	
Smoothing Points	Specifies the degree of data smoothing to be performed on the active component peak before peak detection and integration. The valid range is any odd integer from 1 (no smoothing) through 15 (maximum smoothing). To smooth your component peak data before integration, enter a value in the Smoothing Points box.

Table 93. Avalon peak Integration parameters (Sheet 2 of 2)

Parameter	Description
Event List	
The event list consists of three columns: Time, Event, and Value. ❖ **To change the settings in the Event list** Click **Advanced** to open the Avalon Event List dialog box. For information about the available integration events or adding, changing, or deleting the events from the event list, see "Avalon Event List Dialog Box" on page 265.	
Time	Displays the time of a timed event. This column contains either the term *initial value* or a time value.
Event	Displays initial value (time = 0) and timed integration events.
Value	Displays the value for a integration event.
Auto Calculate Initial Events	This button is available when a raw file is open in the Processing Setup window. When you click this button, the data system automatically determines the best value for each of the seven initial value events on the basis of the data in the current raw file and then displays these values in the Value column of the event list. The data system does not estimate values for timed events; that is, events that have a time value in the Time column. It determines initial values for these events only: Start Threshold, End Threshold, Area Threshold, P-P [Resolution] Threshold, Bunch Factor, Negative Peaks, and Tension. ❖ **To automatically 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.

Avalon Peak Detection Parameters – LC Mode

Table 94 describes the parameters in the Avalon Peak Detection area for the liquid chromatography (LC) mode.

Table 94. Avalon Peak Detection parameters for the liquid chromatography (LC) mode

Parameter	Description
Avalon Peak Detection	
Highest Peak	When you select this option, the data system uses the highest peak in the chromatogram within the specified retention time window for component identification.
Nearest RT	When you select this option, the data system uses the peak with the nearest retention time in the chromatogram to the expected retention time for component identification.

Avalon Peak Detection Parameters – GC Mode

Table 95 describes the parameters in the Avalon Peak Detection area for the gas chromatography (GC) mode.

Table 95. Avalon Peak Detection parameters for the gas chromatography (GC) mode (Sheet 1 of 6)

Parameter	Description
Avalon Peak Detection (GC mode)	
Spectrum	This option is only available in the GC chromatography mode for the data acquired with an MS detector. When you select this option, the data system uses the user-defined reference spectrum for component identification. The data system attempts to match the reference spectrum with a series of unknown spectra and calculates a score value for each comparison. When you select the Spectrum option, a mass-intensity list and the Thresholds area appear (see “Additional parameters for the Spectrum option (Avalon)” on page 355).
Highest Peak	When you select this option, the data system uses the highest peak in the chromatogram within the specified retention time window for component identification, and the Ion Ratio Confirmation window appears. You can use the parameters in the Ion Ratio Confirmation area to confirm the identify of the chromatographic peak on the basis of spectral information (see “Ion Ratio Confirmation (Avalon)” on page 356).

Table 95. Avalon Peak Detection parameters for the gas chromatography (GC) mode (Sheet 2 of 6)

Parameter	Description
Nearest RT	When you select this option, the data system uses the peak with the nearest retention time in the chromatogram to the expected retention time for component identification, and the Ion Ratio Confirmation window appears. You can use the parameters in the Ion Ratio Confirmation area to confirm the identify of the chromatographic peak on the basis of spectral information (see "Ion Ratio Confirmation (Avalon)" on page 356).
Additional parameters for the Spectrum option (Avalon)	
Mass intensity list for the Spectrum option Enter mass-to-charge [*m/z*] and intensity percentages for up to 50 spectrum peaks. The data system uses this data to identify the component. For information about interactively using the spectrum in a representative raw data file to enter the spectral data in the list, see "To enter data in the spectrum table by using an open raw file" on page 36.	
m/z	Each *m/z* value in this column specifies the mass-to-charge [*m/z*] value for one spectral peak in the reference spectrum. The adjacent Intensity (%) box specifies the intensity percentage for this *m/z* value. Range: 0.5–999 999
Intensity	Each intensity percentage in this column specifies the relative intensity for one spectral peak in the reference spectrum. The adjacent *m/z* box specifies the *m/z* value for the spectral peak. Range: 0–100
Thresholds (Spectrum option) The Thresholds area appears when you select the Spectrum option in the GC mode.	
Forward	Specifies 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. Range: 0–1000

Table 95. Avalon Peak Detection parameters for the gas chromatography (GC) mode (Sheet 3 of 6)

Parameter	Description
Reverse	Specifies 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 in a forward match. Range: 0–1000
Match	Specifies a threshold value for match comparisons between the reference spectrum and candidates in the chromatogram. The match threshold is scored on a scale of 0 to 999. The match algorithm is a complex probability factor that is 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. Range: 0–1000
Ion Ratio Confirmation (Avalon) This area appears when you select the Highest Peak or Nearest RT option in the GC mode for data from an MS detector. Use the parameters 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	Selecting this check box activates the parameters in the Ion Ratio Confirmation area.
Ion Ratio Using: Area or Height (read-only)	This read-only parameter shows the currently selected peak quantitation method: area or height. The data system 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.

Table 95. Avalon Peak Detection parameters for the gas chromatography (GC) mode (Sheet 4 of 6)

Parameter	Description
Qualifier ion table	Use this table to enter mass-to-charge [*m/z*] and target ratio tolerances [Window ± %] data for up to five qualifier ions. If you select Area response, the data system 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 ± %), it rejects the quantitation peak. If you select Height response, the data system 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 ± %), it rejects the quantitation peak.
m/z	The value in this column specifies the mass-to-charge [*m/z*] value for a qualifier ion. Range: 0.5–999 999
Target Ratio (%)	The value in this column specifies the Target Ratio (%) value for a qualifier ion. Range for a manual target ratio for the qualifier ion: 0.00–1 000 000
Window (±%)	The value in this column specifies the Target Ratio tolerance for a qualifier ion. Range: 0.00–100.00

Table 95. Avalon Peak Detection parameters for the gas chromatography (GC) mode (Sheet 5 of 6)

Parameter	Description
Window%	
Relative	Selecting this option specifies 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 fails, and the data system sets the IRC Flag to False. If the qualifier ion peak-to-quantitation peak ratio is within range, the ion ratio confirmation test passes, 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	Selecting this option specifies 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-to-quantitation peak ratio is outside this range, the ion ratio confirmation test fails, and the data system sets the IRC Flag to False. If the qualifier ion peak-to-quantitation peak ratio is within range, the ion ratio confirmation test passes, 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.

Table 95. Avalon Peak Detection parameters for the gas chromatography (GC) mode (Sheet 6 of 6)

Parameter	Description
Qualifier Ion Coelution	Specifies the Qualifier Ion Coelution window. Before it runs the ion ratio confirmation test, 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 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 data system rejects the quantitation peak. The data system tests quantitation peaks with matching qualifier ion peaks (in the coelution window) for ion ratio confirmation.

Genesis Detection Page for Quan View

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

After selecting Genesis as the peak detection algorithm on the Identification page of the Quan view, this page appears when you open the Detection page of the Quan view.

> **Note** Click **Advanced** to open the Genesis Advanced Detection Options dialog box where you can set up the advanced detection parameters for the Genesis algorithm.

These topics describe the parameters on the Genesis Detection page for the Processing Setup – Quan view:

- “Quan View – Genesis Detection Page Buttons,” on the next page
- “Genesis Peak Integration Parameters” on page 361
- “Genesis Peak Detection Parameters – LC Mode” on page 364
- “Genesis Peak Detection Parameters – GC Mode” on page 364

For information about changing the chromatography mode, see “Chromatography Options Dialog Box” on page 271.

Quan View – Genesis Detection Page Buttons

Table 92 describes the buttons at the bottom of the Qual view – Detection page.

Table 96. Buttons at the bottom of the Quan view – Detection page for the Genesis algorithm

Parameter	Description
Save As Default	Validates and saves the settings on the current page as default settings. The data system uses these settings for all new processing methods. This option guarantees that the settings for the components are consistent and valid. These default settings are then used for all new components. The data system writes over the previous default values and cannot recover them.
Advanced	For the Genesis peak detection algorithm, this button opens the Genesis Advanced Detection Options dialog box, where you can set up the advanced parameters for the Genesis algorithm. For information about the Genesis Advanced Detection Options dialog box, see "Genesis Advanced Detection Options Dialog Box" on page 281.
Flags	Opens the Data Flags dialog box, where you can set peak area and peak height threshold values. The data system reports these data flags in result files, printed reports, and Quan Browser. For information about the Data Flags dialog box, see "Data Flags Dialog Box" on page 274.

Genesis Peak Integration Parameters

Table 97 describes the parameters in the Genesis Peak Integration area on the Detection page of the Quan view.

Table 97. Genesis peak integration parameters

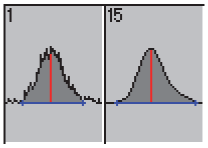
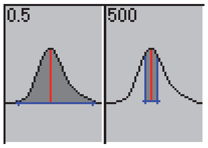
Parameter	Description
Genesis Peak Integration	
Smoothing Points 	Specifies the degree of data smoothing to be performed on the active chromatogram before peak detection and integration. To change this value, type a value in the Smoothing Points box. Default: 7 Range: odd integers from 1 (no smoothing) through 15 (maximum smoothing)
S/N Threshold 	Specifies the signal-to-noise threshold for peak integration. The data system only integrates peaks with a signal-to-noise value that is greater than this value. To change this value, type a value in the S/N Threshold box. Default: 0.5 Range: 0.0–999.0
Enable Valley Detection	Selecting this check box turns on the valley detection integration algorithm and activates the Expected Width parameter. This integration algorithm 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.

Table 97. Genesis peak integration parameters

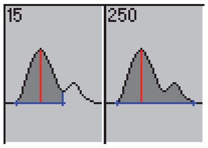
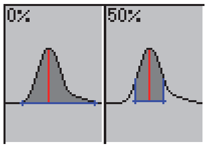
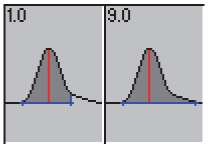
Parameter	Description
Expected Width (sec)  	Specifies the expected peak width, in seconds, for valley detection. This parameter controls the minimum peak width for a peak when the valley detection algorithm is turned on. Selecting the Enable Valley Detection check box makes this box available. When valley detection is turned on, the data system ignores a valley (local minima) that is within the following window: peak apex ± expected width/2 When the data system finds a valley outside the expected peak width window, it terminates the peak at that point. The data system always terminates a peak when the signal reaches the baseline, independent of the value set for the expected peak width. To enter a value for this parameter, select the Enable Valley Detection check box. Then type a value in the Expected Width box. Range: 0.0–999.0
Constrain Peak Width	Selecting this check box turns on the constrain peak width integration algorithm and activates the Peak Height (%) and Tailing Factor boxes.
Peak Height (%)  	Specifies the percent of the total peak height (100%) that determine the start and end points for the peak. To integrate the area under a peak, the data system drops a vertical line to the baseline at these points. The integrated area of a peak is constrained to the peak width between these points. To enter a value for this parameter, select the Constrain Peak Width check box. Then type a value in the Peak Height (%) box. Range: 0.0–100.0
Tailing Factor  	Controls how the data system integrates the tail of a peak. The tailing factor is the maximum ratio of the trailing edge to the leading edge of a constrained peak. To enter a value for this parameter, select the Constrain Peak Width check box. Then type a value in the Tailing Factor box. Range: 0.5–9.0

Table 97. Genesis peak integration parameters

Parameter	**Description**
Min (graphical representation)	Displays a representative drawing of the minimum value for the selected parameter. The location of the cursor defines the selected parameter. For example, if you click the Smoothing Points box, the graphic shows the typical result obtained with the minimum number of smoothing points: a peak with reduced noise. The number in the upper left corner of the graphic is a representative low value for the active parameter. It is not necessarily the minimum value for the parameter.
Max (graphical representation)	Displays a representative drawing of maximum value for the selected parameter. The location of the cursor defines the selected 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. It is not necessarily the maximum value for the parameter.

Genesis Peak Detection Parameters – LC Mode

Table 98 describes the parameters in the Genesis Peak Detection area for the liquid chromatography (LC) mode.

Table 98. Genesis Peak Detection parameters for the liquid chromatography (LC) mode

Parameter	Description
Genesis Peak Detection	
Highest Peak	When you select this option, the data system uses the highest peak in the chromatogram within the specified retention time window for component identification.
Nearest RT	When you select this option, the data system uses the peak with the nearest retention time in the chromatogram to the expected retention time for component identification.
Minimum Peak Height (S/N)	Specifies the minimum peak height on the basis of the signal-to-noise ratio that a peak must meet before the data system recognizes it as a possible chromatographic peak for the selected component. To identify the chromatographic peak for the selected component, the data system ignores chromatographic peaks with a peak height that is less than the specified signal-to-noise threshold value. Range: 0.0 999.0

Genesis Peak Detection Parameters – GC Mode

Table 99 describes the parameters in the Genesis Peak Detection area on the Detection page of the Quan view for the GC mode and mass spectral data.

Table 99. Genesis Peak Detection parameters for the gas chromatography (GC) mode

Parameter	Description
Genesis Peak Detection (GC mode)	
Spectrum	This option is only available in the GC chromatography mode for the data acquired with an MS detector. When you select this option, the data system uses the user-defined reference spectrum for component identification. The data system attempts to match the reference spectrum with a series of unknown spectra and calculates a score value for each comparison. When you select the Spectrum option, a mass intensity list and the Thresholds area appear (see “Additional parameters for the Spectrum option (Genesis)” on page 365).

Table 99. Genesis Peak Detection parameters for the gas chromatography (GC) mode

Parameter	**Description**
Highest Peak	When you select this option, the data system uses the highest peak in the chromatogram within the specified retention time window for component identification, and the Ion Ratio Confirmation window appears. You can use the parameters in the Ion Ratio Confirmation area to confirm the identify of the chromatographic peak on the basis of spectral information (see "Ion Ratio Confirmation (Genesis)" on page 367).
Nearest RT	When you select this option, the data system uses the peak with the nearest retention time in the chromatogram to the expected retention time for component identification, and the Ion Ratio Confirmation window appears. You can use the parameters in the Ion Ratio Confirmation area to confirm the identify of the chromatographic peak on the basis of spectral information (see "Ion Ratio Confirmation (Genesis)" on page 367).
Minimum Peak Height (S/N)	Specifies the minimum peak height on the basis of the signal-to-noise ratio that a peak must meet before the data system recognizes it as a possible chromatographic peak for the selected component. To identify the chromatographic peak for the selected component, the data system ignores chromatographic peaks with a peak height that is less than the specified signal-to-noise threshold value. Range: 0.0 999.0
Additional parameters for the Spectrum option (Genesis)	
Mass intensity list for the Spectrum option Enter mass-to-charge [*m/z*] and intensity percentages for up to 50 spectrum peaks. The data system uses this data to identify the component. For information about interactively using the spectrum in a representative raw data file to enter the spectral data in the list, see "To enter data in the spectrum table by using an open raw file" on page 36.	
m/z	Each *m/z* value in this column specifies the mass-to-charge [*m/z*] value for one spectral peak in the reference spectrum. The adjacent Intensity (%) box specifies the intensity percentage for this *m/z* value. Range: 0.5–999 999

Table 99. Genesis Peak Detection parameters for the gas chromatography (GC) mode

Parameter	Description
Intensity	Each intensity percentage in this column specifies the relative intensity for one spectral peak in the reference spectrum. The adjacent *m/z* box specifies the *m/z* value for the spectral peak. Range: 0–100
Thresholds (Spectrum option) The Thresholds area appears when you select the Spectrum option in the GC mode.	
Forward	Specifies 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. Range: 0–1000
Reverse	Specifies 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 in a forward match. Range: 0–1000
Match	Specifies a threshold value for match comparisons between the reference spectrum and candidates in the chromatogram. The match threshold is scored on a scale of 0 to 999. The match algorithm is a complex probability factor that is 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. Range: 0–1000

Table 99. Genesis Peak Detection parameters for the gas chromatography (GC) mode

Parameter	Description
Ion Ratio Confirmation (Genesis)	
This area appears when you select the Highest Peak or Nearest RT option in the GC mode for data from an MS detector. Use the parameters 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	Selecting this check box activates the parameters in the Ion Ratio Confirmation area.
Ion Ratio Using: Area or Height (read-only)	This read-only parameter shows the currently selected peak quantitation method: area or height. The data system 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-to-charge [*m/z*] and target ratio tolerances [Window ± %] data for up to five qualifier ions. If you select Area response, the data system 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 ± %), it rejects the quantitation peak. If you select Height response, the data system 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 ± %), it rejects the quantitation peak.
m/z	The value in this column specifies the mass-to-charge [*m/z*] value for a qualifier ion. Range: 0.5–999 999
Target Ratio (%)	The value in this column specifies the Target Ratio (%) value for a qualifier ion. Range: 0.00–1 000 000 for a manual target ratio for the qualifier ion

Table 99. Genesis Peak Detection parameters for the gas chromatography (GC) mode

Parameter	Description
Window (±%)	The value in this column specifies the Target Ratio tolerance for a qualifier ion. Range: 0.00–100.00
Window%	
Relative	Selecting this option specifies 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 fails, and the data system sets the IRC Flag to False. If the qualifier ion peak-to-quantitation peak ratio is within range, the ion ratio confirmation test passes, 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	Selecting this option specifies 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-to-quantitation peak ratio is outside this range, the ion ratio confirmation test fails, and the data system sets the IRC Flag to False. If the qualifier ion peak-to-quantitation peak ratio is within range, the ion ratio confirmation test passes, 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.

Table 99. Genesis Peak Detection parameters for the gas chromatography (GC) mode

Parameter	Description
Qualifier Ion Coelution	Specifies the Qualifier Ion Coelution window. Before it runs the ion ratio confirmation test, 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 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 data system rejects the quantitation peak. The data system tests quantitation peaks with matching qualifier ion peaks (in the coelution window) for ion ratio confirmation.

ICIS Detection Page for Quan View

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

After selecting ICIS as the peak detection algorithm on the Identification page of the Quan view, this page appears when you open the Detection page of the Quan view.

Note Click **Advanced** to open the ICIS Advanced Parameters dialog box where you can set up the advanced detection parameters for the ICIS algorithm.

These topics describe the parameters on the ICIS Detection page for the Processing Setup – Quan view:

- “Quan View – ICIS Detection Page Buttons,” on the next page
- “ICIS Peak Integration Parameters” on page 371
- “ICIS Peak Detection Parameters – LC Mode” on page 373
- “ICIS Peak Detection Parameters – GC Mode” on page 373

For information about changing the chromatography mode, see “Chromatography Options Dialog Box” on page 271.

Quan View – ICIS Detection Page Buttons

Table 100 describes the buttons at the bottom of the Qual view – Detection page for the ICIS peak detection algorithm.

Table 100. Buttons at the bottom of the Quan view – Detection page for the Genesis algorithm

Parameter	Description
Save As Default	Validates and saves the settings on the current page as default settings. The data system uses these settings for all new processing methods. This option guarantees that the settings for the components are consistent and valid. These default settings are then used for all new components. The data system writes over the previous default values and cannot recover them.
Advanced	For the ICIS peak detection algorithm, this button opens the ICIS Advanced Parameters dialog box, where you can set up the advanced parameters for the Genesis algorithm. For information about the ICIS Advanced Parameters dialog box, see “ICIS Advanced Parameters Dialog Box” on page 284.
Flags	Opens the Data Flags dialog box, where you can set peak area and peak height threshold values. The data system reports these data flags in result files, printed reports, and Quan Browser. For information about the Data Flags dialog box, see “Data Flags Dialog Box” on page 274.

ICIS Peak Integration Parameters

Table 101 describes the parameters in the ICIS Peak Integration area on the Detection page of the Quan view.

Table 101. ICIS Detection page for Quan view parameters (Sheet 1 of 2)

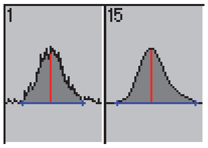
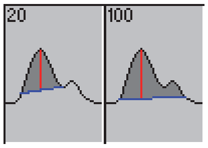
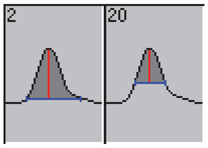
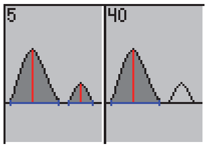
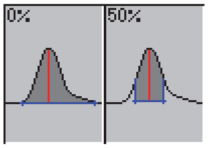
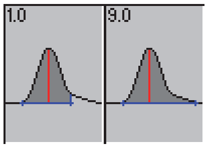
Parameter	Description
ICIS Peak Integration	
Smoothing Points  	Specifies the number of points in the moving average used to smooth the data. Default: 7 Range: 1–15 The ICIS peak detection algorithm uses this value.
Baseline Window  	Specifies the number of scans to review for a local minima. Default: 40 Range: 1–500 The ICIS peak detection algorithm uses this value.
Area Noise Factor  	Specifies the noise-level multiplier used to determine the peak edges after the data system determines the start and end points of a possible peak for the selected component. As you increase this value, the integrated peak area decreases. Default: 5 Range: 1–500 The ICIS peak detection algorithm uses this value.
Peak Noise Factor  	Specifies the noise-level multiplier used to determine the potential peak signal threshold. Default: 10 Range: 1–1000 The ICIS peak detection algorithm uses this value.
Constrain Peak Width	Select this check box to constrain the integrated area of a component peak by specifying a peak height threshold and a tailing factor. When you select the Constrain Peak Width check box, the Peak Height (%) and Tailing Factor boxes become available.

Table 101. ICIS Detection page for Quan view parameters (Sheet 2 of 2)

Parameter	Description
Peak Height (%) 	Specifies the percent of the total peak height (100%) that a signal must be above the baseline before the data system turns integration on or off. To enter a value for this parameter, select the Constrain Peak Width check box. Then type a value in the Peak Height (%) box. Range: 0.0–100.0
Tailing Factor 	Specifies 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 edge of a constrained peak. To enter a value for this parameter, select the Constrain Peak Width check box. Then type a value in the Tailing Factor box. Range: 0.5–9.0
Min (graphical representation)	Displays a representative drawing of the minimum value for the selected parameter. The location of the cursor defines the selected parameter. For example, if you click the Smoothing Points box, the graphic shows the typical result obtained with the minimum number of smoothing points: a peak with reduced noise. The number in the upper left corner of the graphic is a representative low value for the active parameter. It is not necessarily the minimum value for the parameter.
Max (graphical representation)	Displays a representative drawing of maximum value for the selected parameter. The location of the cursor defines the selected 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. It is not necessarily the maximum value for the parameter.

ICIS Peak Detection Parameters – LC Mode

Table 102 describes the parameters in the ICIS Peak Detection area for the liquid chromatography (LC) mode.

Table 102. Genesis Peak Detection parameters for the liquid chromatography (LC) mode

Parameter	Description
Genesis Peak Detection	
Highest Peak	When you select this option, the data system uses the highest peak in the chromatogram within the specified retention time window for component identification.
Nearest RT	When you select this option, the data system uses the peak with the nearest retention time in the chromatogram to the expected retention time for component identification.
Minimum Peak Height (S/N)	Specifies the minimum peak height on the basis of the signal-to-noise ratio that a peak must meet before the data system recognizes it as a possible chromatographic peak for the selected component. To identify the chromatographic peak for the selected component, the data system ignores chromatographic peaks with a peak height that is less than the specified signal-to-noise threshold value. Range: 0.0–999.0

ICIS Peak Detection Parameters – GC Mode

Table 103 describes the parameters in the ICIS Peak Detection area on the Detection page of the Quan view for the GC mode and mass spectral data.

Table 103. ICIS Peak Detection parameters for the gas chromatography (GC) mode (Sheet 1 of 6)

Parameter	Description
Genesis Peak Detection (GC mode)	
Spectrum	This option is only available in the GC chromatography mode for the data acquired with an MS detector. When you select this option, the data system uses the user-defined reference spectrum for component identification. The data system attempts to match the reference spectrum with a series of unknown spectra and calculates a score value for each comparison. When you select the Spectrum option, a mass intensity list and the Thresholds area appear (see "Additional parameters for the Spectrum option (ICIS)" on page 374).

Table 103. ICIS Peak Detection parameters for the gas chromatography (GC) mode (Sheet 2 of 6)

Parameter	Description
Highest Peak	When you select this option, the data system uses the highest peak in the chromatogram within the specified retention time window for component identification and the Ion Ratio Confirmation window appears. You can use the parameters in the Ion Ratio Confirmation area to confirm the identify of the chromatographic peak on the basis of spectral information (see "Ion Ratio Confirmation (ICIS)" on page 376).
Nearest RT	When you select this option, the data system uses the peak with the nearest retention time in the chromatogram to the expected retention time for component identification and the Ion Ratio Confirmation window appears. You can use the parameters in the Ion Ratio Confirmation area to confirm the identify of the chromatographic peak on the basis of spectral information (see "Ion Ratio Confirmation (ICIS)" on page 376).
Minimum Peak Height (S/N)	Specifies the minimum peak height on the basis of the signal-to-noise ratio that a peak must meet before the data system recognizes it as a possible chromatographic peak for the selected component. To identify the chromatographic peak for the selected component, the data system ignores chromatographic peaks with a peak height that is less than the specified signal-to-noise threshold value. Range: 0.0–999.0
Additional parameters for the Spectrum option (ICIS)	
Mass intensity list for the Spectrum option Enter mass-to-charge [*m/z*] and intensity percentages for up to 50 spectrum peaks. The data system uses this data to identify the component. For information about interactively using the spectrum in a representative raw data file to enter the spectral data in the list, see "To enter data in the spectrum table by using an open raw file" on page 36.	
m/z	Each *m/z* value in this column specifies the mass-to-charge [*m/z*] value for one spectral peak in the reference spectrum. The adjacent Intensity (%) box specifies the intensity percentage for this *m/z* value. Range: 0.5–999 999

Table 103. ICIS Peak Detection parameters for the gas chromatography (GC) mode (Sheet 3 of 6)

Parameter	Description
Intensity	Each intensity percentage in this column specifies the relative intensity for one spectral peak in the reference spectrum. The adjacent *m/z* box specifies the *m/z* value for the spectral peak. Range: 0–100
Thresholds (Spectrum option)	
The Thresholds area appears when you select the Spectrum option in the GC mode.	
Forward	Specifies 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. Range: 0–1000
Reverse	Specifies 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 in a forward match. Range: 0–1000
Match	Specifies a threshold value for match comparisons between the reference spectrum and candidates in the chromatogram. The match threshold is scored on a scale of 0 to 999. The match algorithm is a complex probability factor that is 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. Range: 0–1000

Table 103. ICIS Peak Detection parameters for the gas chromatography (GC) mode (Sheet 4 of 6)

Parameter	Description
Ion Ratio Confirmation (ICIS)	
This area appears when you select the Highest Peak or Nearest RT option in the GC mode for data from an MS detector. Use the parameters 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	Selecting this check box activates the parameters in the Ion Ratio Confirmation area.
Ion Ratio Using: Area or Height (read-only)	This read-only parameter shows the currently selected peak quantitation method: area or height. The data system 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-to-charge [*m/z*] and target ratio tolerances [Window ± %] data for up to five qualifier ions. If you select Area response, the data system 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 ± %), it rejects the quantitation peak. If you select Height response, the data system 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 ± %), it rejects the quantitation peak.
m/z	Specifies the mass-to-charge [*m/z*] value for a qualifier ion. Range: 0.5–999 999
Target Ratio (%)	Specifies the Target Ratio (%) value for a qualifier ion. Range for a manual target ratio for the qualifier ion: 0.00–1 000 000

Table 103. ICIS Peak Detection parameters for the gas chromatography (GC) mode (Sheet 5 of 6)

Parameter	Description
Window (±%)	The value in this column specifies the Target Ratio tolerance for a qualifier ion. Range: 0.00–100.00
Window%	
Relative	Selecting this option specifies 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 fails, and the data system sets the IRC Flag to False. If the qualifier ion peak-to-quantitation peak ratio is within range, the ion ratio confirmation test passes, 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	Selecting this option specifies 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-to-quantitation peak ratio is outside this range, the ion ratio confirmation test fails, and the data system sets the IRC Flag to False. If the qualifier ion peak-to-quantitation peak ratio is within range, the ion ratio confirmation test passes, 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.

Table 103. ICIS Peak Detection parameters for the gas chromatography (GC) mode (Sheet 6 of 6)

Parameter	Description
Qualifier Ion Coelution	Specifies the Qualifier Ion Coelution window. Before it runs the ion ratio confirmation test, 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 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 data system rejects the quantitation peak. The data system tests quantitation peaks with matching qualifier ion peaks (in the coelution window) for ion ratio confirmation.

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.

For information about using the Calibration page, see "Setting Up the Calibration Parameters" on page 39.

Table 104 describes the parameters on the Quan view – Calibration page.

Table 104. Calibration page for Quan view parameters (Sheet 1 of 5)

Parameter	Description
Component Type	
Target Compound	Specifies 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 data system activates the options in the Target Compound area.

Table 104. Calibration page for Quan view parameters (Sheet 2 of 5)

Parameter	Description
ISTD	Specifies that the selected component is an internal standard. ❖ **To select a component as an internal standard compound type** 1. Select a component in the Component list. 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	Specifies the amount of the selected component that is added to each sample to provide an internal standard. You can enter amounts with up to three decimals of precision. Select the ISTD Component Type to activate this box.
Units	Specifies the units used for the internal standard amount. For example, ng (nanograms). Select the ISTD Component Type to enable this box.
Target Compounds	
Target Compounds	Specifies the calibration curve parameters for the selected target compound.
ISTD	Lists the components identified as internal standard components. This list is available when you select the internal standard calibration technique, identify one or more components as internal standard components, and select a target component in the Components list. ❖ **To select an internal standard component for a target component** 1. Select the target component of interest in the Components list. 2. Select an internal standard component in the ISTD list.

Table 104. Calibration page for Quan view parameters (Sheet 3 of 5)

Parameter	Description
Isotope % button	Opens the Correction for Isotope Contribution dialog box, where you can set up the calibration corrections for isotope contributions of the internal standard to the target compound and the target compound to the internal standard.
Calibration Curve	Specifies the calibration curve type. The available selections are as follows: • Linear • Quadratic • Linear Log-Log • Quadratic Log-Log • Average RF (response factor) • Point-to-Point • Cubic Spline • Locally Weighted
Units	Specifies 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	Weights all calibration data points equally during the least-squares regression calculation of the calibration curve.
1/X	Specifies 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	Specifies 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.
1/Y	Specifies 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	Specifies 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).

Table 104. Calibration page for Quan view parameters (Sheet 4 of 5)

Parameter	Description
1/s^2	Specifies 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	Select the Ignore option to 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	Select the Force option to make sure that the calibration curve passes through the origin of the data point plot.
Include	Select the Include option to 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	Specifies that the data system use the area of the target compound peak (or the ratio of the areas for the target compound peak and the internal standard compound peak) for the calibration.
Height	Specifies that the data system use the height of the target compound peak (or the ratio of heights for the target compound peak and the internal standard compound peak) for the calibration.

Table 104. Calibration page for Quan view parameters (Sheet 5 of 5)

Parameter	Description
Component	
Component List	Lists the 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 you have 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**.
Buttons	
Save As Default	Validates and saves the settings on the current page as default settings. The data system 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 data system writes over the previous default values and cannot recover them.
Flags	Opens the Calibration and Quantitation Flags dialog box.The data system reports these data flags in result files, printed reports, and Quan Browser. For more information, see “Calibration and Quantitation Flags Dialog Box” on page 269.

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.

For information about setting up the calibration and QC levels, see "Setting Up the Calibration and QC Levels" on page 45.

Table 105 describes the parameters on the Levels page.

Table 105. Levels page for Quan view parameters (Sheet 1 of 2)

Parameter	Description
Readback	
Units	Displays the units set on the Calibration page. The units are also used in reports and in Quan Browser.
Calibration Levels	
Calibration levels shortcut menu	Use this shortcut menu to make changes to the Cal Levels table. This shortcut menu contains the following commands: Delete Rows, Insert Rows, and Copy Levels to All Target Components.
Delete Rows	Deletes the currently selected row of the Cal Levels table.
Insert Row	Inserts a new row in the Cal Levels table.
Copy Levels to All Target Components	Copies the current Cal Levels table to all target components. This action ensures that all target components contain exact duplicates of the current Cal Levels table.
Calibration levels table	
Cal Level	Specifies the calibration level names. The data system can accommodate up to 50 calibration levels. To enter a calibration level, type the new name in the appropriate Cal Level box. To delete a Cal level row, click to the left of the row. The data system highlights the row. Then press DELETE.
Amount	For each target component, specifies the amounts 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.

Table 105. Levels page for Quan view parameters (Sheet 2 of 2)

Parameter	Description
QC Levels	
QC Levels Shortcut Menu	Use this shortcut menu to make changes to the QC Levels table. This shortcut menu contains the following commands: Delete Rows, Insert Rows, and Copy Levels to All Target Components.
Delete Rows	Deletes the currently selected row of the QC Levels table.
Insert Row	Inserts a new row in the QC Levels table.
Copy Levels to All Target Components	Copies the current QC Levels table to all target components. This action ensures that all target components contain exact duplicates of the current QC table.
QC levels table	Enter the QC (quality control) level names, amounts, and % test values. Use QC samples containing known amounts of a component to check the accuracy of an analysis. The data system determines the amount of the target components in the QC samples in the same manner as unknown samples and then determines the difference between the specified amount and the calculated amount.
QC Level	The data system can accommodate up to 50 QC levels. To enter a quality control level, type a name in the appropriate QC Level box. To delete a QC level row, click to the left of the row. The data system highlights the row. Then press DELETE**.**
Amount	For the selected target component, type the amount for each QC level component.
% Test	Type a value for the acceptable difference (as a percent) between the specified amount and the calculated amount for each QC level.
Buttons	
Save As Default	Validates and saves the settings on the current page as default settings. The data system 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.

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.

For information about setting up the system suitability parameters, see "Setting Up the System Suitability Parameters" on page 48.

Table 106 describes the parameters on the System Suitability page.

Table 106. System Suitability page for Quan view parameters (Sheet 1 of 5)

Parameter	Description
Resolution Parameters	
Enable	Selecting this check box activates the Resolution Threshold (%) box. Resolution testing is based on a comparison of the peak height to the 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 (%)	Specifies the resolution threshold. The default value is 90%, and the valid range is 0 to 100%. Resolution threshold is defined as the ratio: $100 \times V/P$ 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

Table 106. System Suitability page for Quan view parameters (Sheet 2 of 5)

Parameter	Description
Symmetry Parameters	
Enable	Selecting this check box activates the system suitability check of peak symmetry. 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. The data system 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 Height (%)	Specifies the peak height where the data system measures the symmetry of target peaks. Default: 50% Range: 0–100%
Symmetry Threshold (%)	Specifies the symmetry threshold value. Default: 90% Range: 0–100%
Peak Classification Parameters	
Enable	Selecting this check box activates the peak classification parameters.
Detect Peak Width	
Peak Height (%)	Specifies the peak height where the data system tests the width of target peaks. Default: 50% Range: 0–100%

Table 106. System Suitability page for Quan view parameters (Sheet 3 of 5)

Parameter	Description
Min Peak Width (sec)	Specifies the minimum peak width at the specified peak height for the peak width suitability test. Default: 1.80 Range: 0.06–29.99
Max Peak Width (sec)	Specifies the maximum peak width at the specified peak height for the peak width suitability test. Default: 3.60 Range: 1.01–30.00
Detect Tailing	
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.	
Peak Height (%)	Specifies the Peak Height where the data system measures the tailing of target peaks. Default: 10% Range: 0–100%
Failure Threshold	Specifies the failure threshold for the tailing suitability test. Default: 2.0 Range: 1.0–50.0

Table 106. System Suitability page for Quan view parameters (Sheet 4 of 5)

Parameter	Description
Detect Column Overload	
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.	
Peak Height (%)	Specifies the peak height at which the data system measures column overloading. Default: 50% Range: 0–100%
Failure Threshold	Specifies the failure threshold value for the column overload suitability test. Default: 1.5 Range: 1.0–20.0
Detect Baseline Clipping	
Number of Peak Widths for Noise Detection	Type a number in the Number of Peak Widths for Noise Detection box for the baseline clipping system suitability test. 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. Default: 1.0 Range: 0.1–10.0
Detect Minimum Signal-To-Noise Ratio	
Signal-To-Noise Ratio	Specifies the minimum signal-to-noise ratio. The data system calculates the signal-to-noise ratio in the quantitation window using only the baseline signal and excludes any extraneous, minor, detected peaks from the calculation. Default: 3 Range: 1–500

Table 106. System Suitability page for Quan view parameters (Sheet 5 of 5)

Parameter	Description
Buttons	
Save As Default	Validates and saves the settings on the current page as default settings. The data system 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 data system 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 107 describes the parameters on the Peak Purity page. The parameters on this page are the same in the Qual and Quan views. Figure 95 on page 340 shows the Peak Purity page in the Qual view.

Table 107. Peak Purity page for Quan view parameters (Sheet 1 of 2)

Parameter	Description
Purity Parameters	
Enable	Selecting this check box activates the Scan Threshold (mAU) and Peak Coverage (%) parameters.
Scan Threshold (mAU)	Specifies a minimum value of intensity for wavelength scans in milliabsorbance units (mAU). A peak purity calculation 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 specified Scan Threshold (mAU) is reached. Use scan threshold for either symmetrical or asymmetrical peaks. Default: 50 mAU Range: 0–1000 mAU (or 1 AU) In a sample with high background or noise, consider starting with a value of 40 mAU.

Table 107. Peak Purity page for Quan view parameters (Sheet 2 of 2)

Parameter	**Description**
Peak Coverage (%)	Specifies a maximum percent value of the width of the integrated peak. A peak purity calculation 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 specified Peak Coverage % is reached. Use peak coverage for symmetrical peaks. Default: 95% Range: 0.0–100.0%
Limit Scan Wavelength	Selecting this check box activates the Range (nm) box. Select this check box to limit the number of wavelengths to include in the peak purity calculation. Then enter a range in the Wavelength Range box.
Range (nm)	Specifies a range of UV-Vis scans (in nanometers). A peak purity calculation 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.

Programs View

Use the Programs view of the Processing Setup window to compile a list of programs or macros to be run by the data system after the analysis of a sample and the processing of the resulting data. The data system runs the programs in the listed order.

For more information about adding programs and macros to a processing method, see "Adding Programs or Macros to Processing Methods" on page 64.

For information about the Programs view toolbar, see "Reports and Programs Views Toolbar" on page 250. For information about the OK, Cancel, and Save As Default buttons, see "OK, Cancel, and Save As Default Buttons" on page 261. For information about using the Programs view, see "Enabling and Setting Up a Program or Macro" on page 65.

The Programs table lists the programs to be run by the data system during post processing.

For information about using the programs table, see Table 108 and these topics:

- "Column Headings" on page 394
- "Macro Arguments" on page 395
- "Printing Raw Files and Layout Files" on page 395

❖ To activate a program or macro

1. For the program or macro that you want to activate, click the Enable column.

   A check box appears.

2. Select the check box.

   When you click elsewhere in the view, the box displays a Yes value.

❖ To select a sample type

1. Click the table cell.

   A check box appears.

2. Select the check box.

   When you click elsewhere in the view, the box displays a Yes value.

❖ To change the status of a table cell from Yes to blank

1. Click the cell.

   A check box appears.

2. Do one of the following:

   - To change the status to Yes, select the check box.
   - To change the status to blank (inactive), clear the check box.

Table 108 describes the parameters for the Programs table in the Program view.

Table 108. Programs table (Sheet 1 of 2)

Parameter	Description
Programs	
Specifies 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	Selecting this check box activates the program or macro. When the program or macro is available, the box displays a Yes value. If it is unavailable, the box is blank.
Sample Type	
Std	Specifies 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.
QC	Specifies 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.
Unk	Specifies 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.
Other	Specifies 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.
Action	Specifies 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.

Table 108. Programs table (Sheet 2 of 2)

Parameter	Description
Program or Macro Name	Specifies the full path of the program or macro that the data system 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 data system displays the new program or macro name. You can also type on the command line. Here is an 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 LCQ™ raw file (L). %R is the macro argument for the current raw file. See "Command Line Arguments" on page 409 or "ExcelExp.exe" on page 412 for more examples.
Sync	Specifies whether to run the selected program synchronously or asynchronously. The data system 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	Specifies any command parameters for the selected program. See the Program or Macro Name box for examples.

Column Headings

Table 109 describes the column headings in the Programs table and their use. The Programs table is part of the Programs view in the Processing Setup window.

Table 109. 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 data system runs a program after a Standard sample analysis.
QC	Determines whether the data system runs the program after a QC sample analysis.
Unk	Determines whether the data system runs the program after an Unknown sample analysis.
Other	Determines whether the data system 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 data system 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 data system exports a Report File formatted according to the selected file extension.

Macro Arguments

You can use the following macros in the command line.

Table 110. Macro arguments

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 data system 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).

Reports View

Use the Reports view of the Processing Setup window to specify how the data system produces reports for samples and sequences. The data system provides several standard report formats. You can also design custom reports in XReport, the Xcalibur report designer. The data system exports results in a number of file formats, including XLS and HTML.

For more information about adding reports to a processing method, see "Adding Report Templates to Processing Methods" on page 59.

The Reports view consists of a menu bar, a toolbar, and two report tables. For information about the Reports view toolbar, see "Reports and Programs Views Toolbar" on page 250. For information about the OK, Cancel, and Save As Default buttons, see "OK, Cancel, and Save As Default Buttons" on page 261.

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 111 and these topics describe the parameters in the Reports view:

- "Sample Report Column Headings" on page 398
- "Summary Reports Column Headings" on page 399
- "Valid File Types for Sample and Summary Reports" on page 399

Table 111. Reports view tables (Sheet 1 of 3)

Parameter	Description
Sample Reports	
This table specifies 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 column	Specifies the 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. Clicking the check box activates the row. When you click anywhere else on the page, the data system replaces the selected check box with the text Yes.

Table 111. Reports view tables (Sheet 2 of 3)

Parameter	Description
Sample Type columns	
Std	Specifies the 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 so you can change the status.
QC	Specifies the 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 so you can change the status.
Unk	Specifies the 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 so you can change the status.
Other	Specifies the 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 so you can change the status.
Save As	Specifies the file export option for the sample report. The data system saves the exported file with the sample file name and the correct extension in the folder where it stores the result files (see "Valid File Types for Sample and Summary Reports" on page 399).
Report Template Name	Specifies the name and location of the report template that the processing method uses 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.
Summary Reports	
This table specifies Summary reports to be issued after processing of a bracketed or non-bracketed sequence. Each row in the Summary 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.

Table 111. Reports view tables (Sheet 3 of 3)

Parameter	Description
Enable	Specifies the 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 so you can change the status.
Save As	Specifies the file export option for the summary report. The data system 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	Specifies the name and location of the report template that the processing method uses to generate the 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.

Sample Report Column Headings

The following table defines columns for sample reports.

Column heading	Use
Enable	Enables a sample report.
Std	Specifies the report for a Standard sample type.
QC	Specifies the report for a QC sample type.
Unk	Specifies the report for an Unknown sample type.
Other	Specifies the report for all other sample types.
Save As	Specifies the file type for saved report.
Report Template Name	Specifies the full path of the template that the data system uses in generating the sample report.

Summary Reports Column Headings

The following table defines columns for summary reports.

Column heading	Use
Enable	Enables 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 data system uses in generating the summary report.

Valid File Types for Sample and Summary Reports

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)

E

Global Dialog Boxes

This appendix describes the Xcalibur dialog boxes that are available from more than one Xcalibur window.

Contents

- Add Programs to Tool Menu Dialog Box
- Add Tool Dialog Box
- Comment Dialog Box
- Customize Toolbar Dialog Box
- Study Name Selector Dialog Box
- File Save – Audit Trail Dialog Box
- File Summary Information Dialog Box
- Password Dialog Box
- Select Directory or Select Data Directory Dialog Box
- Supervisor Permission Dialog Box

Add Programs to Tool Menu Dialog Box

Use the Add Programs to Tool Menu dialog box to add and to remove programs from the Tool menu and to adjust the sequence of the menu.

> **Note** This dialog box is only available from the Tools menu in the Home Page and Qual Browser windows.

Table 112. Add Programs to Tool Menu dialog box parameters

Parameter	Description
Menu Contents	Displays the names of the current list of tools (programs) that have been added to the Tool menu. These names appear when you choose the Tools menu. You can use the Add button, Remove button, Move Up button, and Move Down button in the Add Programs to Tool Menu dialog box to edit the current list of programs.
Menu Text	Specifies the name of the tool (program) selected in the Menu Contents box. To change the name, type the new name in the Menu Text box.
Program	Specifies the command that launches the tool.
Arguments	Add command line arguments.
Initial Directory	Specifies the path that the data system uses to find the tool (program) selected in the Menu Contents box. To change the path, type the new path in the Initial Directory box or click **Browse** and select a directory.
Close	Saves all changes and closes the dialog box.
Add	Opens the Add Tool dialog box, where you can select a program to add to the Tools menu.
Remove	Removes the name of the tool (program) selected in the Menu Contents box from the list of tools.
Move Up	Move the selected tool up in the current list of tools (programs) in the Menu Contents box. This is the sequence displayed when you choose the Tools menu.
Move Down	Moves the selected tool down in the current list of tools (programs) in the Menu Contents box. This is the sequence displayed when you choose the Tools menu.

Add Tool Dialog Box

Use the Add Tool dialog box to specify the path to the program that you want to add to the Tools menu.

Table 113. Add Tool dialog box parameters

Parameter	Description
Program	Type the path and file name of the tool (program) that you want to add to the Tools menu or click **Browse** to select the path and file name.
Browse	Find an existing file.

Comment Dialog Box

The Comment dialog box opens when you try to perform an action or access a feature that requires a comment before continuing.

Table 114. Comment dialog box parameters

Parameter	Description
Your Comment	Type a comment in this box. The comment appears in the Audit Log.

Customize Toolbar Dialog Box

Use the Customize Toolbar dialog box to modify the toolbar. You can add buttons for many menu commands, remove buttons, or change the order of the buttons.

❖ To remove, add, or reposition buttons

1. In the Home Page, Qual Browser, or Quan Browser windows, choose **View > Customize Toolbar**.

2. To remove a button from the toolbar, select the button and drag it away from the toolbar until the ⊘ symbol appears.

3. To reposition a button, drag and drop the button to the location where you want it in the toolbar.

4. To add a button to the toolbar, do the following:
   a. In the Category list, select the category for the button.

      The Commands list displays the selected button category.

   b. In the Commands list, select the button that you want to add to the toolbar, and then drag the button to an appropriate position in the toolbar.

> **Note** This feature is only available in Home Page, Qual Browser, and Quan Browser windows. In Qual Browser, you cannot customize the Amplify toolbar.

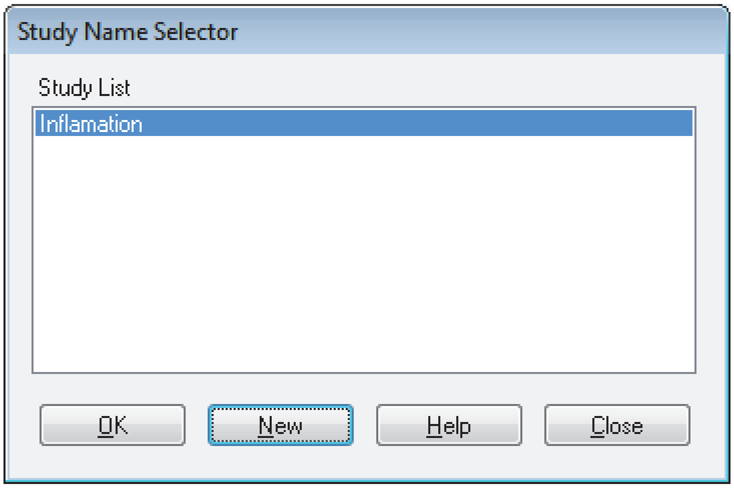
Table 115. Customize Toolbar dialog box parameters

Parameter	Description
Categories	Displays the menu categories available in the toolbar. Select a menu category to view the Commands list and buttons (if available in the toolbar) for that category.
Commands	Displays the commands associated with each menu category and the associated buttons in the toolbar, if available.
Buttons	
Close	Saves all changes and closes the dialog box.
Reset	Resets the toolbar to the default layout.

Study Name Selector Dialog Box

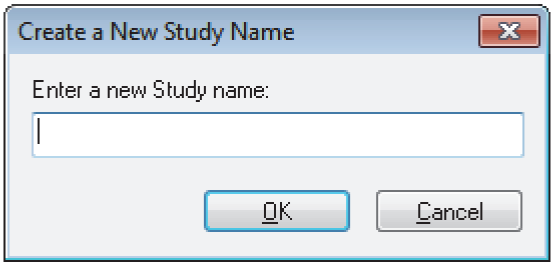
Use the Study Name Selector dialog box (Figure 96) to select a dataset from a predefined list of names. All database entries are then grouped into this dataset. Each application displays the dataset name in the title bar. The format for display is **Dataset: Name**, where Dataset is the name defined by the administrator, and Name is the selected name. Examples are Dataset: Pharmco or Study: Pharmco.

Figure 96. Study Name Selector dialog box



Clicking New opens the Create a New Study Name dialog box (Figure 97).

Figure 97. Create a New Study Name dialog box


Create a New Study Name

Enter a new Study name:

The title of the Study Name Selector dialog box might be different if the administrator chooses to use another name for a dataset. For example, it might be titled Dataset Name Selector or Job Name Selector.

Table 116. Dataset Name Selector dialog box parameters

Parameter	Description
Study List	Displays the list of predefined dataset names. When the dialog box opens, the list of predefined dataset names appears in this order: 1. The last dataset name used appears at the top of the list. 2. The dataset names from the Dataset List page of the Configuration dialog box appears. 3. If the system settings permit, the most recent dataset names stored in the database fill the list until it reaches the maximum number of entries. 4. If a blank name is permitted, the time [Blank] appears in the list.
Button	
New	Opens the Create a New Dataset Name dialog box, where you can enter a name for a new dataset and save the name in the database for future use. The new dataset name appears in the Dataset Name List.

File Save – Audit Trail Dialog Box

The File Save – Audit Trail dialog box requires that you enter information about the current file changes before you save the file.

Table 117. File Save – Audit Trail dialog box parameters

Parameter	Description
User	Type a string of up to 24 alphanumeric characters that identify the operator. To include reference text that identifies the operator, type the text in the User box.
Comment	Type a comment about the active file.
What Changed	Type information about the changes to the active file. This information is part of the Xcalibur auditing system.

When you have entered the audit information, click **Continue** to save the file.

If you have not entered the audit trail information, a dialog box opens with the following message:

> ***Please enter your user name and a description into the audit log.***

You must enter this information before you can save the file.

File Summary Information Dialog Box

Use the File Summary Information dialog box to obtain information and provide reference information about the current file.

Table 118. File Summary Information dialog box parameters

Parameter	Description
Header	Displays the date and time that the file was created, the date and time that the file was last modified (if applicable), the user name of the person who last saved the file, and the number of times that the file has been saved.
Comment	Contains user-specified information. You can edit the text directly in the box.

Password Dialog Box

The Password dialog box opens when you try to perform an action or access a feature for which the administrator has required that you enter your user name and password.

Table 119. Password dialog box parameters

Parameter	Description
Name	Enter your user name in this box.
Enter Password	Enter your password in this box.
Your Comment	Enter your comment in this box. The comment will appear in the Audit Log. The Your Comment field appears only if the administrator has required that you enter a comment to perform this action.

Select Directory or Select Data Directory Dialog Box

Use the Select Directory dialog box or the Select Data Directory dialog box to select a directory on the Xcalibur computer hard drive. If you are connected to another computer over a network, you can also select a directory on another computer that you have access to. The Xcalibur data system displays the current path below the text: Directory selected. An example of a directory for an Xcalibur method is c:\Xcalibur\methods.

The title text that appears in the title bar of this dialog box varies, depending on what you are doing when you activate the dialog box.

Table 120. Select Directory dialog box parameters

Parameter	Description
Directory Selected	Displays named groups of files called subdirectories and folders. Select the directory that contains the file that you want to open.
Drives	Displays the letter designations of all of the hard drives that your computer currently has access to. You can gain access to additional drives by connecting to a network.
Disk Space/No Chart	Displays the amount of disk space available on the default path disk drive.
Network	Opens the Map Network Drive dialog box, where you can map a network folder.

Supervisor Permission Dialog Box

The Supervisor Permission dialog box opens when you try to perform an action or access a feature that first requires the supervisor to enter his or her user name and password.

Table 121. Supervisor Permission dialog box parameters

Parameter	Description
Name	Enter your user name in this box as supervisor.
Enter Password	Enter your password in this box as supervisor.
Your Comment	Enter a comment in this box. The comment appears in the Audit Log. The Your Comment field appears only if the administrator has required that you enter a comment to perform this action.

Executable Programs and Command Line Arguments

This chapter describes specific tools that work with the Xcalibur data system.

Contents

- Command Line Arguments
- ExcelExp.exe
- XConvert.exe

Command Line Arguments

Use command line arguments to open a file, create a new file, or print a file automatically from a script or command line. You can add these functions to the command lines in the following locations:

- In the Microsoft Windows Run application, choose **Start > Run** from the Windows taskbar. When the Run dialog box opens, use the Open box.
- In the Sequence Setup view of the Home Page window, choose **Actions > Run This Sample** or **Actions > Run Sequence**. When the Run Sequence dialog box opens, use the Pre Acquisition or Post Acquisition command line boxes.
- In the Programs view of the Processing Setup window, use the Program or Macro Name column.
- In the Microsoft Windows Command Prompt, choose **Start > Programs > Accessories > Command Prompt** from the Windows taskbar.

The following is standard syntax for these command lines:

To open an application, type the following:

path application

To create a new file in an application, type the following:

path application path new filename

To print a file from an application, type the following:

path application /p path filename

where:

path is the absolute pathname.

new filename is the name that you would like to apply to your new file.

filename is the name of an existing file.

application is the application name. The possible applications are as follows:

- HomePage – Home Page window and Sequence Setup view
- InstSetup – Instrument Setup window
- ProcSetup – Processing Setup window
- QuanBrowser – Quan Browser window
- QualBrowser – Qual Browser window

For example, use this syntax to print the file drugx_01.raw:

C:\Xcalibur\system\programs\QualBrowser /p C:\Xcalibur\examples\data\drugx_01.raw

You can omit the application path (*path*) if you are running the command line from within the data system. For example, to print the file drugx_01.raw, use:

QualBrowser /p C:\Xcalibur\examples\data\drugx_01.raw

If you are running the command line from the Processing Setup window, the program warns you when you type an invalid program name or path.

The following table lists the possible command lines. If you have installed the Xcalibur data system to the default location, the *path* before the application is **C:\Xcalibur\system\programs**.

Table 122. Command lines by file type (Sheet 1 of 2)

File Type	Example parameters and results
.raw	pathQuanBrowser pathfile.raw Opens the file in the Quan Browser window.
	*path*QuanBrowser /p *pathfile*.raw Opens the file in the Quan Browser window, prints the spectrum and chromatogram, and then closes the Quan Browser window.
	*path*QualBrowser *pathfile*.raw Opens the file in the Qual Browser window.
	path\QualBrowser /p *pathfile*.raw Opens the file in the Qual Browser window, prints the spectrum and chromatogram, and then closes the Qual Browser window.
.sld	*path*HomePage *pathfile*.sld Opens the file in the Home Page window – Sequence Setup view.
	*path*HomePage /p *pathfile*.sld Opens the file in the Sequence Setup view and displays the Print Selection dialog box. After you click OK, the sequence is printed.
.pmd	*path*ProcSetup *pathfile*.pmd Opens the file in the Processing Setup window.
	path\ProcSetup /p *pathfile*.pmd Opens the file in the Processing Setup window and displays the Print dialog box. After you click **Print**, the processing method is printed.
.meth	*path*InstSetup *pathfile*.meth Opens the file in the Instrument Setup window.

Table 122. Command lines by file type (Sheet 2 of 2)

File Type	Example parameters and results
.rst	*path*QuanBrowser *pathfile*.rst Opens the file in the Quan Browser window.
	*path*QualBrowser *pathfile*.rst Opens the file in the Qual Browser window.
	*path*QualBrowser /p *pathfile*.rst Opens the file in the Qual Browser window, prints the spectrum and chromatogram, and then closes the Qual Browser window.

ExcelExp.exe

You can create and export summary reports and result file exports that can be opened directly in Microsoft Excel using the ExcelExp program [ExcelExp.exe].

Note ExcelExp.exe has no user interface, so you can only access it through its command line.

These topics provide information about how to use the ExcelExp program:

- Command Line Format
- Path Names (/F)
- Export File Formats (/T)
- Command Prompt Examples
- Processing Method Example

Command Line Format

The command line for this program has three fields: Export Type, Data Source Path Name, and Export File Type. The Xcalibur data system names the output file name on the basis of the data source file name and places it in the same directory as the data source file.

ExcelExp.exe /E*export type* /*data source path* /T*export file type*

/E - Set export type

/F - Path name of file to summarize/export

/T - Set export file format

Export Types (/E):

SUMMARY (for example, /ESUMMARY)

RESULT (for example, /ERESULT)

Path Names (/F)

For SUMMARY, the path name must be the path name of a sequence (.sld) file.

For RESULT, the path name must be the path name of a result (.rst) file.

Export File Formats (/T)

XLS (for example, /TXLS)

Note For RESULT exports, the export file will have a .crf extension. You can open this file directly in Microsoft Excel.

TXT (for example, /TTXT)

CSV (for example, /TCSV)

Use the XLS format whenever possible.

Command Prompt Examples

Choose **Start > Run** to open the Run dialog box, or choose **Start > Programs > Accessories > Command Prompt** to open the Command Prompt dialog box.

- To create a summary report for the steroids sample data set, type the following:

  ```
  c:\xcalibur\system\programs\ExcelExp.exe /ESUMMARY
  /Fc:\xcalibur\examples\methods\steroid.sld /TXLS
  ```

- To create a result file dump of the steroids15 result file from the Xcalibur xcalibur\examples\data folder, type the following:

  ```
  c:\xcalibur\system\programs\ExcelExp.exe /ERESULT
  /Fc:\xcalibur\examples\data\steroids15.rst /TXLS
  ```

Processing Method Example

❖ To add the ExcelExp.exe program to a processing method

1. From the Road Map view of the Home Page window, choose **GoTo > Processing Setup**.

   The Processing Setup window opens.

2. Open the Programs view by doing one of the following:
   - Click the **Programs** icon, ⚙, in the View bar.
   - Choose **View > Programs** from the menu bar.

3. Select the **Enable** check box to activate a row.

4. Double-click the **Program or Macro Name** box and browse to ExcelExp.exe.

   ```
   C:\Xcalibur\system\programs\ExcelExp.exe
   ```

5. Type program parameters in the Parameters box; for example, type the following:

   ```
   /ERESULT /F%F /TXLS
   ```

   Note If you use ExcelExp.exe as a Programs entry in a processing method, use the place holder %F. At the time the program is run, the %F is replaced with the current result file name. In addition, avoid running /ESUMMARY from ExcelExp.exe. It is better to create summary reports by batch processing from the Sequence Setup window by choosing Actions > Batch Reprocess. Select the Print Summary Reports check box to print a summary report for all of the samples in the current sequence.

6. Save the processing method.

XConvert.exe

This Xcalibur utility program converts source files of one data format to destination files having a different data format.

Table 123. Data format conversion

Source files	**Extension**
Xcalibur	(*.raw)
ICIS	(*.dat)
GCQ	(*.ms)
Magnum	(*.ms)
ANDI	(*.cdf)
Mass Lab 2	(*.raw)
Lasermat	(*.*)
Destination files	**Extension**
Xcalibur	(*.raw)
ICIS	(*.dat)
ANDI	(*.cdf)
Text files	(*.txt)

Note The Xcalibur data system does not currently support all interconversion combinations and posts a message whenever an unsupported conversion is requested.

These topics provide information about how to use the file conversion utility:

- File Converter Application
- Automatic File Conversion

File Converter Application

You can open the Thermo File Converter application from the Xcalibur data system.

❖ To open the Thermo File Converter application

From the Road Map view of the Home Page window, choose **Tools > File Converter**.

The Thermo File Converter application opens. You can exit the Xcalibur data system without exiting the Thermo File Converter application. For instructions on using the File Converter application, see “Converting File Formats” on page 140.

Automatic File Conversion

You can automatically convert and store files as they are created in the data system by adding the XConvert.exe program to a processing method as an executable action during data processing or by adding the appropriate command to a command line.

❖ To add the XConvert.exe program to a processing method

1. From the Road Map view of the Home Page window, choose **GoTo > Processing Setup**.

   The Processing Setup window opens.

2. Open the Programs view by doing one of the following:
   - Click the **Programs** icon, , in the View bar.
   - Choose **View > Programs** from the menu bar.
3. Select the **Enable** check box to activate a row.
4. In the Actions list, select **Run Program**.
5. Double-click the **Program or Macro Name** box and browse to XConvert.exe.

   drive:\Xcalibur\system\programs\XConvert.exe

6. Type program parameters in the Parameters box.

❖ To convert files by using a command line

Type the following in the command line:

Path\XConvert /S*Source Type* /D*Destination Type Source Path*/*File* /O *Destination Directory*

where:

/S*Source Type*, /D*Destination Type*, and *Source Path*/*File* are mandatory. If you are using this command line in the Programs column of the Processing Setup window, you can omit the path to XConvert.

These are the currently supported source and destination types:

- Source Type: Xcalibur (.raw) file [L], ICIS (.dat) file [I], ANDI (.cdf) file [A]
- Destination Type: Xcalibur (.raw) file [L], ICIS (.dat) file [I], ANDI (.cdf) file [A], Text (.txt) file [T]

Follow these examples when using a command line:

- To convert a file (myfile.raw), located in the last specified source directory, from Xcalibur (.raw) file format to ICIS (.dat) file format, use the following command line:

  C:\Xcalibur\system\programs\XConvert %R /SL /DI

  where:

  %R is the current raw file in the path

- To convert a file (myfile.raw) located in C:\Xcalibur\data from Xcalibur (.raw) file format to ANDI (.cdf) file format, use the following command line:

  C:\Xcalibur\system\programs\XConvert /DA /SL %R

  where:

  %R is the current raw file in the path

- To convert a file (myfile.raw) located in C:\Xcalibur\data from ICIS (.dat) file format to Xcalibur (.raw) file format with the resulting .raw file being stored in C:\temp, use the following command line:

  C:\Xcalibur\system\programs\XConvert /SI /DL C:\Xcalibur\data\myfile.dat /O C:\temp

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