

Thermo Xcalibur

Getting Started (Quantitative Analysis)

XCALI-97207 Revision B September 2010

DOCUMENTATION
SURVEY

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Release history: Revision A, January 2009; Revision B, September 2010

Software version: Thermo Xcalibur version 2.1 and above.

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Preface

This guide contains a set of tutorials that show how to quantitatively process a set of raw data files using the Thermo Xcalibur™ mass spectrometry data system. Refer to the *Quantitative Analysis User Guide* for details about data acquisition.

This guide also contains Xcalibur system configuration and other administration and reference information.

Use these tutorials to process a set of raw data files:

1. [Creating a Processing Method](#)
2. [Batch Processing Data Files](#)
3. [Working with Results Files in Quan Browser](#)
4. [Previewing, Specifying, and Printing Reports](#)

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.



Related Documentation

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

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

Special Notices

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

Special notices include the following:

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

Note Highlights information of general interest.

Tip Highlights helpful information that can make a task easier.

Contacting Us

There are several ways to contact Thermo 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
Web site	www.thermo.com/ms

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Go to mssupport.thermo.com and click **Customer Manuals** in the left margin of the window.

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- Fill out a reader survey online at <http://www.surveymonkey.com/s/PQM6P62>.
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Part

1

Tutorials

Xcalibur Overview

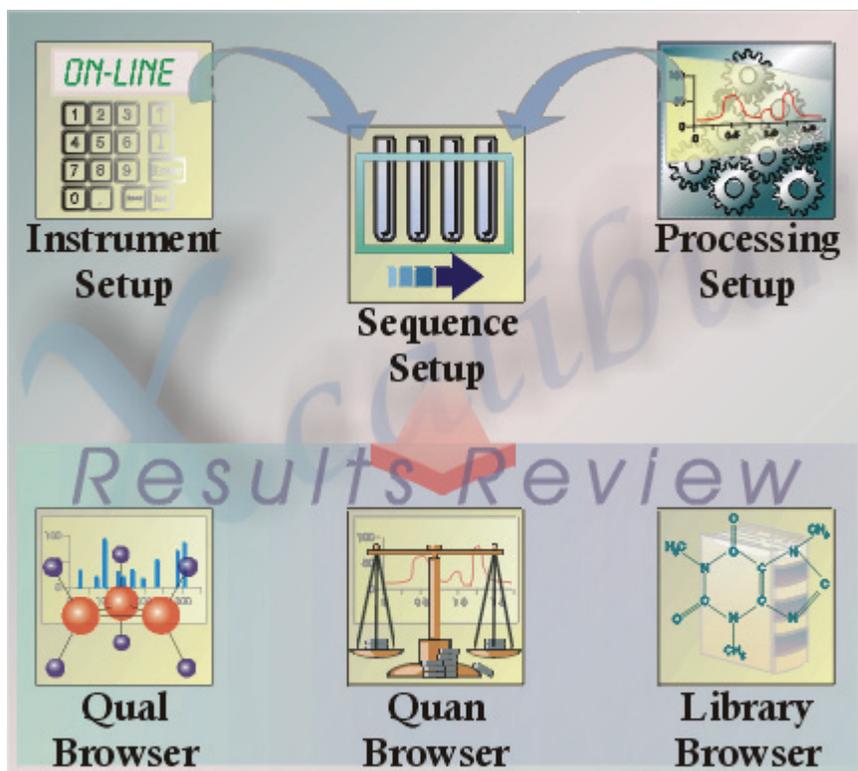
This book provides tutorials that show how to quantitatively process a set of raw data files. View these diagrams for an overview of the Xcalibur quantitative analysis process.

Contents

- [Figure 1](#): View of the Xcalibur application, Home Page – Road Map (with buttons to take you to views for performing acquiring, processing, and data viewing functions)
- [Figure 2](#): Acquiring the sample set (flow diagram)
- [Figure 3](#): Processing acquired data (flow diagram)
- [Figure 4](#): Automatic acquisition and processing using Xcalibur system and your system software (flow diagram)

Figure 1 shows the view when you open the Xcalibur application. Each button takes you to a separate view where you can perform functions involved in acquiring, processing, and viewing data.

Figure 1. Navigating the Xcalibur Roadmap



For more information about these functions of the Xcalibur process, refer to the following documents stored in C:\Xcalibur\system\programs:

Function	Document	File name
Instrument Setup	<i>Acquisition and Processing User Guide</i>	XCAL_Pro_Seq.pdf
Sequence Setup		
Processing Setup		
Quan Browser	<i>Quantitative Analysis User Guide</i>	XCAL_Quan_UG
Qual Browser	<i>Qualitative Analysis User Guide</i>	XCAL_Qual_UG
Library Browser	<i>Creating and Searching Libraries User Guide</i>	XCAL_Libraries_UG

Figure 2 provides a flow diagram for acquiring the sample set.

For information about working with samples to get data beyond the information in this guide, refer to the documents that came with your hardware and the *Acquisition and Processing User Guide*.

Figure 2. Acquiring quantitation data

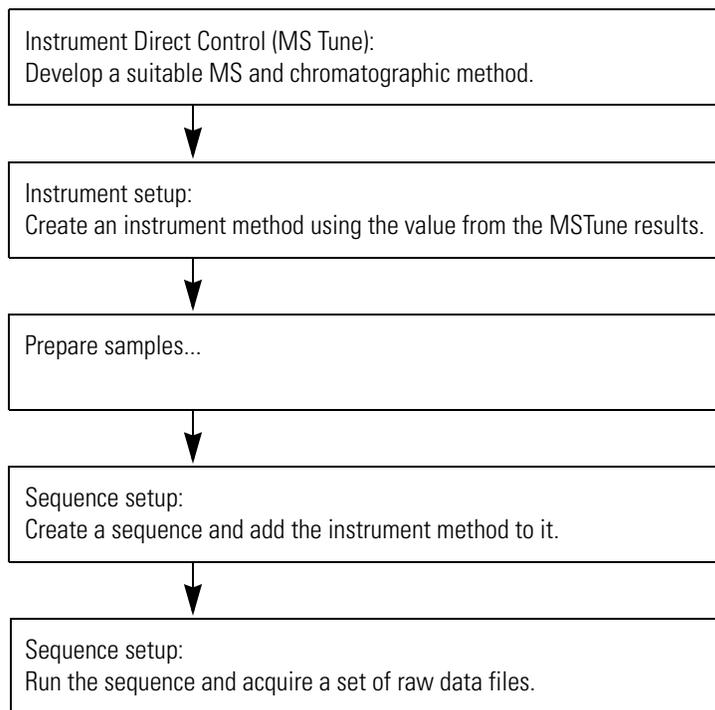


Figure 3 provides a flow diagram for processing data once you have acquired it.

For information about using sequences and processes to process your data beyond the information in this manual, refer to the *Acquisition and Processing User Guide*.

Figure 3. Processing previously acquired quantitation data

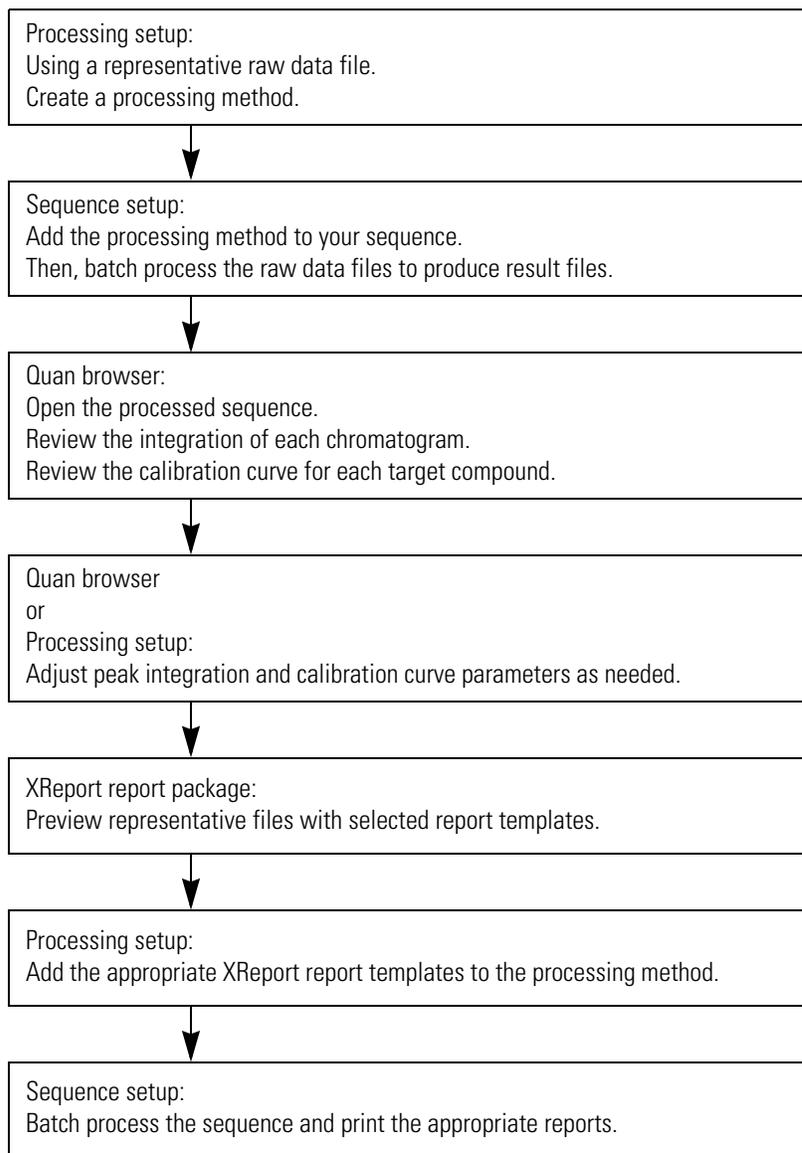
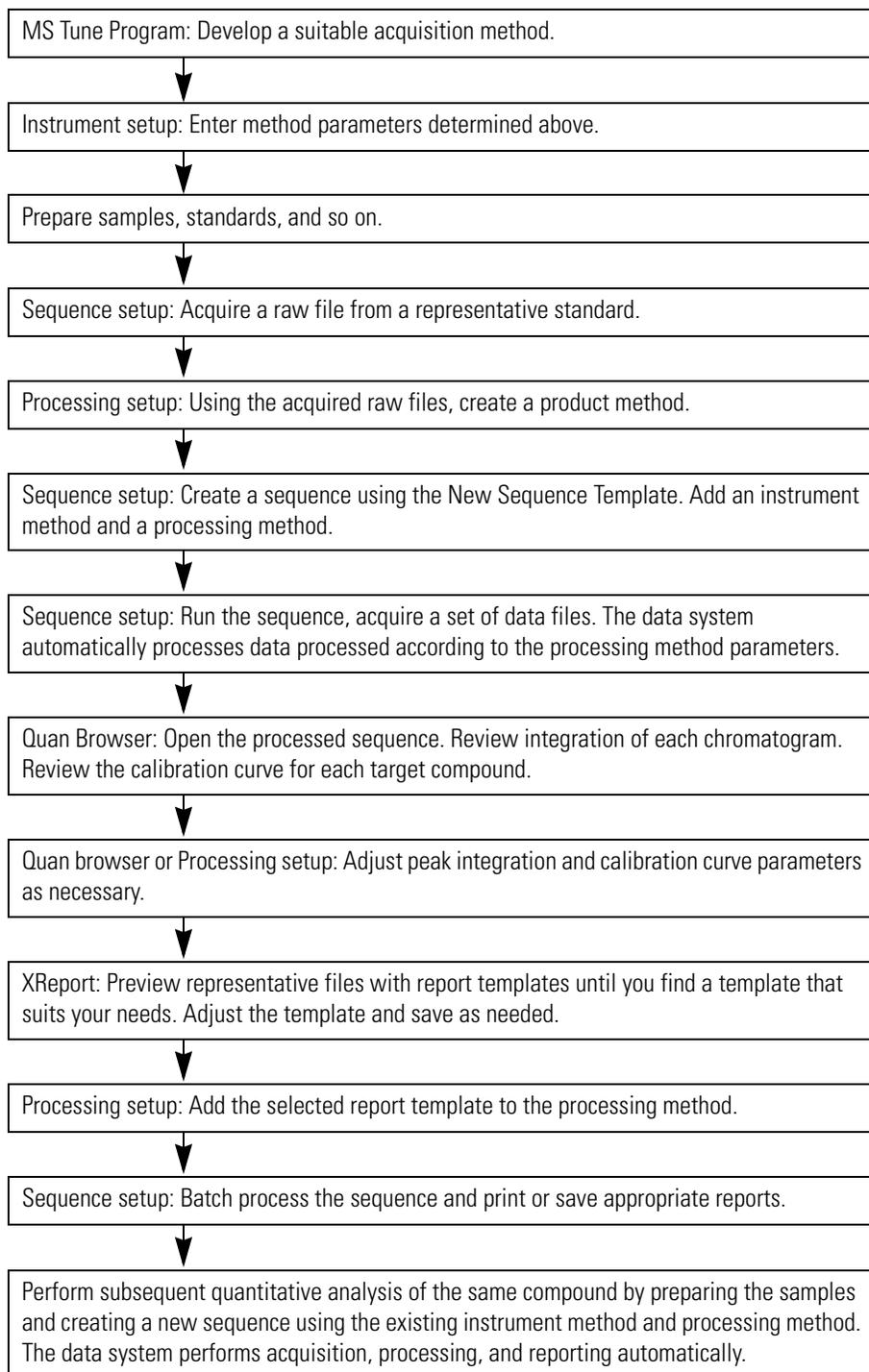


Figure 4 provides a flow diagram of how to do acquisition and processing automatically using the Xcalibur data system and the software that came with your hardware.

Figure 4. Acquiring and processing data automatically



Creating a Processing Method

Use the following procedures to create a processing method for quantifying data using the raw data files associated with the C:\Xcalibur\examples\methods\drugx.sld sequence file.

Note This tutorial does not discuss using system suitability parameters to test the chromatographic peaks. To add report templates to the processing method, see [Chapter 5](#), “Previewing, Specifying, and Printing Reports.”

Create a processing method that quantifies the target compound in the drugx data set by performing these procedures in sequence.

Contents

- [Opening the Processing Setup Window](#)
- [Specifying Quan View Options](#)
- [Opening a Raw Data File](#)
- [Specifying Identification Settings for Analysis Components](#)
- [Entering Peak Integration and Detection Parameters](#)
- [Selecting Calibration Settings](#)
- [Specifying Calibration Levels and QC Levels](#)
- [Saving the Processing Method](#)

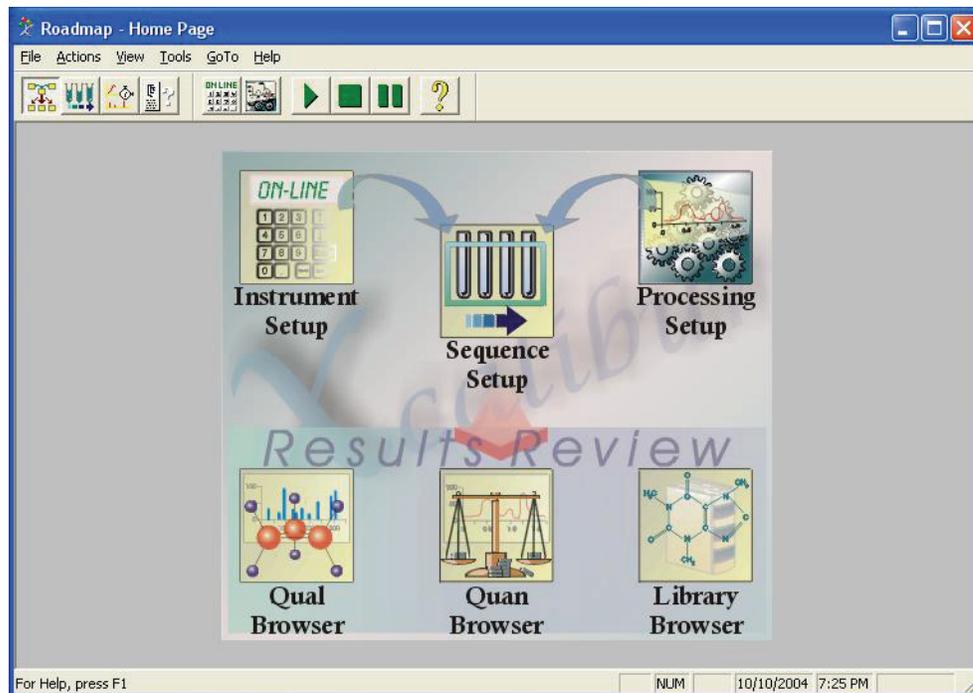
Opening the Processing Setup Window

Create a process in the Processing Setup window.

❖ To open the Processing Setup window

1. Click  on the Road Map on the Xcalibur Home Page (see [Figure 5](#)) or choose **GoTo > Processing Setup**.

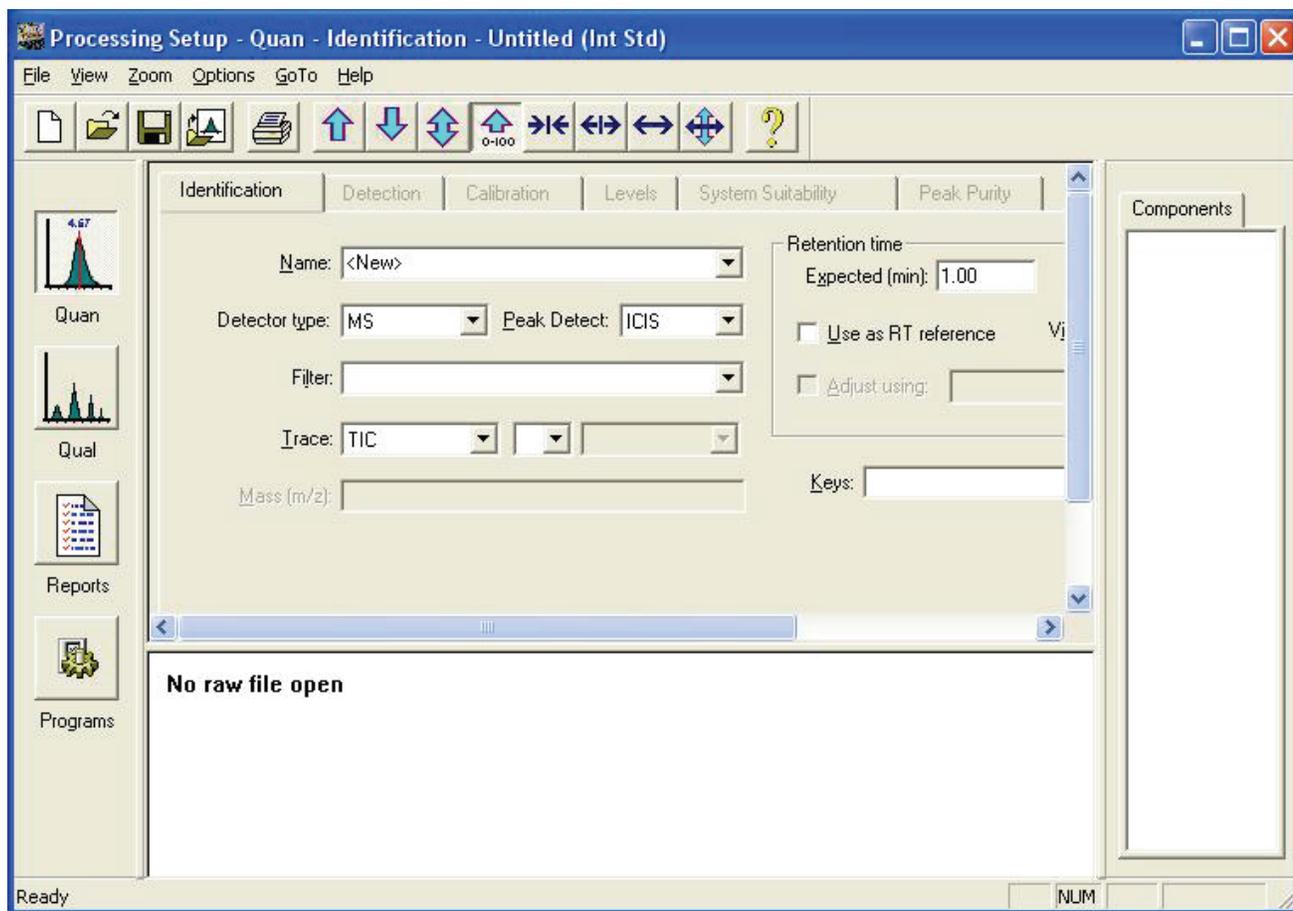
Figure 5. Roadmap view of the Xcalibur Home Page window



2. Click  to display the Quan view if it is not already displayed.

3. Click the **Identification** tab. The Identification page for Quan view opens (see Figure 6).

Figure 6. Identification page for Quan view



4. If the data system automatically loads a method, choose **File > New** to start with a fresh display.

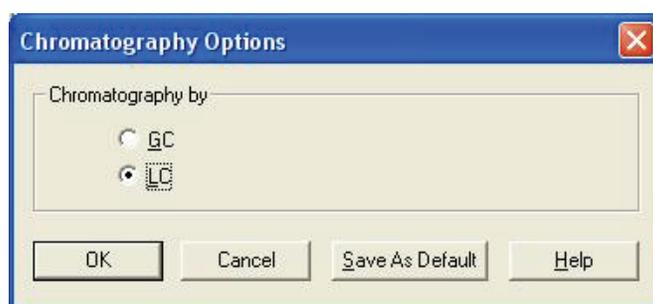
Specifying Quan View Options

The Options menu commands in the Processing Setup window vary depending on the current view. From the Quan view in Processing Setup, specify the type of chromatography and the type of calibration technique used. LC/MS collected the data set used in this tutorial, and the internal standard calibration technique quantified the drugx target compound.

❖ To specify chromatography by LC

1. Choose **Options > Chromatography By** in the Processing Setup window. The Chromatography Options dialog box opens (see [Figure 7](#)).

Figure 7. Chromatography Options dialog box

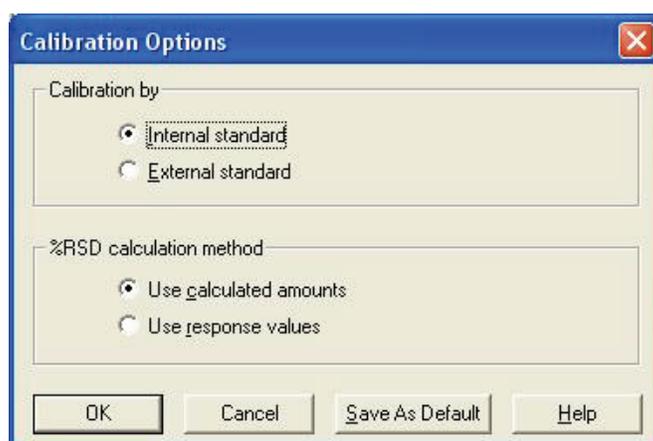


2. To specify chromatography by LC, select the **LC** option.
3. Click **OK** to close the dialog box.

❖ To specify the internal standard calibration technique

1. Choose **Options > Calibration Options** in the Processing Setup window. The Calibration Options dialog box opens (see [Figure 8](#)).

Figure 8. Calibration Options dialog box



2. To specify calibration by internal standard, select the **Internal Standard** option.
3. Click **OK** to close the dialog box.

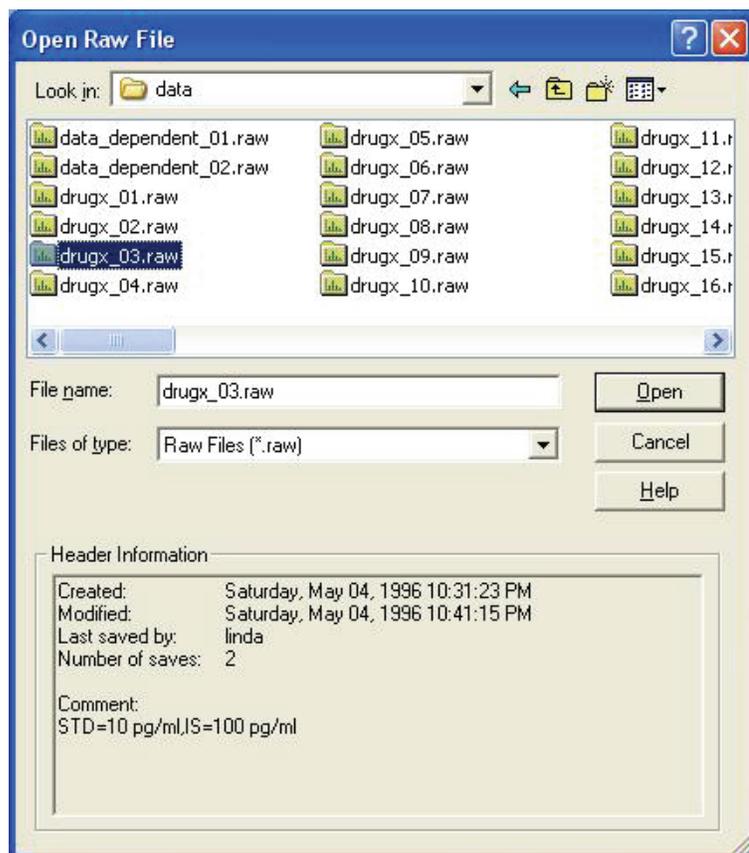
Opening a Raw Data File

Open a representative raw file from the data set to determine appropriate peak detection and integration parameters for the processing method. In this tutorial, use the drugx_03.raw file. In general, select a raw file corresponding to a low-concentration calibration standard.

❖ To open a raw data file in Quan view

1. Click  or choose **File > Open Raw File**. The Open Raw File dialog box opens (see [Figure 9](#)).

Figure 9. Open Raw File dialog box



2. Browse to the following file name and location:

C:\Xcalibur\examples\data\drugx_03.raw.

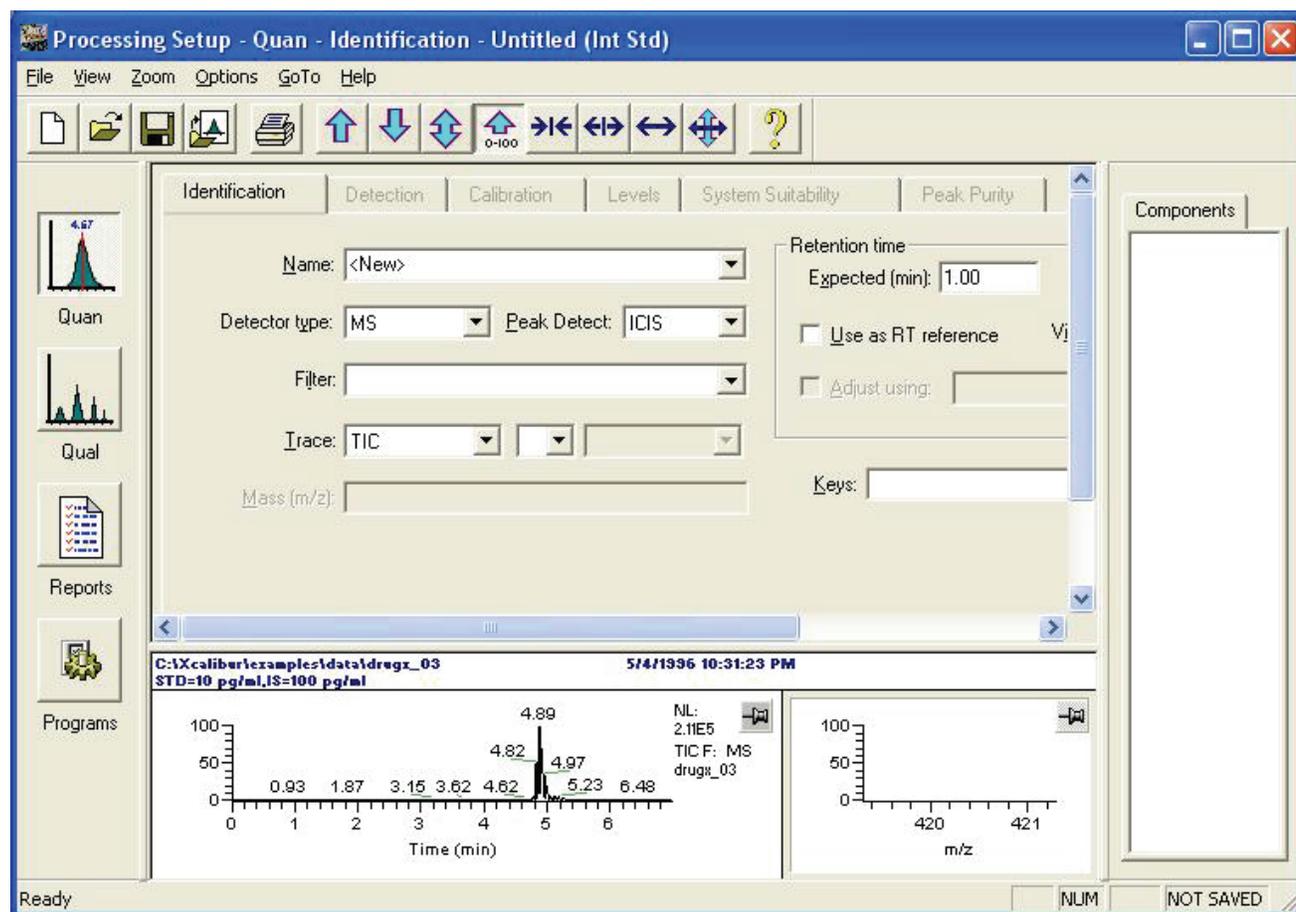
3. Select **drugx_03.raw** and click **Open**.

Processing Setup opens the drugx_03.raw file and displays the unfiltered total ion chromatogram (see [Figure 10](#)).

2 Creating a Processing Method

Opening a Raw Data File

Figure 10. Identification page, showing the total ion current (TIC) chromatogram of drugx_03.raw



Note If you save a processing method when a raw file is open, the raw file name is saved in the processing method. To have the Xcalibur data system automatically open the associated raw file whenever you open the processing method, select the **On** button for the Auto-Open Raw File option in the Settings dialog box. To open this dialog box in the Quan view of Processing Setup, open a processing method and choose **Options > Settings**.

Specifying Identification Settings for Analysis Components

This section describes how to identify target compounds and internal standards and contains the following topics:

- [Specifying Identification Settings for the Internal Standard](#)

For the internal standard calibration technique, each calibration standard contains one or more target compounds and one or more internal standards.

- [Specifying Identification Settings for the Target Compound](#)

In this section, use the Identification page for Quan view in Processing Setup to name the components of the sample, display spectra, and specify retention time and peak identification criteria.

The data set used in this tutorial contains one target compound and one internal standard. The target compound is drugx. The internal standard is D4.

Specifying Identification Settings for the Internal Standard

Processing Setup needs component identification information to associate the internal standard with a chromatographic peak. To identify the internal standard, perform the following procedures in sequence.

1. [Naming the Internal Standard](#)
2. [Selecting the Detector Type](#)
3. [Selecting the Peak Detection Type](#)
4. [Matching Scan Filters with Components](#)
5. [Selecting the Trace Type](#)
6. [Entering the Retention Time Automatically](#)

2 Creating a Processing Method

Specifying Identification Settings for Analysis Components

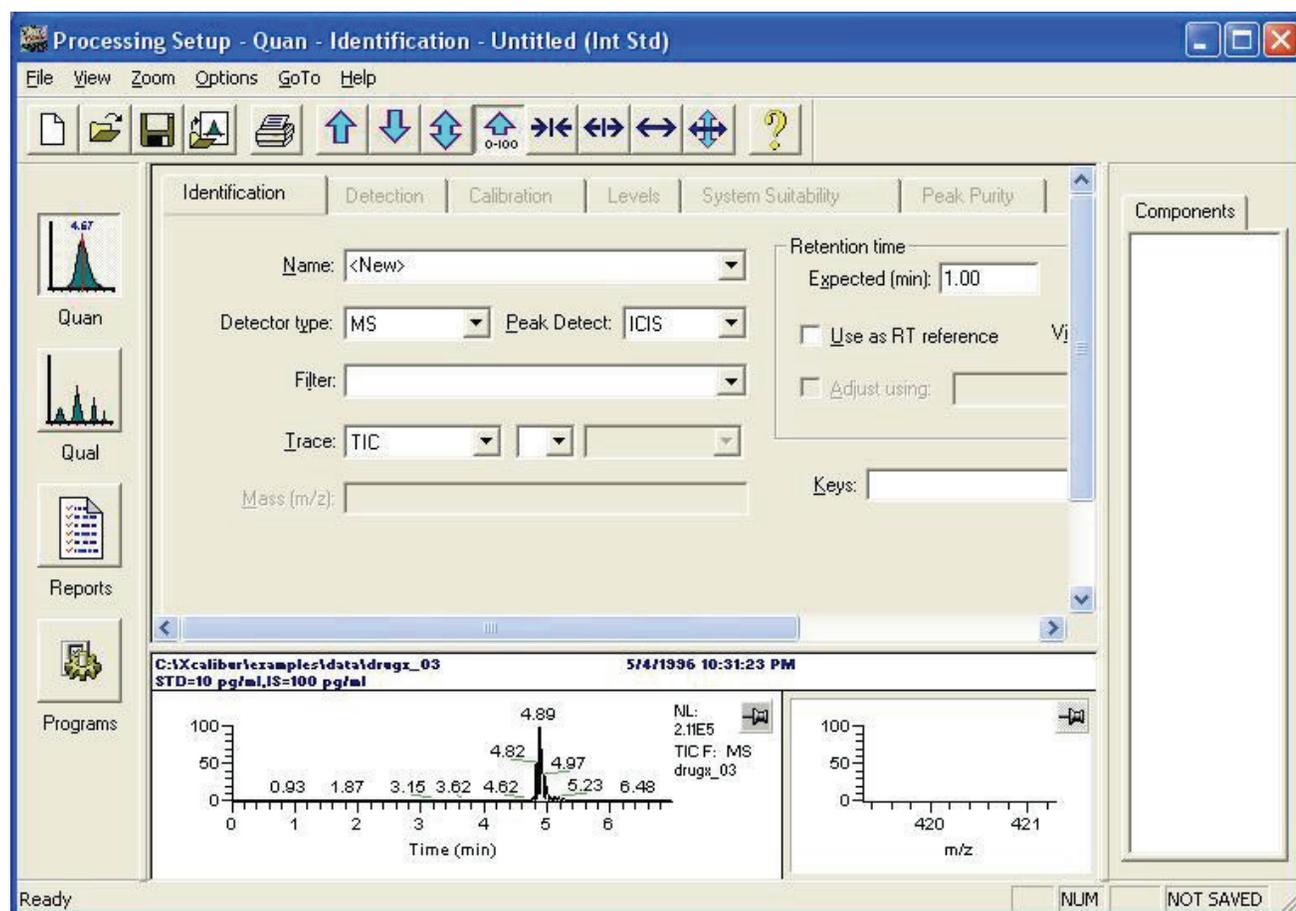
Naming the Internal Standard

Use the Name list on the Identification page to name the components of the sample. When you change settings, Processing Setup changes the settings for the named component only.

❖ To enter the name of the internal standard in the Name list

1. Select **New** in the Name list and type **D4**, the name of the internal standard (see Figure 11).

Figure 11. Identification page



2. Click **OK** to save the new name.

Note To delete a component, highlight the component name in the Component list at the right. Choose **Options > Delete component name**.

Selecting the Detector Type

Use the Detector Type list on the Identification page to specify the type of detector you used to obtain the raw file.

❖ To specify the Detector type

Select **MS** in the Detector Type list.

Selecting the Peak Detection Type

Use the Peak Detect list on the Identification page to specify the type of peak detection algorithm to use (ICIS, Genesis, or Avalon) to analyze raw data.

These algorithms do the following:

- Apply smoothing
- Construct a chromatogram using the scan or mass filters
- Assign peak numbers
- Generate a peak list
- Determine the peak start and peak end points

All algorithms provide component peak detection and chromatographic peak detection. Select the ICIS or Genesis algorithms for MS data. Select the Avalon algorithm for PDA, UV, and analog data.

❖ To specify the Peak Detection type

Select **ICIS** in the Peak Detect list.

Matching Scan Filters with Components

The Xcalibur data system creates unique scan filters to acquire data according to the type of experiment specified in the instrument method. When you load a raw file, the data system lists the scan filters associated with the raw file in the Filter box. In this example, the application acquired selected reaction monitoring (SRM) data on the following, using alternating product ion scans (drugx and D4, respectively):

- a proprietary drug of molecular weight 465 u (Parent ion m/z 465; product ion m/z 420)
- a deuterated internal standard of molecular weight 469 u (parent ion m/z 469; product ion m/z 424)

To calibrate and quantify drugx, filter the total ion current chromatogram.

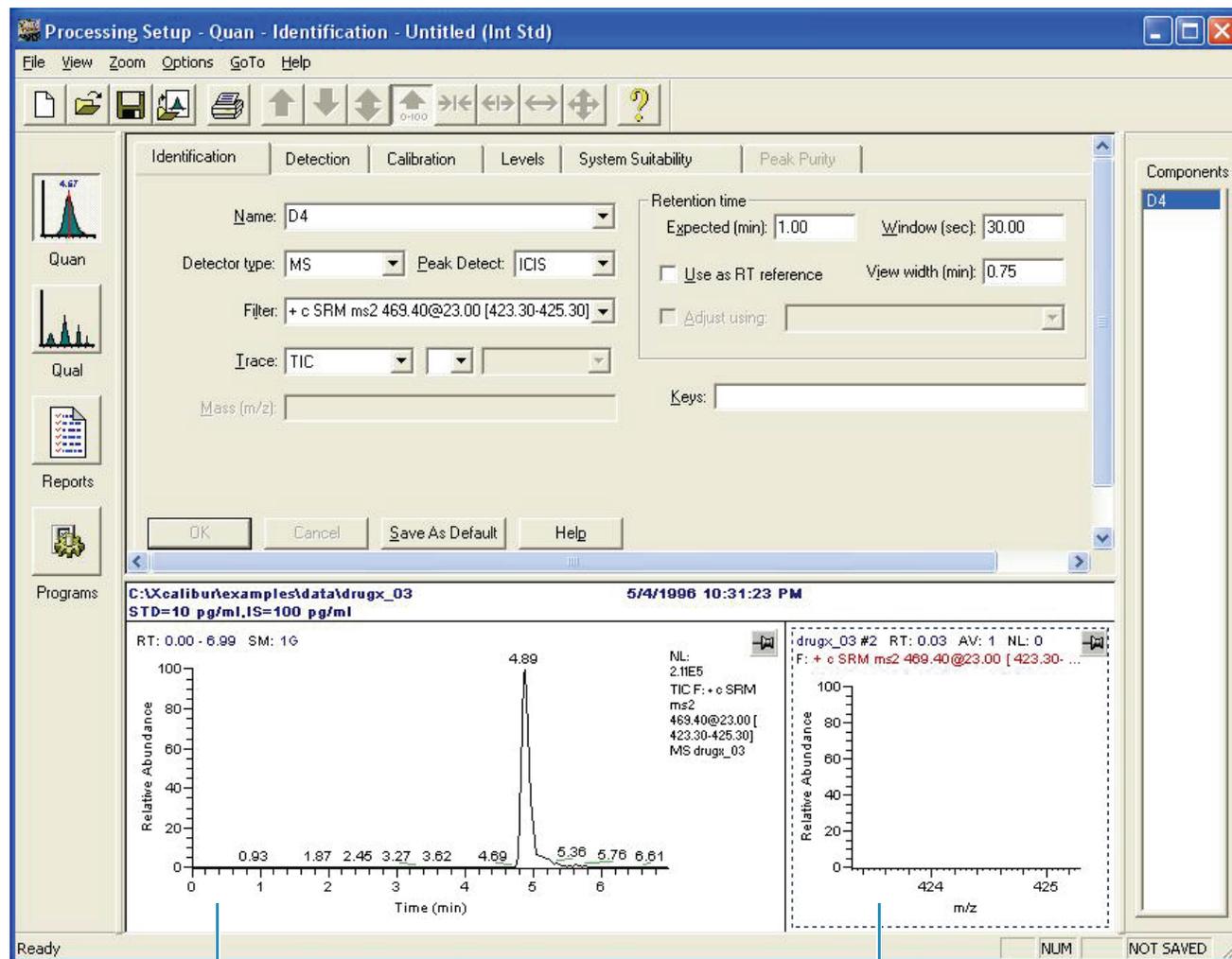
2 Creating a Processing Method

Specifying Identification Settings for Analysis Components

❖ To match D4 with its scan filter

1. From the Filter list for the drugx_03.raw file, select
+ c SRM ms2 469.40@23.00[423.30-425.30] as the scan filter for D4.
2. Click **OK** to display the mass chromatogram for D4 (see Figure 12).

Figure 12. Scan filtered chromatogram and mass spectrum for D4



Chromatogram Plot view

Spectrum Plot view

Selecting the Trace Type

Use the Trace list on the Identification page for Quan view to specify the type of chromatogram to use for processing.

❖ To specify the type of chromatogram

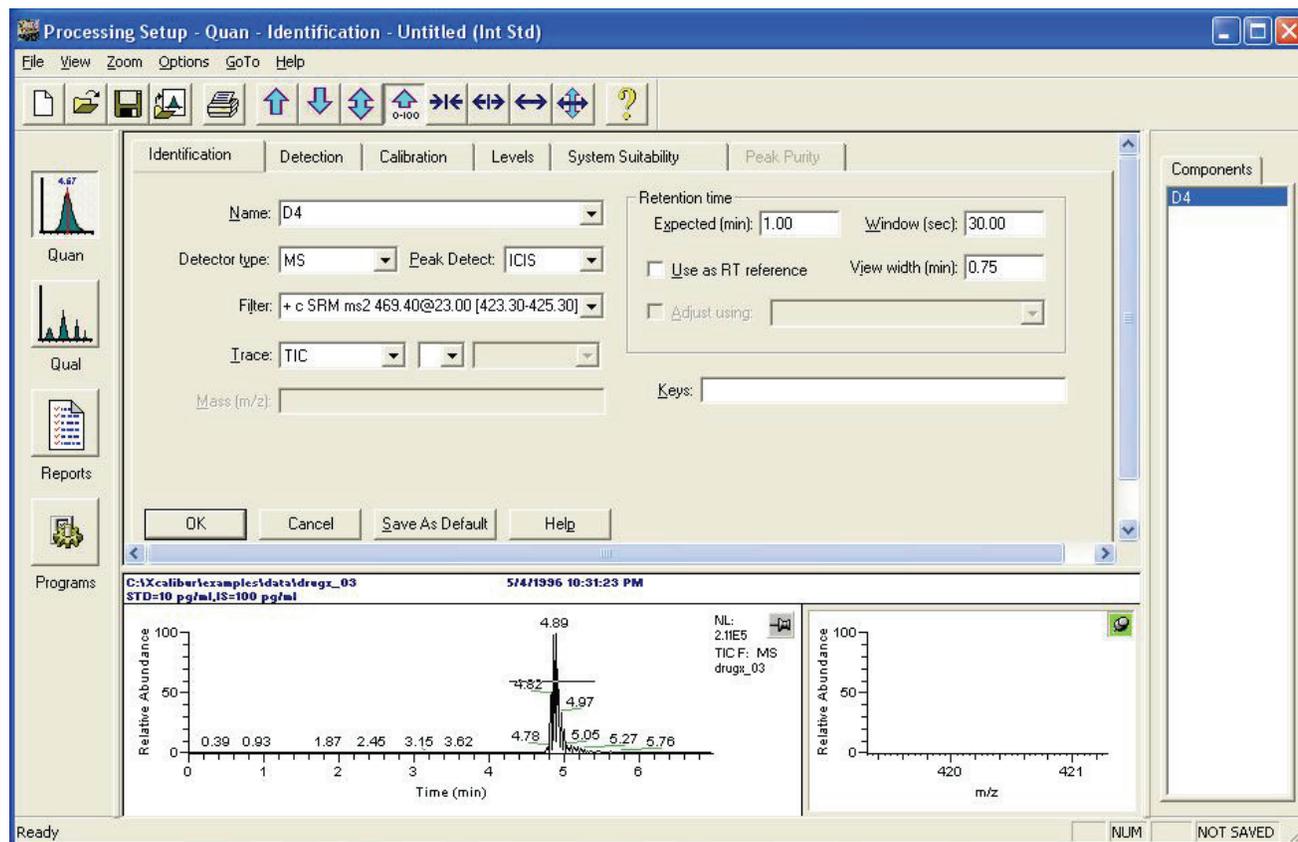
In the Trace list, select **TIC** to specify total ion current.

Entering the Retention Time Automatically

❖ **To automatically enter the retention time of a chromatographic peak**

1. To activate the Spectrum Plot view, click  in the upper right corner (see [Figure 12](#)).
 The pin background turns green  and appears to be pinned to the screen.
2. Click and drag the cursor in the Chromatogram Plot view across the chromatogram peak as shown in [Figure 13](#). The horizontal line across the center of the peak shows the area selected by the mouse movement.

Figure 13. Selecting the scan corresponding to the peak maximum

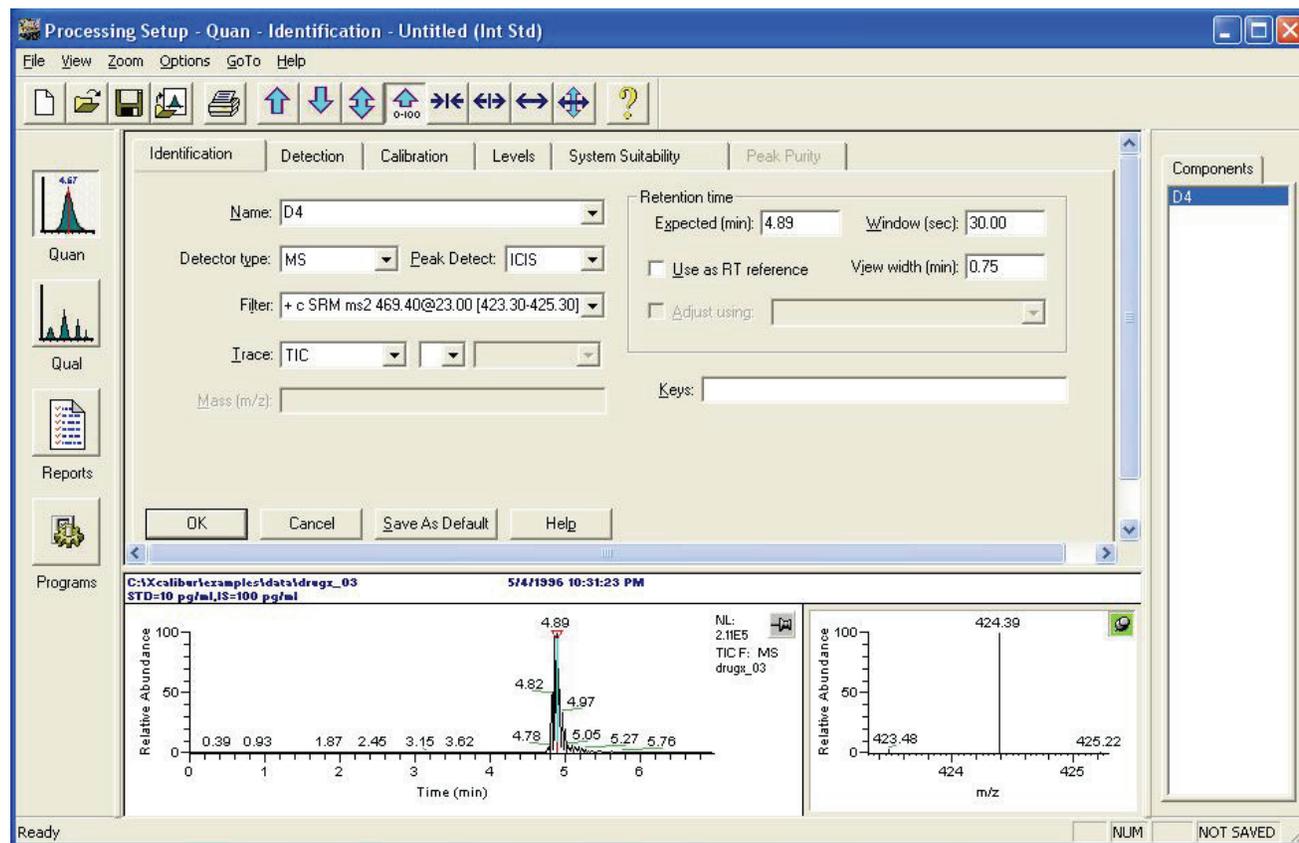


3. Release the mouse button. Processing Setup performs the following events automatically.
 - Selects the retention time of the peak maximum and highlights the selected scan in the LC peak with a red marker in the Chromatogram Plot view.
 - Enters the retention time corresponding to the selected scan in the Expected box in the Retention Time area.
 - Displays the mass spectrum of the product ions in the Spectrum Plot view (see [Figure 14](#)).

2 Creating a Processing Method

Specifying Identification Settings for Analysis Components

Figure 14. Identification page with a retention time marker (vertical line)



4. To use the actual retention time of D4 as the retention time reference for the other component in the drugx chromatogram, select the **Use as RT Reference** check box.

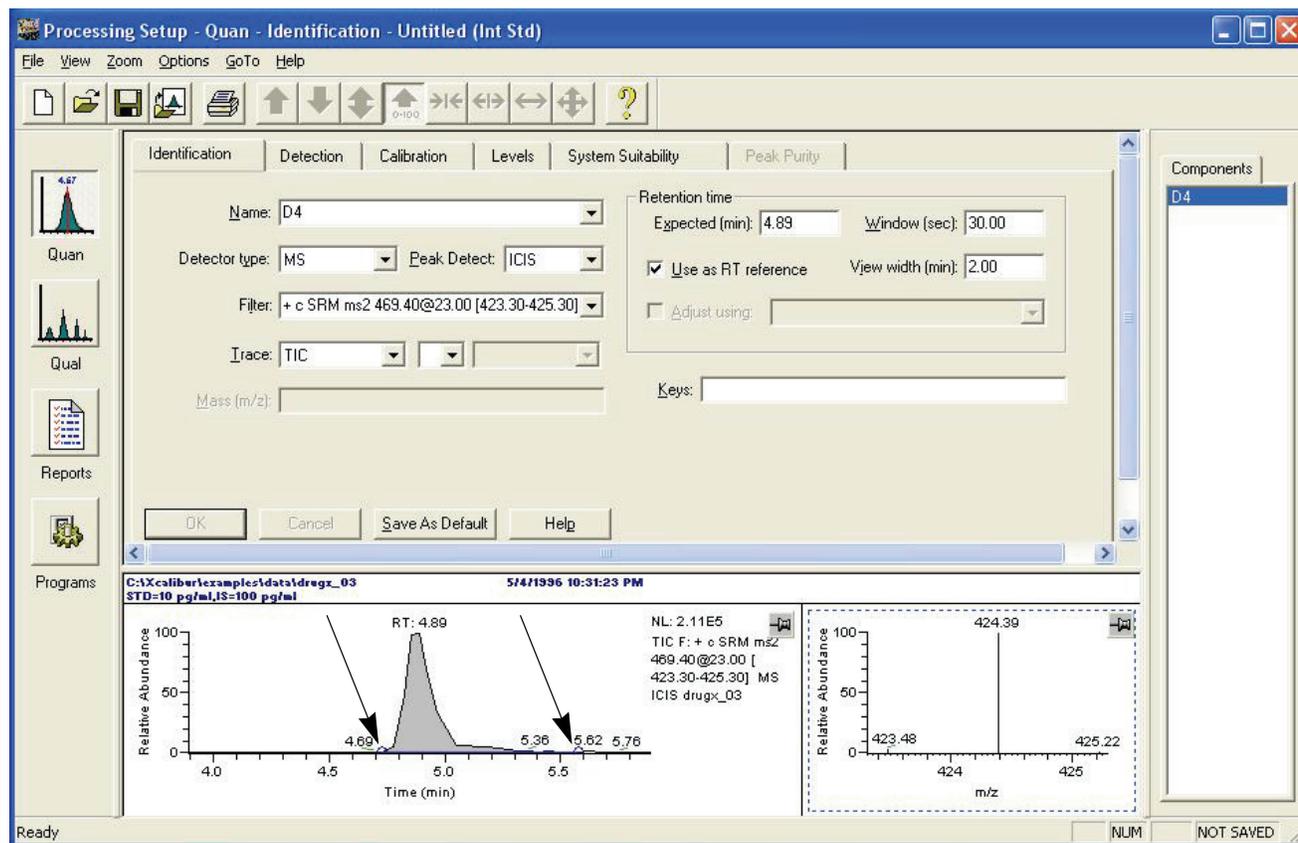
Note To adjust the expected retention time of a component relative to the reference component, select the **Adjust Using** check box. See step 12 on page 20.

Leave the Window box number at **30** seconds. This parameter controls the width of the window that the algorithm searches to locate the component. In this case the algorithm searches 15 seconds on either side of RT 4.89 to find D4.

5. Type **2.00** into the View Width box. View width controls how much of the chromatogram time range the application displays when you view the components.
6. To save the component identification information for D4, click **OK**.

In the Chromatogram view, the data system displays the Time portion of the chromatogram from 3.9 to 5.9 minutes based on a selection of 2.00 as the View width for a peak with an expected retention time of 4.9 min. Processing Setup automatically shades the integrated portion of the peak gray and displays blue integration markers at the starting and ending points of the peak integration. The baseline is indicated by a blue line that connects the integration markers (see Figure 15). Arrows point to the integration markers.

Figure 15. Area of peak integration (grayed) and the integration markers



7. Inspect the integrated peak and verify the following:

- The retention time on the peak agrees with that in the Expected box in the Retention Time area.
- The scan filter in the Filter box is matched to the correct component in the Components list.

If the peak has not been identified, repeat this procedure. Click the pin (📌) in the Spectrum Plot view (the pane to the right of the Chromatogram Plot view) before performing step 2 on page 17.

If the peak has been identified properly, you are ready to specify the peak identification parameters for the target compound.

Tip When you are entering many components with similar peak integration parameters, first enter all of the identification parameters for one of the components. Click **Save As Default**. These parameters then become the default values for new components.

Specifying Identification Settings for the Target Compound

❖ To specify the settings for the target compound

1. Select **New** in the Name list. The Apply Changes dialog box opens if you have warnings enabled. Click **Yes** to apply changes.
2. To specify the name of the target compound, type **drugx**.
3. Click **OK** to save the new name.
4. Select **MS** in the Detector Type list if it is not already selected.
5. Select **ICIS** in the Peak Detect list box.
6. To match the target compound with its scan filter, open the Filter list to display the available scan filters in the drugx_03.raw file.
7. Select **+ c SRM ms2 465.30@23.00[419.30-421.30]** to select the scan filter for drugx.
8. Click **OK** to apply the scan filter to the total ion current. Processing Setup automatically displays the mass chromatogram corresponding to the target compound.
9. Select **TIC** (total ion current) in the Trace list if it is not already selected.
10. To display the mass spectrum of the currently active component and automatically enter the retention time of the LC peak, do the following:
 - a. To activate the Spectrum Plot view, click the currently grayed pin in its upper right corner.

The pin background turns green () and appears to be pinned to the screen.
 - b. Click and drag the cursor in the Chromatogram Plot view across the chromatogram peak.
 - c. Release the mouse button.

Processing Setup automatically performs the following events:

- Selects the retention time of the peak maximum and highlights the selected scan in the LC peak with a red marker in the Chromatogram Plot view.
 - Enters the retention time corresponding to the selected scan in the Expected box in the Retention Time area.
11. Type **2.00** into the View Width box.
 12. To adjust the expected retention time of drugx by changes in the actual retention time of D4, do the following:
 - a. Select the **Adjust Using** check box.

The Adjust Using list becomes active.

b. Select **D4** in the Adjust Using list.

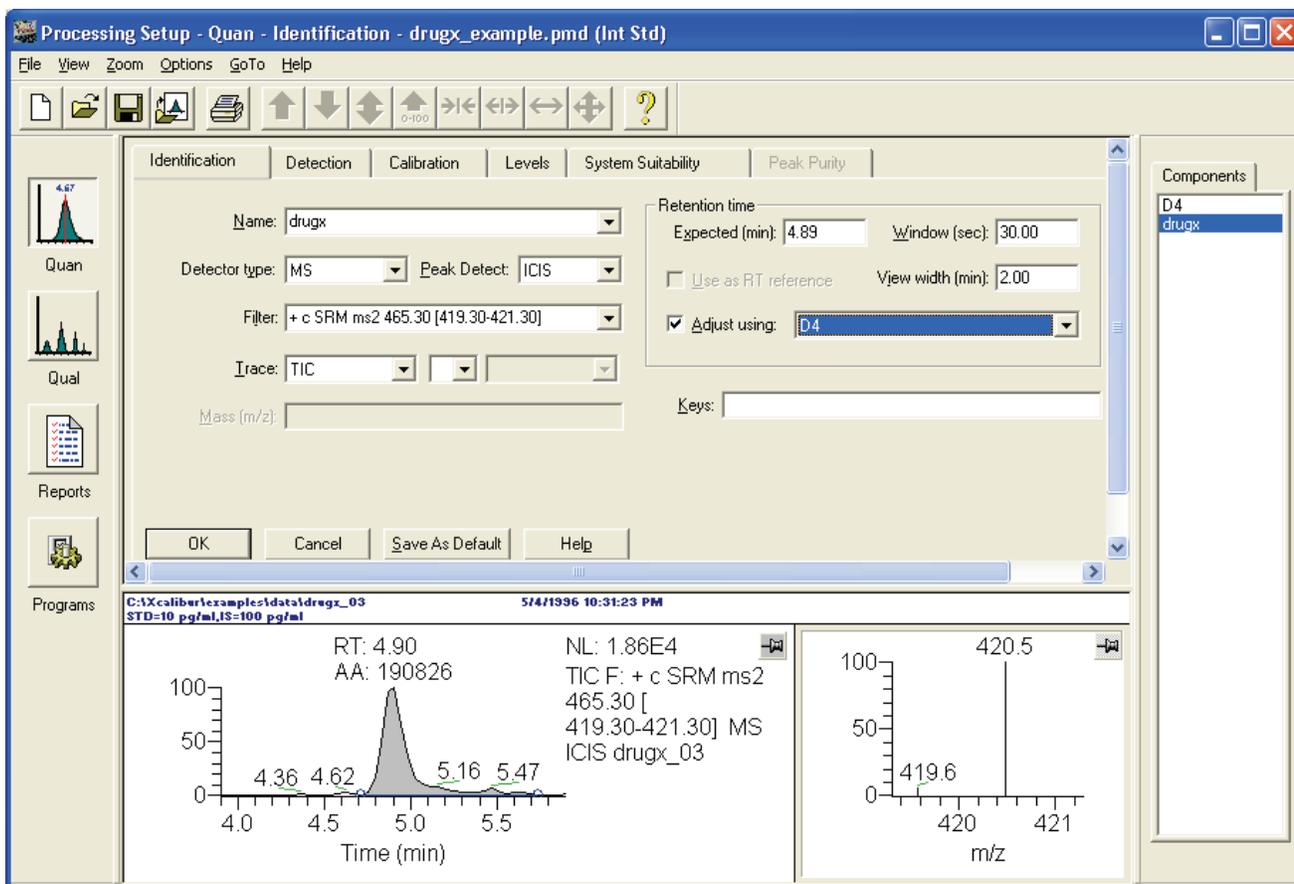
You selected D4 as the retention time reference component in step 4 on page 18.

13. Leave the window value at **30** seconds.

14. To accept the peak identification settings for drugx, click **OK** (see Figure 16).

In the Chromatogram Plot view, Processing Setup displays the 3.9 to 5.9 minute portion of the chromatogram because you selected 2.00 as the View width for a peak with an expected retention time of 4.9 minutes. Processing Setup automatically shades the integrated portion of the peak gray and displays blue integration markers at the starting and ending points of the peak integration. The baseline is indicated by a blue line that connects the integration markers.

Figure 16. Peak identification settings for drugx



2 Creating a Processing Method

Entering Peak Integration and Detection Parameters

Entering Peak Integration and Detection Parameters

Use the Detection page for Quan view in Processing Setup to enter peak integration and detection parameters.

To enter peak integration and detection parameters, perform these procedures in order.

1. [Entering Peak Integration Parameters](#)
2. [Entering Peak Detection Parameters](#)

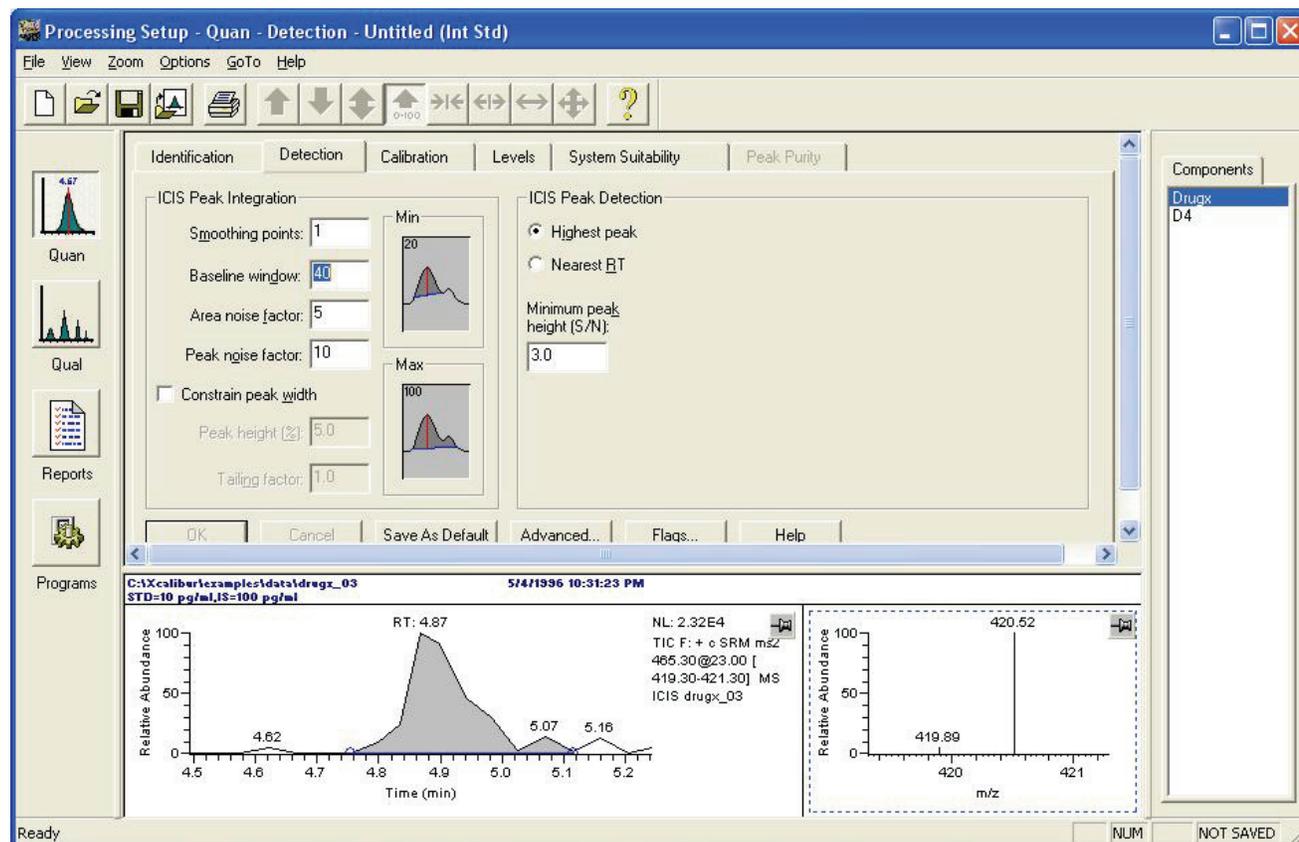
Entering Peak Integration Parameters

Enter peak integration parameters to specify how the data system determines the area of each peak in the chromatogram. Processing Setup provides peak integration parameter options in the Peak Integration area on the Detection page.

❖ To enter the ICIS peak integration parameters for the internal standard and the target compound

1. Click the **Detection** tab (Figure 17). The Detection page for Quan view opens.

Figure 17. Detection page for Quan view



2. To select the D4 internal standard in the Components list, select **D4**.
3. Type **5** in the Smoothing Points box in the ICIS Peak Integration area.

Based on the peak view, type the number of points used in the moving average used to smooth data in the Smoothing Points box. The valid range is 1 (no smoothing) to 15 (maximum smoothing).
4. To set the maximum number of scans that the application reviews for a local minimum to 40, type **40** in the Baseline Window box. The valid range is 1 through 500.
5. To specify an area noise factor of 5, type **5** in the Area Noise Factor box. The area noise factor is a noise level multiplier used to determine the location of a peak edge after the location of the possible peak. The valid range is 1 to 500.
6. Type **10** in the Peak Noise Factor box. The peak noise factor is a noise level multiplier used to determine the potential peak signal threshold. The valid range is 1 to 1000.
7. Clear the **Constrain Peak Width** check box.

Use the constrain peak width option to control how much of the peak is integrated by specifying a peak height threshold and a tailing factor. Select the **Constrain Peak Width** check box to activate this box. The valid range for Peak Width threshold is 0.0 to 100.0%. The valid range for Tailing Factor is 0.5 through 9.0.

To save the peak integration parameters, click **OK**.

8. To select the target compound, click **drugx** in the Components list. Repeat steps 2 through 7 for the target compound.

Entering Peak Detection Parameters

Peak detection parameters specify how the Xcalibur data system selects a peak within the specified retention time window for a component.

❖ To enter the peak detection parameters for the internal standard and the target compound

1. To select the D4 internal standard, click **D4** in the Components list.
2. To associate D4 with the highest peak in the chromatogram, select the **Highest Peak** option in the ICIS Peak Detection area (see [Figure 19](#) on [page 25](#)).
3. To have the data system ignore all peaks that do not have a signal-to-noise ratio of 3 or greater, type **3** in the Minimum Peak Height (S/N) box. The valid range is 0.0 (all peaks) through 999.0.
4. Verify that the advanced peak detection parameters are set to their default values.
 - a. Click . The ICIS Advanced Parameters dialog box opens.

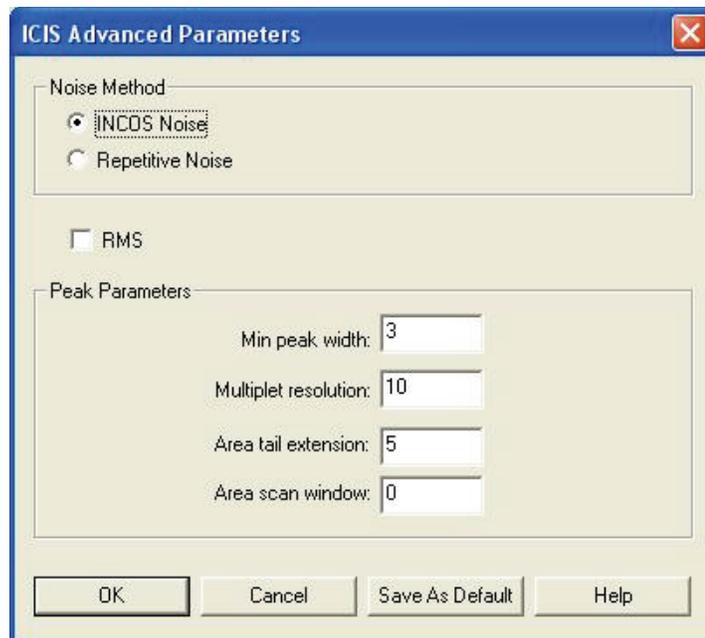
2 Creating a Processing Method

Entering Peak Integration and Detection Parameters

Use the ICIS Advanced Parameters dialog box to specify advanced component detection criteria. These additional criteria can be used if the standard detection criteria do not provide the desired results. Refer to the *Acquisition and Processing User Guide* for information on the parameters in the ICIS Advanced Parameters dialog box.

- b. Inspect the ICIS Advanced Parameters dialog box. Make sure the settings are the same as those in [Figure 18](#).

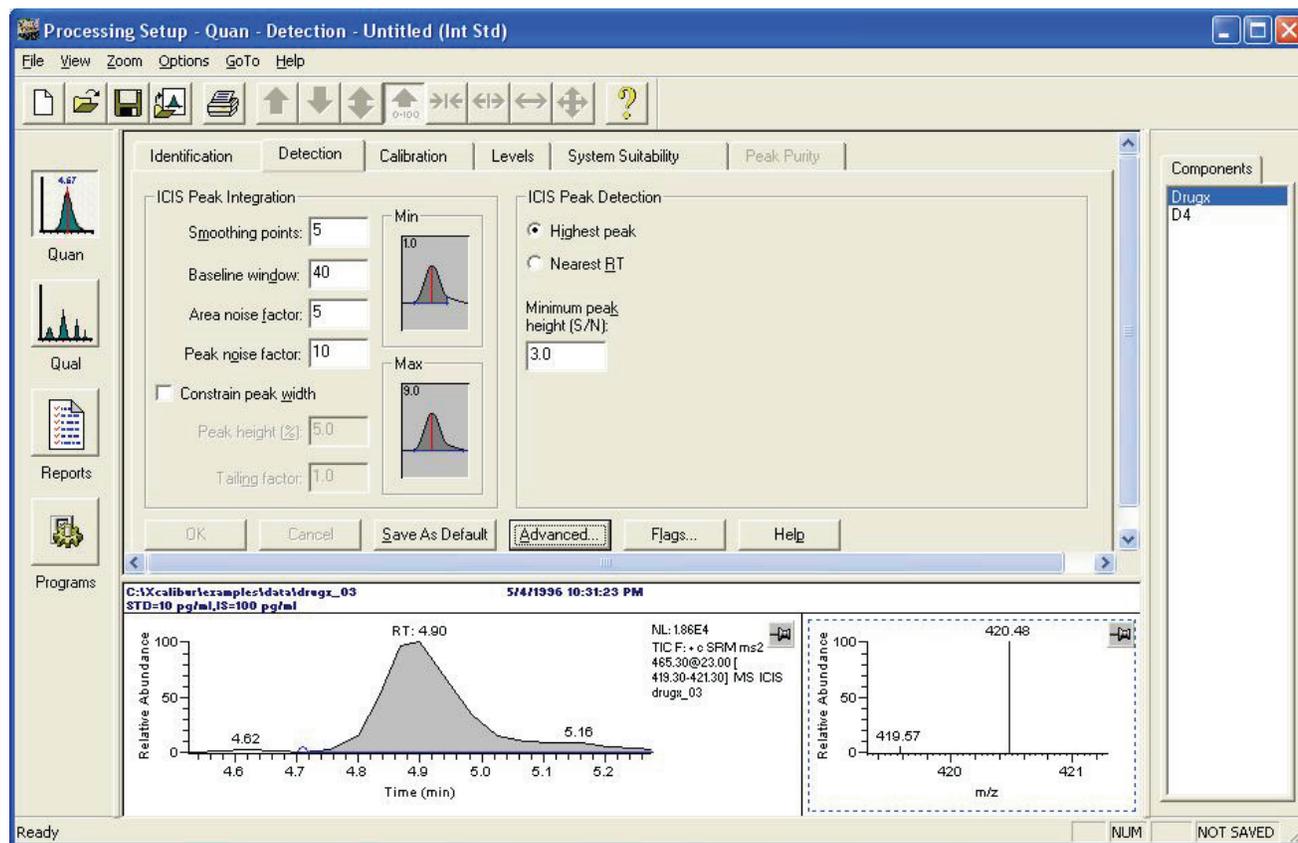
Figure 18. ICIS Advanced Parameters dialog box, showing default settings



- c. Click **OK** to close the dialog box.
5. To save the peak detection parameters, click **OK**.
6. To select the target compound, click **drugx** in the Components list. Repeat steps 2 through 5 for the target compound.

The Detection page should look like the one shown in [Figure 19](#).

Figure 19. Detection page, showing settings for drugx and D4



Selecting Calibration Settings

In Processing Setup, use the Calibration page for Quan view to specify the calibration curve type. When using the internal standard calibration technique, use this page to associate the internal standard with a target compound and to specify the amount of internal standard used to spike the calibration standards and unknowns.

❖ To select the calibration settings

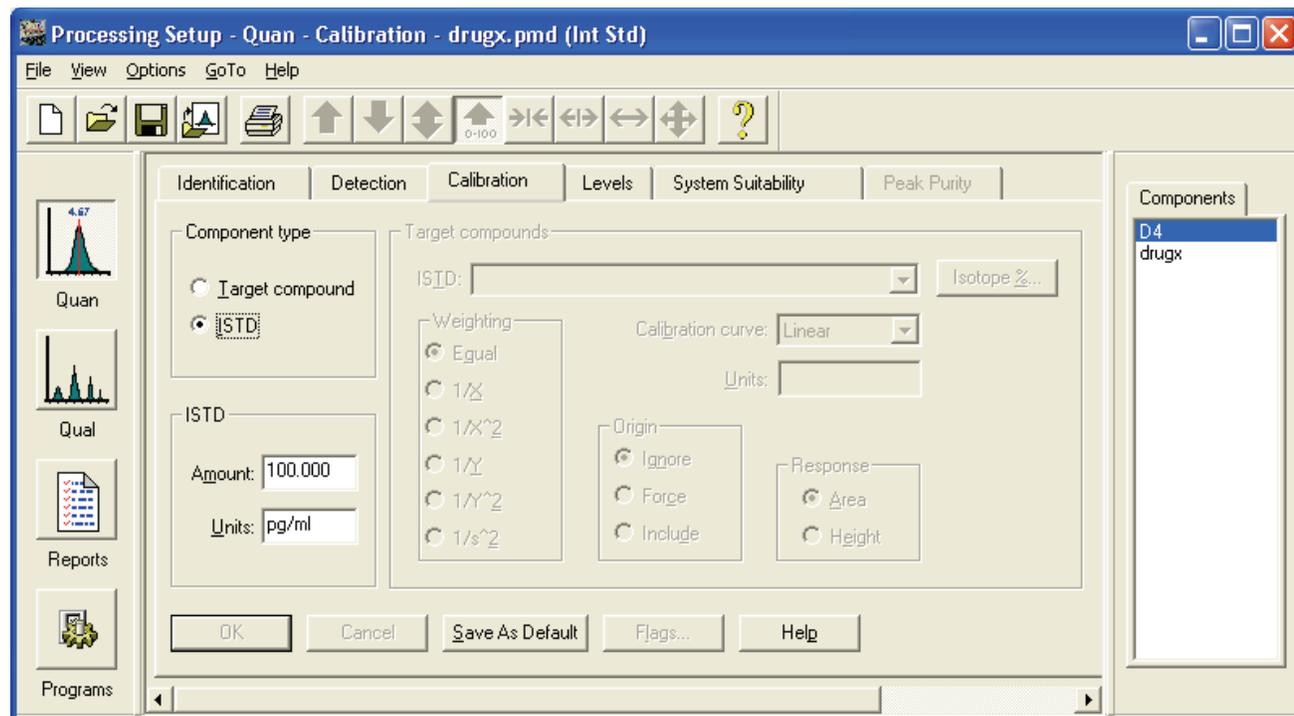
1. Click the **Calibration** tab. The Calibration page for Quan view opens.
2. To enter the calibration settings for the D4 internal standard, click **D4** in the Components list.
3. To select D4 as the internal standard, select the **ISTD** option in the Component Type area.
4. To specify an internal standard amount of 100 pg/mL, type **100** in the Amount box in the ISTD (Internal Standard) area.
5. To specify pg/mL as the units of concentration, type **pg/mL** in the Units box.

2 Creating a Processing Method

Selecting Calibration Settings

- To save the settings for D4, click **OK**. The Calibration page should look like [Figure 20](#). This procedure does not discuss setting parameters on the System Suitability or Peak Purity pages. For information about setting these parameters, refer to the *Acquisition and Processing User Guide*.

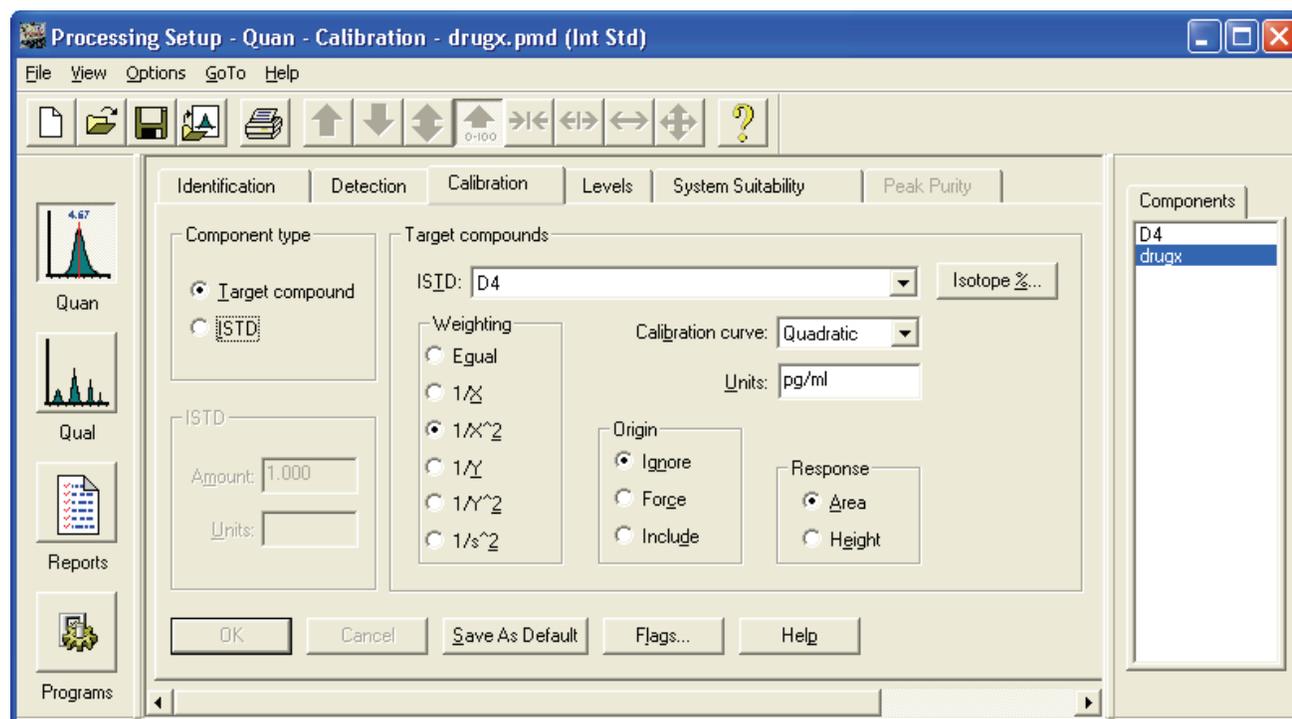
Figure 20. Calibration page, showing the settings for the D4 internal standard



❖ To enter the calibration settings for the drugx target compound

1. Select **drugx** in the Components list.
2. To specify drugx as a target compound, select the **Target Compound** option in the Component Type area.
3. Select **D4** in the ISTD list as the internal standard in the Target Compound area.
4. To specify a quadratic fit calibration curve, select **Quadratic** in the Calibration Curve list.
5. To specify the units of concentration, type **pg/10 μ l** in the Units box.
6. To specify a weighting of $1/X^2$, select **1/X²** in the Weighting area.
7. To exclude the origin as a data point when fitting the calibration curve, select **Ignore** in the Origin area.
8. To use the area of the peak to determine response, select **Area** in the Response area.
9. To save the settings, click **OK**. The Calibration page should look like the one shown in [Figure 21](#).

Figure 21. Settings for the drugx target compound



Specifying Calibration Levels and QC Levels

In Processing Setup, use the Levels page for Quan view to specify the amount of target compound (analyte) in each calibration level. The Xcalibur data system uses the calibration levels information to construct the calibration curve as it processes a sequence. Also specify the amount of target compound in the QC check standards. The application uses the QC standards to check the stability of the LC/MS instrument during a sequence run.

This section contains the following topics.

- [Specifying the Calibration Levels of the Target Compound](#)
- [Specifying the QC Levels](#)

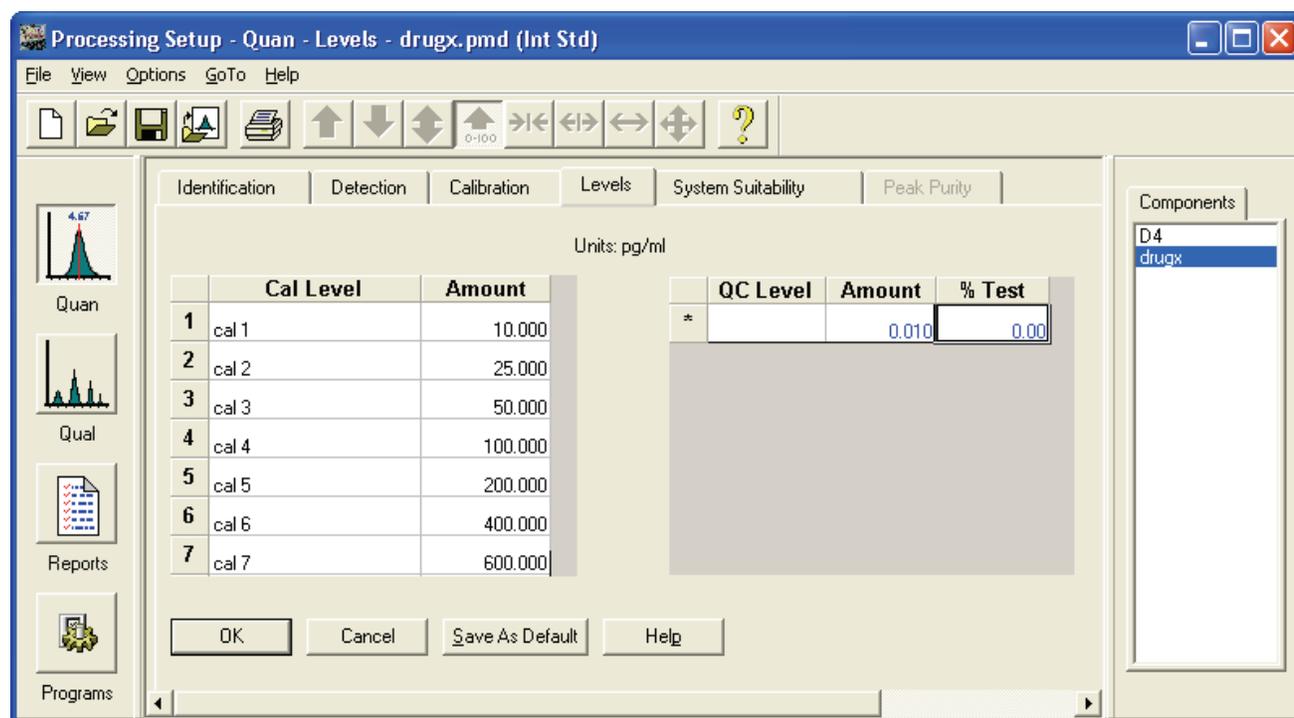
Specifying the Calibration Levels of the Target Compound

❖ To specify the levels of the target compound

1. Select **drugx** in the Components list from the Quan view of the Processing Setup window.
2. Select the **Levels** tab. The Levels page for Quan view opens (see [Figure 22](#)).

Note If you select D4 and then try to open the Levels page, a warning box appears. The Levels page is not available for ISTD components.

Figure 22. Levels page for Quan view



3. Enter the calibration level information for the target compound:
 - a. To specify the name of the first calibration level, type **cal 1** in the first Cal Level box.
 - b. Press the TAB key to advance the cursor to the first Amount box.
 - c. To specify an injection amount of 10 pg, type **10** in the box.
 - d. To create a new row and to advance the cursor to the second Cal Level box, press the TAB key twice.
 - e. Repeat this procedure until you fill in the nine calibration levels as shown in [Table 1](#). The table shows the number of picograms of drugx injected in 10 µL of the corresponding calibration solution.

Table 1. Calibration Level table

Cal Level	Amount
cal 1	10
cal 2	25
cal 3	50
cal 4	100
cal 5	200
cal 6	400
cal 7	600
cal 8	800
cal 9	1000

Specifying the QC Levels

❖ To specify the QC levels

1. To specify the name of the first QC level, type **QC 1** in the first QC Level box.
2. To advance the cursor to the first Amount box, press the TAB key.
3. To specify an injection amount of 10 pg, type **10** in the box.
4. Press the TAB key to advance the cursor to the first %Test box.
5. To specify a 20% test value, type **20** in the box.

Note The %Test values for QCs in this example are shown in [Table 2](#). The data system uses the criteria in this example to determine whether QCs pass. Use any %Test parameters appropriate for a specific application.

6. To create a new row and advance the cursor to the second QC Level box, press the TAB key twice.
7. Repeat this procedure until you fill in the three QC levels as shown in [Table 2](#).

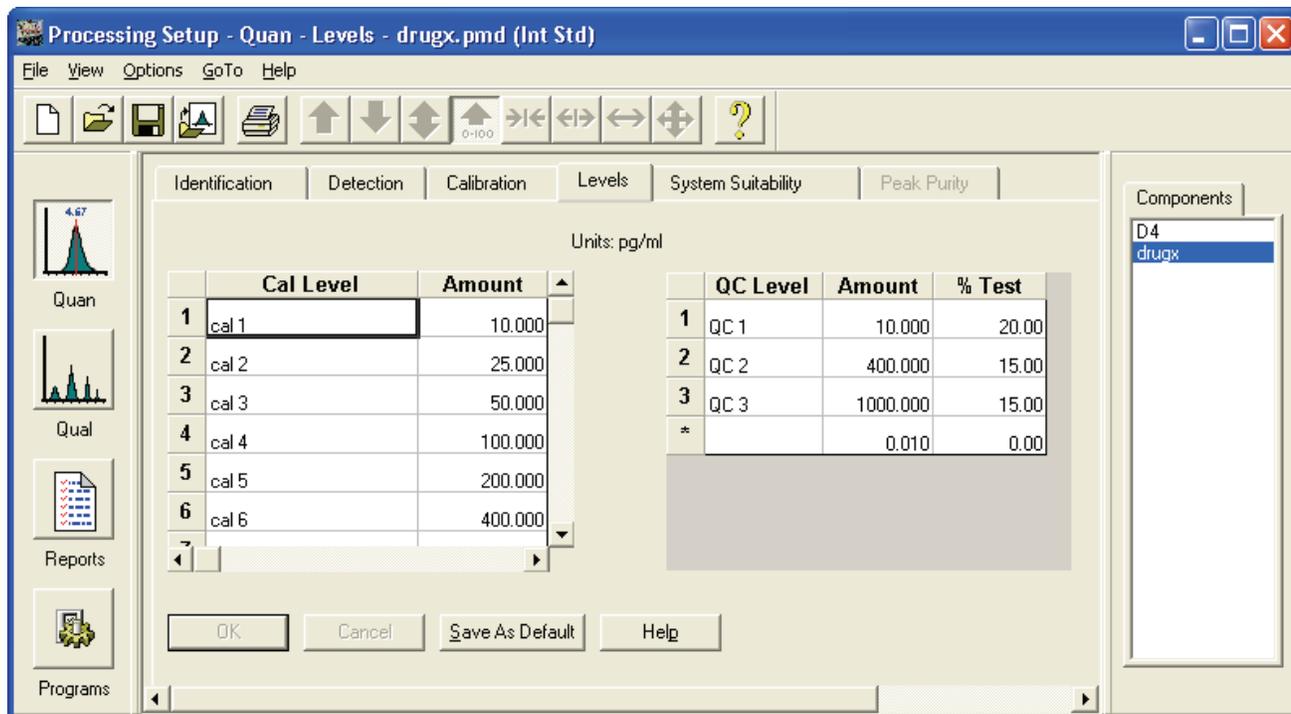
Table 2. QC Level table, showing QC levels, amounts (in pg/injection), and % Test for drugx

QC Level	Amount	% Test
QC 1	10	20
QC 2	400	15
QC 3	1000	15

8. To save the calibration and QC level settings, click **OK**.

The Levels page should look like the one shown in [Figure 23](#).

Figure 23. Levels page, showing the completed Calibration Level and QC Level tables



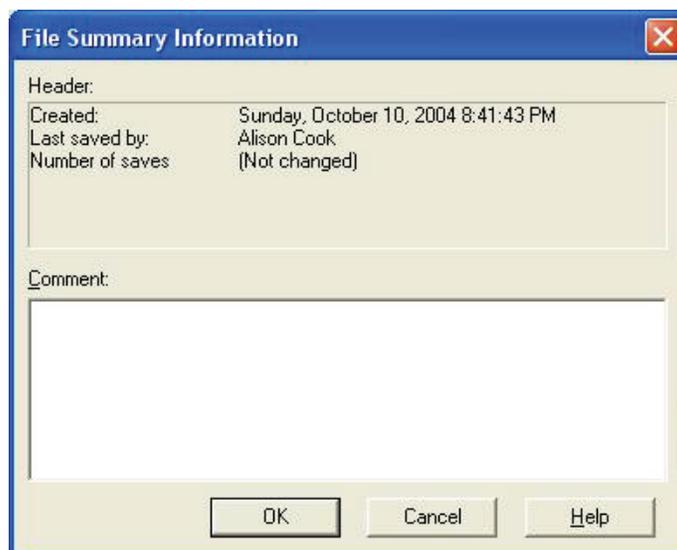
Saving the Processing Method

Before you exit the Processing Setup window, save the processing method.

❖ **To save the processing method**

1. Choose **File > Save As**. The File Summary Information dialog box opens.
2. Type **Processing method for drugx example** in the Comment box (see [Figure 24](#)).

Figure 24. File Summary Information dialog box



3. Click **OK**. The Save As dialog box opens.
4. Browse to the C:\Xcalibur\examples\methods folder or the directory where you saved the the data system examples.
5. Type **drugx_example.pmd** in the File Name box.
6. To save the processing method and close the dialog box, click **Save**.

Batch Processing Data Files

After creating a processing method, add it to the sequence used to acquire the drugx data set. After the Xcalibur data system batch processes the sequence containing the processing method, the software creates a result file for each raw file.

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

This tutorial describes how to add a processing method to a sequence and how to batch process a sequence using the drugx raw data files.

Contents

- [Adding a Processing Method to a Sequence](#)
- [Batch Processing the Sequence to Produce Results Files](#)

Adding a Processing Method to a Sequence

A sequence is a list containing sample acquisition and processing information. Sequence files in the Xcalibur data system have an .sld file extension. Sequences in the application use two types of methods: an instrument method and a processing method. Use the instrument method to acquire data files and use the processing method to process the information contained in the data files after they are acquired.

To quantify the drugx target compound in the example data files, add the drugx_example.pmd processing method to the existing drugx.sld sequence.

Note For additional information about setting up a sequence for quantitative analysis, go to the *Quantitative Analysis User Guide*.

❖ To add the processing method to the sequence

1. If you are working in Processing Setup, choose **GoTo > Xcalibur Home Page**. The Xcalibur Home Page window opens (see [Figure 25](#)).

Figure 25. GoTo menu in Processing Setup



2. To open the Sequence Setup view, click .
3. Choose **File > Open**.
4. Browse to the C:\Xcalibur\examples\methods\drugx.sld sequence file.
5. Select **drugx.sld** and click **Open**.

Sequence Setup displays the drugx.sld sequence (see [Figure 26](#)).

Figure 26. Sequence Setup view, showing the sequence drugx.sld saved on the C:\ drive

	Sample Type	File Name	implate	Path	Inst Meth	Proc Meth	Position	Inj Vol	Level
1	Std Bracket	drugx_01	01	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx	102	50.00	cal 1
2	Std Bracket	drugx_02	02	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx	103	50.00	cal 1
3	Std Bracket	drugx_03	03	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx	104	50.00	cal 1
4	Std Bracket	drugx_04	04	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx	105	50.00	cal 2
5	Std Bracket	drugx_05	05	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx	108	50.00	cal 3
6	Std Bracket	drugx_06	06	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx	109	50.00	cal 4
7	Std Bracket	drugx_07	07	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx	110	50.00	cal 5
8	Std Bracket	drugx_08	08	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx	111	50.00	cal 6
9	Std Bracket	drugx_09	09	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx	112	50.00	cal 7
10	Std Bracket	drugx_10	10	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx	113	50.00	cal 8
11	Std Bracket	drugx_11	11	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx	114	50.00	cal 9
12	Std Bracket	drugx_12	12	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx	115	50.00	cal 9
13	Std Bracket	drugx_13	13	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx	116	50.00	cal 9
14	QC	drugx_14	14	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx	121	50.00	QC 1
15	QC	drugx_15	15	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx	122	50.00	QC 1
16	QC	drugx_16	16	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx	123	50.00	QC 1
17	QC	drugx_17	17	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx	124	50.00	QC 1
18	QC	drugx_18	18	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx	125	50.00	QC 1
19	QC	drugx_19	19	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx	126	50.00	QC 1
20	QC	drugx_20	20	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx	133	50.00	QC 2
21	QC	drugx_21	21	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx	134	50.00	QC 2
22	QC	drugx_22	22	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx	135	50.00	QC 2
23	QC	drugx_23	23	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx	136	50.00	QC 2
24	QC	drugx_24	24	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx	137	50.00	QC 2
25	QC	drugx_25	25	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx	138	50.00	QC 2
26	QC	drugx_26	26	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx	139	50.00	QC 3
27	QC	drugx_27	27	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx	140	50.00	QC 3
28	QC	drugx_28	28	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx	141	50.00	QC 3
29	QC	drugx_29	29	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx	142	50.00	QC 3
30	QC	drugx_30	30	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx	143	50.00	QC 3
31	QC	drugx_31	31	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx	144	50.00	QC 3
*								0.00	

6. To change the processing method to C:\Xcalibur\examples\methods\drugx_example.pmd in the sequence:
 - a. Double-click the top cell (cell number 1) in the Proc Meth column. The Select Processing Method dialog box opens.
 - b. Browse to the C:\Xcalibur\examples\methods\drugx_example.pmd processing method.
 - c. Select **drugx_example.pmd** and click **Open** to enter the C:\Xcalibur\examples\methods\drugx_example.pmd processing method in all the rows of the sequence.
7. To change some of the QC sample types to unknown sample types, click row 14 of the Sample Type column and select the **Unknown** sample type from the list. Repeat this procedure to select the Unknown sample type for rows 15 to 18, 20 to 24, 26 to 30.

3 Batch Processing Data Files

Adding a Processing Method to a Sequence

The sequence should now look like the one shown in [Figure 27](#).

Figure 27. Drugx sequence, with drugx_example.pmd selected as the processing method

	Sample Type	File Name	Sample ID	Path	Inst Meth	Proc Meth	Position	Inj Vol	Level
1	Std Bracket	drugx_01	01	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx_example	102	50.00	cal 1
2	Std Bracket	drugx_02	02	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx_example	103	50.00	cal 1
3	Std Bracket	drugx_03	03	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx_example	104	50.00	cal 1
4	Std Bracket	drugx_04	04	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx_example	105	50.00	cal 2
5	Std Bracket	drugx_05	05	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx_example	108	50.00	cal 3
6	Std Bracket	drugx_06	06	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx_example	109	50.00	cal 4
7	Std Bracket	drugx_07	07	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx_example	110	50.00	cal 5
8	Std Bracket	drugx_08	08	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx_example	111	50.00	cal 6
9	Std Bracket	drugx_09	09	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx_example	112	50.00	cal 7
10	Std Bracket	drugx_10	10	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx_example	113	50.00	cal 8
11	Std Bracket	drugx_11	11	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx_example	114	50.00	cal 9
12	Std Bracket	drugx_12	12	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx_example	115	50.00	cal 9
13	Std Bracket	drugx_13	13	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx_example	116	50.00	cal 9
14	Unknown	drugx_14	14	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx_example	121	50.00	
15	Unknown	drugx_15	15	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx_example	122	50.00	
16	Unknown	drugx_16	16	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx_example	123	50.00	
17	Unknown	drugx_17	17	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx_example	124	50.00	
18	Unknown	drugx_18	18	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx_example	125	50.00	
19	QC	drugx_19	19	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx_example	126	50.00	QC 1
20	Unknown	drugx_20	20	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx_example	133	50.00	
21	Unknown	drugx_21	21	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx_example	134	50.00	
22	Unknown	drugx_22	22	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx_example	135	50.00	
23	Unknown	drugx_23	23	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx_example	136	50.00	
24	Unknown	drugx_24	24	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx_example	137	50.00	
25	QC	drugx_25	25	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx_example	138	50.00	QC 2
26	Unknown	drugx_26	26	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx_example	139	50.00	
27	Unknown	drugx_27	27	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx_example	140	50.00	
28	Unknown	drugx_28	28	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx_example	141	50.00	
29	Unknown	drugx_29	29	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx_example	142	50.00	
30	Unknown	drugx_30	30	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx_example	143	50.00	
31	QC	drugx_31	31	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx_example	144	50.00	QC 3
*								0.00	

- To save the sequence, choose **File > Save As**. Type **sample Drugx_Example sequence** in the Comment box (see [Figure 28](#)).

Figure 28. File Summary Information dialog box

File Summary Information

Header:

Created: Friday, January 07, 2005 3:27:37 PM

Last saved by:

Number of saves (Not changed)

Comment:

sample DrugX_Example sequence

OK Cancel Help

9. Click **OK**. The Save As dialog box opens.
10. Type **drugx_example** in the File Name box and click **Save**. The sequence is saved as C:\Xcalibur\examples\methods\drugx_example.sld.

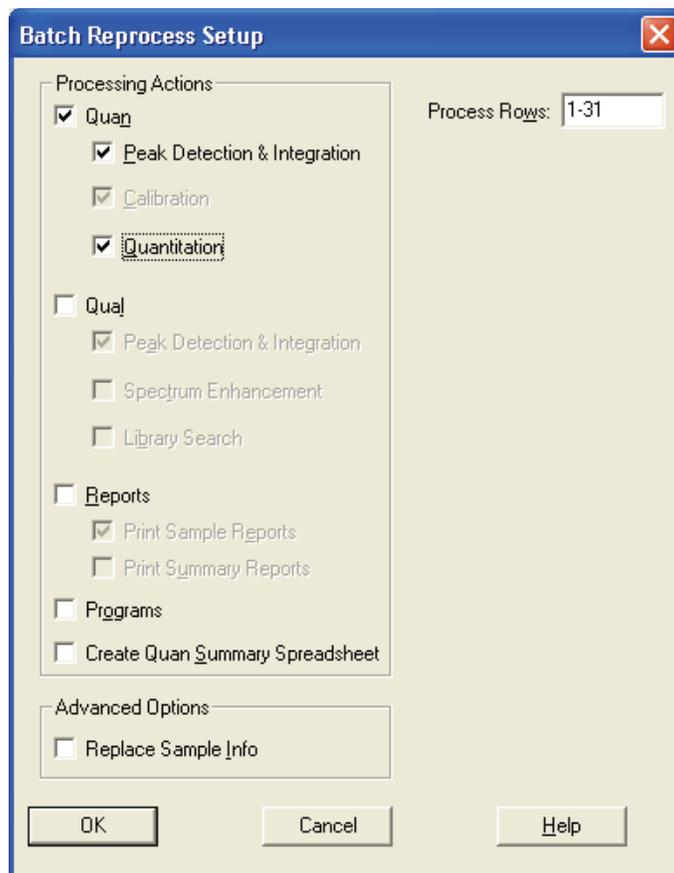
Batch Processing the Sequence to Produce Results Files

After adding a processing method to the sequence, batch process data files to produce results files that can be viewed in Quan Browser.

❖ To batch process the sequence and perform a quantitative analysis on the raw data files

1. Click  or choose **Actions > Batch Reprocess**. The Batch Reprocess Setup dialog box opens.

Figure 29. Batch Reprocess Setup dialog box



2. To set the batch process options as shown in [Figure 29](#), select the **Quan**, **Peak Detection & Integration**, and **Quantitation** check boxes.
3. Type **1-31** in the Process Rows box.

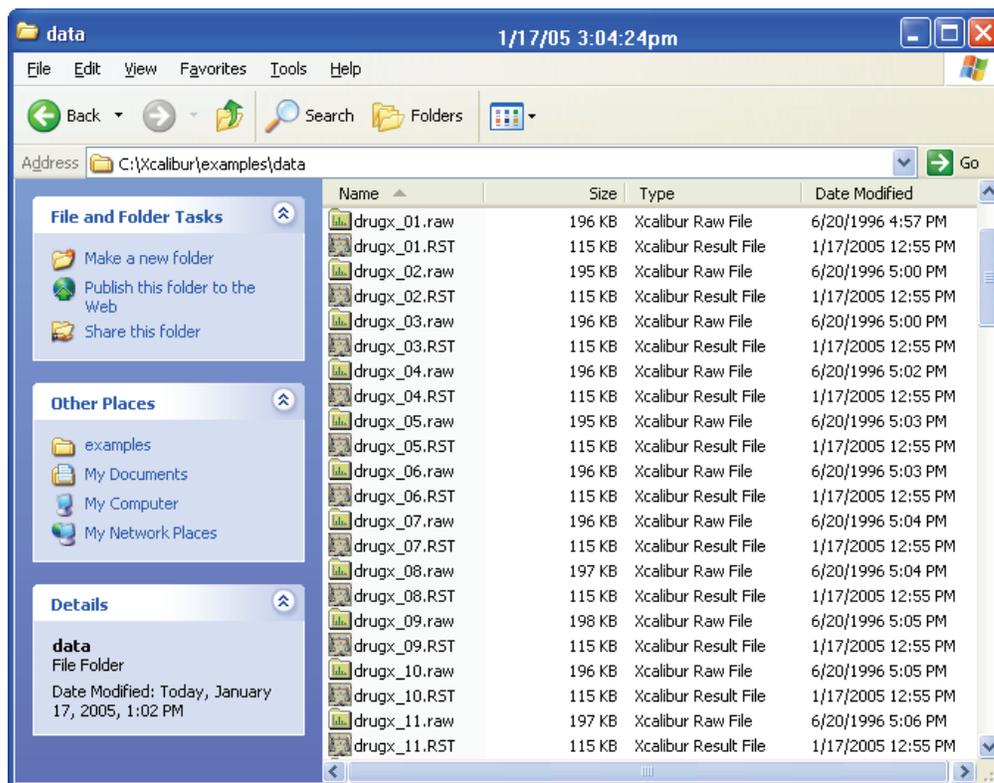
3 Batch Processing Data Files

Batch Processing the Sequence to Produce Results Files

4. To start batch processing, click **OK**.

The data system creates a results data file for each raw data file in the C:\Xcalibur\examples\data\ folder (see [Figure 30](#)).

Figure 30. Explore directory, showing the location of the raw data files [.raw] and the result data files [.rst]



Note The Xcalibur application exports the results data files to the folder where the raw files are located. In this example, the results data files and the raw data files are in C:\Xcalibur\examples\data\.

Working with Results Files in Quan Browser

After adding a processing method to the sequence and then batch processing the sequence, review the results files and the calibration curve for the drugx target component in the Quan Browser window. In addition, you can modify the identification, detection, integration, and some of the calibration parameters contained in the processing method.

This tutorial describes how to review quantitation data and how to modify portions of the processing method in Quan Browser.

Contents

- [Reviewing Sequence Files in Quan Browser](#)
- [Modifying the Processing Method in Quan Browser](#)

Reviewing Sequence Files in Quan Browser

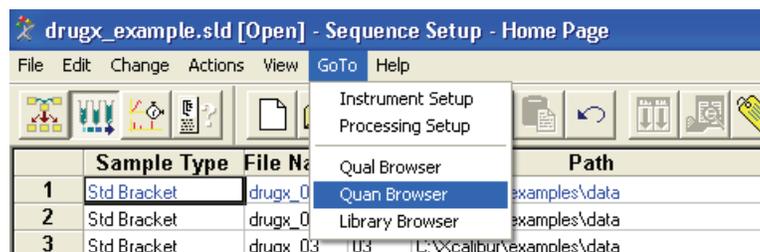
Review the quantitative analysis results of the processed drugx sample set from the Quan Browser window.

Note For additional information about using Quan Browser, go to the *Quantitative Analysis User Guide*.

❖ To review the results after you batch process a sequence

- To open the sequence in the Quan Browser window, choose one of these options:
 - If you are in the Xcalibur Home Page view, click **Quan Browser**.
 - If you are working in the Sequence Setup view, choose **GoTo > Quan Browser** (see [Figure 31](#)).

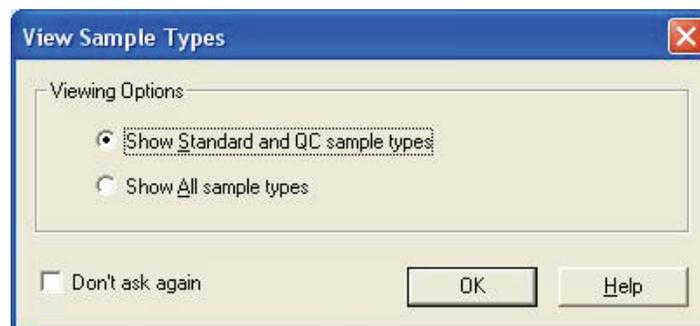
Figure 31. GoTo menu in Sequence Setup



The Open dialog box for sequence list files (*.sld) opens.

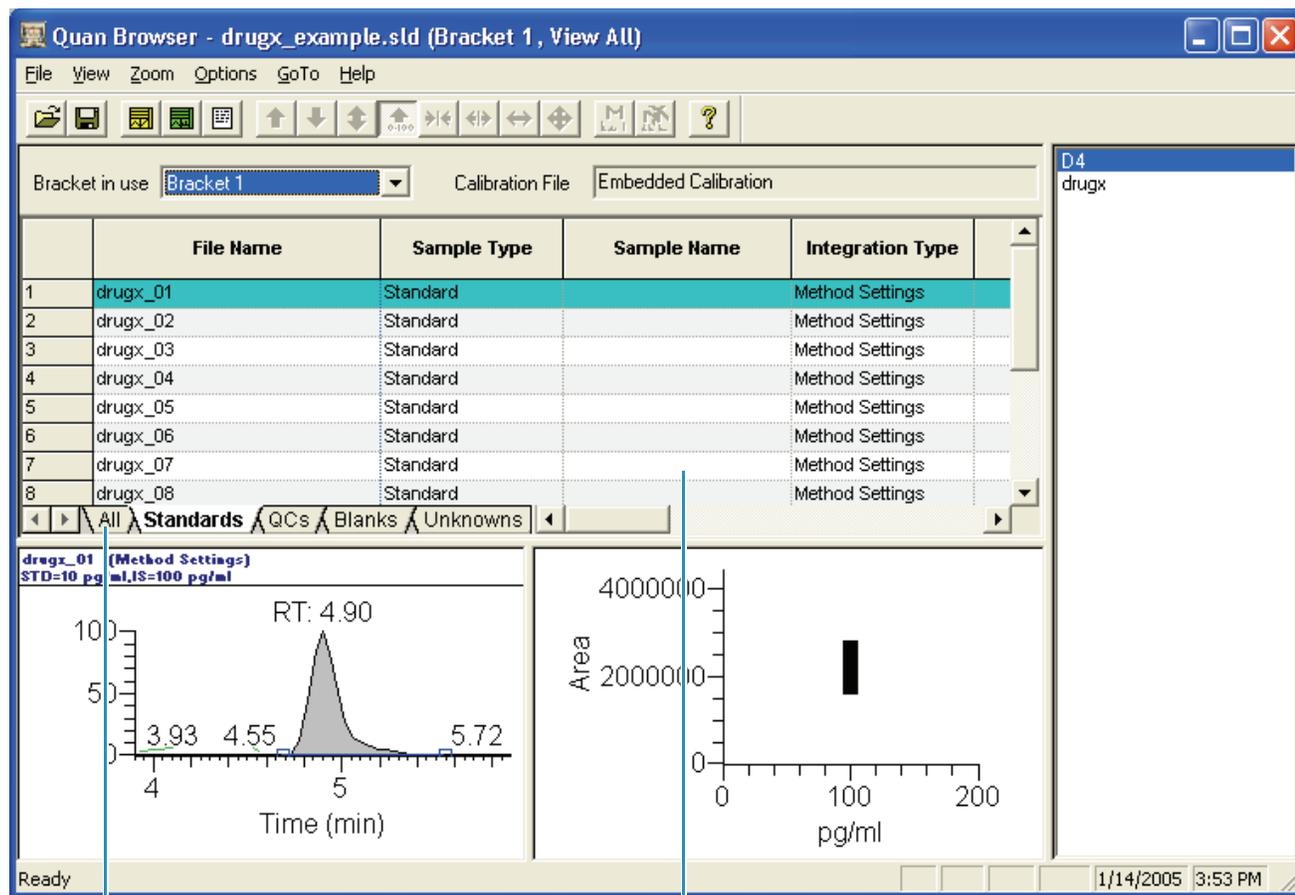
- Browse through the directories to find the C:\Xcalibur\examples\methods\drugx_example.sld sequence.
- Select **drugx_example.sld** and click **Open**. The View Sample Types dialog box opens (see [Figure 32](#)).

Figure 32. View Sample Types dialog box



- Select the **Show Standard and QC Sample Types** option and click **OK**. The drugx_example.sld sequence opens in the Quan Browser window (see [Figure 33](#)).

Figure 33. Quan Browser window, internal standard D4 selected, showing the All tab



All tab

Results grid view

5. To display all of the data files, click the **All** tab at the bottom of the Results Grid view (indicated in Figure 33).
6. To select the first data file, click the first row in the Results Grid view.
7. Check the entries for each component in the selected result grid row for peak detection and integration problems. Make sure that the selected data file corresponds to the correct level and sample type. If necessary, modify the peak identification, detection, or integration parameters in the processing method.

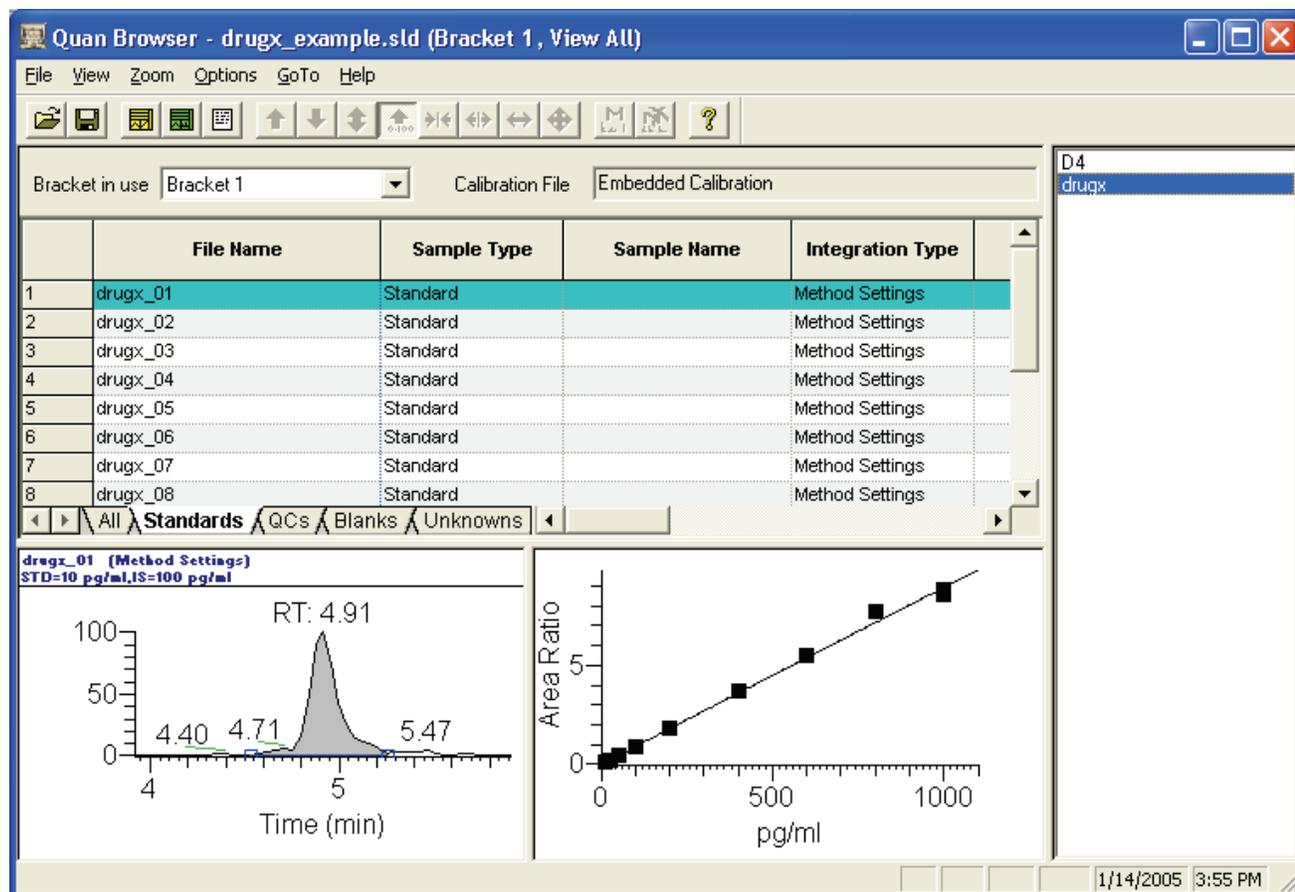
Note Modify the processing method in either Processing Setup or Quan Browser. In Quan Browser, modify the calibration curve and calibration levels settings of the processing method in the Calibration Settings dialog box. To open the Calibration Settings dialog box, right-click the Calibration Curve view and choose **Calibration Settings** from the shortcut menu. To save the modified processing method, choose **File > Export Method** in the Quan Browser window. For more information about processing methods, see Chapter 2, “Creating a Processing Method.”

4 Working with Results Files in Quan Browser

Reviewing Sequence Files in Quan Browser

8. Inspect the component peak in the Chromatogram Plot view. Verify that the Xcalibur data system found the peak. The application shades found peaks gray and marks the starting and ending points with square integration markers. Make sure that the application integrated the peak properly and that the shaded area accurately represents the contribution of the component to the chromatogram. If necessary, modify the peak detection or integration parameters of the processing method.
9. Click the next row in the Results Grid view to select the next data file. Perform steps 7 and 8 for each data file.
10. Select **drugx** in the Components list to display the results for the target compound. Perform steps 7 and 8 for the target compound for each data file.
11. Inspect the calibration curve in the Calibration Curve Plot view. Evaluate the calibration curve according to the criteria used in the local laboratory. If necessary, modify the calibration curve parameters of the processing method (see Figure 34). For more information about modifying processing methods, see Chapter 2, “Creating a Processing Method.”

Figure 34. Quan Browser window, with the target compound drugx selected



Modifying the Processing Method in Quan Browser

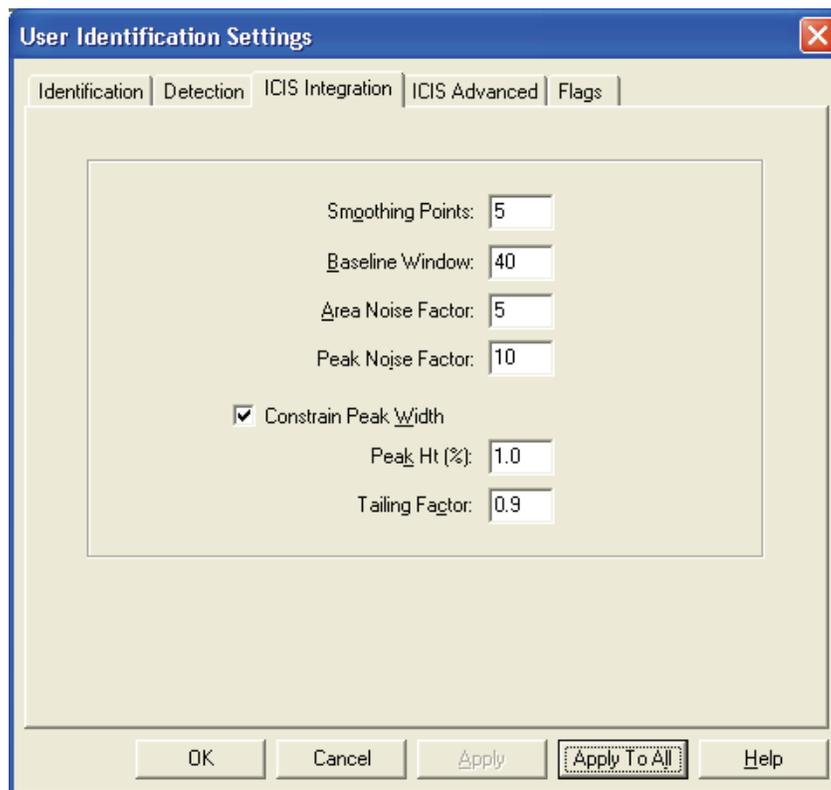
You can modify some sections of the processing method in Quan Browser, including the identification, detection, and integration parameters for the peaks in the components list or several of the calibration curve parameters. You cannot modify the amounts for the calibration levels, but you can exclude calibration points from the calibration curve.

❖ To modify the processing method

1. Select **drugx** from the component list on the right side of the Quan Browser window.
2. To modify an identification, detection, or integration parameter, such as Constrain Peak Width, right-click the Chromatogram Plot view to open a shortcut menu and choose **User Peak Detection Settings**.

The User Identification Settings dialog box opens (see [Figure 35](#)).

Figure 35. User Identification Settings dialog box



- a. Click the **ICIS Integration** tab. The ICIS Integration page opens.
- b. Select the **Constrain Peak Width** check box.
- c. Type **1** in the Peak Ht[%] box.
- d. Type **0.9** in the Tailing Factor box.
- e. Click **Apply To All** to update the integration of the results files in the sequence.

4 Working with Results Files in Quan Browser

Modifying the Processing Method in Quan Browser

The Processing dialog box opens and processes the results files in the open sequence. View the result of this new setting in the Chromatogram Plot view.

Note This new integration setting is temporary unless you save it to the processing method by exporting the method.

3. To modify the calibration curve, do the following:
 - a. Right-click the Calibration Curve Plot view to open a shortcut menu.
 - b. Choose **Calibration Settings**. The Calibration Options dialog box opens.
 - c. Click the **Curve** tab. The Curve page opens.
 - d. Select **Linear** from the Calibration Curve Type list.
 - e. To display the new curve fit in the Calibration Curve Plot view, click **Apply**.
 - f. Click **OK** to close the dialog box.
4. To save the modifications as a new processing method, do the following:
 - a. Choose **File > Export Method**.
The Save As dialog box opens.
 - b. Type **drugx_example_2** in the File Name box.
 - c. Browse to the C:\Xcalibur\examples\methods folder in the Directories box.
 - d. Click **OK**.

Previewing, Specifying, and Printing Reports

To print reports as you batch process a sequence, specify one or more report templates in the processing method.

This tutorial describes how to review, specify, and print reports.

Contents

- [Previewing Reports in XReport](#)
- [Specifying Report Templates in the Processing Method](#)
- [Printing Reports](#)

Previewing Reports in XReport

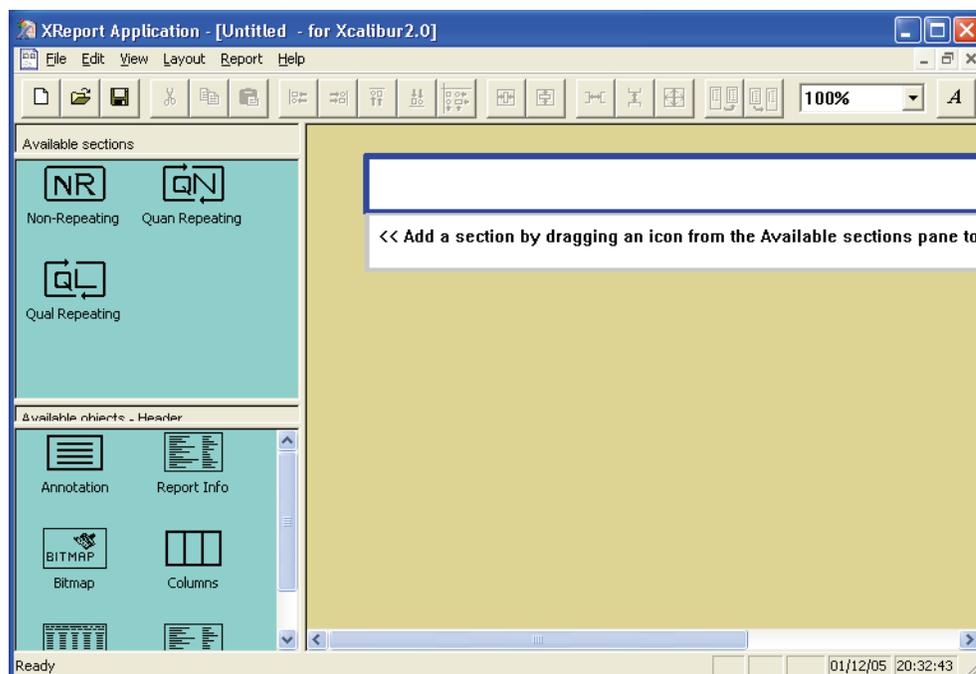
Before adding a report template to the processing method or before using the processing method to print reports, preview the results of the selected template with representative data in XReport. Previewing a report helps to print reports with adequate information and efficient formatting.

❖ To preview a representative display of the report template

1. To start the XReport application, double-click  on the desktop or choose **Start > Programs > Thermo Xcalibur > XReport** from the computer taskbar.

XReport opens and creates a new template (see [Figure 36](#)).

Figure 36. XReport Application window showing a new blank report template

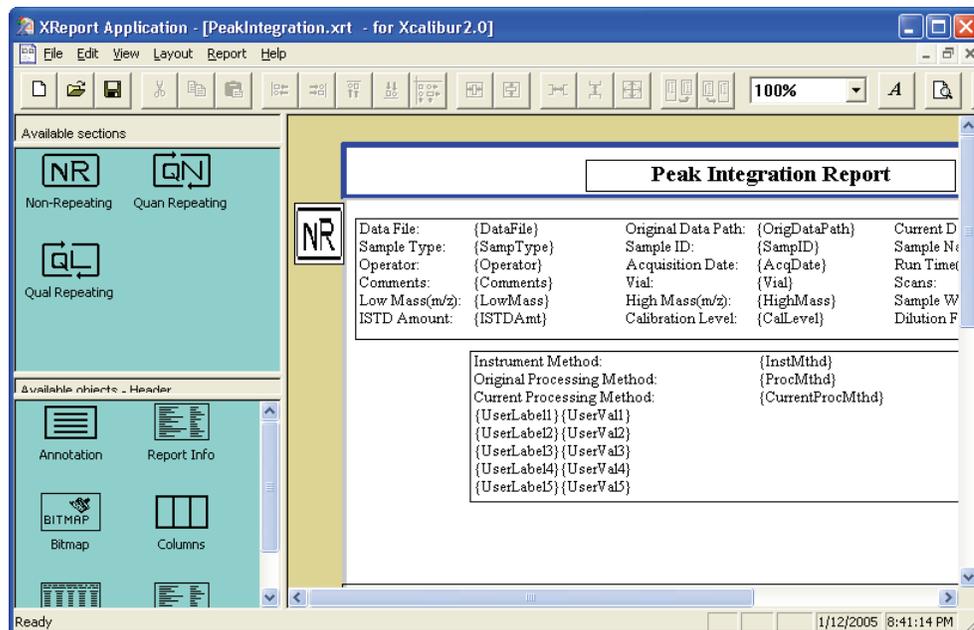


2. Choose **File > Open**. The XReport Templates dialog box opens.

3. Select **PeakIntegration.xrt** and click **Open**.

XReport opens the PeakIntegration.xrt report template (see [Figure 37](#)).

Figure 37. PeakIntegration.xrt report template

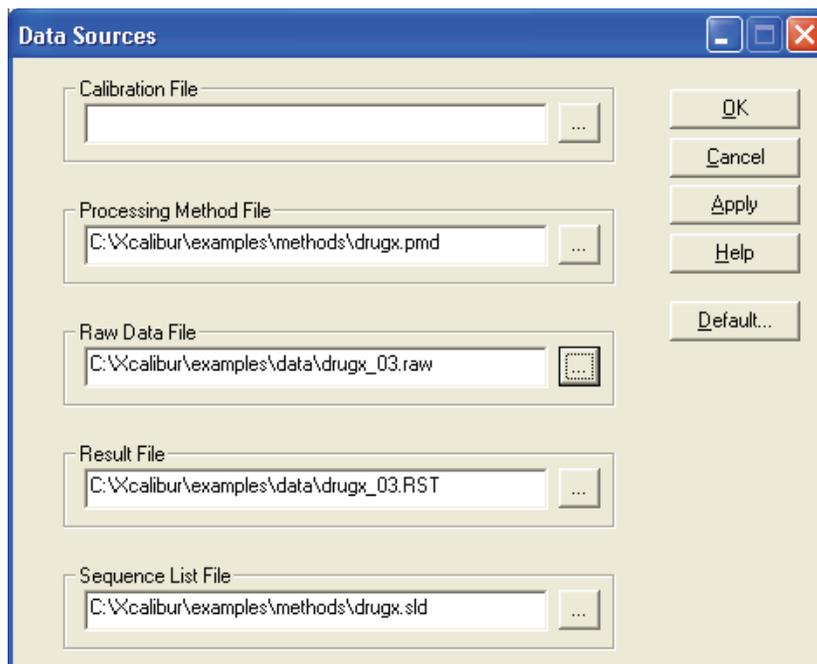


4. To select a representative data file to test the peak integration, choose **Report > Data Sources**. The Data Sources dialog box opens. Enter source information.
 - a. Click  in the Raw Data File area. The Select Raw File dialog box opens.
 - b. Select **drugx_03.raw** and click **Open**.
 - c. Click  in the Result File area.
 - d. Select **drugx_03.RST** and click **Open**. All selections in the dialog box should look like those in [Figure 38](#).
 - e. Click **OK**.

5 Previewing, Specifying, and Printing Reports

Previewing Reports in XReport

Figure 38. Data Sources dialog box



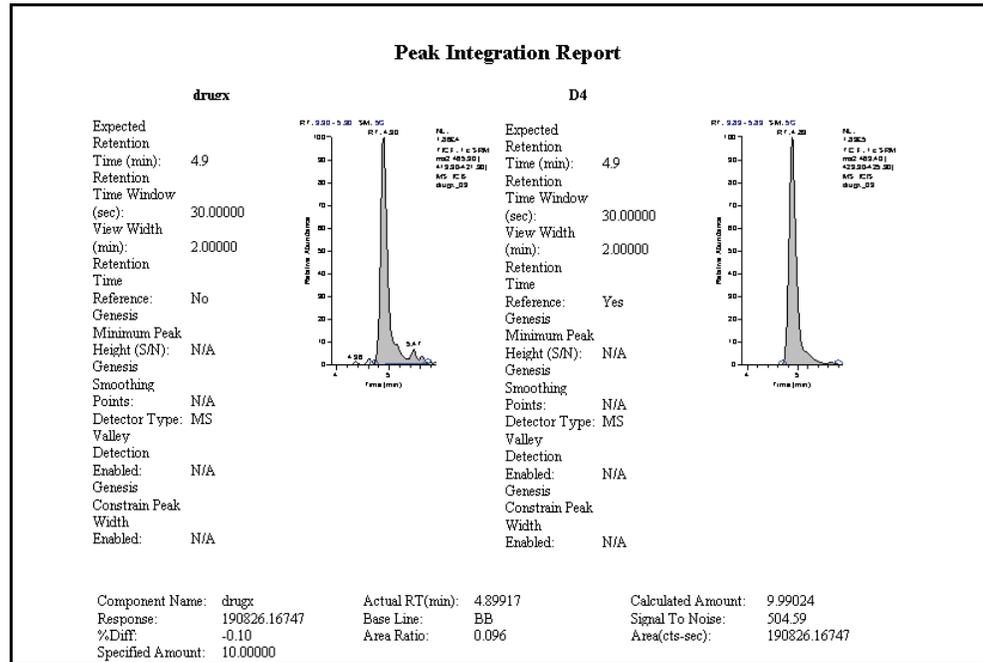
5. Choose **Report > Resolve Report** from the XReport main window.

The peak integration report opens, displaying the data from the drugx.rst file (see [Figure 39](#) and [Figure 40](#)).

Figure 39. Peak Integration Report, page 1

Peak Integration Report			
Data File:	drugx_03	Original Data Path:	C:\LCQ\Data\mrw_27_417\Sat_0504_WD1
Sample Type:	Std Update	Sample ID:	04
Operator:	linda	Acquisition Date:	05/04/96 10:31:23 PM
Comments:	STD=10 pg/ml,IS=100 pg/ml	Vial:	104
Low Mass(m/z):	419.30	High Mass(m/z):	425.30
ISTD Amount:	0.000	Calibration Level:	
Instrument Method:		Current Data Path:	C:\Xcalibur\example\data
Original Processing Method:		Sample Name:	
Current Processing Method:		Run Time(min):	6.98
Study		Scans:	314
Client		Sample Weight:	0.00
Laboratory		Dilution Factor:	1.00
Company			
Phone			

Figure 40. Peak Integration Report, page 2



6. Close the report.
7. Choose **File > Open**. The XReport Templates dialog box opens.
8. Select **CompCalReport_ICIS.xrt** and click **Open**.
 XReport opens the CompCalReport_ICIS.xrt report template.
9. To select a representative sequence file to test the component calibration report:
 - a. Choose **Report > Data Sources**. The Data Sources dialog box opens (see Figure 38 on page 48).
 - b. Click  in the Sequence List File area.
 The Select Sequence File dialog box opens.
 - c. Select the drugx_example.sld file and click **Open**.
 - d. Click OK to close the Data Sources dialog box.
10. Choose **Report > Resolve Report**.

The Xcalibur application combines the data with the report template and opens the component calibration report, displaying the data from the drugx_example.sld sequence file. The component calibration report for the drugx_example.sld sequence file is six pages long. Page 5, containing the calibration curve for drugx, is shown in Figure 41. Page 6, which shows the calculated amounts for drugx, is shown in Figure 42.

Figure 41. Component calibration report, showing the calibration curve for drugx, the target compound

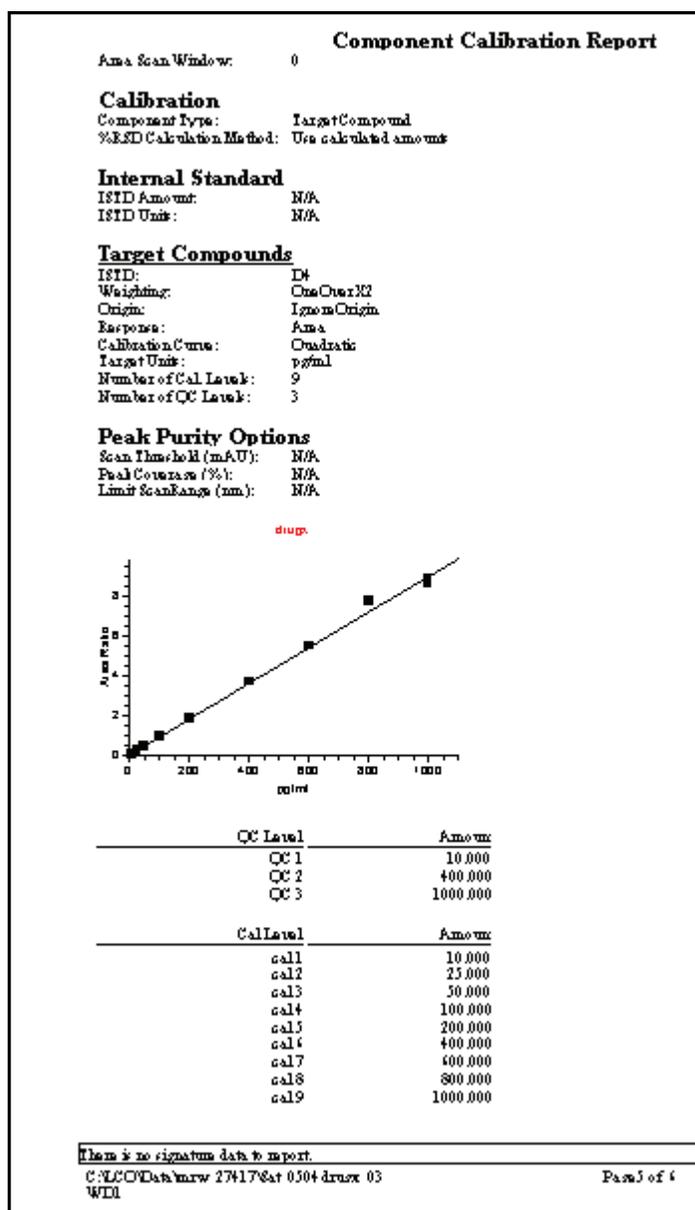


Figure 42. Component calibration report, showing the calculated amounts for drugx, the target compound

Component Calibration Report							
Sample ID	Area	Area Ratio	ISTD Area	Specified Amount	Calculated Amount	% Diff	% RSD
01	188710.251	0.091	2078851.260	10.00000pg/ml	9.47181pg/ml	-5.28	9.960
02	211511.636	0.107	1982388.747	10.00000pg/ml	11.23365pg/ml	12.34	9.960
03	180306.351	0.091	1976747.831	10.00000pg/ml	9.52022pg/ml	-4.80	9.960
04	451037.533	0.222	2031139.035	25.00000pg/ml	24.00399pg/ml	-3.98	0.000
05	885012.506	0.434	2038543.922	50.00000pg/ml	47.49013pg/ml	-5.02	0.000
06	1863855.738	0.922	2021162.567	100.00000pg/ml	101.58703pg/ml	1.59	0.000
07	3971164.797	1.835	2163988.136	200.00000pg/ml	202.97623pg/ml	1.49	0.000
08	8383333.830	3.697	2267325.391	400.00000pg/ml	410.58494pg/ml	2.65	0.000
09	12075236.424	5.487	2200807.986	600.00000pg/ml	611.04911pg/ml	1.84	0.000
10	17476372.702	7.709	2267013.730	800.00000pg/ml	861.41090pg/ml	7.68	0.000
11	21056082.091	8.604	2447194.337	1000.00000pg/ml	962.70426pg/ml	-3.73	1.570
12	21901731.830	8.608	2544250.852	1000.00000pg/ml	963.17444pg/ml	-3.68	1.570
13	22971424.038	8.839	2598948.309	1000.00000pg/ml	989.28833pg/ml	-1.07	1.570
14	311190.520	0.138	2259271.484	N/A	14.66965pg/ml	N/A	N/A
15	225704.696	0.115	1962050.435	N/A	12.15669pg/ml	N/A	N/A
16	227047.300	0.109	2090424.803	N/A	11.44590pg/ml	N/A	N/A
17	217023.171	0.107	2026948.538	N/A	11.27500pg/ml	N/A	N/A
18	213032.790	0.102	2080418.832	N/A	10.75815pg/ml	N/A	N/A
19	206836.121	0.118	1749375.294	10.00000pg/ml	12.51077pg/ml	25.11	0.000
20	7961931.521	3.821	2083738.522	N/A	424.39301pg/ml	N/A	N/A
21	7930753.486	3.871	2048563.176	N/A	430.02691pg/ml	N/A	N/A
22	8884407.016	3.997	2222893.049	N/A	444.05120pg/ml	N/A	N/A
23	8677072.992	3.641	2383086.126	N/A	404.28797pg/ml	N/A	N/A
24	7716769.166	3.553	2171640.815	N/A	394.49148pg/ml	N/A	N/A
25	9381228.456	3.640	2578958.562	400.00000pg/ml	404.21187pg/ml	1.05	0.000
26	23285379.393	9.252	2516922.507	N/A	1036.11383pg/ml	N/A	N/A
27	22265730.639	8.916	2497326.380	N/A	998.02890pg/ml	N/A	N/A
28	19445064.013	8.191	2374075.563	N/A	915.87370pg/ml	N/A	N/A
29	22924140.919	8.654	2648831.276	N/A	968.39931pg/ml	N/A	N/A
30	20196941.490	8.934	2260567.165	N/A	1000.14155pg/ml	N/A	N/A
31	22277135.870	9.103	2447197.670	1000.00000pg/ml	1019.27271pg/ml	1.93	0.000

There is no signature data to report.

C:\LCQ\DATA\raw 27417\Sat 0504 drugx 03 Page 6 of 6
WD1

Specifying Report Templates in the Processing Method

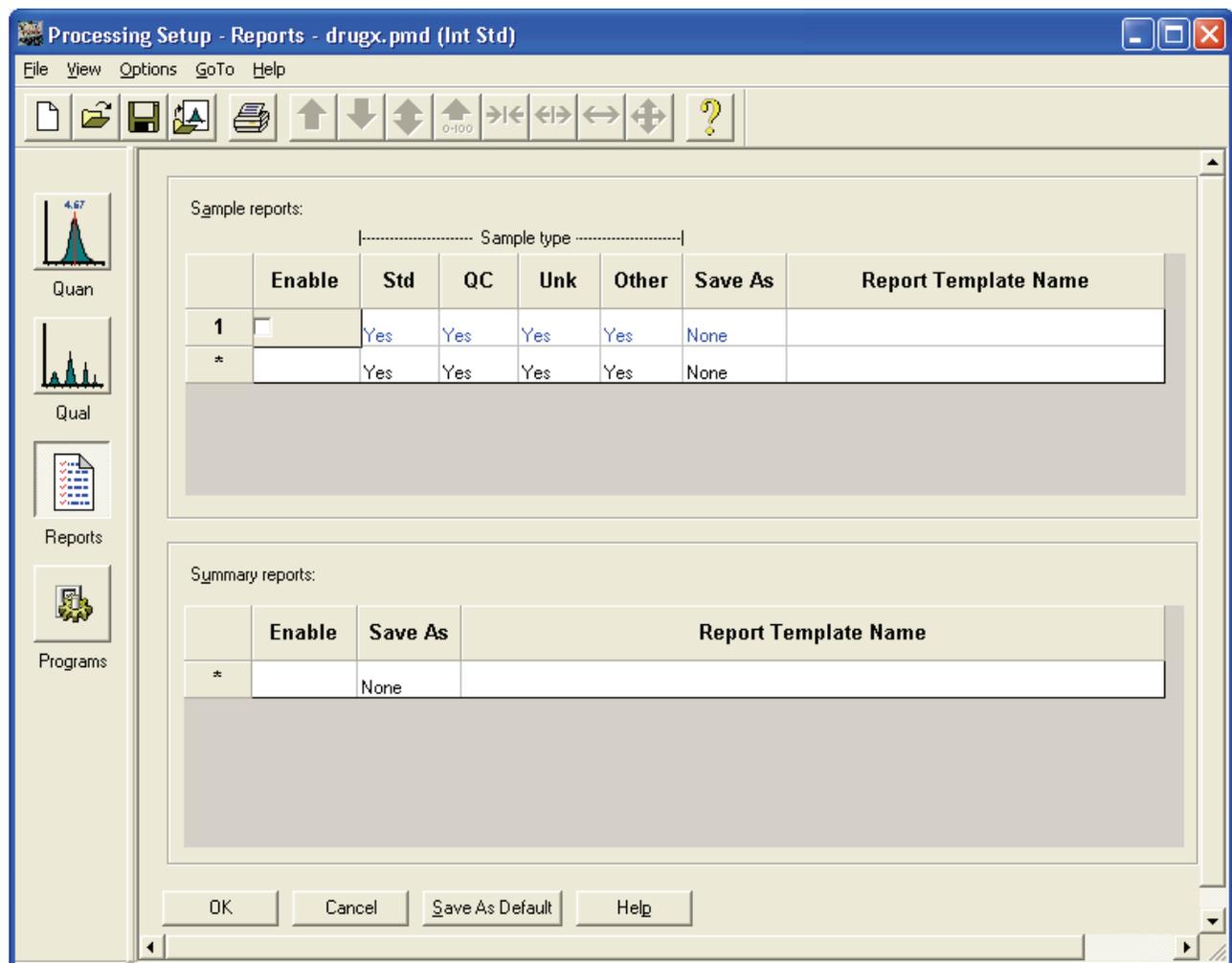
The Xcalibur data system contains a set of report templates that provide formats for reports of results. To change the layout of a report or to create a completely new template, use the XReport application to create personal custom report templates. For instructions on creating custom reports, refer to the *XReport User Guide*.

Specify the report templates to use from the Reports view of Processing Setup.

After previewing the results of combining a sample data set with the report templates, do the following:

1. Click  from the view bar in the left pane. The Reports view opens (see [Figure 43](#)).

Figure 43. Reports view of the Processing Setup window



2. In the Sample Reports table, click the first row under the Enable column. The **Enable** check box is selected.
3. Double-click the first row under the Save As column. The Save As list opens. To save the report as a .doc file, select **Doc**.

The data system saves reports generated from the processing method in the same directory as the source data files and names files in the format *data file name_template name.xxx*, where *data file name* is the name of the data file and *template name* is the name of the template used to generate the report, and *.xxx* is the suffix (for example, .doc or .pdf) indicating the file type. If more than one report is generated from the same data file and template, XReports adds a date stamp before the suffix.

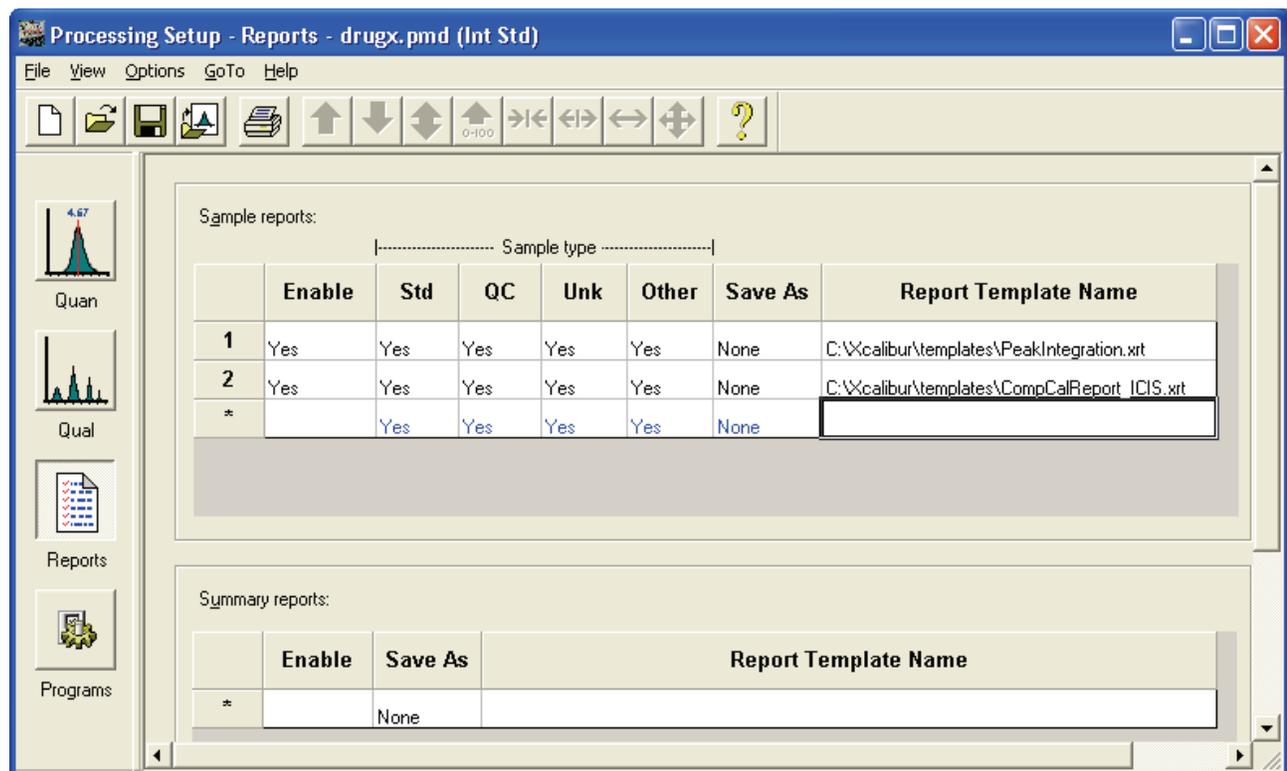
4. In the Sample Reports table, double-click the first row under the Report Template Name column.

The Browse for Sample Report Template dialog box opens.

5. To choose the sample peak integration report template, select **PeakIntegration.xrt** and click **Open**.
6. In the Sample Reports table, click the second row under the Enable column to display the Enable check box. Select the **Enable** check box.
7. Click the second row of the table under the Save As column. The Save As list opens. To save the report as a .doc file, select **Doc**.
8. Double-click the second row of the table under the Report Template Name column.
The Browse for Sample Report Template dialog box opens.
9. To choose the sample component calibration report template, select **CompCalReport_ICIS.xrt** and click **Open**.
10. Click **OK** to save the settings.

The Report view should look like [Figure 44](#).

Figure 44. Selecting peak integration report and component calibration report templates



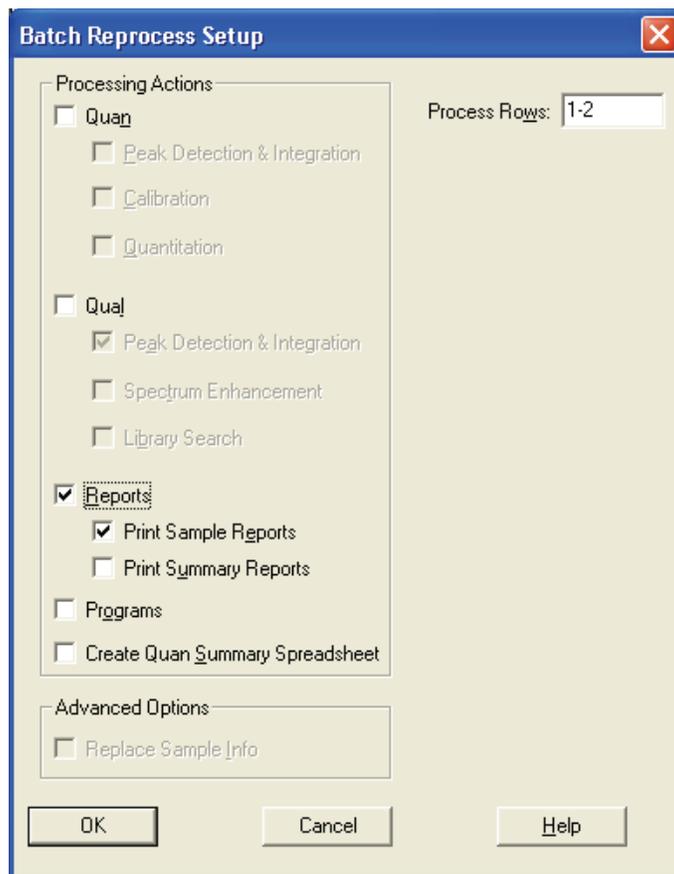
Printing Reports

Sequence Setup uses the report templates that you specified in the Reports view of Processing Setup to print reports as you batch process a sequence.

❖ To print reports

1. Click  on the Xcalibur Home Page. The Sequence Setup view opens.
2. To open the `drugx_example.sld` sequence (if it is not already open), click  on the toolbar (or choose **File > Open**). The Open dialog box opens.
3. Browse through the directories to find the `C:\Xcalibur\examples\methods\drugx_example.sld` sequence.
4. Select **drugx_example.sld** and click **Open**. The `drug_example.sld` sequence opens.
5. Choose **Actions > Batch Reprocess**. The Batch Reprocess Setup dialog box opens (see [Figure 45](#)).

Figure 45. Batch Reprocess Setup dialog box showing selections for printing reports



6. Select the **Reports** check box (see [Figure 45](#)). Select the **Print Sample Reports** check box.
7. Type **1-2** in the Process Rows box.
8. Click **OK** to start batch processing and report generation. The data system prints the reports for the first two data files in the sequence.

For more information on performing quantitative analysis, refer to the *Quantitative Analysis User Guide*.

For more information on XReport, go to the *XReport User Guide*.

System Configuration and Administration

Configuring and Setting Up Xcalibur System Components

To configure and set up Xcalibur system components for use, read these topics.

Contents

- [Configuring Xcalibur Software](#)
- [Converting File Formats](#)
- [Confirming the Properties of Finnigan Security Server](#)

Configuring Xcalibur Software

Configure the Xcalibur application using the Xcalibur Configuration dialog box. Use the pages in the dialog box to define the location of data, methods, and report templates on your data system; to edit customer information; to select the fonts that you want to use; and to select error handling options.

To configure Xcalibur software, do these procedures:

1. [Opening the Xcalibur Configuration Dialog Box](#)
2. [Selecting Default Folders](#)
3. [Updating Customer Information](#)
4. [Configuring Fonts](#)
5. [Selecting a Default Peak Detection Algorithm](#)
6. [Selecting Default Mass Options](#)
7. [Selecting Default Labeling and Scaling Options](#)
8. [Selecting Error Handling Options](#)
9. [Defining the Dataset List](#)

Opening the Xcalibur Configuration Dialog Box

❖ To open the Xcalibur Configuration dialog box

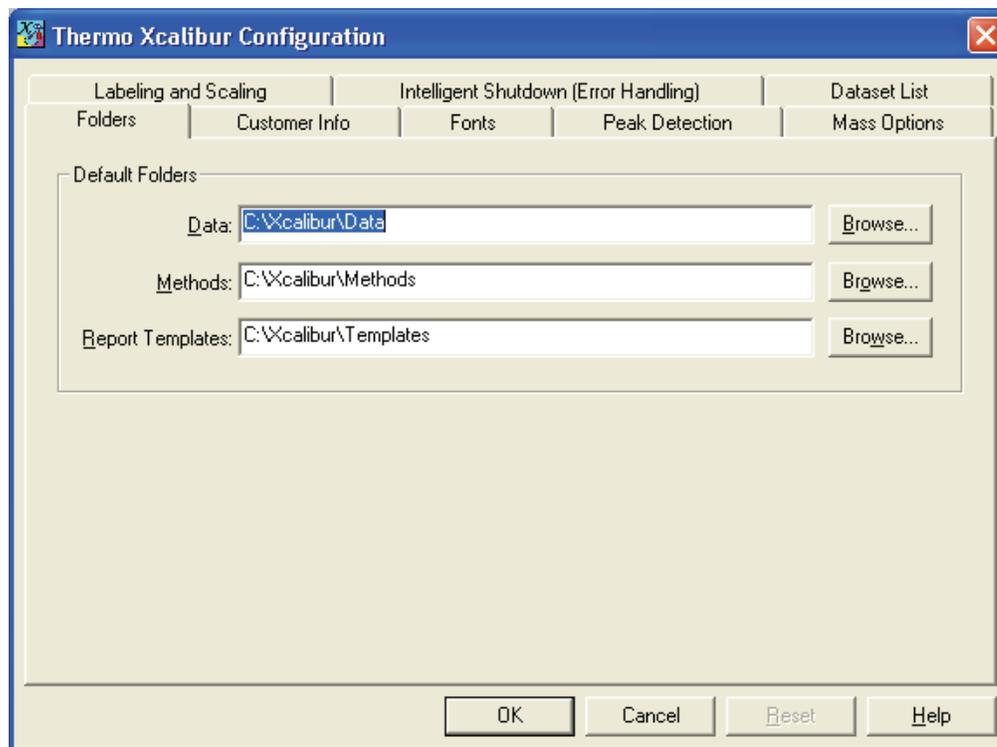
1. Choose **Start > Programs > Thermo Xcalibur > Xcalibur** from the Windows™ desktop. The Home Page window opens.
2. Choose **Tools > Configuration** from the Roadmap view of the Home Page window. The Xcalibur Configuration dialog box opens.

Selecting Default Folders

❖ To select Xcalibur default folders

1. Click the **Folders** tab. The Folders page of the Xcalibur Configuration dialog box opens (see Figure 46).

Figure 46. Folders page



2. To specify the default folder for your Xcalibur Data, click **Browse** and select the folder.
3. To specify the default folder for your Methods, click **Browse** and select the folder.
4. To specify the default folder for your Report Templates, click **Browse** and select the folder.
5. To save your settings, click **OK**.

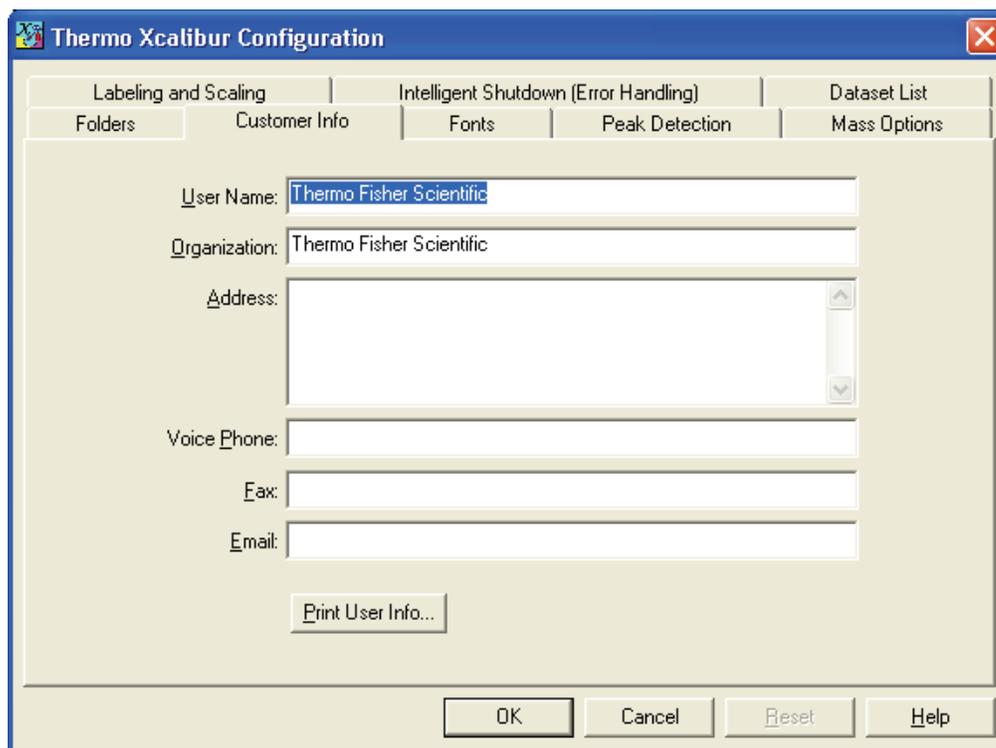
Updating Customer Information

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. Click the **Customer Info** tab. The Customer Info page of the Xcalibur Configuration dialog box opens (see [Figure 47](#)).

Figure 47. Customer Info page



The screenshot shows the 'Thermo Xcalibur Configuration' dialog box with the 'Customer Info' tab selected. The dialog box has a blue title bar and a standard Windows-style window with a close button (X) in the top right corner. The main area is divided into several tabs: 'Labeling and Scaling', 'Intelligent Shutdown (Error Handling)', 'Dataset List', 'Folders', 'Customer Info', 'Fonts', 'Peak Detection', and 'Mass Options'. The 'Customer Info' tab is active, displaying the following fields: 'User Name:' with the value 'Thermo Fisher Scientific', 'Organization:' with the value 'Thermo Fisher Scientific', 'Address:' (empty), 'Voice Phone:' (empty), 'Fax:' (empty), and 'Email:' (empty). Below these fields is a 'Print User Info...' button. At the bottom of the dialog box are four buttons: 'OK', 'Cancel', 'Reset', and 'Help'.

2. If the information on the Customer Info page is incomplete or incorrect, type the new information.
3. To save your settings, click **OK**.

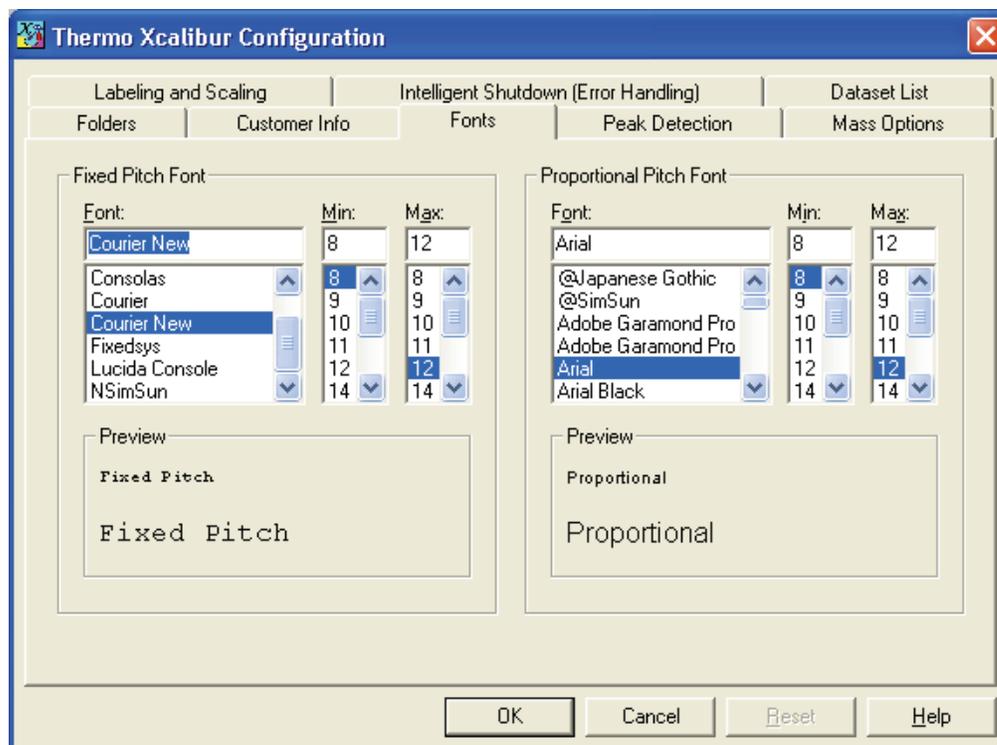
Configuring Fonts

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. Click the **Fonts** tab. The Fonts page of the Xcalibur Configuration dialog box opens (see Figure 48).

Figure 48. Fonts page



2. [Optional] To select a fixed pitch font, select a font name in the Fixed Pitch Font list. The selected font name is displayed at the top of the list.
 - a. Enter the minimum size of the selected font in the Min list.
 - b. Enter the maximum size of the selected font in the Max list.
 - c. View the font sample, minimum size (top) and maximum size (bottom), in the Fixed Pitch Font Preview area.
3. [Optional] To select a proportional font, select a font name in the Proportional Pitch Font list. The selected font name is displayed at the top of the list.
 - a. Enter the minimum size of the selected font in the Min list.

- b. Enter the maximum size of the selected font in the Max list.
- c. View the font sample, minimum size (top) and maximum size (bottom), in the Proportional Pitch Font Preview area.

Note In the Spectrum list view, if the Xcalibur application 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.

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

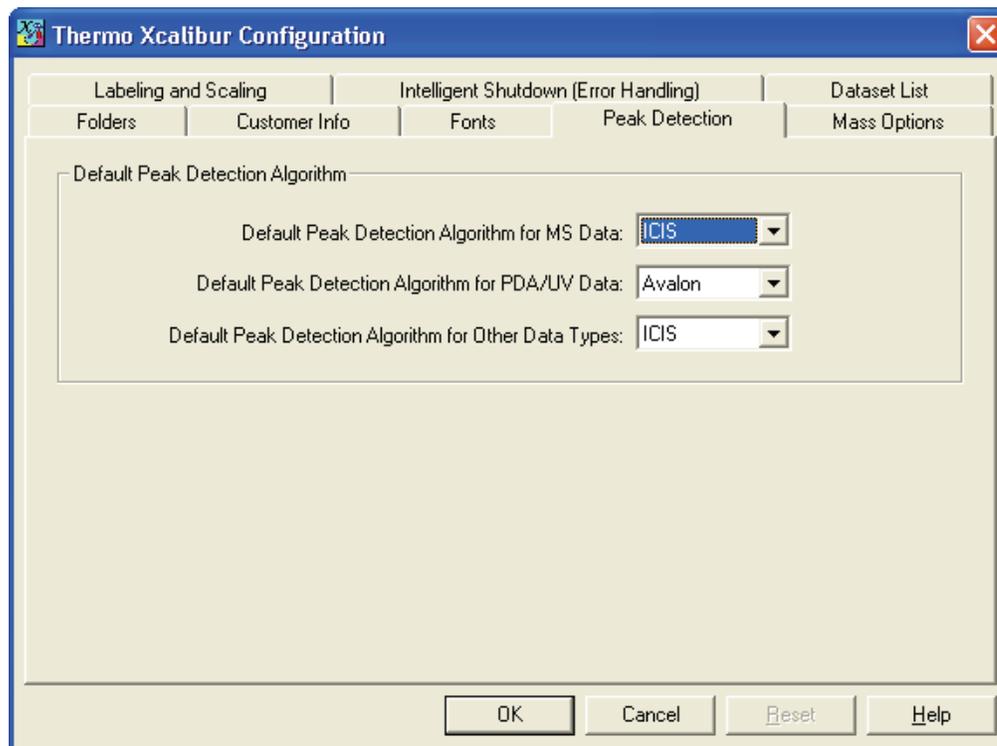
Selecting a Default Peak Detection Algorithm

Use the Peak Detection page of the Xcalibur Configuration dialog box to view or change the default peak detection algorithms for all data types.

❖ To specify peak detection parameters

1. Click the **Peak Detection** tab. The Peak Detection page of the Xcalibur Configuration dialog box opens (see [Figure 49](#)).

Figure 49. Peak Detection page



2. To select the Default Peak Detection Algorithm for MS Data, click an algorithm name from the corresponding list.
3. To select the Default Peak Detection Algorithm for PDA/UV Data, click an algorithm name from the corresponding list.
4. To select the Default Peak Detection Algorithm for Other Data Types, click an algorithm name from the corresponding list.
5. To save your settings, click **OK**.

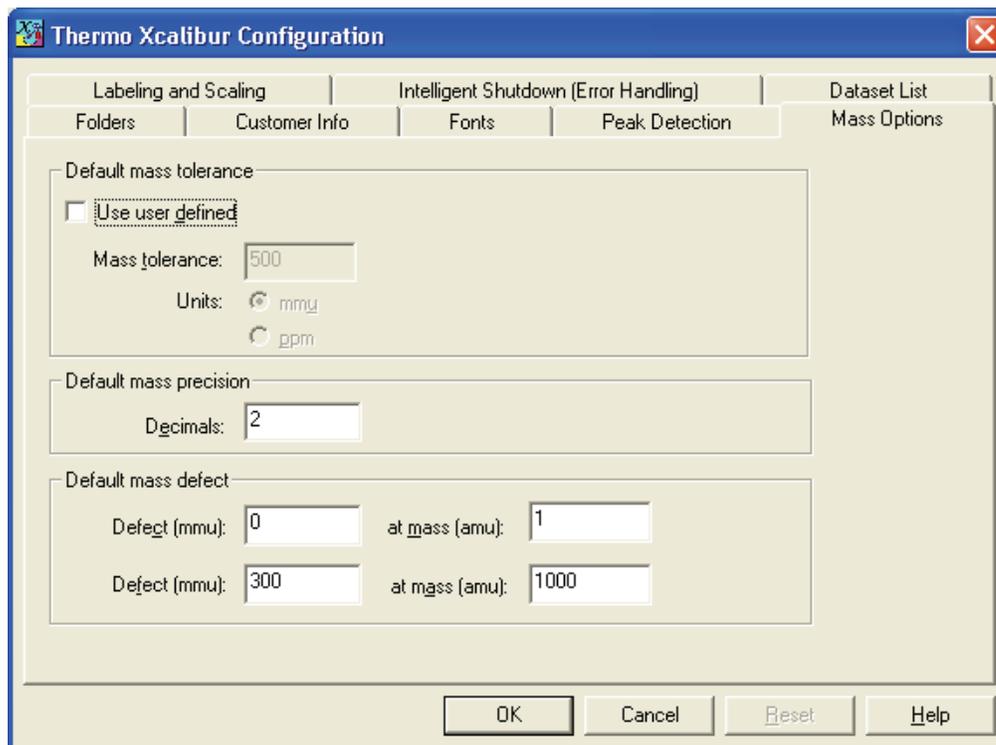
Selecting Default Mass Options

Use the Mass Options page of the Xcalibur Configuration dialog box to view or specify default parameter values that affect mass calculations and library searches.

❖ To specify mass options

1. Click the **Mass Options** tab. The Mass Options page of the Xcalibur Configuration dialog box opens (see [Figure 50](#)).

Figure 50. Mass Options page



2. Specify a default value for mass tolerance:
 - a. Select the **Use User Defined** check box in the Default Mass Tolerance area. This activates the Mass Tolerance box.
 - b. Type a value from **0.1** to **50000** in the Mass Tolerance box.
 - c. Select either **mmu** (millimass units) or **ppm** (parts per million) from the Units options.
3. To specify a default value for mass precision, type a value from **0** to **5** in the Decimals box.
4. 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 **10000** 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.
5. 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 **10000** 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.
6. To save your settings, click **OK**.

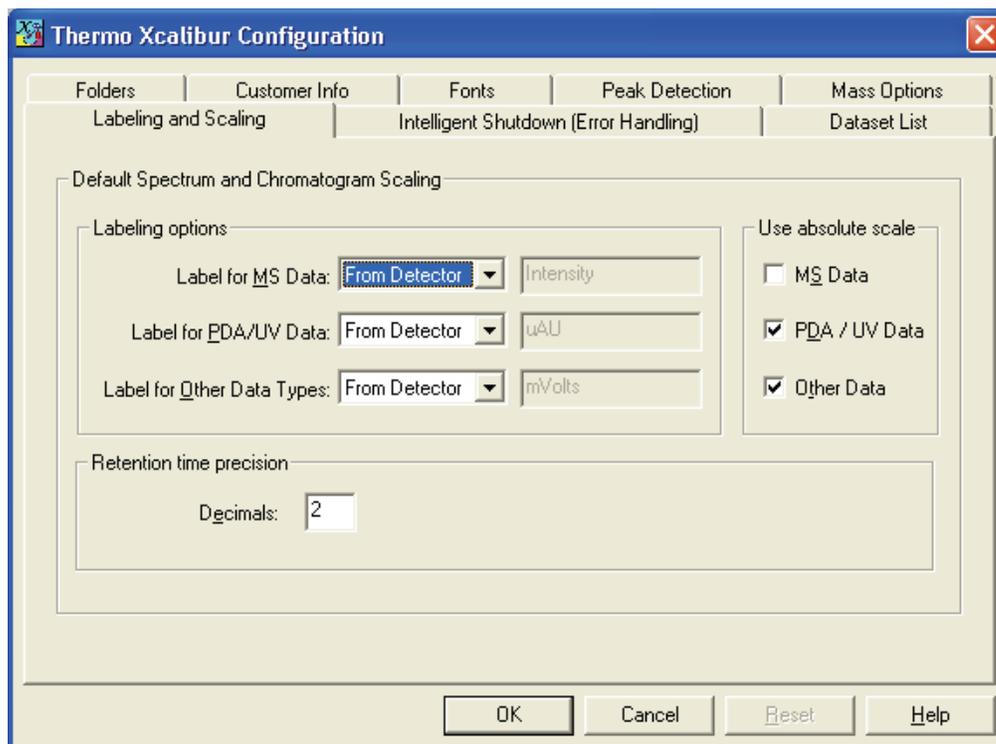
Selecting Default Labeling and Scaling Options

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 spectrum and chromatogram plots.

❖ 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 (see [Figure 51](#)).

Figure 51. Labeling and Scaling page



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**, enter 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**, enter 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**, enter 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 your settings, click **OK**.

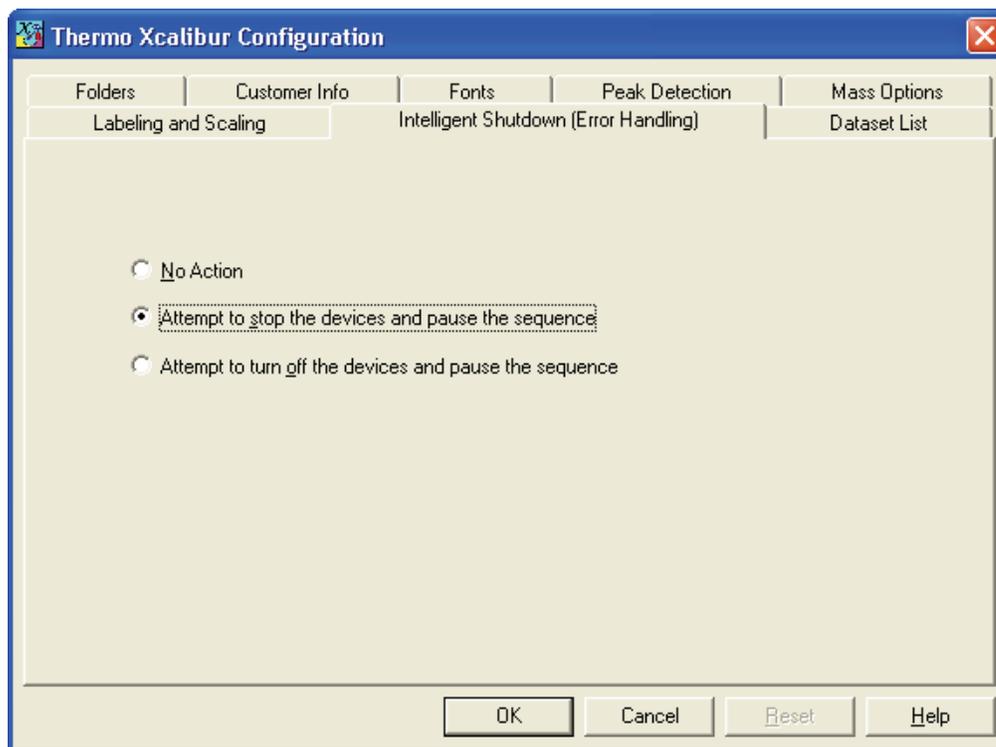
Selecting Error Handling Options

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.

❖ 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 (see [Figure 52](#)).

Figure 52. Intelligent Shutdown (Error Handling page)



2. Select the error handling option, **Attempt to Stop the Devices and Pause the Sequence**.
3. To save your settings, click **OK**.

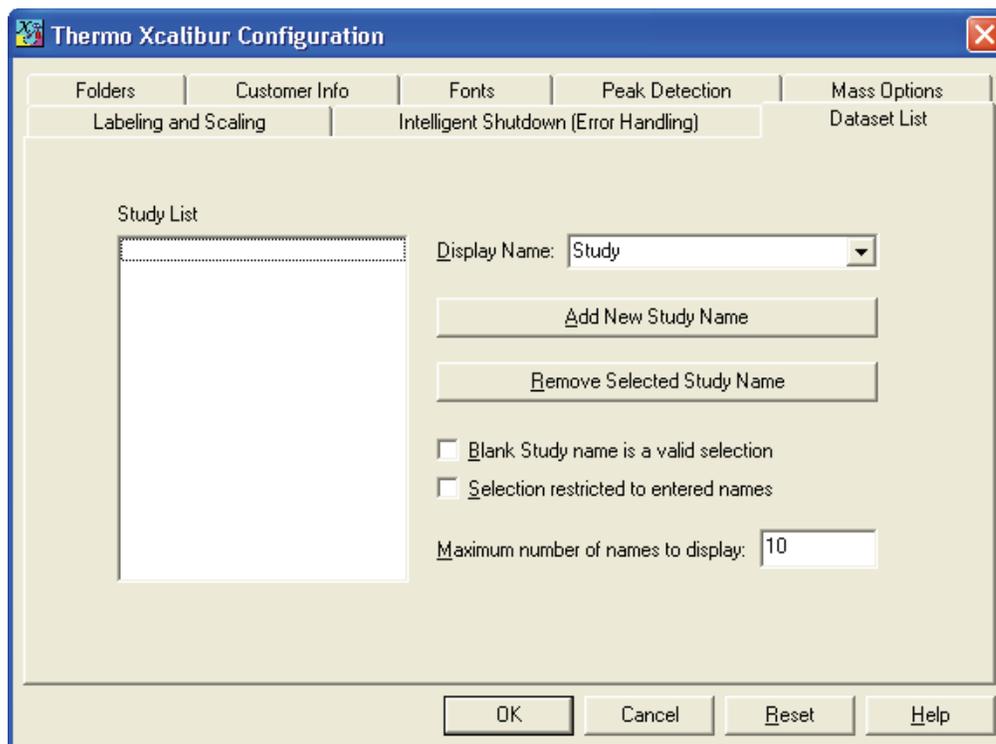
Defining the Dataset List

As 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.

❖ To define the list of dataset names

1. Click the **Dataset List** tab. The Dataset List page of the Xcalibur Configuration dialog box opens (see [Figure 53](#)).

Figure 53. Dataset List page



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 by doing the following:
 - 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.

3. If necessary, repeat steps a and b to add more names to the list.
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:
 - 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:
 - 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.

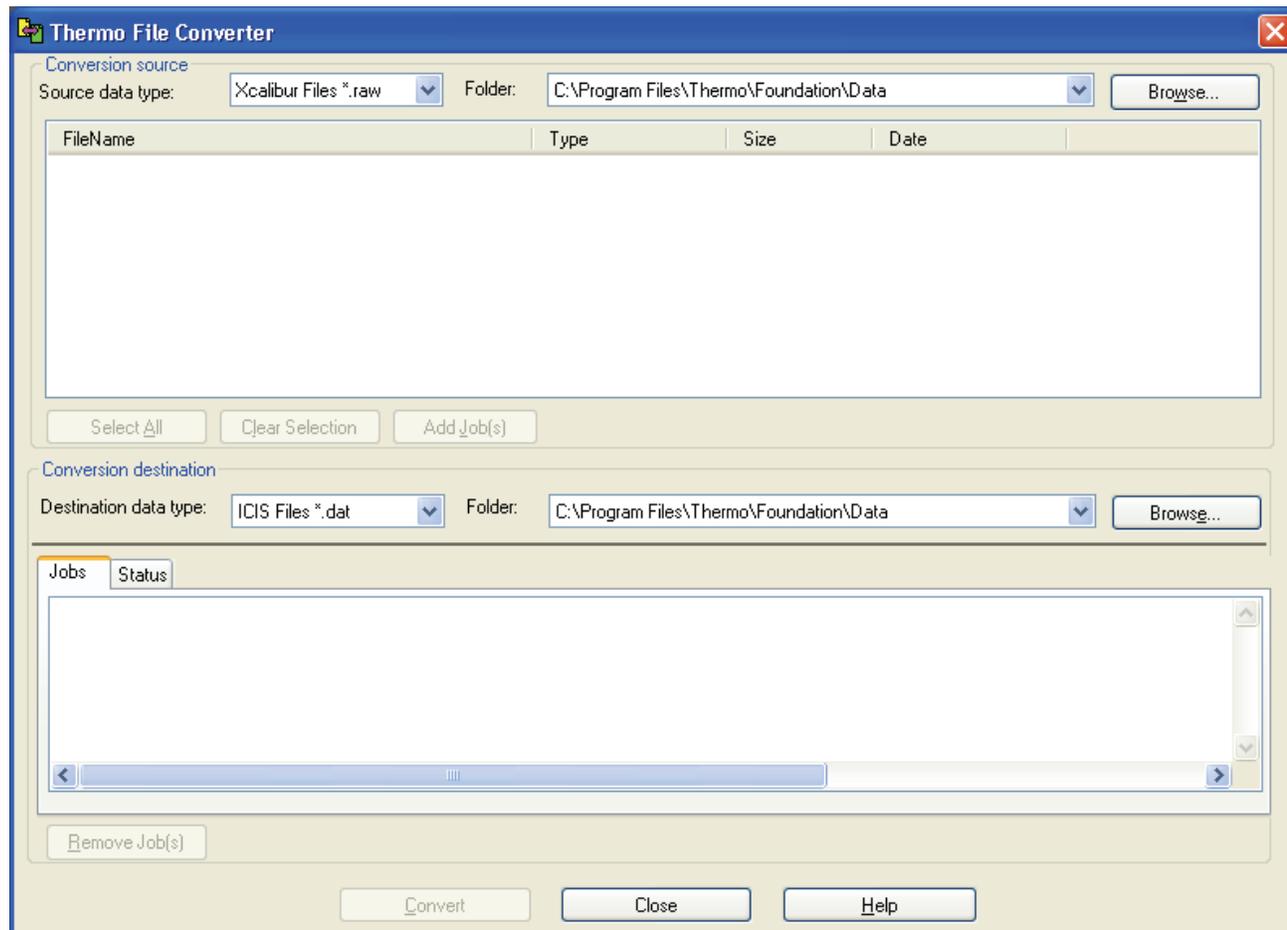
- Clear this check box to specify that the names listed in the Study List as well as those obtained from the database appear in the Dataset Name Selector dialog box.
7. To specify the maximum number of names to display in the Dataset Name Selector dialog box, type a number in the Maximum Number of Names to Display box.
 8. To save your settings, click **OK**.

Converting File Formats

❖ To convert files from one file format to another using the Thermo File Converter dialog box

1. Choose **Tools > File Converter** from the Roadmap view of the Home Page window. The [Thermo File Converter Dialog Box](#) opens (see [Figure 54](#)).

Figure 54. Thermo File Converter dialog box



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.

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 application 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**. 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 you want to convert, select 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 progress by clicking the Status tab in the Conversion Destination area.

The Xcalibur application continues file conversion processing until all files are converted and stored in the specified destination folder.

- To convert other source files with a different format, go to step 8.
- If you are done converting files, go to step 9.

8. To convert a different source data type, click **Clear Selection** to clear all files displayed in the Conversion Source list.

Repeat steps 2 through 7 for the other source data type.

9. To close the File Converter dialog box, click **Close**.

Confirming the Properties of Finnigan Security Server

The authorization and auditing functions of an application such as the Xcalibur data system installed on the Thermo Foundation application rely on two system services: the Finnigan Security Server and the Thermo Foundation DatabaseService. These services are installed when you install the application software. They automatically start whenever a user restarts a workstation.

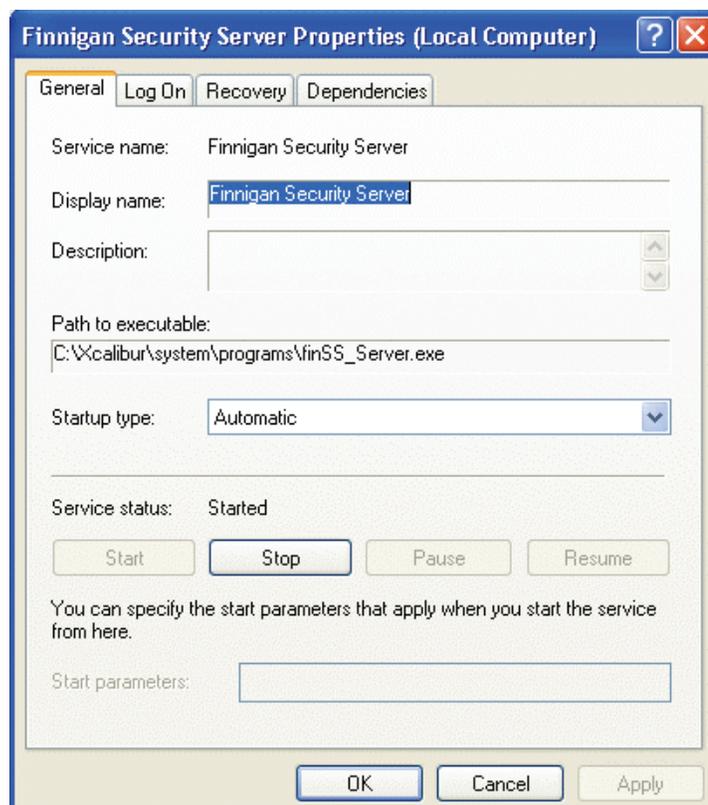
The main function of the Finnigan Security Server, which is installed with the Xcalibur software, is user authentication. If certain events require authentication, the Finnigan Security Server verifies the user names and passwords entered.

Note For information related to the Thermo Foundation DatabaseService, refer to the *Thermo Foundation Administrator Guide*.

❖ To confirm that the properties of the Finnigan Security Server is set correctly

1. To open the Services window, choose **Start > Control Panel** from your computer taskbar, double-click **Administrative Tools**, and double-click **Services**.
2. Confirm properties for the Finnigan Security Server:
 - a. Right-click **Finnigan Security Server** and choose **Properties** from the shortcut menu. The Finnigan Security Server Properties dialog box opens (see [Figure 55](#)).

Figure 55. General page

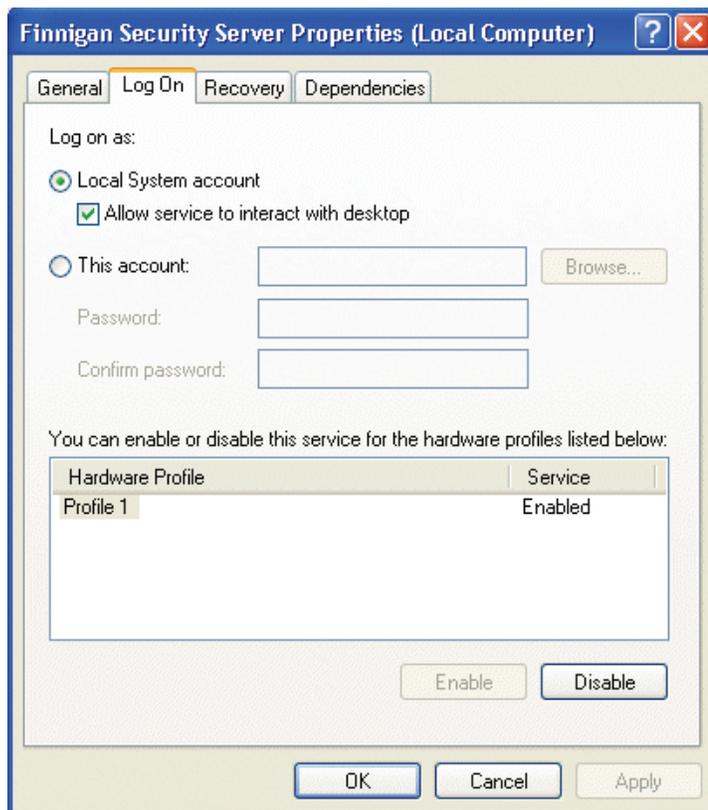


6 Configuring and Setting Up Xcalibur System Components

Confirming the Properties of Finnigan Security Server

- 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 (see Figure 56).

Figure 56. Log On page



- 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.

Xcalibur System Administration Reference

This appendix provides reference information to configure and manage the Xcalibur data system.

Contents

- [Configuring the Xcalibur Data System](#)
- [Configuring the System](#)
- [Configuring Instruments](#)
- [Instrument Setup](#)

Configuring the Xcalibur Data System

On the pages of the Xcalibur Configuration dialog box, enter configuration information for the Xcalibur data system.

Xcalibur Configuration Dialog Box

The Xcalibur Configuration dialog box has these pages:

- [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](#)

Customer Info Page

Use the Customer Information page of the Xcalibur Configuration dialog box to confirm and update the following Xcalibur software license information.

Table 3. Xcalibur software license parameters

Parameter	Description
User Name	View or change the name assigned to the Xcalibur license agreement. To change the user name, log on to your computer as an administrator.
Organization	View or change the organization assigned to the Xcalibur license agreement. To change the organization, log on to your computer as an administrator.
Address	View the address assigned to the Xcalibur license agreement. Commas separate the sections of the address, for example: City, State, and Country.
Voice Phone	View the voice telephone number assigned to the Xcalibur license agreement.
Fax	View the fax telephone number assigned to the Xcalibur license agreement.
Email	View the e-mail address assigned to the Xcalibur license agreement.
Print User Info	Print 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 to the user when choosing a dataset. Only the administrator can access this feature.

Note The names of several parameters on this page change when you select a new Display Name (see below). 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 4. Dataset List page parameters (Sheet 1 of 2)

Parameter	Description
Dataset List	View or change the dataset names that have been entered. The names are stored in the registry. To add a new dataset name to the list, click Add New Dataset Name .
Display Name	View or change the name that the data system uses for a dataset. You can type in 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 parameter Dataset List changes to Study List.

Table 4. Dataset List page parameters (Sheet 2 of 2)

Parameter	Description
Add New Dataset Name	Enter a new dataset name. The new dataset name is added to the Dataset List and stored in the registry.
Remove Selected Dataset Name	Remove the currently selected name from the Dataset List and from the registry. This action does not remove the name from the database if the name has already been used.
Blank Dataset Name is a Valid Selection	Set to allow a user to select a blank name when asked to select a dataset. Clear to require the user to select a valid dataset.
Selection Restricted to Entered Names	Select to list only the names listed in the Dataset List in the Dataset Name Selector dialog box. Clear to show the names listed in the Dataset List as well as those obtained from the database in the Dataset Name Selector dialog box.
Maximum Number of Names to Display	View or change 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.

Table 5. Folders page parameters

Parameter	Description
Default Folders	
Data	View or change the current default path to the folder that contains your Xcalibur data. To change the path, click Browse and select the folder to hold your data. When you click OK , the data system changes the default path in the Data box to the new path.
Methods	View or change the current default path to the folder that contains your Xcalibur methods. To change the path, click Browse and select the folder to hold your data. When you click OK , the data system changes the default path in the Methods box to the new path.
Report Templates	View or change the current default path to the folder that contains your Xcalibur report templates. To change the path, click Browse and select the folder to hold 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 Xcalibur application.

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 6. Fonts page parameters (Sheet 1 of 2)

Parameter	Description
Fixed Pitch Font	
Font	View or change 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	View or change 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 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	View or change 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 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.
Fixed Pitch Font Preview	
Preview	View the following examples: <ul style="list-style-type: none"> • Example text with fixed pitch font at minimum size. • Example text with fixed pitch font at maximum size.

Table 6. Fonts page parameters (Sheet 2 of 2)

Parameter	Description
Proportional Pitch Font	
Font	View or change 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 Xcalibur application 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	View or change 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	View or change 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	View the following examples: <ul style="list-style-type: none"> • Example text with fixed pitch font at minimum size. • Example text with fixed 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 the Xcalibur data system makes when an error occurs during data acquisition.

Table 7. Intelligent Shutdown page parameters

Parameter	Description
No Action	When an error occurs during data acquisition, set the data system to take no action and try to continue to the next sample.
Attempt to Stop the Devices and Pause the Sequence	When an error occurs during data acquisition, set the data system to send a stop command to all devices and pause the acquisition sequence before the next injection.
Attempt to Turn Off the Devices and Pause the Sequence	When an error occurs during data acquisition, set the data system to send a Turn off device command to all devices and pause the acquisition sequence before the next injection.

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.

Table 8. 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 Xcalibur application 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	Specify 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	Specify 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 uAU as a label.

Table 8. Labeling and Scaling page parameters (Sheet 2 of 2)

Parameter	Description
Label for Other Data Types	Specify in this list 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	
Specify 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	Specify that the default (global) settings use absolute scaling with MS data.
PDA/UV Data	Specify that the default (global) settings use absolute scaling with PDA/UV data.
Other Data	Specify the default (global) settings for data types other than MS and PDA/UV.
Retention Time Precision	
Decimals	Specify 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 Xcalibur application uses these defaults throughout to acquire and display your data. If you do not select the Use User Defined check box, then the application uses the values for mass options that are stored in the open raw file in the data system.

(Use the Masses dialog box in Processing Setup, Qual Browser, and Quan Browser to change the default settings for tolerance and precision in those applications.)

Table 9. Mass Options page parameters (Sheet 1 of 2)

Parameter	Description
Default Mass Tolerance	
Use User Defined	Activate the user-defined default settings for mass tolerance and mass units.
Mass Tolerance	Specify the user-defined default setting for mass tolerance. To activate the user-defined settings, select the Use User Defined check box. Then, enter a value from 0.1 to 50000 . The Xcalibur application 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 application then creates a new default layout file with this mass tolerance value.

Table 9. Mass Options page parameters (Sheet 2 of 2)

Parameter	Description
Units	Specify the default units that are used in processing mass spectral data. To activate the user-defined settings, select the Use User Defined check box. Then, select either the mmu option or the ppm option.
Default Mass Precision	
Decimals	Specify the default number of decimals 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 Xcalibur application. 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	
View or change 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 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 you specify for the default mass defect are applied throughout the Xcalibur application if no other value is available in the currently open method or raw file.	
Defect (mmu)	Specify default values (in millimass units) for 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)	Specify 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.

Table 10. Peak Detection page parameters

Parameter	Description
Default Peak Detection Algorithm	
Default Peak Detection Algorithm for MS Data	Select ICIS , Genesis , or Avalon as the default peak detection algorithm for MS data.
Default Peak Detection Algorithm for PDA/UV Data	Select ICIS , Genesis , or Avalon as the default peak detection algorithm for PDA/UV data.
Default Peak Detection Algorithm for Other Data Types (Data types other than MS and PDA/UV)	Select ICIS , Genesis , or Avalon as the default peak detection algorithm for data types other than MS, PDA, or UV data.

Configuring the System

The Xcalibur data system provides the following system configuration dialog boxes:

- [Add Programs to Tool Menu Dialog Box](#)
- [Add Tool Dialog Box](#)
- [Comment Dialog Box](#)
- [Customize Toolbar Dialog Box](#)
- [Dataset Name Selector Dialog Box](#)
- [Thermo File Converter Dialog Box](#)
- [File Save – Audit Trail Dialog Box](#)
- [File Summary Information Dialog Box](#)
- [Password Dialog Box](#)
- [Print Selection Dialog Box](#)
- [Select Directory/Select Data Directory Dialog Box](#)
- [Supervisor Permission Dialog Box](#)
- [View Audit Trail Dialog Box](#)
- [Spectrum Ranges Dialog Box](#)

Add Programs to Tool Menu Dialog Box

Use the Add Programs to Tool Menu dialog box to add and to remove application programs from the Tool menu and to adjust the sequence of the menu.

Table 11. Add Programs to Tool Menu dialog box parameters

Parameter	Description
Menu Contents	View 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	View or change 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	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.
Arguments	Add command line arguments.
Initial Directory	View or change 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.
Close	Save all changes and close the current page or dialog box.
Add	Add a tool (program) to the Tools menu.
Remove	Remove the name of the tool (program) selected in the Menu Contents box from the list of tools.
Move Up	Select a tool and move it up in the current sequence of tools (programs) in the Menu Contents box. This is the sequence displayed when you choose the Tools menu.
Move Down	Select a tool and move it down in the current sequence 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 12. 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 13. Comment dialog box parameters

Parameter	Description
Your Comment	Enter your 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.

Note This feature is only available in Sequence Setup, Qual Browser, and Quan Browser. In Qual Browser, you cannot customize the Amplify toolbar.

Table 14. Customize Toolbar dialog box parameters

Parameter	Description
Categories	View the menu categories available on the toolbar. Select a menu category to view the Commands list and buttons (if available on the toolbar) for that category.
Commands	View the commands associated with each menu category and the associated buttons on the toolbar if available.
Buttons	
Close	Save all changes and close the current page or dialog box.
Reset	Return the setting for the current selection to the value that was displayed when you selected the setting. The Reset command button only works on boxes.

Dataset Name Selector Dialog Box

Use the Dataset Name Selector dialog box 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.

The title of this dialog box might be different if the administrator chooses to use another name for a dataset. For example, it might be titled Study Name Selector or Job Name Selector.

Table 15. Dataset Name Selector dialog box parameters

Parameter	Description
Dataset Name List	Displays the list of predefined dataset names. When the dialog box opens, the list of predefined dataset names appears in this order: <ol style="list-style-type: none">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	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.

Thermo File Converter Dialog Box

Use the Thermo File Converter dialog box to convert one data file type to another data file type.

Note

- The Xcalibur data system does not currently support all interconversion combinations and posts a message whenever an unsupported conversion is requested.
- 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 from two locations: the Pre Acquisition or Post Acquisition run line of the Run Sequence dialog box located in the Sequence Setup view of the Home Page window, or from the Program or Macro Name run line of the Run Sequence dialog box located in the Programs view of the Processing Setup window.

The Xcalibur data system provides file interconversions for the following file types.

Table 16. File interconversions for data file types

File type	File extension
Xcalibur	*.raw
ICIS	*.dat
GCQ	*.ms
Magnum	*.ms
ANDI	*.cdf
AutoMass	*.spa
MassLab2	*.raw
LaserMAT	*.*

❖ To convert a file

1. Select the source and destination directories, and the conversion type in the [Thermo File Converter Dialog Box](#).
2. Click **Convert**. The data system automatically performs the file conversion and creates a new file. The Status page displays the conversion status of each job.

Table 17. Thermo File Converter dialog box parameters (Sheet 1 of 3)

Parameter	Description
Conversion Source	
Source Data Type	<p>View 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:</p> <ul style="list-style-type: none"> • 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 (*.*) <p>The source data type is selected from the Destination Data Type list.</p>
Folder	<p>View or change 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.</p>
Conversion Source table	<p>View the file name, type, size, and date of the files located in the directory specified in the Folder list and of the type specified in the Source Data Type list.</p>
Browse	<p>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.</p> <p>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.</p>
Select All	<p>Select all of the files that appear in the Conversion Source table. The data system highlights all of the files.</p>
Clear Selection	<p>Clear the currently selected files.</p> <p>This button is only active when you select one or more files in the Conversion Source table.</p>

Table 17. Thermo File Converter dialog box parameters (Sheet 2 of 3)

Parameter	Description
Add Job(s)	<p>Add the specified conversion job to the Jobs page of the Conversion Destination area. Each file conversion is considered a separate job.</p> <p>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:</p> <p style="padding-left: 40px;">C:\Xcalibur\examples\data\drugx_06.raw</p> <p style="padding-left: 40px;">C:\Xcalibur\examples\data\drugx_06.cdf</p> <p>The Add Job(s) button is only active when one or more files have been selected 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.</p>
Conversion Destination	
Destination Data Type	<p>View the data type that you want the source data files converted to. The following data types can be selected from the Destination Data Type list:</p> <ul style="list-style-type: none"> • ICIS Files (*.dat) • ANDI Files (*.cdf) • Text Files (*.txt) <p>The software selects the data type that a source data type file can be converted from in the Source Data Type list.</p>
Folder	View the path to the destination folder to hold your converted file. The list contains all the paths that you have recently selected. To select another folder to store your converted files, click Browse in the Conversion Destination area.
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.
Jobs page	<p>This page in the Conversion Destination area displays the jobs that have been selected for conversion. The job display format is as follows:</p> <p style="padding-left: 40px;">C:\Xcalibur\examples\data\drugx_06.raw</p> <p style="padding-left: 40px;">C:\Xcalibur\examples\data\drugx_06.cdf</p> <p>To remove a job prior to running the conversion, select the job and click Remove Job(s).</p>
Remove Job(s)	Removes jobs that are selected for removal from the Jobs page. You must remove a job prior to converting it.

Table 17. Thermo File Converter dialog box parameters (Sheet 3 of 3)

Parameter	Description
Status page	<p>This page in the Conversion Destination area displays the status of jobs that have been converted. The format is as follows:</p> <p style="padding-left: 40px;">Successfully converted C:\Xcalibur\examples\data\drugx_06.raw to C:\Xcalibur\examples\data\drugx_06.cdf</p> <p>This page also displays the status of unsuccessful conversions.</p>
Other Buttons	
Convert	<p>Starts 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:</p> <p style="padding-left: 40px;">Successfully converted C:\Xcalibur\examples\data\drugx_06.raw to C:\Xcalibur\examples\data\drugx_06.cdf</p> <p>This page also displays the status of unsuccessful conversions.</p>

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 18. File Save – Audit Trail dialog box parameters

Parameter	Description
User	Enter 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	View and enter useful information about the active file.
What Changed	View Xcalibur-generated information about changes to the active file. This information is part of the Xcalibur audit system.

When you have entered the above 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 19. File Summary Information dialog box parameters

Parameter	Description
Header	The header information includes 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	View or change a description of the active file and any comments that have been entered. 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 20. 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.

Print Selection Dialog Box

Table 21. Print Selection dialog box parameters

Parameter	Description
Select the Printing Output	
Vial Position List	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	Print selected rows in a sequence.
Displayed Columns Only	Print the currently displayed columns of the active sequence. To change the sequence columns displayed, choose Change > Column Arrangement .

Select Directory/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 22. Select Directory dialog box parameters

Parameter	Description
Directory Selected	View named groups of files called subdirectories and folders. Select the directory that contains the file you want to open.
Drives	View 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	View the amount of disk space available on the default path disk drive.
Network	Connect your computer to any drive on a network that you have access to.

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 23. 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.

View Audit Trail Dialog Box

Table 24. View Audit Trail dialog box parameters

Parameter	Description
Date/Time	View the month/day/year and time that the active file was changed. This information is used for the Xcalibur audit system.
User ID	View the user identification number of the current user. This information is part of the Xcalibur audit system.
Logon ID	View the Logon identification of the current user. This information is part of the Xcalibur audit system.
What Changed	View Xcalibur-generated information about changes to the active file. This information is part of the Xcalibur audit system.
User Comment	View comments made by the user describing the modification to the active file. This information is part of the Xcalibur audit system.

Spectrum Ranges Dialog Box

Use the Spectrum Ranges dialog box to view and edit the mass range, time, and other properties of a spectrum plot:

- In Qual Browser, for all plots in the active spectrum view.
- On the Home Page, for the active spectrum plot in Real Time Plot mode.

You can also apply automatic processing options such as smoothing and background subtraction. The dialog box consists of two pages:

- Ranges Page, Spectrum Ranges dialog box
- Automatic Processing Page, Spectrum Ranges dialog box

Configuring Instruments

Use these dialog boxes to configure your instruments.

- [Instrument Configuration Dialog Box](#)
- [Out of Date Instrument Drivers Detected Dialog Box](#)

Instrument Configuration Dialog Box

Use the Instrument Configuration dialog box to review all available devices and configure the devices that you want to install using the following controls.

Table 25. Instrument Configuration dialog box parameters (Sheet 1 of 2)

Parameter	Description
Device Types	
	View or change the category of device types currently displayed in the Available Devices area. The default option is All. The other options allow you to select a subset of all of the devices as follows:
All:	Displays all configurable Xcalibur devices.
AS:	Displays all configurable Xcalibur autosampler devices.
Detector:	Displays all configurable detector devices.
GC:	Displays all configurable Xcalibur gas chromatograph devices.
LC:	Displays all configurable Xcalibur liquid chromatograph devices.
MS:	Displays all configurable Xcalibur mass spectrometer devices.
Other:	Displays all other Xcalibur configurable devices.
Available Devices	
	This area displays buttons for all available devices of the type selected in the Device Types list. For example if All is displayed in the Device Types list, this area displays all Xcalibur configurable devices.
Available Device	View available instruments. Each button displayed in the Available Devices area represents an instrument that can be configured as an Xcalibur device. The buttons that are displayed depend upon the selection in the Device Types list. To select an Xcalibur device for configuration, click the button corresponding to the device to be configured and click Add .
Add	Add the device you have selected in the Available Devices area to the Configured Devices area. A device must be present in the Configured Devices area to begin the process of configuring the device.

Table 25. Instrument Configuration dialog box parameters (Sheet 2 of 2)

Parameter	Description
Configured Devices	
	View all of the devices that have been added from the devices listed in the Available Devices group box.
	A device must be present in the Configured Devices area to begin the process of configuring the device.
Remove	Remove the device you have selected from the Configured Devices area. Each button displayed in the Configured Devices area represents an instrument that has been selected for configuration as an Xcalibur device but might or might not have been configured. To configure a device listed in the Configured Devices area, click the button of the device to be configured, and then click Configure to open the appropriate configuration dialog box.
Configure	Open the appropriate configuration dialog box for the device you have selected in the Configured Devices area. For example, to configure an LCQ MS detector, click LCQ in the Configured Devices area, and then click Configure . The LCQ Configuration dialog box opens.
Other Controls	
Done	Close the Instrument Configuration dialog box after you have configured Xcalibur devices.

Out of Date Instrument Drivers Detected Dialog Box

This dialog box opens only when you select **Start > Programs > Thermo Foundation 1.0 > Instrument Configuration**. The Instrument Configuration view opens. If your Xcalibur software is out of date, Xcalibur displays the following message:

The device drivers for the following instruments are not compatible with the installed version of Xcalibur. You must install the current drivers before you can use these instruments.

If this message appears, install the latest software for the instruments listed. This software is located on an Xcalibur CD-ROM. Run the appropriate setup file to load the new software. Run Setup.exe from the appropriate instrument directory on the CD-ROM.

Note The Xcalibur data system and inlets are shipped on a separate CD-ROM from the Xcalibur software used for the MS detectors and mass spectrometers. When a new version of Xcalibur is released, usually you must update the software for both the Data system and inlets software as well as the MS detectors and mass spectrometers for all configured instruments.

Table 26. Out of Date Instrument Drivers Detected dialog box parameters

Parameter	Description
Instrument	View currently installed instruments with out-of-date software. Installed in this context indicates that the Setup.exe files for the listed instruments have been previously run from the appropriate directory of an Xcalibur CD-ROM.
In Use	View the status of the instrument displayed in the Instrument list: In Use (Yes) or Not In Use (blank). In Use devices appear in the Configured Devices area of the Instrument Configuration view.
Version	View the current version of the instrument that is displayed in the same row of the Instrument list. Make sure the version to be installed is more recent than the current version.

Instrument Setup

After selecting which instruments you want the Xcalibur data system to control using the Instrument Configuration program, use Instrument Setup to specify your instrument settings.

- [File Menu for the Instrument Setup Window](#)
- [Instrument menu for the Instrument Setup Window](#)
- [Help Menu for the Instrument Setup Window](#)
- [Instrument Setup Window Toolbar](#)

The Instrument Setup window displays the setup parameters required for each instrument that you select on the View bar. These might include your autosampler, chromatograph, MS detector or mass spectrometer, divert valve, syringe pump, contact closure timing sequence, and/or all other Xcalibur-supported instruments that you have configured.

You can create new methods, modify existing methods, and save method files. You can import previously collected 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.

The Instrument Setup window displays the icons of all of the Xcalibur instruments you have selected using the Instrument Configuration dialog box. (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.

To enter the setup parameters for a particular instrument, click the icon for that instrument. The Xcalibur data system displays one or more pages of parameters to be set for the one you selected.

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 program.

Menus

Instrument Setup contains the following menus:

- [File Menu for the Instrument Setup Window](#)

Instrument

- [Instrument menu for the Instrument Setup Window](#)

The *Instrument* menu changes when you use the View bar to select an instrument. Each instrument-specific menu contains instrument-specific menu commands.

- [Help Menu for the Instrument Setup Window](#)

Toolbar

Instrument Setup toolbar

File Menu for the Instrument Setup Window

Table 27. File menu commands

Command	Description
New	Create a new file having the appropriate extension.
Open 	Find and open a file that already exists.
Save 	Open 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	Edit user and description information, 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.
Summary Information	Edit user and description information, as well as view header information about the active file.
Change Dataset Name	Select a dataset from a predefined list of names. The text of this menu item might be different if the administrator chose to use another name for a dataset. For example, this menu item might be Change Job Name.
Audit Trail	View all auditable events and changes made to data files in the current application.
Print 	Print your method.
Print Preview	View your page setup so that you can see what it looks like before printing it.
Print Setup	Select the following printing options: printer, form, orientation, and one- or two-sided printing.
Most Recently Used Files	View the paths and names of the last four files used. These 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, it is opened.
Exit	Close 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 for the Instrument Setup Window

The Xcalibur data system groups commands that deal with instrument-specific controls in the [Instrument] menu. You can activate [Instrument] commands from either the mouse or keyboard.

Help Menu for the Instrument Setup Window

Table 28. Help menu commands

Command	Description
[Instrument] Help	Open the Configuration and Setup Help for the selected instrument.
Instrument Setup Help	Open Xcalibur Help and display Help for the Instrument Setup window.
Help On Current Item	View Help for the Instrument Setup page that is currently displayed.
[Instrument] Contents and Index	View the Contents, Index, and Find Help pages for the selected instrument.
Xcalibur Help	Open Xcalibur Help.
Glossary	Open the glossary.
How To Use Help	Open Help that describes how to use the Help viewer.
About Instrument Setup	View the installed version number of the Instrument Setup program and the Thermo Fisher Scientific copyright notice.

Instrument Setup Window Toolbar

Table 29. Toolbar for the Instrument Setup window

Button	Description
 New	Create a new instrument method.
 Open	Find and open an existing file.
 Save	Enter audit information about the active file if your method has been saved before and click Continue to save the file. 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	Print the parameters in your instrument method.
 Home Page	View the Home Page window – Roadmap view.
 Help	View Help for the Instrument Setup page that is currently displayed.

Using Xcalibur Files and Samples

These tutorials analyze a sample set example provided with the Xcalibur data system and located in the C:\Xcalibur\examples\data directory. The target compound is a proprietary pharmaceutical product. The data was collected in the applications laboratory at Thermo Fisher Scientific, San Jose, using LC and MS/MS techniques in the electrospray ionization (ESI) mode.

The pharmaceutical product is called drugx. An isotopically labeled internal standard (ISTD) was used to quantify the pharmaceutical. The internal standard called D4 is a deuterated analogue of drugx that has four deuterium atoms exchanged for hydrogen atoms in the compound.

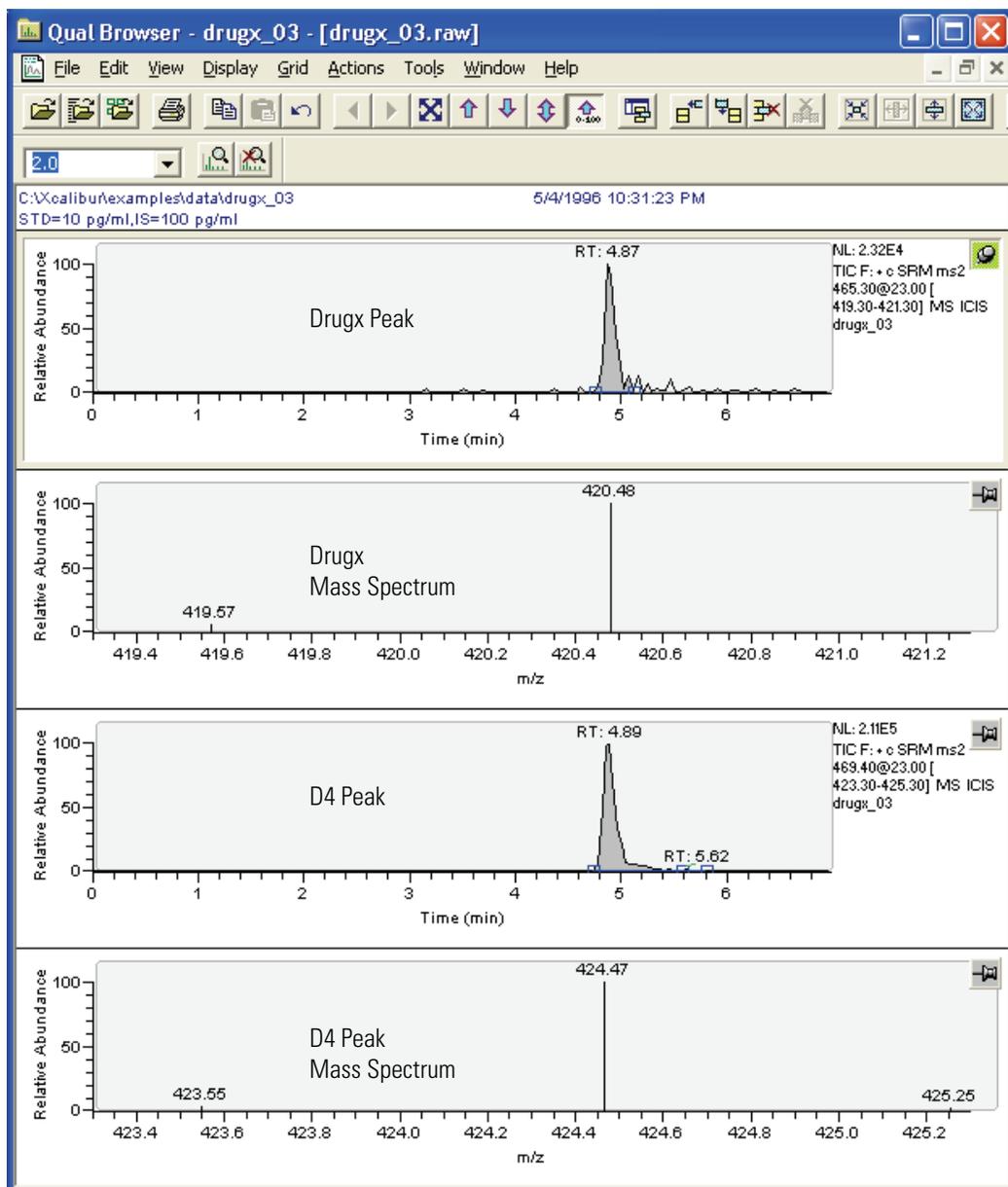
The calibration standards were prepared by spiking human plasma with drugx to give nine calibration levels with concentrations of 10, 25, 50, 100, 200, 400, 600, 800, and 1000 pg/mL. Triplicate samples were run at the high (1000 pg/mL) and low (10 pg/mL) ends of the curve with single samples run in between.

The QC samples were prepared similarly by spiking human plasma with drugx to give three QC levels with concentrations of 10, 400, and 1000 pg/mL. Six replicates per QC level were run.

The calibration and QC standards were spiked with 100 pg/mL of the D4 internal standard.

Figure 57 displays the scan filter chromatograms and mass spectra for a drugx.raw data file.

Figure 57. Chromatograms and mass spectra for drugx and D4



Home Page Reference

Use the Home Page window to control or access all Xcalibur application functions and features from three main views. Visibility and control of Xcalibur features are based on the current configuration of instrument components.

Contents

- [Views](#)
- [Menus](#)
- [Toolbars](#)
- [Xcalibur Dialog Boxes](#)

Views

- [Information View](#)
- [Roadmap View](#)
- [Real Time Plot View](#)

The [Information View](#) has two tabbed pages and is located on the left side of the window. It can be displayed alongside any of the three main views.



[Roadmap View](#)



[Sequence Setup](#)



[Real Time Plot](#)

You can access the following pre-acquisition programs from the Home page:



[Instrument Setup](#)



[Working with Processes and Sequences](#)

You can also access the following post-acquisition programs from the Home page:



[Qual Browser](#)



[Quan Browser](#)



[Library Browser](#)

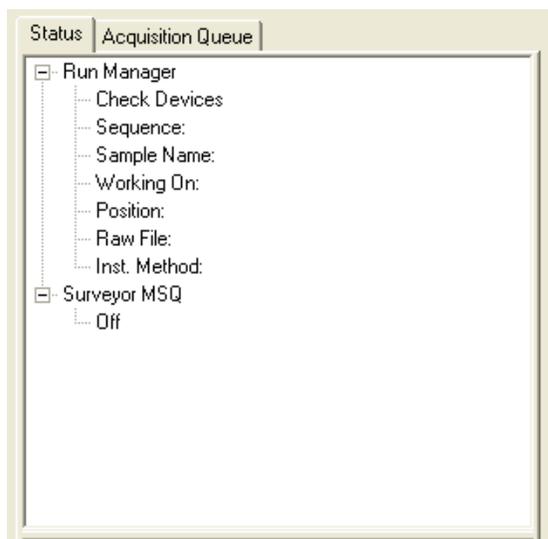
Information View

The Information view consists of the following two pages:

- [Status Page for the Information View](#)
- [Acquisition Queue Page for the 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 for the Information View



The Status page of the Information view provides the following overall summary of the Xcalibur data system status:

- Run Manager
 - Check Devices
 - Sequence
 - Sample Name
 - Working On
 - Position
 - Raw File
 - Instrument Method
- Instruments

The readback status of each Xcalibur-configured instrument appears on the Status page.

When you click an instrument, the Xcalibur data system displays current readings for the instrument on tabbed pages below the Run Manager pane. Set these parameters in the software that controls your instrument.

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 for the Information View

The Acquisition Queue page of the Information view displays all of the sequences that are required for 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 Xcalibur application places a large “X” to the left of each completed sequence row as samples are processed.

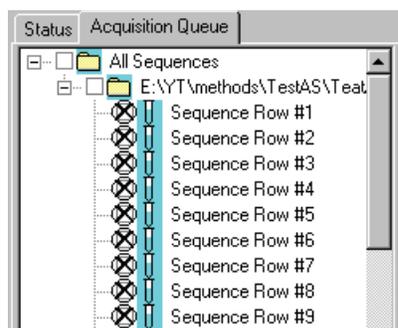
Sequences are stored in the All Sequences folder, and sequence rows are stored in the Sequence folder specified by their paths, for example: C:\methods\Test.sld.

The sequences and sequence rows 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 when it is selected or not selected.

❖ To remove a selected list or sequence row from the acquisition queue

1. Click the sequence or sequence row to select it. The Xcalibur application places a small “x” 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.

The following example shows processed samples, as indicated by the large “X” to the left of each numbered sequence row:



Note This 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.

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 buttons to open the window for that application. Then, click the Help command in the menu bar to display Help for any of the windows: Information View, Sequence Setup, Processing Setup, Qual Browser Reference, Quan Browser Reference, and Library Reference.

You can also display menus by right-clicking the icons. The menus contain commands such as Go To and Open Last Used Instrument Method.

Menu Bar

[File Menu](#)[View Menu](#)[GoTo Menu](#)[Actions Menu](#)[Tools Menu](#)[Help Menu](#)

Toolbars

[View Toolbar](#)[Sequence Editor Toolbar](#)[Roadmap Toolbar](#)[Plot Toolbar](#)

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. The chromatograms can be displayed 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 or toolbar. Control the way information appears in the Real Time Plot view using the Plot toolbar.

Menu Bar

The Real Time Plot view menu bar contains the following menus:

[File Menu](#)[View Menu](#)[Help Menu](#)[Actions Menu](#)[GoTo Menu](#)

Toolbars

[View Toolbar](#)[Sequence Editor Toolbar](#)[Roadmap Toolbar](#)[Plot Toolbar](#)

Menus

The Xcalibur Home page has the following menus. Click an item for a detailed description of options that are available on that menu. The menus and menu commands change depending on whether you display the Roadmap view, Sequence Setup view, or Real Time Plot view.

- [File Menu](#)
- [Change Menu](#)
- [View Menu](#)
- [GoTo Menu](#)
- [Edit Menu](#)
- [Actions Menu](#)
- [Tools Menu](#)
- [Help Menu](#)

File Menu

The commands in the Home Page window File menu change depending on which of the following views are displayed:

- [Roadmap and Real Time Plot](#)
- [Sequence Setup](#)

Roadmap and Real Time Plot

Table 30. File menu – Roadmap and Real Time Plot command

Command	Description
Exit	Close the window.
	The Home Page window must be open to operate the Xcalibur data system and to communicate with Xcalibur components.

Sequence Setup

Table 31. File menu – Sequence Setup commands

Command	Description
New 	Create a new file with the appropriate extension.
Open 	Find and open an existing file.
Save 	Enter audit information about the active file and save the file in a specific location (drive and directory). After you have entered audit information, click the OK button. The Save As dialog box opens.
Save As	Name a new file, enter file summary information, and save the file in a specific location (drive and directory).
Summary Information	View, change, or delete file summary information about the active file.
Import Sequence	Locate (drive and directory) and open a stored sequence.
Export Sequence	Specify a new location (drive and directory) for the active sequence.
Change Dataset Name	Select a dataset from a predefined list of names. The text of this menu item might be different if the administrator chose to use another name for a dataset. For example, this menu item might be Change Job Name.
View Audit Trail	View all auditable events and changes made to data files in the current application.
Print 	Print a sequentially numbered vial position list from the active sequence, selected rows in a sequence, or currently displayed columns of the active sequence.
Print Preview	View what you want to print so that you can see what it looks like before you print it.
Page Setup	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	Close the active window. If you exit before clicking OK from an active dialog box, the data system prompts you to save your changes.

Note Instrument Setup and Processing Setup are separate windows that have their own menus.

Change Menu

The Change menu is available only in the Sequence Setup view of the Home Page window.

Table 32. Change menu commands

Command	Description
User Labels 	Change the heading captions of five information boxes on the Sequence Setup view. The default caption headings are Study, Client, Laboratory, Company, and Phone.
Tray Name	Select the Autosampler Tray Type for the current sequence.
Column Arrangement 	View or hide specific sequence columns. ❖ To select the columns of a displayed sequence <ol style="list-style-type: none">1. Select the columns from the Available Columns list.2. Click Add. ❖ To remove the columns of a displayed sequence <ol style="list-style-type: none">1. Select the columns from the Displayed Columns list.2. Click Remove.
Transfer Row Info 	Match samples by Sample ID or Position.

Note Instrument Setup and Processing Setup are separate windows that have their own menus.

View Menu

The View menu commands in the Home Page window change depending on the following displayed views:

- [Real Time Plot](#)
- [Roadmap and Sequence Setup](#)

Real Time Plot

Table 33. View menu – Real Time Plot commands (Sheet 1 of 3)

Command	Description
Controls	
Lock Display	<p>Unlock the data from the instrument. With the data unlocked, you can use Home Page window buttons on the toolbar or menu commands to review previously acquired data. During the time that you are in the unlocked mode, the Xcalibur data system continues to gather and save all data. In the unlocked mode, the lock icon in the toolbar appears pushed out and the Lock Display command has no check mark.</p> <p>To relock the data to the instrument, choose Options > Lock Display.</p> <p>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 the locked mode, the lock icon in the toolbar appears to be pressed in and the Lock Display command has a check mark.</p> <p>You can click  in the Home Page window toolbar to lock the data to and unlock the data from the instrument.</p> <p>To unlock the data from the instrument, you can also click the chromatogram or spectrum views.</p>
Reset Display	<p>Reset the display parameters to the settings defined in the Instrument Setup Method selected for the sample in the sequence after you have changed Home Page window display parameters using Home Page commands.</p> <p>The Instrument Setup Method selected for the sample in the sequence 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 Instrument Setup Method selected. While the sample is running, you can change display parameters using Home Page window menu commands.</p>
Ranges	<p>Set up the mass range, time, average scan, filter, and background subtraction for the spectrum that the Xcalibur data system displays in the Home Page window.</p>

Table 33. View menu – Real Time Plot commands (Sheet 2 of 3)

Command	Description
Zoom	
Zoom In Y 	To show more detail, zoom in on the Y-axis by a factor of two (2) from the current baseline. For example, you can change the Y-axis range from 0–100 to 0–50.
Zoom Out Y 	To show more data, zoom out on the Y-axis by a factor of two (2). For example, you can change the Y-axis range from 0–25 to 0–50.
Normalize 	Normalize the intensity scale of the data display to a fixed range on the Y-axis, from 0–25% to 0–100%.
Zoom In X 	To show more detail, zoom in on the X-axis by a factor of two (2). For example, you can change the X-axis range from 0–20 to 5–15.
Zoom Out X 	To show more data, zoom out on the X-axis by a factor of two (2) from the center. For example, you can change the X-axis range from 7.5–12.5 to 5–15.
Display All 	View all data on the X-axis or all text in a report. For example, you can change the X-axis range from 7.5–12.5 to 0–20.
Pan	
Next Scan 	View the next mass scan with its scan number.
Previous Scan 	View the previous mass scan with its scan number.
Display Options	Select the style, color, label [chromatogram and spectrum only], axis, normalization, and smooth [chromatogram only] options for your chromatogram, spectrum, or map.
Roadmap View 	View or hide the Xcalibur Roadmap view. This view displays a schematic representation of all Xcalibur software windows and their relationships. This view can be displayed on the right side of the Home Page window. When you select the command, the view appears if it was previously hidden or hides if it was previously displayed.
Sequence Setup View 	Create, edit, save, or open a sample sequence.

Table 33. View menu – Real Time Plot commands (Sheet 3 of 3)

Command	Description
Real Time Plot View 	View 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 <ul style="list-style-type: none"> • 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 	Monitor the Run Manager status, Xcalibur component statuses, 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	Perform file maintenance and manage the sample sequence using the Sequence Editor toolbar with the Sequence Setup view.
Plot Toolbar	Use the Plot toolbar to <ul style="list-style-type: none"> • 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	Add command icons to and delete command icons from the Home Page toolbars.

Roadmap and Sequence Setup

Table 34. View menu – Roadmap and Sequence Setup commands

Command	Description
Roadmap View 	View or hide the Xcalibur Roadmap view. This view displays a schematic representation of all Xcalibur windows and their relationships. This view can be displayed on the right side of the Home Page window. When you select the command, the view appears if it was previously hidden or hides if it was previously displayed.
Sequence Setup View 	Create, edit, save, or open a sample sequence.
Real Time Plot View 	View 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 	Monitor the Run Manager status, Xcalibur component statuses, 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	Perform file maintenance and manage the sample sequence.
Plot Toolbar	Use the Plot toolbar to <ul style="list-style-type: none"> • 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	Add command icons to and delete command icons from the Home Page toolbars.

Note [Instrument Setup](#) and Processing Setup are separate windows that have their own menus.

GoTo Menu

Table 35. GoTo menu commands

Command	Description
	Open the Instrument Setup window.
	Open the Processing Setup window.
	Open the Qual Browser Reference window.
	Open the Quan Browser Reference window.
	Open the Library Reference window.

Note [Instrument Setup](#) and Processing Setup are separate windows that have their own menus.

Edit Menu

The Edit menu is available only in the Sequence Setup view of the Home Page window.

Table 36. Edit menu commands (Sheet 1 of 3)

Command	Description
Undo 	<p>Cancel your previous action.</p> <p>For example, if you have just deleted an entry or annotation, click  to replace the deleted entry or annotation.</p> <p>Click  to delete an entry or annotation you just finished.</p> <p> cancels only one previous action.</p>
Clear	Remove the text in selected sequence boxes or entire sequence rows. Select boxes by clicking or clicking and dragging. Select a sample row by clicking the row number (far left column). Select multiple adjacent rows by clicking and dragging up or down the sample number column. The Xcalibur data system highlights the selected rows. Then, choose Edit > Clear . The data system clears the text from the selected boxes. It clears the current Sample Type to Sample Type: Unknown.
Copy 	Copy selected rows or columns from the sequence to the clipboard.

Table 36. Edit menu commands (Sheet 2 of 3)

Command	Description
Paste 	Paste copied sequence rows or columns from the clipboard to the screen.
Insert Row	<p>Insert one new row at a time anywhere in the current sequence.</p> <p>❖ To insert a row</p> <ol style="list-style-type: none"> 1. Select the row directly below the line to be inserted by clicking its row number (far left column). The Xcalibur application highlights the selected row. 2. Choose Edit > Insert Row. The following message appears: <p style="text-align: center;">Insert above line <i>X</i>?</p> 3. Click Yes or press the INSERT key on the keyboard to insert a row. Click No to cancel the Insert Row command.
Delete Row	<p>Delete one or more adjacent rows from the current sequence.</p> <p>❖ To delete a row</p> <ol style="list-style-type: none"> 1. Select a row to be deleted by clicking a row number (far left column) or select multiple adjacent rows to be deleted by clicking and dragging up or down the sample number column. The Xcalibur application highlights the selected rows. 2. Choose the Delete Row command. The following message appears: <p style="text-align: center;">Delete Rows <i>X</i> to <i>X</i>?</p> 3. Click Yes to delete the rows or press the DELETE key on the keyboard. Click No to cancel the Delete Row command.
Go To Row	<p>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.</p> <p>❖ To go to a row in the current sequence</p> <ol style="list-style-type: none"> 1. Type the number of the line in the Go To Line Number box. 2. Click OK.

Table 36. Edit menu commands (Sheet 3 of 3)

Command	Description
Fill Down 	Copy information from a sample row to a series of rows and avoid repetitive cut-and-paste operations. ❖ To copy information from one row to a series of rows Select the sequence information that you want to copy to the sample rows below the selected sample row. The Xcalibur data system automatically fills the rows below the selected row with the selected entries. It only fills rows directly below the selected row.
Browse File Name 	Select a path and file name that exist on your computer or network. The Xcalibur data system enters the selected path and file name in the active File Name box. This command is only active when the cursor is in a Sequence Setup File Name box.

Note [Instrument Setup](#) and Processing Setup are separate windows that have their own menus.

Actions Menu

The Actions menu commands in the Home Page window change depending on which of the following views are displayed:

- [Roadmap and Real Time Plot](#)
- [Sequence Setup](#)

Roadmap and Real Time Plot

Table 37. Actions menu – Roadmap and Real Time Plot commands (Sheet 1 of 3)

Command	Description
Check Disk Space 	Determine how much available disk space you have on your disk drive or drives. Click this icon in the toolbar if this icon has been added to the toolbar.
Start Analysis 	Start the next run in the Sequence queue. This command is only available under these conditions: <ul style="list-style-type: none"> • when an autosampler is configured • when an MS Detector contact closure interface is configured • when the Start When Ready check box is clear in the Start Options area of the Run This Sample dialog box or the Run Sequence dialog box Make sure the data system is in the Ready state.

Table 37. Actions menu – Roadmap and Real Time Plot commands (Sheet 2 of 3)

Command	Description
Stop Analysis 	<p>Stop the current analysis. When the current sample has stopped, the data system creates a raw file for the terminated sample that contains all raw data acquired prior to the time of the Stop Analysis command. The application then enters the Paused state, as indicated by the flashing red message to the right of the Sequence box in the Current area in the Status view of the Home Page window.</p> <p>To start the next sample in the Sequence queue after a Stop Analysis command, use the Start Analysis command or click the (depressed) Pause/Resume Analysis button in the toolbar.</p>
Pause Analysis 	<ul style="list-style-type: none"> Pause Pause sample list processing when the button appears in the up (not depressed) position. The Xcalibur data system changes the appearance of the button from the up (not depressed) to the down (depressed) state. If a sample list has been downloaded or if sample data acquisition has started, the data system completes the current sample and creates a raw file for the sample. The data system then enters the Paused state, as indicated by the flashing red Paused to the right of the Sequence box in the Current area in the Status view of the Home Page window. Resume Resume sequence processing. The application starts the next sample in the Sequence queue.
Devices On	<p>Put 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.</p> <p>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.</p>
Devices Standby	<p>Put 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.</p> <p>This option has the same effect as choosing the Standby option in the After Sequence Set System area in the Run Sequence dialog box.</p>

Table 37. Actions menu – Roadmap and Real Time Plot commands (Sheet 3 of 3)

Command	Description
Devices Off	<p>Put 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.</p> <p>This option has the same effect as choosing the Off option in the After Sequence Set System area in the Run Sequence dialog box.</p> <p>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.</p>
Automatic Devices On	<p>Set the Xcalibur data system to automatically turn on all devices controlled by the application before starting a data acquisition.</p> <p>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.</p> <p>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:</p> <p style="padding-left: 40px;">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.</p>
Reinstate Warnings	<p>Restore the display of messages that you have turned off by selecting the Don’t Ask Again check box.</p> <p>Periodically, the Xcalibur application displays a message or dialog box that includes the following:</p> <p style="padding-left: 40px;"><input type="checkbox"/> Don’t ask again.</p> <p>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.</p> <p>To turn off warnings, select this check box:</p> <p style="padding-left: 40px;"><input checked="" type="checkbox"/> Don’t ask again</p>

Sequence Setup

Table 38. Actions menu – Sequence Setup commands (Sheet 1 of 3)

Command	Description
Check Disk Space 	Determine how much available disk space you have on a disk drive.
Run This Sample 	Collect data for one or more consecutive samples selected from the active sequence.
Run Sequence 	Collect data for one or more consecutive samples selected from the active sequence.
Batch Reprocess 	Reprocess data for samples selected from the active sequence.
Open [Method] File 	Edit either an instrument method or a processing method selected from the Sequence Setup view. <ul style="list-style-type: none"> • If 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 view and displays the selected file so that you can edit parameters. • If 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 parameters. This command is only active if you select an instrument method or a processing method.
Start Analysis 	Start the next run in the Sequence queue. <p>This command is only available under these conditions:</p> <ul style="list-style-type: none"> • when an autosampler is configured • when an MS Detector contact closure interface is configured • when the Start When Ready check box is clear in the Start Options area of the Run This Sample dialog box or the Run Sequence dialog box Make sure the Xcalibur application is in the Ready state.

Table 38. Actions menu – Sequence Setup commands (Sheet 2 of 3)

Command	Description
Stop Analysis 	<p>Stop the current analysis. When the current sample has stopped, the Xcalibur data system creates a raw file for the terminated sample that contains all raw data acquired prior to the time of the Stop Analysis command. The application then enters the Paused state, as indicated by the flashing red message to the right of the Sequence box in the Current area in the Status view of the Home Page window.</p> <p>To start the next sample in the Sequence queue after a Stop Analysis command, use the Start Analysis command or click the (depressed) Pause/Resume Analysis button in the toolbar.</p>
Pause Analysis 	<ul style="list-style-type: none"> Pause Pause sample list processing when the button appears in the up (not depressed) position. The Xcalibur data system changes the appearance of the button from the up (not depressed) to the down (depressed) state. If a sample list has been downloaded or if sample data acquisition has started, the data system completes the current sample and creates a raw file for the sample. The data system then enters the Paused state, as indicated by the flashing red Paused to the right of the Sequence box in the Current area in the Status view of the Home Page window. Resume Resume sequence processing. The application starts the next sample in the Sequence queue.
Devices On	<p>Put 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.</p> <p>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.</p>
Devices Standby	<p>Set the system to 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.</p> <p>This option has the same effect as choosing the Standby option in the After Sequence Set System area in the Run Sequence dialog box.</p>

Table 38. Actions menu – Sequence Setup commands (Sheet 3 of 3)

Command	Description
Devices Off	<p>Put 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.</p> <p>This option has the same effect as choosing the Off option in the After Sequence Set System area in the Run Sequence dialog box.</p> <p>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.</p>
Automatic Devices On	<p>Set the Xcalibur data system to automatically turn on all devices controlled by the data system before starting a data acquisition.</p> <p>If this command has a check mark to its left, the application automatically turns on all devices that are in the Off or Standby state.</p> <p>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:</p> <p style="padding-left: 40px;">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.</p>
Reinstate Warnings	<p>Restore the display of messages that you have turned off by selecting the Don’t Ask Again check box.</p> <p>Periodically, the Xcalibur application displays a message or dialog box that includes the following:</p> <p style="padding-left: 40px;"><input type="checkbox"/> Don’t ask again.</p> <p>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.</p> <p>To turn off warnings, select this check box:</p> <p style="padding-left: 40px;"><input checked="" type="checkbox"/> Don’t ask again</p>

Note [Instrument Setup](#) and Processing Setup are separate windows that have their own menus.

Tools Menu

The Tools menu is available only in the Roadmap view of the Home Page window.

Table 39. Tools menu commands

Command	Description
Configuration	Configure Xcalibur default folders, enter customer information, and change Xcalibur fixed pitch and proportional pitch fonts.
 Queue Manager	Monitor processing status.
 File Converter	Convert files from one file type to another file type.
LCQuan	Review quantitative analysis results in the LCQuan™ window.
Library Manager	Manage NIST libraries used with NIST searching software and convert libraries between the ICIS/GCQ/ITS 40, MassLab, NIST, and ANDI-MS formats.
Add Tools	Add to or remove programs from the Home Page window menu bar. The Xcalibur application 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.

Note [Instrument Setup](#) and Processing Setup are separate windows that have their own menus.

Help Menu

Table 40. Help menu commands

Command	Description
Home Page Help	Open Xcalibur Help and display help for the Home Page window.
View Help	Open Xcalibur Help and display help for the current view.
Xcalibur Help	Open Xcalibur Help.
Glossary	Open the glossary.
How To Use Online Help	Open Help that describes how to use the Help viewer.
About Home Page	Open the About Home Page dialog box. The About Home Page dialog box displays the installed version number of the Home Page program and the product copyright notice.

Note [Instrument Setup](#) and Processing Setup are separate windows that have their own menus.

Toolbars

The Xcalibur Home page has the following toolbars. Click an item for a detailed description of options available on that menu.

- [View Toolbar](#)
- [Roadmap Toolbar](#)
- [Sequence Editor Toolbar](#)
- [Plot Toolbar](#)

View Toolbar

Table 41. View toolbar buttons

Button	Description
 Roadmap View	View a schematic representation of all Xcalibur windows and their relationships. This view can be displayed on the right side of the Home Page window. The view appears if it was previously hidden or hides if it was previously displayed.
 Sequence View	Create, edit, save, or open a sample sequence.
 Real Time Plot View	View chromatogram and spectrum data for the current sample. Use the Plot tool 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.
 Information View	Monitor Run Manager status, Xcalibur component statuses, and the acquisition queue. The Information View has two tabbed pages and is located on the left side of the window. It can be displayed alongside any of the three main views.

Roadmap Toolbar

Table 42. Roadmap toolbar buttons (Sheet 1 of 2)

Button	Description
 Instrument Setup	Set up instruments for the Xcalibur application.
 Processing Setup	Create or modify an Xcalibur process.

Table 42. Roadmap toolbar buttons (Sheet 2 of 2)

Button	Description
	<p>Start Analysis</p> <p>Start the next run in the Sequence queue.</p> <p>You can review the sample list queue at any time using the Acquisition Queue page of the Home Page Information view.</p> <p>This button on the toolbar is only available when an autosampler is configured, a LC/MS Detector contact closure interface is configured, and the Start When Ready check box is clear in the Start Options area of the Run Sequence dialog box. Make sure the Xcalibur data system is in the Ready state.</p>
	<p>Stop Analysis</p> <p>Stop the current sample run immediately. The Xcalibur application creates a raw file for the terminated sample that contains all raw data prior to the time of the Stop Analysis command. The data system then enters the Paused state, as indicated by the flashing red Paused message to the right of the Sequence box in the Current area in the Status view of the Home Page window.</p> <p>To start the next sample in the sample list queue after a Stop Analysis command, use the Start Analysis command or click the (depressed) Pause/Resume Analysis button in the toolbar.</p> <p>You can review the sample list queue at any time using the Acquisition Queue page of the Information view.</p>
	<p>Pause/Resume Sequence Queue</p> <ul style="list-style-type: none"> <p>• Pause</p> <p>Pause sample list processing when the button appears in the up (not depressed) position.</p> <p>The Xcalibur data system changes the appearance of the button from the up (not depressed) to the down (depressed) state. If a sample list has been downloaded or if sample data acquisition has started, the data system completes the current sample and creates a raw file for the sample. The application then enters the Paused state, as indicated by the flashing red Paused to the right of the Sequence box in the Current area in the Status view of the Home Page window.</p> <p>• Resume</p> <p>Resume sample list processing with the next sample in the sample list queue. The button changes in appearance from the down (depressed) to the up (not depressed) state to indicate that the data system is resuming sample list processing.</p> <p>You can review the sample list queue at any time using the Acquisition Queue page of the Home Page Information view.</p>
	<p>Xcalibur Help</p> <p>View the contents window for Xcalibur Help.</p>

Sequence Editor Toolbar

Table 43. Sequence Editor toolbar buttons (Sheet 1 of 3)

Button	Description
 New Sequence	Create a new sequence.
 Open	Find and open a file that already exists.
 Save	Save the current sequence. If you have not previously saved the current sequence, the Save As dialog box opens. Specify a location and name for the current sequence.
 Print	Select print range and print quality.
 Copy	Copy selected rows or columns from the sequence to the clipboard.
 Paste	Paste copied sequence rows or columns from the clipboard to the screen.
 Undo	<p>Cancel your previous action.</p> <p>For example, if you have just deleted an entry or annotation, click  to replace the deleted entry or annotation.</p> <p>Click  to delete an entry or annotation you just finished.</p> <p> cancels only one previous action.</p>
 Fill Down	<p>Copy sequence information from one selected sample row to one or more other sample rows without the need for repetitive cut-and-paste operations.</p> <p>❖ To fill information in rows</p> <ol style="list-style-type: none"> 1. Select the sequence information that you want to copy to the sample rows below the selected sample row. 2. Click the Fill Down button in the Sequence Setup Editor toolbar. The Fill Down dialog box opens. The Xcalibur application automatically fills the rows below the selected row with the selected entries. It only fills the rows directly below the selected row.
 Browse File Name	Select a path and file name that already exist on your computer or network. The Xcalibur data system enters the selected path and file name in the active File Name box. This button is only active when the cursor is in a Sequence Setup File Name box.
 User Labels	Change the heading captions of five information boxes on the Sequence Setup view. The default caption headings are Study, Client, Laboratory, Company, and Phone.

Table 43. Sequence Editor toolbar buttons (Sheet 2 of 3)

Button		Description
	Column Arrangement	<p>View or hide specific sequence columns.</p> <p>❖ To add a displayed column</p> <ol style="list-style-type: none"> 1. Click the column name in the Available Columns list and click Add. The Xcalibur application moves the column name to the Displayed Columns list. 2. Click OK. The data system adds the column to the sequence. <p>❖ To delete a displayed column</p> <ol style="list-style-type: none"> 1. Click the column name in the Displayed Columns list and click Remove. The data system moves the column name to the Available Columns list. 2. Click OK. The data system removes the column from the sequence.
	Transfer Row Info	Match samples by either sample ID or by position.
	Disk Space	Determine how much available disk space you have on your disk drive or drives.
	Run Sample	Collect data for one or more consecutive samples selected from the active sequence.
	Run Sequence	Collect data for one or more consecutive samples selected from the active sequence.
	Batch Reprocess	Reprocess data for samples selected from the active sequence.
	Start Analysis	<p>Start the next run in the Sequence queue.</p> <p>You can review the sample list queue at any time using the Acquisition Queue page of the Home Page Information view.</p> <p>This button on the toolbar is only available when an autosampler is configured, a LC/MS Detector contact closure interface is configured, and the Start When Ready check box is clear in the Start Options area of the Run Sequence dialog box. Make sure the data system is in the Ready state.</p>
	Stop Analysis	<p>Stop the current analysis. When the current sample has stopped, the Xcalibur application creates a raw file for the terminated sample that contains all raw data acquired prior to the time of the Stop Analysis command. The application then enters the Paused state, as indicated by the flashing red message to the right of the Sequence box in the Current area in the Status view of the Home Page window.</p> <p>To start the next sample in the Sequence queue after a Stop Analysis command, use the Start Analysis command or click the (depressed) Pause/Resume Analysis button in the toolbar.</p>

Table 43. Sequence Editor toolbar buttons (Sheet 3 of 3)

Button	Description
 Pause/Resume Sequence Queue	<ul style="list-style-type: none"> Pause Pause sample list processing when the button appears in the up (not depressed) position. The Xcalibur data system changes the appearance of the button from the up (not depressed) to the down (depressed) state. If a sample list has been downloaded or if sample data acquisition has started, the data system completes the current sample and creates a raw file for the sample. It then enters the Paused state, as indicated by the flashing red Paused to the right of the Sequence box in the Current area in the Status view of the Home Page window. Resume Resume sample list processing with the next sample in the sample list queue. The button changes in appearance from the down (depressed) to the up (not depressed) state to indicate that the data system is resuming sample list processing. <p>You can review the sample list queue at any time using the Acquisition Queue page of the Home Page Information view.</p>
 Help	Opens Xcalibur Help and display the contents window for the Sequence Setup view.

Plot Toolbar

Table 44. Plot toolbar buttons (Sheet 1 of 2)

Button	Description
	<p>Start Analysis</p> <p>Start the next run in the Sequence queue.</p> <p>You can review the sample list queue at any time using the Acquisition Queue page of the Home Page Information view.</p> <p>This button on the toolbar is only available when an autosampler is configured, a LC/MS Detector contact closure interface is configured, and the Start When Ready check box is clear in the Start Options area of the Run Sequence dialog box. Make sure the data system is in the Ready state.</p>
	<p>Stop Analysis</p> <p>Stop the current analysis. When the current sample has stopped, the data system creates a raw file for the terminated sample that contains all raw data acquired prior to the time of the Stop Analysis command. The data system then enters the Paused state, as indicated by the flashing red message to the right of the Sequence box in the Current area in the Status view of the Home Page window.</p> <p>To start the next sample in the Sequence queue after a Stop Analysis command, use the Start Analysis command or click the (depressed) Pause/Resume Analysis button in the toolbar.</p>
	<p>Pause/Resume Analysis</p> <ul style="list-style-type: none"> <p>Pause</p> <p>Pause sample list processing when the button appears in the up (not depressed) position.</p> <p>The Xcalibur data system changes the appearance of the button from the up (not depressed) to the down (depressed) state. If a sample list has been downloaded or if sample data acquisition has started, the data system completes the current sample and creates a raw file for the sample. The system then enters the Paused state, as indicated by the flashing red Paused to the right of the Sequence box in the Current area in the Status view of the Home Page window.</p> <p>Resume</p> <p>Resume sample list processing with the next sample in the sample list queue. The button changes in appearance from the down (depressed) to the up (not depressed) state to indicate that the data system is resuming sample list processing.</p> <p>You can review the sample list queue at any time using the Acquisition Queue page of the Home Page Information view.</p>
	<p>Zoom In Y</p> <p>To show more detail, zoom in on the Y-axis by a factor of two (2) from the current baseline. For example, you can change the Y-axis range from 0–100 to 0–50.</p>
	<p>Zoom Out Y</p> <p>To show more data, zoom out on the Y-axis by a factor of two (2). For example, you can change the Y-axis range from 0–25 to 0–50.</p>

Table 44. Plot toolbar buttons (Sheet 2 of 2)

Button	Description
 Normalize	Normalize the intensity scale of the data display to a fixed range on the Y-axis, from 0–25% to 0–100%.
 Zoom In X	To show more detail, zoom in on the X-axis by a factor of two (2). For example, you can change the X-axis range can from 0–20 to 5–15.
 Zoom Out X	To show more data, zoom out on the X-axis by a factor of two (2) from the center. For example, you can change the X-axis range from 7.5–12.5 to 5–15.
 Display All	View all data on the X-axis or all text in a report. For example, you can change the X-axis range from 7.5–12.5 to 0–20.
 Show Previous Scan	View the previous mass scan with its scan number.
 Show Next Scan	View the next mass scan with its scan number.
 Lock Display	<p>Unlock the data from the instrument so that you can use Xcalibur buttons on the toolbar or menu commands to review the data. During the time that you are in the unlocked mode, the data system continues to gather and save all data. In the unlocked mode, the lock icon in the toolbar appears pushed out.</p> <p>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 the locked mode, the lock icon in the toolbar appears to be pressed in.</p> <p>To relock the data to the instrument, click  in the Plot toolbar.</p>
 Help	Opens Xcalibur Help and displays the contents window for the Roadmap view of the Home Page. This window displays procedures, and information topics.

Xcalibur Dialog Boxes

- [Chromatogram Ranges Dialog Box](#)
- [Spectrum Ranges Dialog Box](#)

Chromatogram Ranges Dialog Box

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 *Qualitative Analysis User Guide*.

Spectrum Ranges Dialog Box

Use the Spectrum Ranges dialog box to view and edit the mass range, time, and other properties of a spectrum plot:

- In Qual Browser, for all plots in the active spectrum view
- On the Home Page, for the active spectrum plot in Real Time Plot mode

You can also apply automatic processing options such as smoothing and background subtraction.

For more information about the Spectrum Ranges dialog box, refer to the *Qualitative Analysis User Guide*.

Xcalibur Reference Tools

Read this chapter for information about specific tools that work with the Xcalibur data system.

Contents

- [Command Line Arguments](#)
- [ExcelExp.exe](#)
- [Command Line Format](#)
- [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 do these functions from command lines in the following locations:

- From the Microsoft Windows Run application (choose **Start > Run** from the Windows taskbar).
- From 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.
- From the Programs view of the Processing Setup window, by using the Program or Macro Name column.
- From 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:

path application

To create a new file in an application:

path application path new filename

To print a file from an application:

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:

- **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 software to the default location, the *path* before the application is **C:\Xcalibur\system\programs**.

Table 45. Command lines by file type (Sheet 1 of 2)

File Type	Example parameters and results
.raw	<i>pathQuanBrowser pathfile.raw</i> Opens the file in the Quan Browser window.
	<i>pathQuanBrowser /p pathfile.raw</i> Opens the file in the Quan Browser window, prints the spectrum and chromatogram, and then closes the Quan Browser window.
	<i>pathQualBrowser pathfile.raw</i> Opens the file in the Qual Browser window.
	<i>path\QualBrowser /p pathfile.raw</i> Opens the file in the Qual Browser window, prints the spectrum and chromatogram, and then closes the Qual Browser window.
.sld	<i>pathHomePage pathfile.sld</i> Opens the file in the Home Page window – Sequence Setup view.
	<i>pathHomePage /p pathfile.sld</i> Opens the file in the Sequence Setup view, and displays the Print Selection dialog box. After you click OK , the sequence is printed.
.pmd	<i>pathProcSetup pathfile.pmd</i> Opens the file in the Processing Setup window.
	<i>path\ProcSetup /p pathfile.pmd</i> Opens the file in the Processing Setup window, and displays the Print dialog box. After you click Print , the processing method is printed.
.meth	<i>pathInstSetup pathfile.meth</i> Opens the file in the Instrument Setup window.

Table 45. Command lines by file type (Sheet 2 of 2)

File Type	Example parameters and results
.rst	<i>pathQuanBrowser pathfile.rst</i> Opens the file in the Quan Browser window.
	<i>pathQualBrowser pathfile.rst</i> Opens the file in the Qual Browser window.
	<i>pathQualBrowser /p pathfile.rst</i> 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 results file exports that can be opened directly in Microsoft Excel using the ExcelExp program [ExcelExp.exe].

Note ExcelExp.exe has no user interface and can only be accessed through its command line.

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 based on the data source file name and places it in the same directory as the data source file.

ExcelExp.exe /Export type /data source path /Texport 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, this must be the path name of a sequence file (.sld).

For RESULT, this must be the path name of a results file (.rst).

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:

```
c:\xcalibur\system\programs\ExcelExp.exe /ESUMMARY
/Fc:\xcalibur\examples\methods\steroid.sld /TXLS
```

- To create a result file dump of the steroids15 results file from the Xcalibur xcalibur\examples\data folder:

```
c:\xcalibur\system\programs\ExcelExp.exe /ERESULT
/Fc:\xcalibur\examples\data\steroids15.rst /TXLS
```

Processing Setup Example

❖ To create a processing setup

1. From the Road Map view of the Home Page window, choose **GoTo > Processing Setup**. The Processing Setup window opens.
2. Click the **Programs** button in the View bar. The Programs view opens. Select the **Enable** check box to activate a row.
3. Double-click the **Program or Macro Name** box and browse to ExcelExp.exe (see path in the next step).
4. Type program parameters in the Parameters box.

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 results 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.

Program or Macro Name box:

c:\xcalibur\system\programs\ExcelExp.exe

Parameters box:

/ERESULT /F%F /TXLS

XConvert.exe

This Xcalibur utility program converts source files of one data format to destination files having a different data format.

Table 46. Data format conversion (Sheet 1 of 2)

Source files	Extension
Xcalibur	(* .raw)
ICIS	(* .dat)
GCQ	(* .ms)
Magnum	(* .ms)
ANDI	(* .cdf)
Mass Lab 2	(* .raw)
Lasermat	(* .*)

Table 46. Data format conversion (Sheet 2 of 2)

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.

Execution

From the Road Map view of the Home Page window, choose **Tools > File Converter**. The [Thermo File Converter Dialog Box](#) opens. This is the same dialog box that opens if you double-click XConvert.exe located in the Xcalibur > System > Programs directory.

You can also run XConvert.exe from the following command lines:

From 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.

From the Programs view of the Processing Setup window, use the Program or Macro Name command line box.

Automatic File Conversion

You can automatically convert and store files as they are created in the data system using the Xcalibur Convert.exe application and by selecting Run Program in the Action list.

The command line format is:

Path\XConvert /SSource Type /DDestination Type Source Path/File /O Destination Directory.

where */SSource Type*, */DDestination 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]

Examples:

- 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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