



thermo scientific

Thermo Xcalibur

Getting Started Guide

Processing Quantitative Data

Software Version 4.6

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ThermoFisher
SCIENTIFIC

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

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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 *Xcalibur Data Acquisition and Processing User Guide* for information about modifying the data system configuration, setting up the instrument configuration from within the Foundation platform, creating instrument methods and sequences for data acquisition, and for more detailed information about creating processing methods and batch reprocessing. Refer to the *Xcalibur Quan Browser User Guide* for more information about reviewing quantitation data.

Note You can modify the Xcalibur data system configuration by using the Thermo Xcalibur Configuration dialog box. Configuration options include the location of the default directories for your data files, methods, and report templates; the font size and type and the unit labels displayed in the preview views; the default mass tolerance, mass precision, and mass defect used to process the data files, and so on.

Use these tutorials to process a set of raw data files provided with the data system:

1. [Tutorial 1: Creating a Processing Method](#)
2. [Tutorial 2: Batch Reprocessing Data Files](#)
3. [Tutorial 3: Working with Result Files in Quan Browser](#)
4. [Tutorial 4: Reviewing, Specifying, and Printing Reports](#)

Contents

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

Related Documentation

Thermo Fisher Scientific provides the following documentation for the Xcalibur data system:

- *Xcalibur Quick Start Guide*
- *Xcalibur Getting Started Guide*
- *Xcalibur Data Acquisition and Processing User Guide*
- *Xcalibur Quan Browser User Guide*
- *Xcalibur Qual Browser User Guide*
- *Xcalibur Library Browser User Guide*
- *XReport User Guide*
- Help from within the data system

❖ To view the product manuals

- To access the Xcalibur manual set, do one of the following:
 - From the computer taskbar, choose **Start > Thermo Scientific Xcalibur > Thermo Scientific Xcalibur Manuals**.
 - From the Xcalibur home page – Roadmap view, choose **Help > Manuals**.
- To access the manual set for the Thermo Scientific mass spectrometer from the computer taskbar, choose **Start > Thermo Instruments > mass spectrometer**.

❖ To view the Help

You can open the Help in these ways:

- To open the Help for the Xcalibur data system, choose **Help > Xcalibur Help**. The Help opens to the Welcome page.
- To open the Help for an Xcalibur window, choose **Help > Window Help**, where *Window* is the current active window: home page, Instrument Setup, Processing Setup, Qual Browser, Quan Browser, or Library Browser.
- To open the Help for a specific page or dialog box of the Xcalibur user interface, click **Help**, choose **Help > Help on Current Item**, or press the F1 key.

❖ To download user documentation from the Thermo Scientific website

1. Go to www.thermoscientific.com.
2. In the Search box, type the product name and press ENTER.
3. In the left pane, select **Documents & Videos**, and then under Refine By Category, click **Operations and Maintenance**.

4. (Optional) Narrow the search results or modify the display as applicable:
 - For all related user manuals and quick references, click **Operator Manuals**.
 - For installation and preinstallation requirements guides, click **Installation Instructions**.
 - For documents translated into a specific language, use the Refine By Language feature.
 - Use the Sort By options or the Refine Your Search box (above the search results display).
5. Download the document as follows:
 - a. Click the document title or click **Download** to open the file.
 - b. Save the file.

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

Contact	Email	Telephone	QR Code
U.S. Technical Support	us.techsupport.analyze@thermofisher.com	(U.S.) 1 (800) 532-4752	
U.S. Customer Service and Sales	us.customer-support.analyze@thermofisher.com	(U.S.) 1 (800) 532-4752	
Global Support	<ul style="list-style-type: none"> ❖ To find global contact information or customize your request <ol style="list-style-type: none"> 1. Go to thermofisher.com. 2. Click Contact Us, select the country, and then select the type of support you need. 3. At the prompt, type the product name. 4. Use the phone number or complete the online form. ❖ To find product support, knowledge bases, and resources <p>Go to thermofisher.com/us/en/home/technical-resources.</p> ❖ To find product information <p>Go to thermofisher.com/us/en/home/brands/thermo-scientific.</p> 		

Introduction

This book provides tutorials that show how to quantitatively process a set of raw data files. For an overview of the Xcalibur data system and the data set used in the tutorials, review these topics.

Contents

- [Opening the Data System and Working with the Roadmap View](#)
- [Overview of the Xcalibur Data System](#)
- [Data Acquisition Flow Diagram](#)
- [Data Processing Flow Diagram](#)
- [Automated Data Acquisition and Processing Flow Diagram](#)
- [Xcalibur Example Files](#)

Opening the Data System and Working with the Roadmap View

To open and close the data system and to work with the Roadmap view, see these topics:

- [Opening, Navigating, and Closing the Data System](#)
- [Adding Application Pages to the Roadmap View](#)
- [Using the XApp Store to Explore Available Thermo Scientific Applications](#)

Opening, Navigating, and Closing the Data System


The Xcalibur data system provides access to all of your installed Thermo Scientific™ applications and the Thermo Scientific applications that are available in the XApp Store.

❖ To open the Xcalibur data system

Do one of the following:

- From the Windows taskbar, choose **Start > Thermo Scientific Xcalibur > Xcalibur**.

—or—

- On the computer desktop, double-click the **Xcalibur** icon, .

The home page window opens with the Info view on the left and the Roadmap view (open to the XApps page) on the right.


❖ To navigate the Xcalibur data system

To navigate the home page views (Roadmap, Sequence Setup, Real Time Plot, and Info), use the View menu or the View toolbar, .

To navigate the Xcalibur applications, use the Roadmap view or the Go To menu.

❖ To close the Xcalibur data system

Do one of the following:

- Click the **Close** icon, , in the upper right corner of the Xcalibur window.

—or—

- Right-click the **Xcalibur** icon in the taskbar and choose **Close Window** from the shortcut menu.

The XApps page provides access to the Xcalibur data system and other Thermo Scientific applications that are installed on the data system computer. The XApp Store page—which opens when you click the XApp Store tab—provides access to Thermo Scientific applications that are available for purchase.

The Status page of the Info view displays the instrument status, and the Acquisition Queue page displays the status of the injection sequences that you submit. For information about working with the Info view, refer to the *Xcalibur Data Acquisition and Processing User Guide*.

The XApps page contains the following icons (Figure 1):

- The first row contains icons for the Instrument Setup window, the Sequence Setup view, and the FreeStyle™ application.
- The remaining icons for the Xcalibur applications and other installed Thermo Scientific applications populate the page in alphabetical order from left to right and top to bottom.
- The last row contains icons for the mzCloud™, Planet Orbitrap, and Thermo Fisher Cloud websites.

The data system automatically detects the installed applications. If the XApp Store contains a later version of an installed application, a star (★) appears in the upper right corner of the application icon. You cannot hide or rearrange the icons on the XApps page.

Figure 1. Xcalibur home page with the Info and Roadmap views




Indicates that a later version of this application is available in the XApp Store.

Clicking the double chevron below the application icon opens a menu.

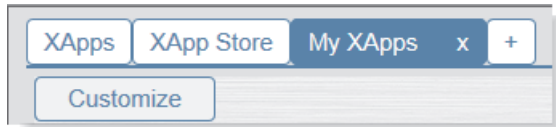
Adding Application Pages to the Roadmap View

You can customize the Roadmap view by adding pages that provide access to your preferred set of Thermo Scientific applications.

❖ To add application pages to the Roadmap view

In the Roadmap view, click the **My XApps** icon, .

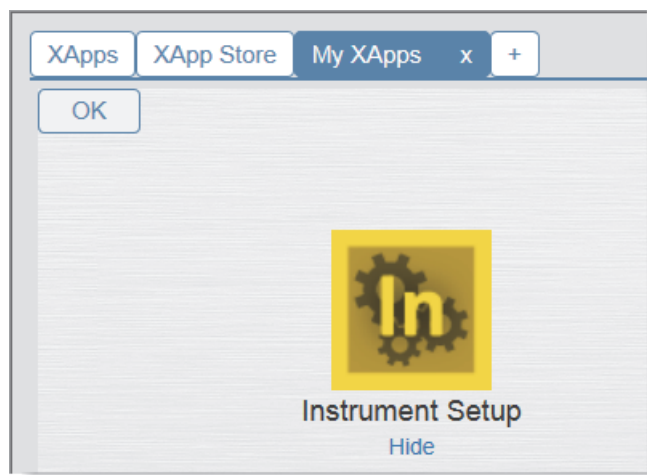
A new My XApps page opens with the same icons as the XApps page.



❖ To hide applications on a custom page

1. Click **Customize**.

“Hide” appears below each application icon and the OK button replaces the Customize button.



2. To hide an application, click **Hide**.

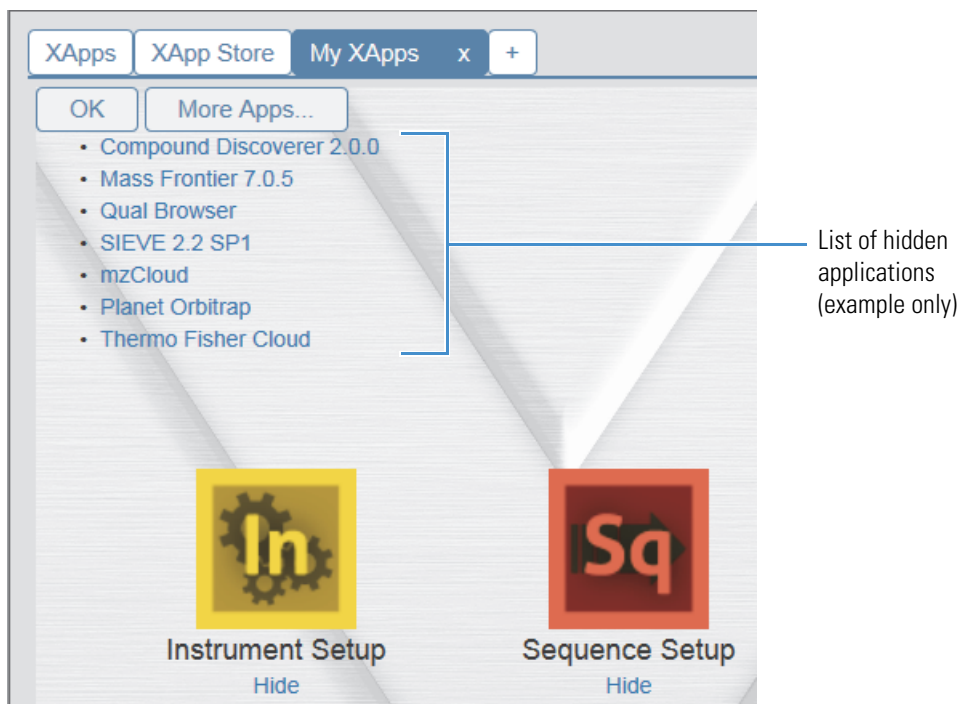
The application icon disappears from the page. Once you hide at least one application, the More Apps button appears to the right of the OK button.

3. Click **OK** to save the changes.

❖ To show installed applications on a custom page


1. Click **More Apps**.

A list of the hidden applications appears below the button. If the More Apps button is not visible, the custom page already contains icons for all the installed applications.



2. From the More Apps list, select the hidden application that you want to show on your custom page.

❖ To rename a MyXApps tab

1. Double-click the **MyXApps** tab ().
2. Select the tab text.
3. Type a new name.
4. Click ✓.

Using the XApp Store to Explore Available Thermo Scientific Applications

Use the XApp Store to access information about and install trial versions of Thermo Scientific applications.

❖ To open the XApp Store

Click the **XApp Store** tab in the Xcalibur Roadmap view.

❖ To view product information

On the XApp Store page, click **More Information** below the product name.

The product's website page opens.

❖ To be contacted by a sales representative

1. On the XApp Store page, click **How to Order** below the product name.

The product's Contact Us website page opens.

2. Fill in the form and click **Send**.

❖ To view and save the system requirements for an application

1. On the XApp Store page, click **System Requirements** below the product name.

The *Product Name* System Requirements document opens as a PDF file.

2. To save the PDF file to a local folder, do the following:

- a. Click the **Tools** icon, , and choose **File > Save As**.

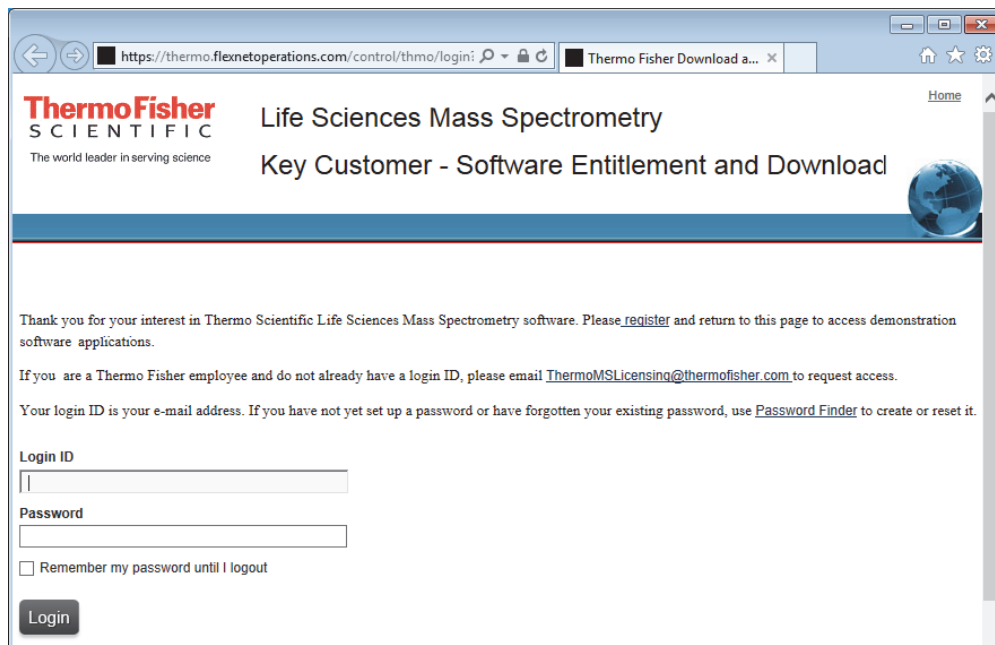
The Save As dialog box opens. The File Name box contains the document's default file name.

- b. Select the folder where you want to store the PDF file and click **Save**.

❖ To install a trial version of an available application

1. On the XApp Store page, click **Try** to the right of the application that you want to install.

The Thermo Scientific Life Sciences and Mass Spectrometry (LSMS) website for software downloads opens to the Login page ([Figure 2](#)).

Figure 2. Login page for software LSMS downloads

The screenshot shows a web browser window with the URL <https://thermo.flexnetoperations.com/control/thmo/login>. The page header includes the Thermo Fisher Scientific logo and the text "Life Sciences Mass Spectrometry" and "Key Customer - Software Entitlement and Download". A "Home" link and a globe icon are also present. The main content area contains the following text:

Thank you for your interest in Thermo Scientific Life Sciences Mass Spectrometry software. Please [register](#) and return to this page to access demonstration software applications.

If you are a Thermo Fisher employee and do not already have a login ID, please email ThermoMSLicensing@thermofisher.com to request access.

Your login ID is your e-mail address. If you have not yet set up a password or have forgotten your existing password, use [Password Finder](#) to create or reset it.

Below the text are the following form fields:

- Login ID:
- Password:
- Remember my password until I logout
- Login button

2. If you do not have a login ID, click **Register** to create one.
3. After you receive a confirmation email, log in.
The Product Information page opens.
4. Select the application that you want to install.
The demo page for the selected application opens.
5. Download the *Product Name and version* zip folder.

Overview of the Xcalibur Data System

To acquire and process raw data files, use the Instrument Setup and Processing Setup windows and the Sequence Setup view.

Instrument Setup	Use this window to create instrument methods with the chromatographic settings for your chromatography system and the data acquisition parameters for your mass spectrometer. You can also access an additional command menu for each instrument from this window.
Sequence Setup	Use this view of the home page window to set up the injection and processing sequence for your sample set. For data acquisition, the sequence must contain one or more instrument methods, the sample positions in the autosampler, and the injection volume for each sample. For data processing, the sequence must contain one or more processing methods.
Processing Setup	Use this window to create processing methods for your data sets. Processing methods contain the information required to extract qualitative or quantitative results from the raw data. This information includes the parameter settings for baseline integration, peak identification, and analyte quantification. Processing methods also specify the templates to be used to report the results.

Use the browser windows to review unprocessed raw data files (RAW files) or result files (RST files) created during batch processing.

For information about setting up the instrument method for your LC, GC, LC/MS, or GC/MS system, refer to the Help provided in the Instrument Setup window for each configured device.

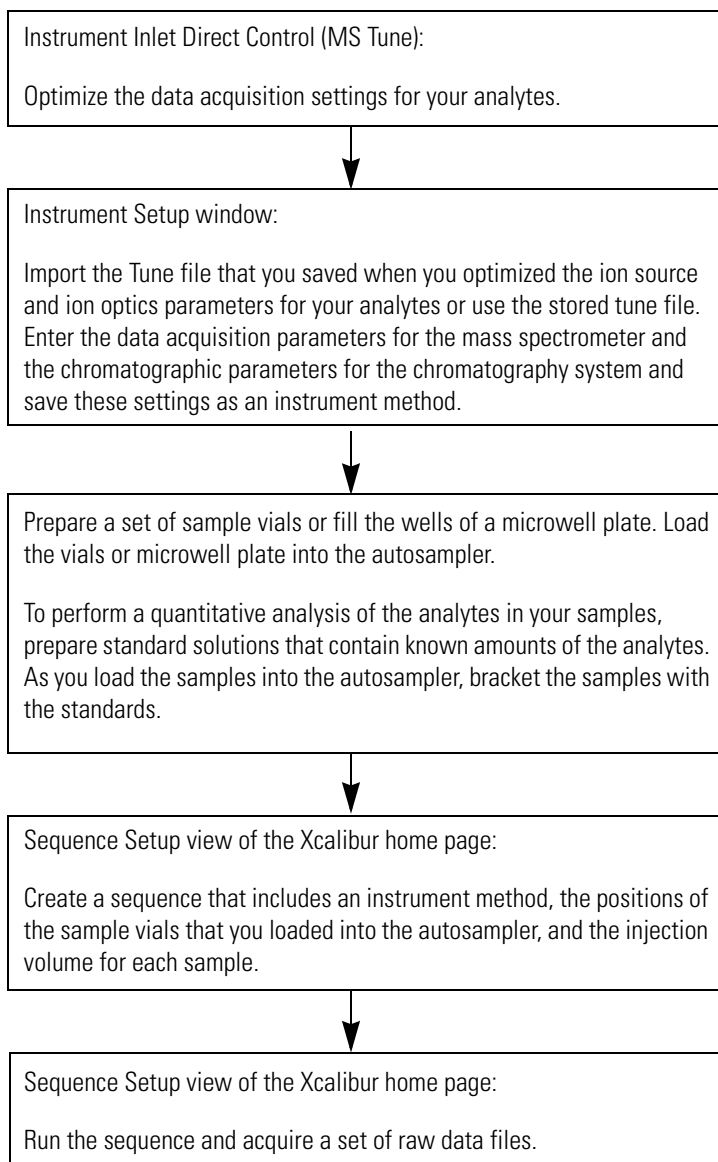
In addition to Help, Thermo Fisher Scientific provides hardware manuals and getting started guides for your Thermo Scientific mass spectrometer, and user guides or getting started guides for your Thermo Scientific LC system. For third-party LC systems that the Xcalibur data system controls, Thermo Fisher Scientific provides getting connected guides.

Data Acquisition Flow Diagram

Figure 3 provides a flow diagram for acquiring the sample set.

For information about creating an instrument method for your LC/MS system, refer to the Help systems and the getting started guides for the liquid chromatography (LC) instruments and the mass spectrometer (MS).

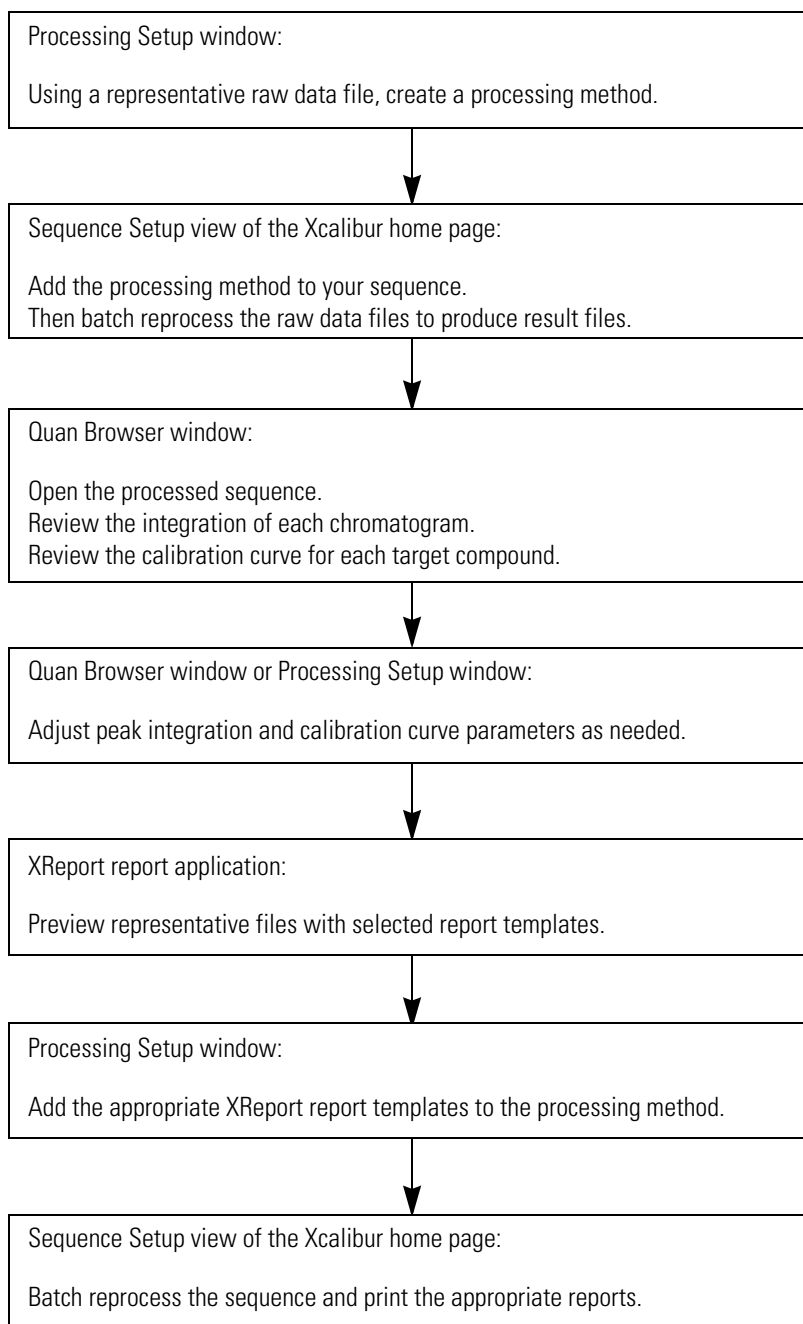
Figure 3. Acquiring data files



Data Processing Flow Diagram

Figure 4 provides a flow diagram for processing data once you have acquired it. For information about acquiring the raw data, refer to the *Xcalibur Data Acquisition and Processing User Guide*.

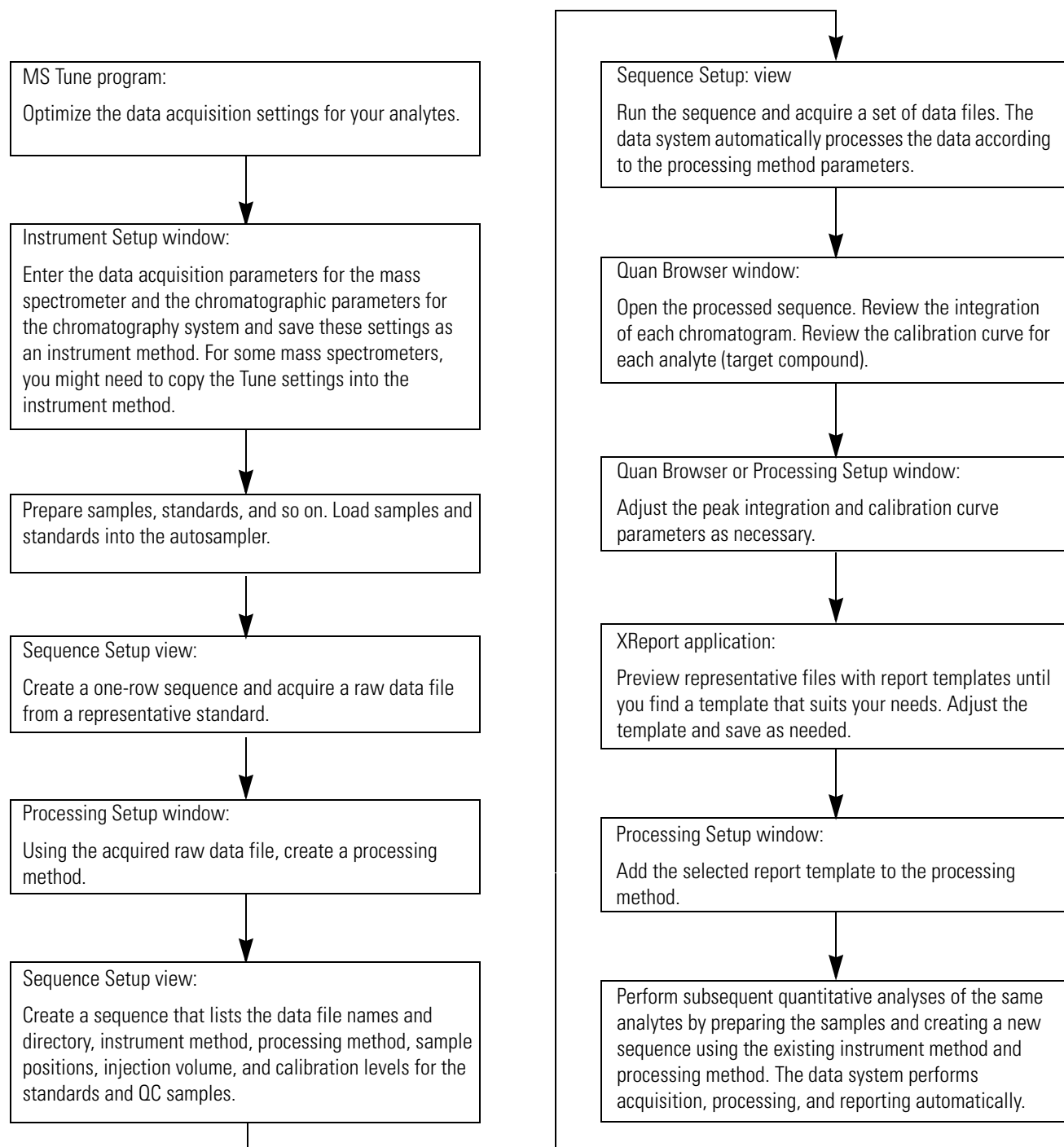
Figure 4. Processing previously acquired quantitation data



Automated Data Acquisition and Processing Flow Diagram

Figure 5 provides a flow diagram of how to do acquisition and processing automatically using the Xcalibur data system and the instrument control software provided with your mass spectrometer and chromatography system.

Figure 5. Acquiring and processing quantitative data automatically



Xcalibur Example Files

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

The lab used the internal standard calibration technique to quantify the pharmaceutical compound called drugx. The internal standard compound called D4 is a deuterated analogue of drugx that has four deuterium atoms exchanged for hydrogen atoms in the compound.

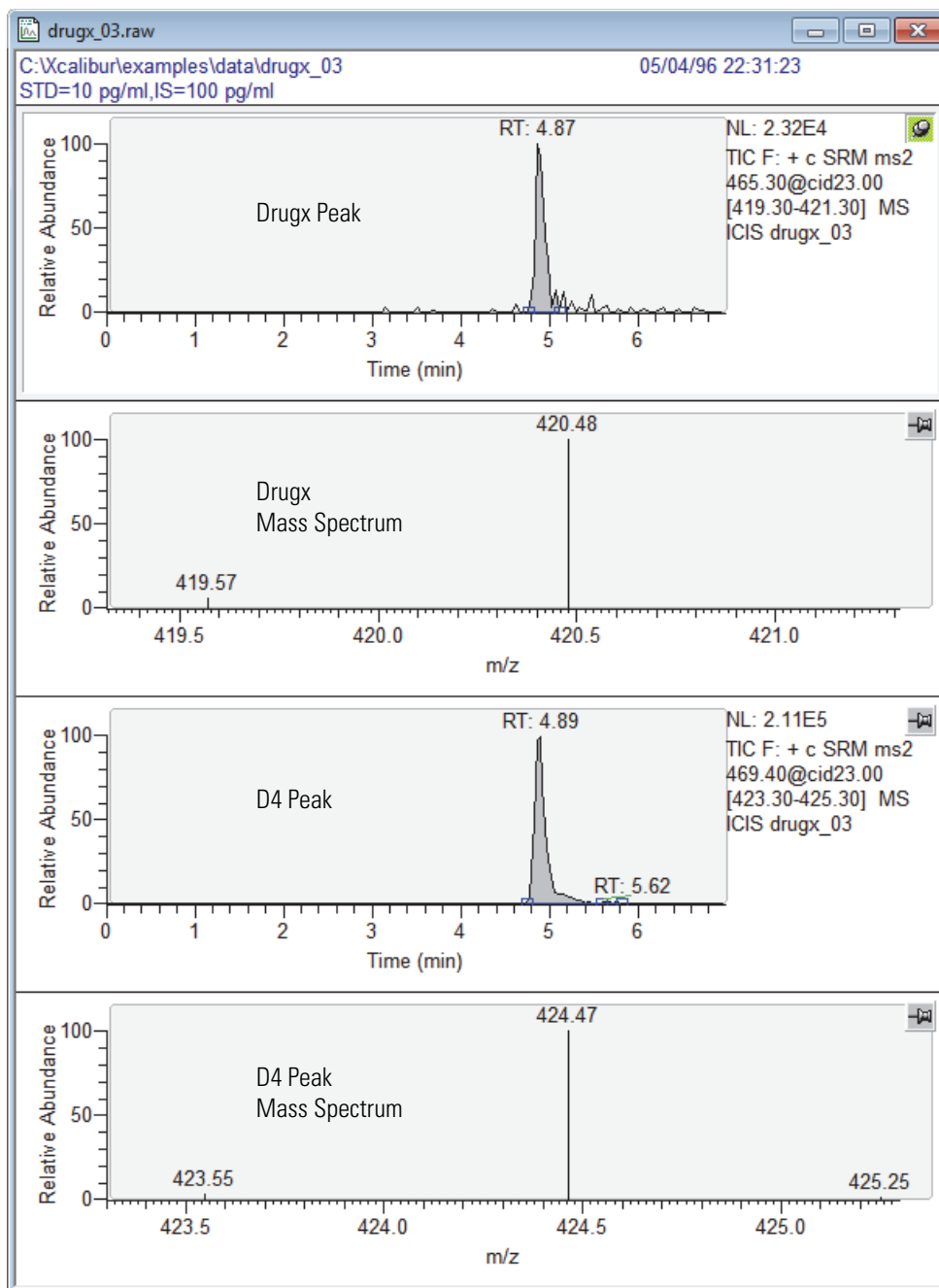
The calibration standards were prepared by spiking human plasma with drugx to give nine calibration levels with concentrations of 10, 25, 50, 100, 200, 400, 600, 800, and 1000 pg/mL. The lab ran triplicate samples at the high (1000 pg/mL) and low (10 pg/mL) ends of the curve with single samples run in 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 6](#) displays the scan filter chromatograms and mass spectra for a drugx.raw data file.

Figure 6. Chromatograms and mass spectra for drugx and D4



1 Introduction

Xcalibur Example Files

Tutorial 1: Creating a Processing Method

Use the following procedures to create a processing method for quantifying data using the raw data files associated with the drugx sequence file, drugx.sld, in the following directory:

drive:\Xcalibur\examples\methods

This tutorial does not discuss using system suitability parameters to verify the performance of the chromatographic column or the validity of the chromatographic peaks. To add report templates to the processing method, see [Chapter 5, “Tutorial 4: Reviewing, Specifying, and Printing Reports.”](#)

Create a processing method that quantifies the target compound (analyte) in the drugx data set by following these procedures in the order listed.

Contents


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

Opening the Processing Setup Window

Use the Processing Setup window to create a processing method. Use the Quan view of the Processing Setup window to set up the calibration information for your the target components (analytes) of a quantitative analysis.

❖ To open the Quan view of the Processing Setup window

1. Open the Xcalibur data system as follows:


- On the computer desktop, double-click the **Xcalibur** shortcut icon, .

–or–

- From the computer taskbar, choose **Start > Thermo Scientific Xcalibur > Xcalibur**.

The Xcalibur data system opens to the home page window.


2. Open the Processing Setup window as follows:

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

–or–

- From the menu bar, choose **GoTo > Processing Setup**.

3. If the Quan view is not already displayed, open it as follows:

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

–or–

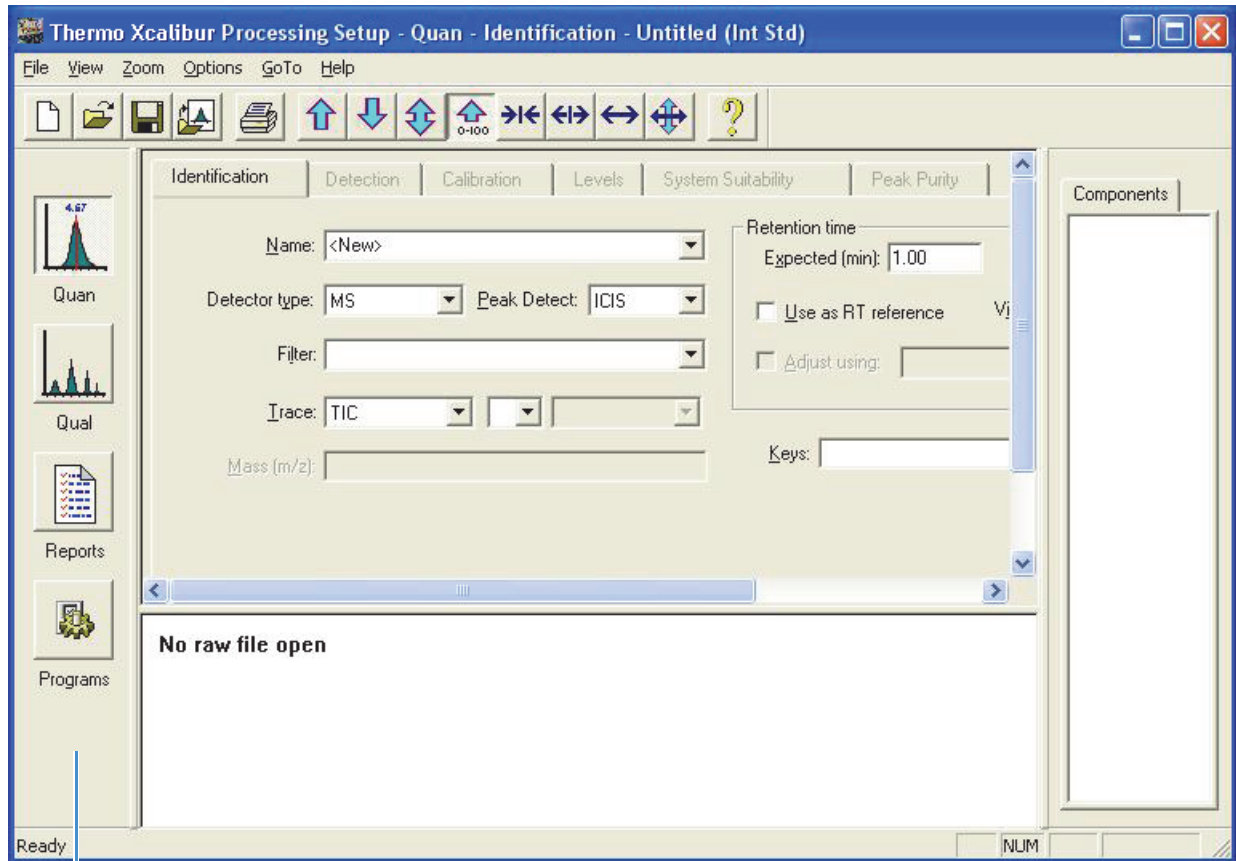
- On the menu bar, choose **View > View Quan**.

Tip The View bar is a vertical panel of icons on the left side of the window. If the View bar is not displayed, choose **View > View Bar** to display it on the left side of the Processing Setup window.

4. Click the **Identification** tab.

The Identification page opens (Figure 7).

Figure 7. Identification page for the Quan view of the Processing Setup window



View bar

5. If the data system automatically loads a processing method, choose **File > New** to start a new processing method.

Specifying the Quan View Options

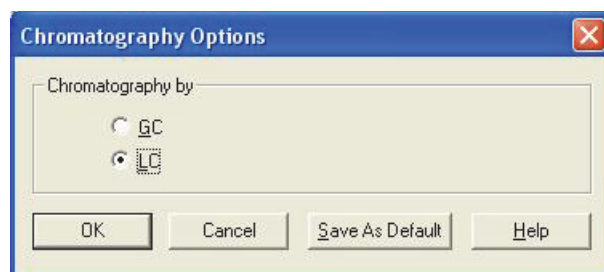
The chemists at Thermo Fisher Scientific acquired the data set used in this tutorial with an LC/MS system, and they used the internal standard calibration technique to quantify the drugx target compound.

❖ To specify chromatography by LC

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

The Chromatography Options dialog box opens (Figure 8).

Figure 8. Chromatography Options dialog box



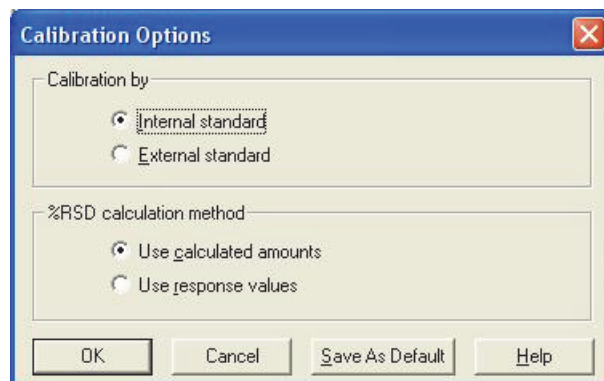
2. To specify chromatography by LC, select the **LC** option.
3. Click **OK** to save the settings and close the dialog box.

❖ To specify the internal standard calibration technique

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

The Calibration Options dialog box opens (Figure 9).

Figure 9. 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 data file from the data set to determine appropriate peak detection and integration settings for the processing method. In this tutorial, use the drugx_03.raw file. In general, select a raw data file corresponding to a low-concentration calibration standard.

❖ To open a raw data file in the Quan view of the Processing Setup window

1. Do one of the following:

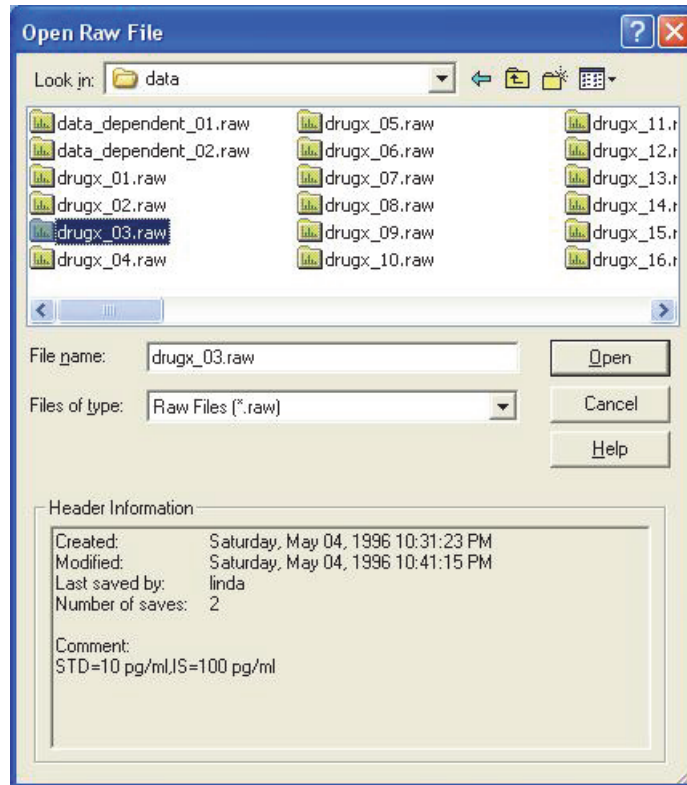
- In the toolbar, click the **Open Raw** icon, .

–or–

- From the menu bar, choose **File > Open Raw File**.

The Open Raw File dialog box opens (Figure 10).

Figure 10. Open Raw File dialog box



2. Browse to the following location:

drive:\Xcalibur\examples\data

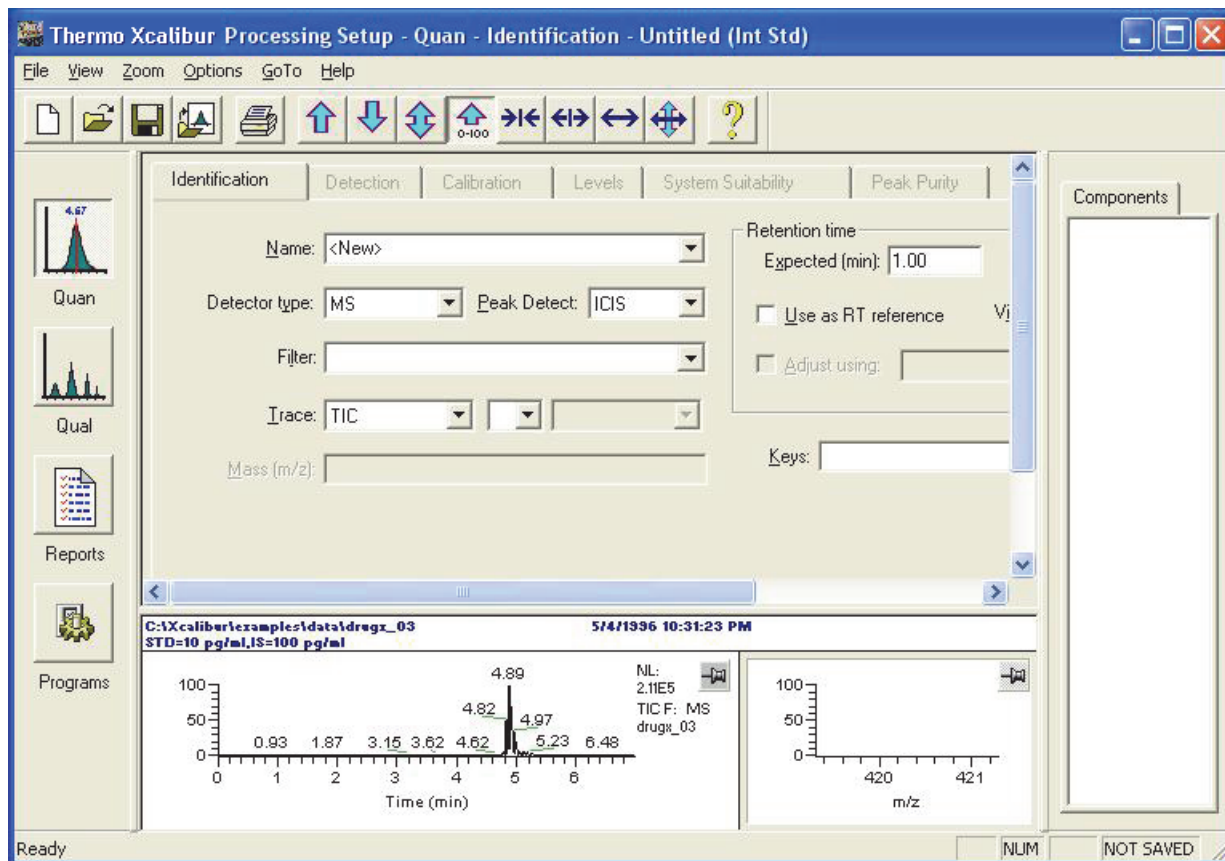
2 Tutorial 1: Creating a Processing Method

Opening a Raw Data File

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

Processing Setup opens the drugx_03.raw file (Figure 11).

Figure 11. Identification page with the total ion current (TIC) chromatogram of drugx_03.raw



Tip If you save a processing method when a raw data file is open, the raw data file name is saved in the processing method. To have the Xcalibur data system automatically open the associated raw data file whenever you open the processing method, select the **On** option in the Auto-Open Raw File area of the Settings dialog box.

To open this dialog box in the Processing Setup window, choose **Options > Settings**.

Specifying the Identification Settings for Analysis Components

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

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

For the internal standard calibration technique, each calibration standard contains one or more target compounds and one or more internal standards. The data set used in this tutorial contains one target compound and one internal standard. The target compound is drugx. The internal standard compound is D4.

Specifying the Identification Settings for the Internal Standard

A processing method needs component identification information to associate each sample component with a chromatographic peak. Use the Identification page for the Quan view in the Processing Setup window to name the sample components and to specify the retention time and peak identification criteria.

To identify the internal standard, follow these procedures:

- [Specifying the Name of the Internal Standard](#)
- [Selecting the Detector Type](#)
- [Selecting the Peak Detection Algorithm](#)
- [Matching Scan Filters with Components](#)
- [Selecting the Trace Type](#)
- [Entering the Retention Time of the Component Automatically](#)

2 Tutorial 1: Creating a Processing Method

Specifying the Identification Settings for Analysis Components

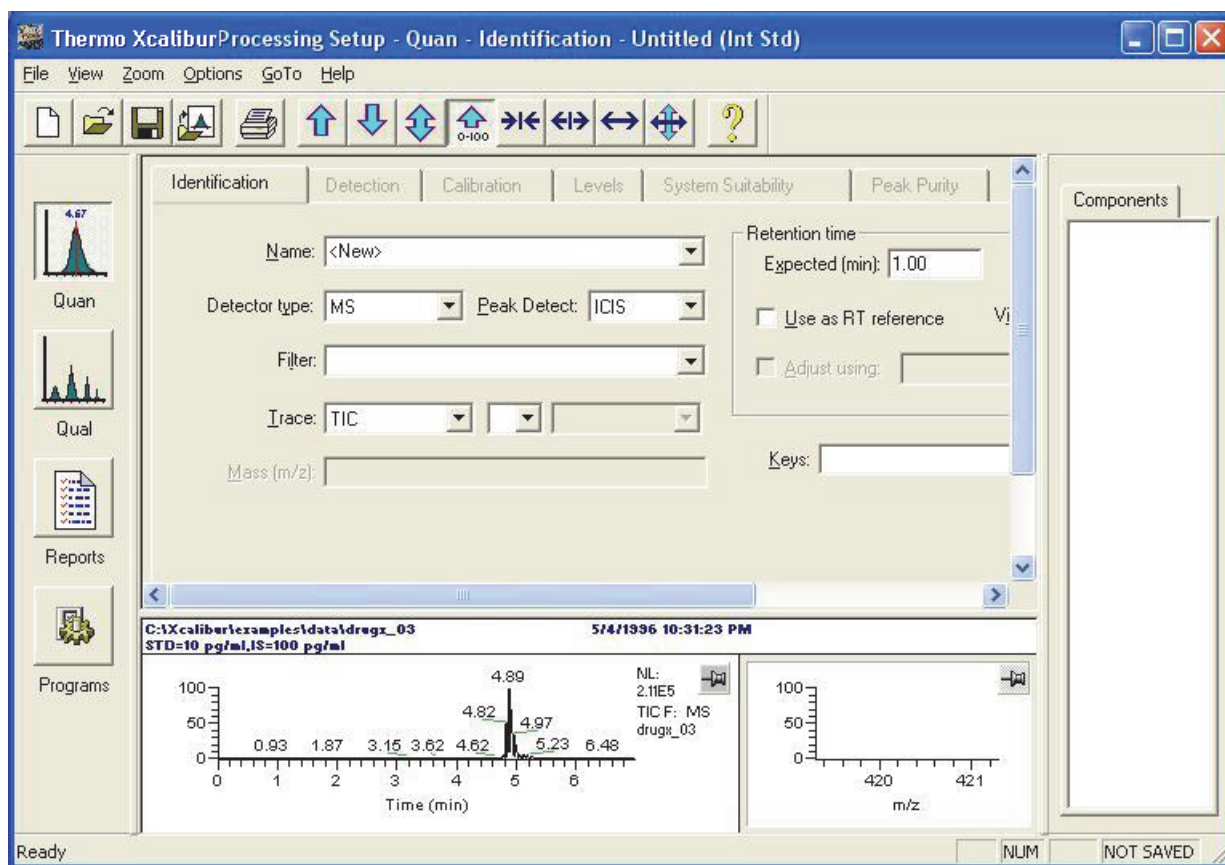
Specifying the Name of the Internal Standard

Use the Name list on the Identification page to name the components in the sample. The parameter settings on the Identification page are specific to the component selected in the Components list on the right side of the window.

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

1. In the Name list, select **<New>**, and then type **D4**, the name of the internal standard (Figure 12).

Figure 12. Identification page without named components



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

The name appears in the Components list.

Note To delete a component, highlight the component name in the Components list on the right side of the window. Then, choose **Options > Delete component name**.

Selecting the Detector Type

Use the Detector Type list on the Identification page to specify the type of detector used to acquire the raw data file. The available selections are MS (mass spectrometer), Analog, A/D card, PDA (photodiode array detector), and UV (UV-Vis detector).

❖ To specify the type of detector used to acquire the data

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

Selecting the Peak Detection Algorithm

Use the Peak Detect list on the Identification page to specify the 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 algorithm

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 data file, the data system lists the scan filters associated with the raw data file in the Filter box. In this example, the application acquired selected reaction monitoring (SRM) data on the following compounds, using alternating product ion scans (drugx and D4, respectively):

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

To quantify drugx, use the following filtered mass chromatograms for drugx and its internal standard, D4.

drug x (analyte)	TIC F: + c SRM ms2 465.30@23.00[419.30–421.30]
D4 (internal standard)	TIC F: + c SRM ms2 469.40@23.00[423.30–425.30]

❖ To match the internal standard, D4, with its scan filter

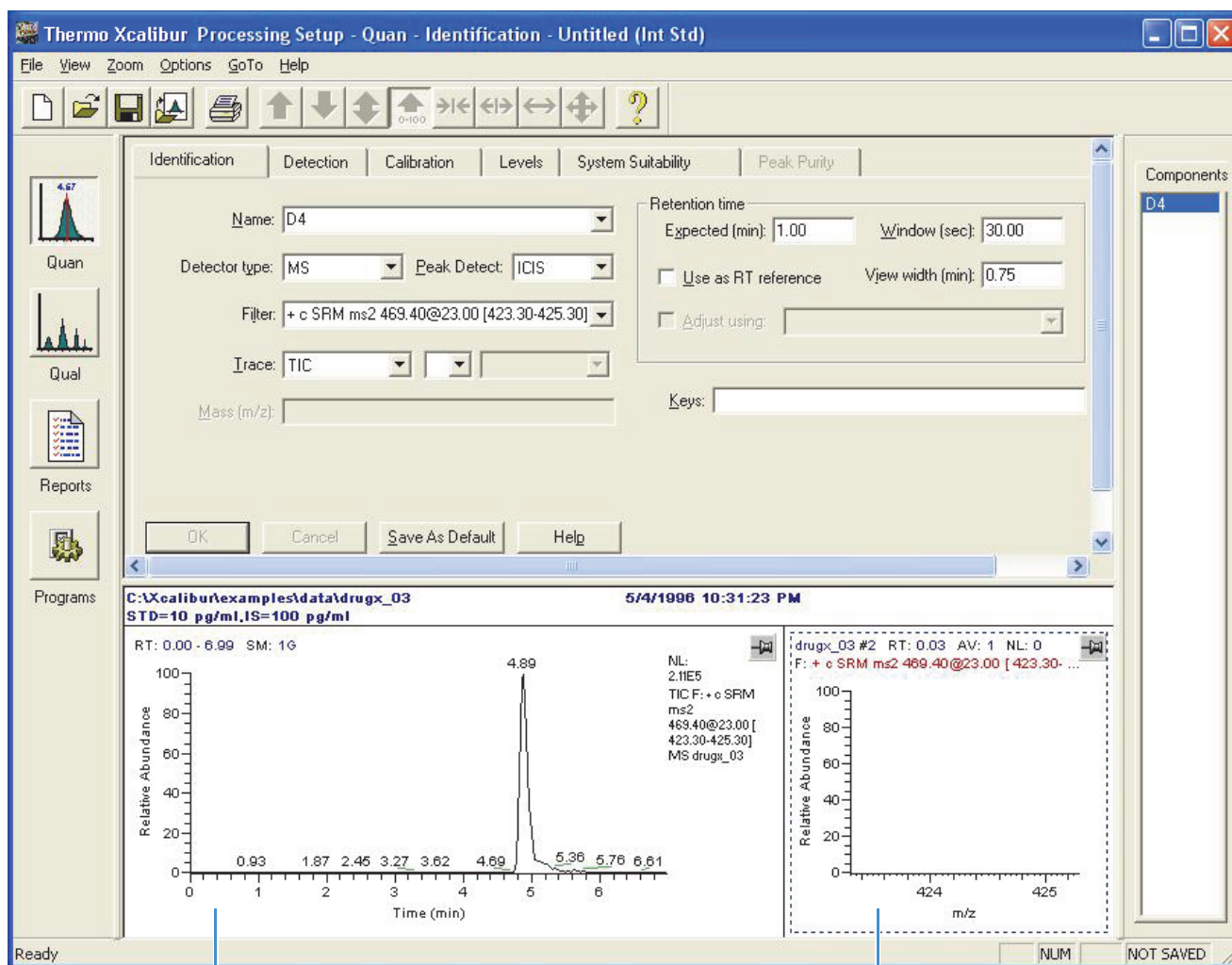
1. From the Filter list for the drugx_03.raw file, select the following scan filter for D4:

+ c SRM ms2 469.40@23.00[423.30–425.30]

Note The scan filter indicates a positive, centroid profile, selected reaction monitoring experiment type (SRM), MS/MS scan, precursor ion scan of m/z 469.40 at 23.0 units of CID energy with a product mass-to-charge range of 423.30–425.30.

2. Click **OK** to display the mass chromatogram for D4 ([Figure 13](#)).

Figure 13. Scan filter mass 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 of the Component Automatically

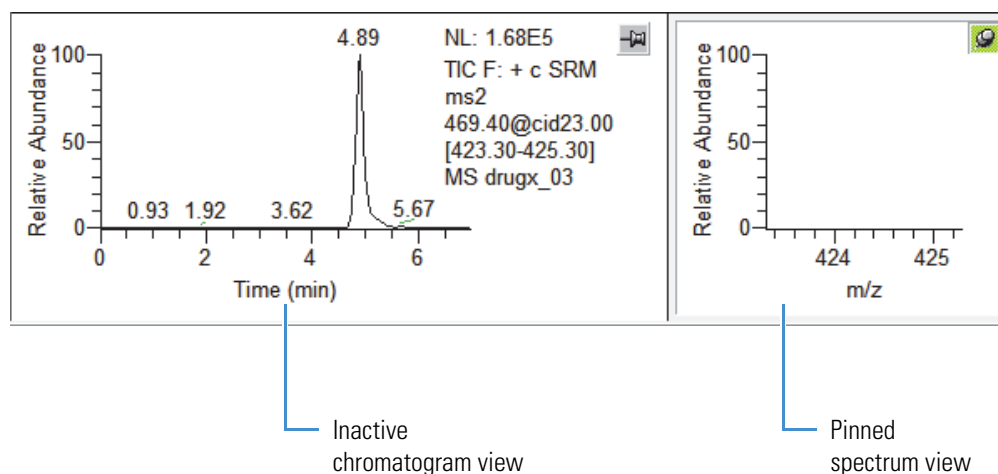
You can enter the expected retention time and retention time window for a component manually by typing the values in their respective boxes or automatically by working with the chromatogram and spectrum views.

❖ To automatically enter the retention time of a chromatographic peak

1. To make the spectrum view the active and pinned view, click the pin icon, , in the upper right corner of the cell ([Figure 14](#)).

The pin background turns green  and appears to be pinned to the screen.

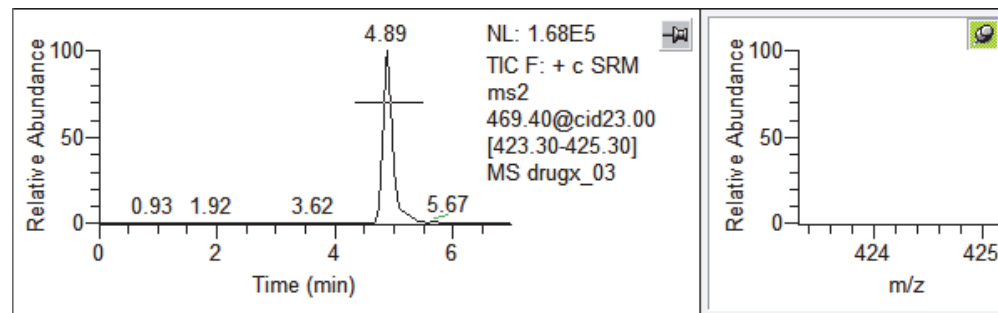
Figure 14. Inactive chromatogram view and pinned spectrum view



2. In the chromatogram view, drag the cursor across the chromatogram peak as shown in [Figure 15](#).

The horizontal line across the center of the peak shows the time range selected by the mouse movement.

Figure 15. Selecting the scan (time point) corresponding to the peak maximum

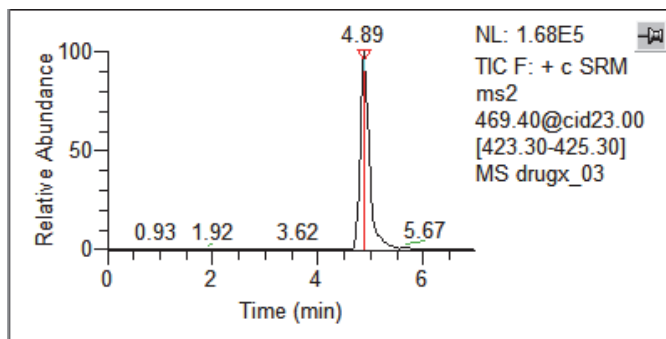


3. Release the mouse button.

The data system automatically does the following:

- Selects the retention time of the peak apex and highlights the selected scan with a vertical red marker in the chromatogram view (Figure 16).

Figure 16. Vertical red marker at the peak apex

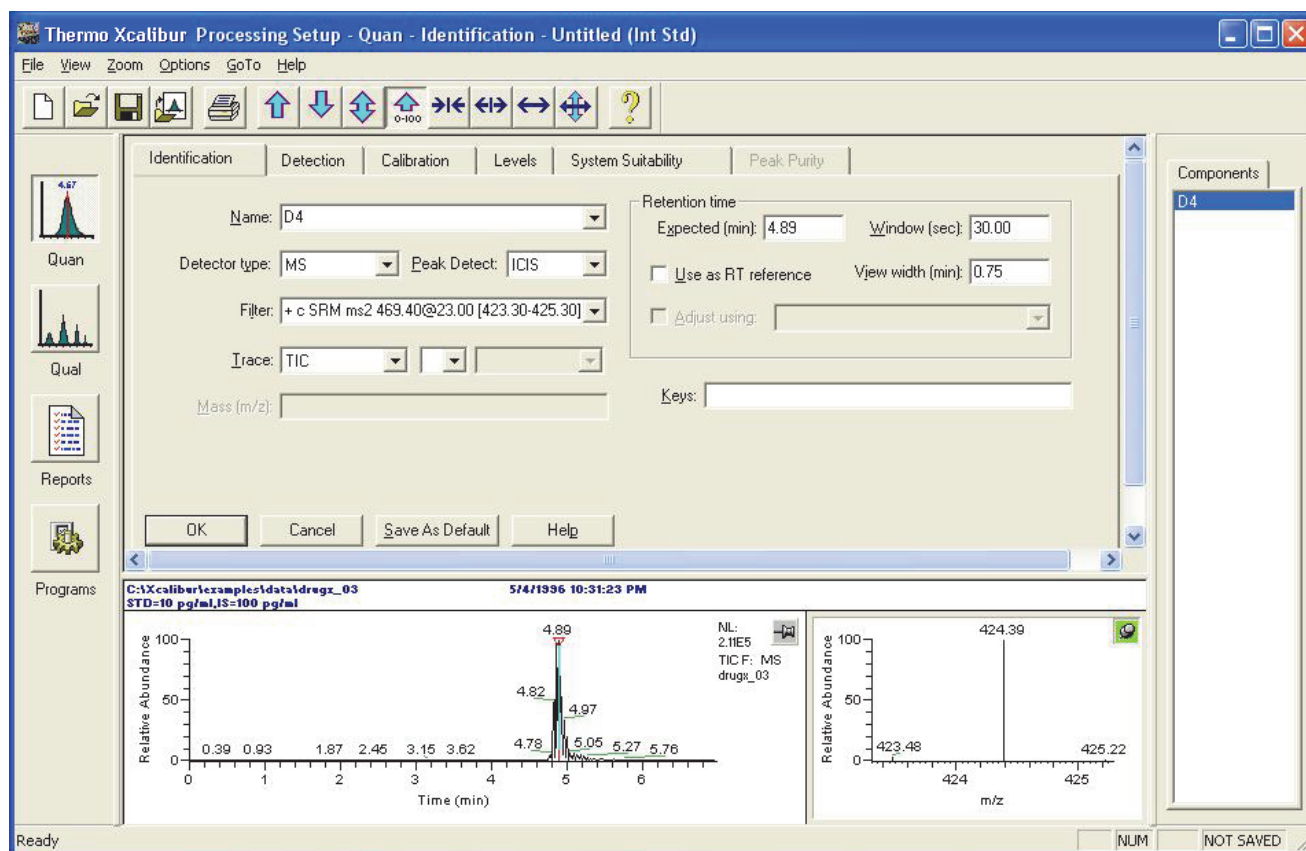


- Displays the retention time corresponding to the selected scan in the Expected box in the Retention Time area (Figure 17).
- Displays the mass spectrum of the product ions in the spectrum view (Figure 17).

2 Tutorial 1: Creating a Processing Method

Specifying the Identification Settings for Analysis Components

Figure 17. Identification page with a retention time marker (vertical line) and associated mass spectrum



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 8](#) of the next procedure, [Specifying the Identification Settings for the Target Compound](#).

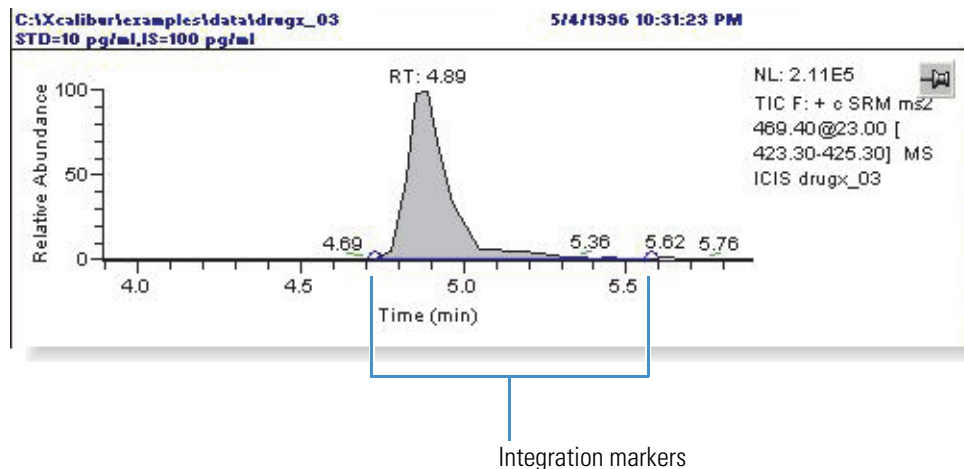
- Leave the Window box number at **30** seconds. This parameter controls the width of the window that the algorithm searches to locate the component. In this case the algorithm searches 15 seconds on either side of RT 4.89 minutes to find the D4 peak.
5. Type **2.00** in the View Width box.

View width controls how much of the chromatogram time range the application displays when you view the components in the chromatogram view.

6. To save the component identification information for D4, click **OK**.


The chromatogram view displays the time portion of the chromatogram from 3.9 to 5.9 minutes based on a selection of 2.00 minutes as the view width for a peak with an expected retention time of 4.9 min. Integrated peaks are shaded in gray with blue integration markers at the starting and ending points of the peak. The baseline is indicated by a blue line that connects the integration markers (Figure 18).

Figure 18. 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 icon, , in the spectrum view (the pane to the right of the chromatogram plot view) before performing [step 2](#) on [page 26](#).

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 the Identification Settings for the Target Compound

The procedure for identifying the target compound is the same as that for identifying the internal standard. In the following procedure, you use the internal standard that you identified in [Specifying the Identification Settings for the Internal Standard](#) as the retention time reference component.

❖ To specify the identification settings for the target compound

1. To specify a name for the target compound, do the following:

- a. Select **<New>** in the Name list.

The Apply Changes dialog box opens if you have warnings enabled.

- b. Click **Yes** to apply changes.
- c. To specify the name of the target compound, type **drugx**.
- d. Click **OK** to save the new name.

The target compound name appears in the Components list.


2. Select **MS** in the Detector Type list if it is not already selected.
3. Select **ICIS** in the Peak Detect list.
4. To match the target compound with its scan filter, do the following:

- a. In the Filter list, select the following filter for drugx:

+ c SRM ms2 465.30@23.00[419.30-421.30]

- b. Click **OK** to apply the scan filter to the total ion current.

Processing Setup automatically displays the mass chromatogram corresponding to the target compound.

5. Select **TIC** (total ion current) in the Trace list if it is not already selected.
6. To display the mass spectrum of the currently active component and automatically enter the retention time of the target compound peak, do the following:
 - a. To make the spectrum view the active and pinned view, click the pin icon, , in the upper right corner of the cell.

The pin background turns green  and appears to be pinned to the screen.

- b. Drag the cursor in the chromatogram view across the chromatographic peak.
- c. Release the mouse button.

The data system automatically does the following:

- Selects the retention time of the peak apex and highlights the selected scan with a red marker in the chromatogram view.
- Enters the retention time corresponding to the selected scan in the Expected box in the Retention Time area.

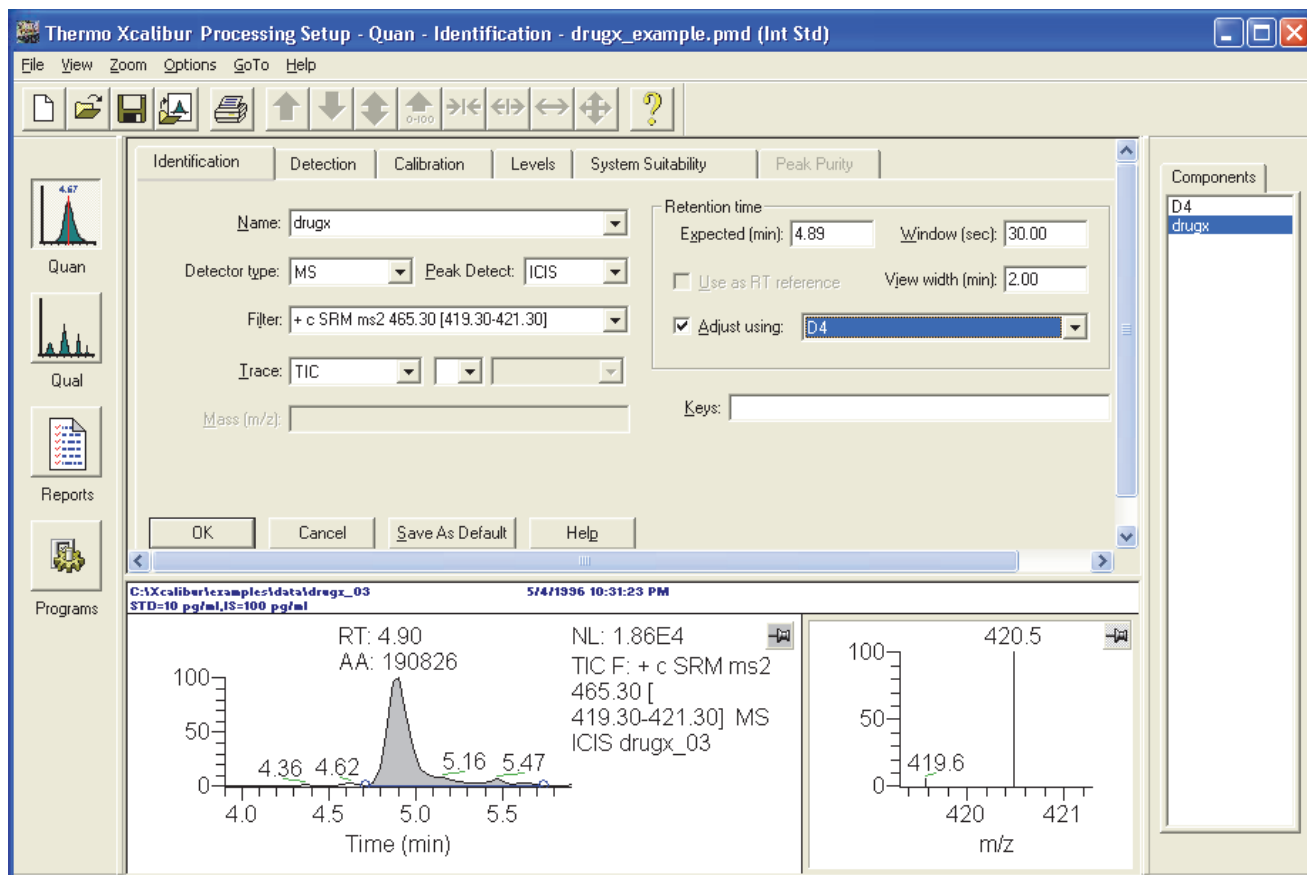
7. Type **2.00** into the View Width box.
8. To adjust the expected retention time of drugx by changes in the actual retention time of D4, do the following:
 - a. Select the **Adjust Using** check box.
The Adjust Using list becomes available.
 - b. Select **D4** in the Adjust Using list.

You selected D4, the internal standard, as the retention time reference component in [step 4](#) of the previous procedure, [Specifying the Identification Settings for the Internal Standard](#).

9. Leave the value in the Window box at **30** seconds.
10. To accept the peak identification settings for drugx, click **OK**.

The chromatogram view displays the time portion of the chromatogram from 3.9 to 5.9 minutes based on a selection of 2.00 minutes as the view width for a peak with an expected retention time of 4.9 min. Integrated peaks are shaded in gray with blue integration markers at the starting and ending points of the peak. The baseline is indicated by a blue line that connects the integration markers ([Figure 19](#)).

Figure 19. Peak identification settings for drugx, the target compound



Entering Peak Integration and Detection Parameters

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

To enter peak integration and detection parameters, follow these procedures in order:

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

Entering the Peak Integration Parameters

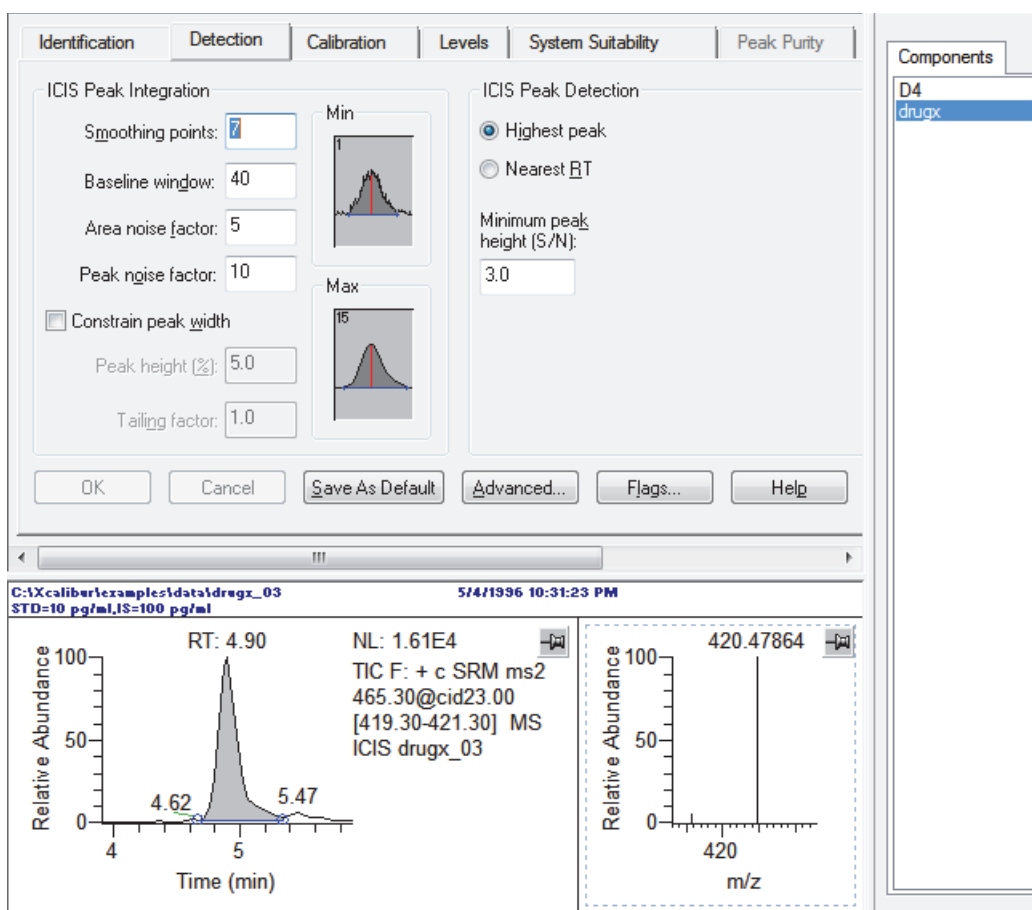
Enter peak integration parameters to specify how the data system determines the area of each peak in the chromatogram. Processing Setup provides peak integration parameter options in the Peak Integration area on the Detection page.

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

1. Click the **Detection** tab.

The Detection page for the Quan view opens (Figure 20).

Figure 20. Detection page for the Quan view of the Processing Setup window



2. In the Components list, select **D4**.
3. To enter the peak integration settings for the selected component, do the following:
 - a. Type **5** in the Smoothing Points box in the ICIS Peak Integration area.

Based on the peak view, type the number of points in the moving average that are used to smooth data in the Smoothing Points box. The valid range is 1 (no smoothing) to 15 (maximum smoothing).

- b. 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.

- c. 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.

- d. 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.

- e. Clear the **Constrain Peak Width** check box.

Note This tutorial does not use the constrain peak width option.

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 make the Peak Height (%) and Tailing Factor parameters available. The valid range for the peak height threshold is 0.0 to 100.0%. The valid range for the tailing factor is 0.5 to 9.0.

4. To save the peak integration parameters for D4, click **OK**.
5. To enter the peak integration settings for the target compound, do the following:
 - a. Select **drugx** in the Components list.
 - b. Repeat [step 3](#) of this procedure.
 - c. To save the peak integration parameters for drugx, click **OK**.

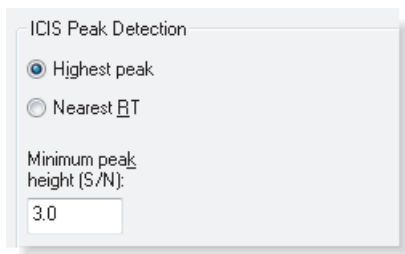
Entering the Peak Detection Parameters

Peak detection parameters specify how the Xcalibur data system selects a chromatographic 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. In the Components list, select **D4**, the internal standard for the target component drugx.
2. To associate the selected component with the highest peak in the filtered chromatogram, select the **Highest Peak** option in the ICIS Peak Detection area ([Figure 21](#)).

Figure 21. Highest Peak option selected



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.

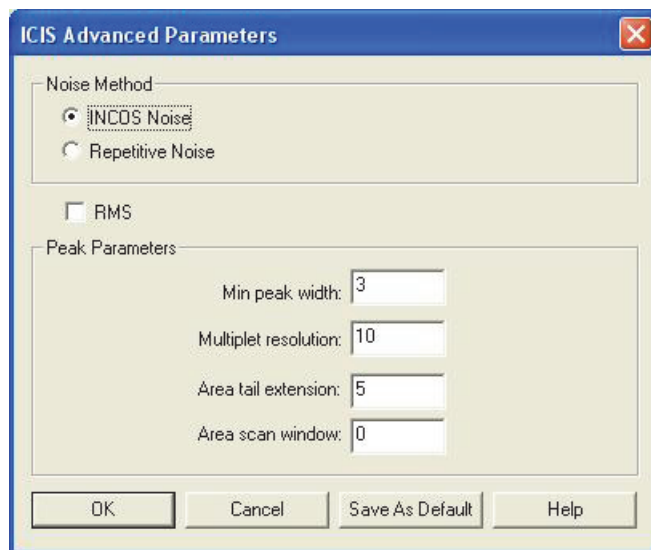
4. Verify that the advanced peak detection parameters are set to their default values as follows:
 - a. Click **Advanced**.

The ICIS Advanced Parameters dialog box opens (Figure 22).

Use the ICIS Advanced Parameters dialog box to specify advanced component detection criteria if the standard detection criteria do not provide the desired results. Refer to the *Xcalibur Data Acquisition and Processing User Guide* for information on the parameters in the ICIS Advanced Parameters dialog box. The application applies the settings in the ICIS Advanced Parameters dialog box on a per component basis.

- b. Inspect the settings in the ICIS Advanced Parameters dialog box. Make sure the settings are the same as those in Figure 22.

Figure 22. ICIS Advanced Parameters dialog box, showing the default settings



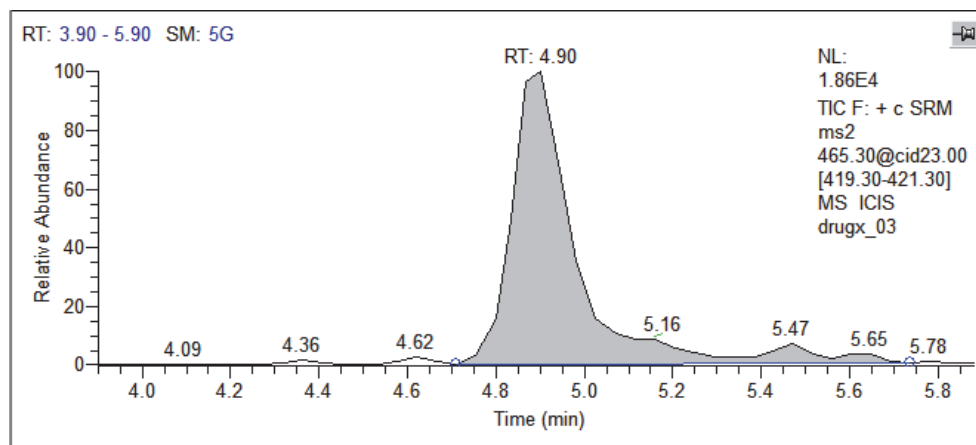
- c. Click **OK** to close the ICIS Advanced Parameters dialog box.

5. To save the peak detection parameters, click **OK**.
6. In the Components list, select **drugx**, the target compound (analyte) for this analysis.
7. Repeat [step 2](#) through [step 5](#) of this procedure for drugx, the target compound.
8. On the Detection page, verify the following settings for drugx and D4. Select one component in the Components list and check the settings. Then, select the other component in the Components list and check the settings.

Parameter	Setting
ICIS Peak Integration	
Smoothing Points	5
Baseline Window	40
Area Noise Factor	5
Peak Noise Factor	10
Constrain Peak Width	Clear
ICIS Peak Detection	
Highest Peak	Selected
Minimum Peak Height (S/N)	3

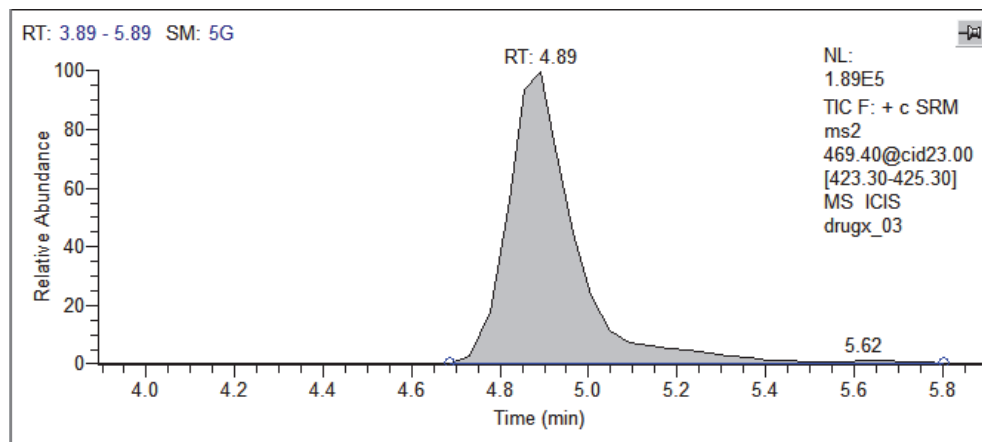
9. Verify that the scan filter chromatogram for drugx matches [Figure 23](#).

Figure 23. Scan filter chromatogram for drugx



10. Verify that the scan filter chromatogram for D4 matches [Figure 24](#).

Figure 24. Scan filter chromatogram for D4



Selecting the Calibration Settings

In the Processing Setup window, use the Calibration page of the 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.

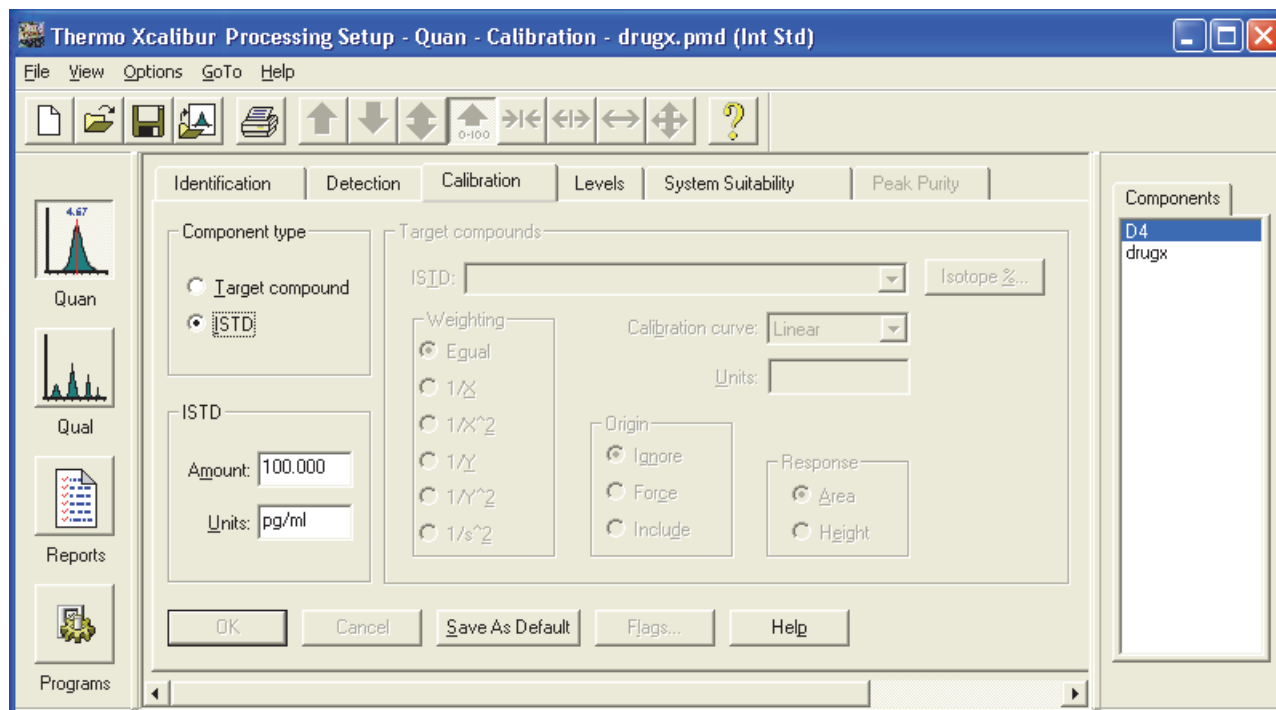
The Calibration page of the Quan view opens.

2. To enter the calibration settings for the internal standard, component D4, do the following:
 - a. In the Components list, click **D4**.
 - b. To select D4 as the internal standard, select the **ISTD** option in the Component Type area.
 - c. To specify an internal standard amount of 100 pg/mL, type **100** in the Amount box in the ISTD (Internal Standard) area.
 - d. To specify pg/mL as the units of concentration, type **pg/mL** in the Units box.
3. To save the settings for D4, click **OK**.
4. Verify that the calibration settings for component D4 match those in [Figure 25](#).

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Selecting the Calibration Settings

Figure 25. Calibration page, showing the settings for the D4 internal standard



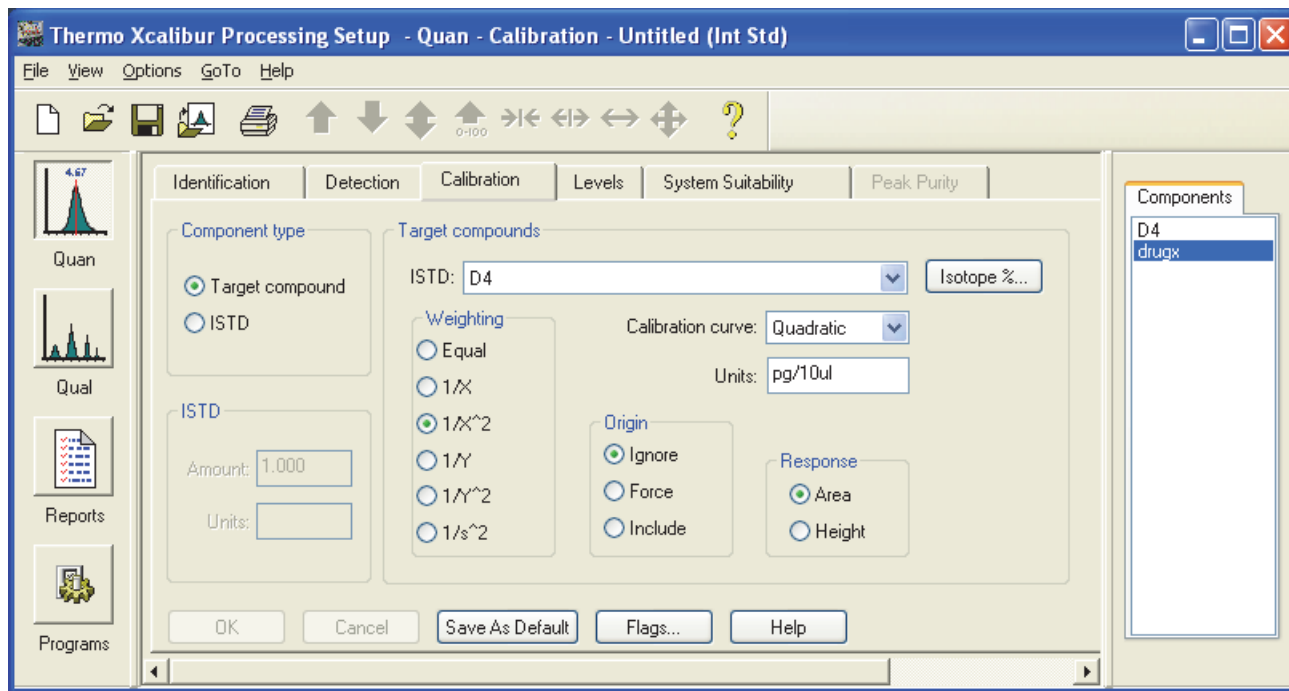
This procedure does not discuss setting parameters on the System Suitability or Peak Purity pages. For information about setting these parameters, refer to the *Xcalibur Data Acquisition and Processing User Guide*.

❖ 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. To specify D4 as the internal standard for the target compound, select **D4** in the ISTD list in the Target Compounds 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 µL** in the Units box.
6. To specify a weighting of $1/X^2$, select the **1/X²** option in the Weighting area.
7. To exclude the origin as a data point when fitting the calibration curve, select the **Ignore** option in the Origin area.
8. To use the area of the peak to determine response, select the **Area** option in the Response area.
9. To save the settings, click **OK**.

10. Verify that the calibration settings for the drugx (target component) are the same as those in Figure 26.

Figure 26. Settings for the drugx target compound



Specifying Calibration Levels and QC Levels

In Processing Setup, use the Levels page of the Quan view to specify the amount of target compound 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.

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

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

Specifying the Calibration Levels of the Target Compound

Use the Levels page to set up the calibration levels for the target compound.

❖ **To specify the calibration levels of the target compound**

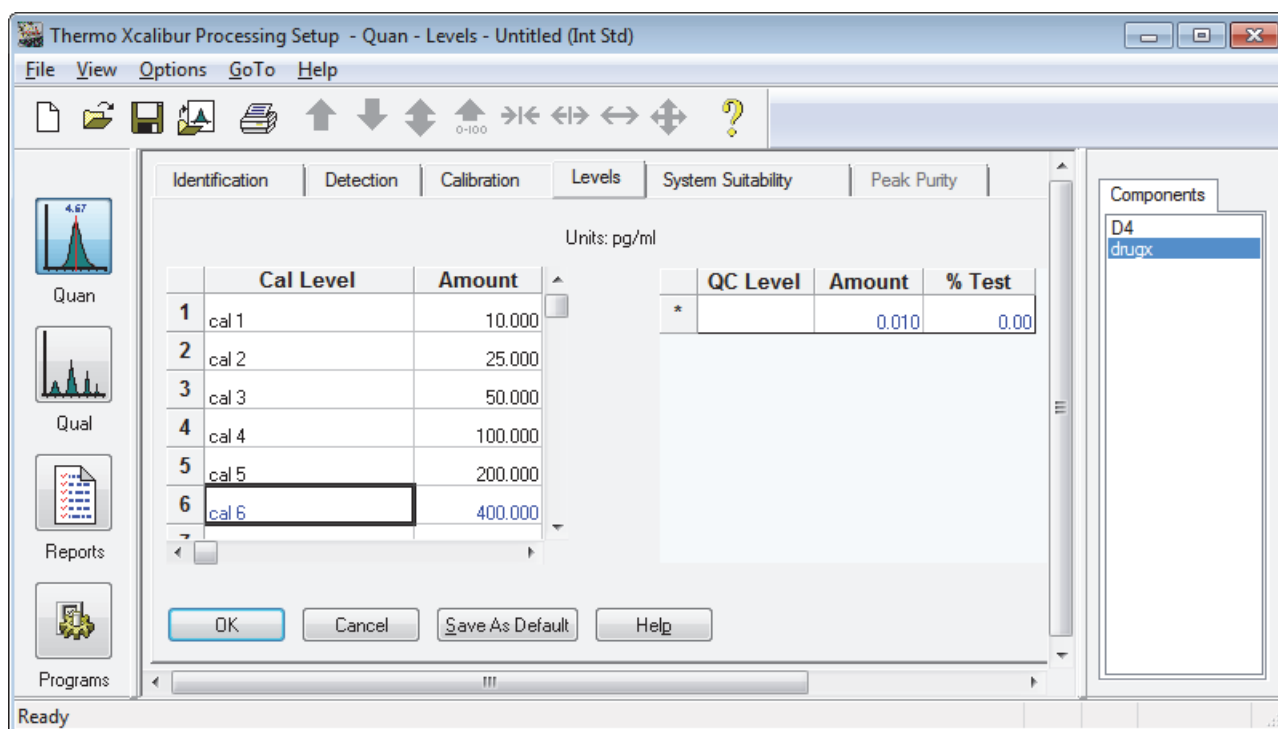
1. In the Quan view of the Processing Setup window, select **drugx** in the Components list.
2. Click the **Levels** tab.

The Levels page for Quan view opens (Figure 27).

Note If you select D4 and then try to open the Levels page, a warning message appears.

The Levels page is not available for ISTD components.

Figure 27. Levels page for Quan view



3. Enter the calibration level information for the target compound as follows:
 - a. To specify a name for the first calibration level, type **cal 1** in the Cal Level column of the first row. Then, press the TAB key to advance the cursor to the Amount column.
 - b. To specify an injection amount of 10 pg, type **10** in the Amount column.
 - c. To create a new row and to advance the cursor to the next Cal Level box, press the TAB key twice.

- d. Repeat this procedure for each of 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
1	cal 1	10
2	cal 2	25
3	cal 3	50
4	cal 4	100
5	cal 5	200
6	cal 6	400
7	cal 7	600
8	cal 8	800
9	cal 9	1000

Specifying the QC Levels

Use the QC levels table on the Levels page to set up the quality control specifications.

❖ To specify the QC levels

1. To specify the name of the first QC level, type **QC 1** in the QC Level column of the first row. Then, press the TAB key to advance the cursor to the Amount column.
2. To specify an injection amount of 10 pg, type **10** in the Amount column. Then, press the TAB key to advance the cursor to the %Test column.
3. To specify an acceptable difference of 20%, type **20** in the %Test column.

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.

For your applications, type a value in the %Test column for the acceptable difference (as a percent) between the specified amount and the calculated amount of each QC level.

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

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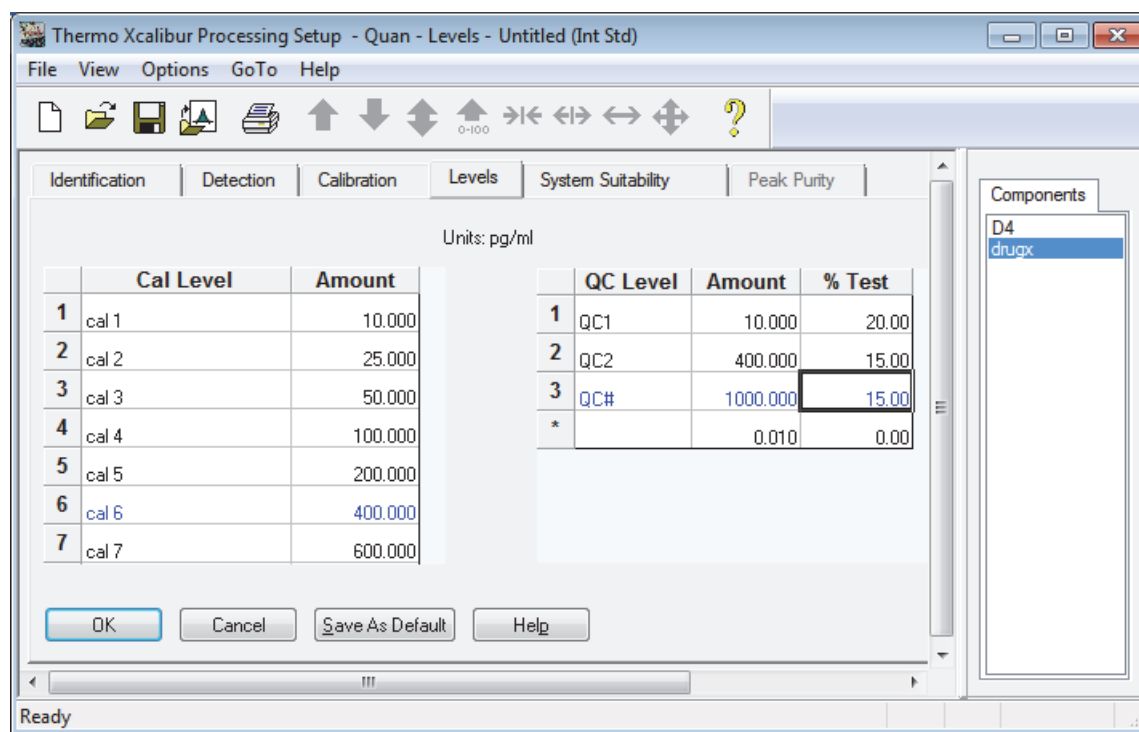
Saving the Processing Method

Table 2. QC sample specifications

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

6. To save the calibration and QC level settings, click **OK**.
7. Verify that the entries in the calibration standard and quality control tables are the same as those in [Figure 28](#).

Figure 28. Levels page, showing the completed calibration and quality control tables



Saving the Processing Method

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

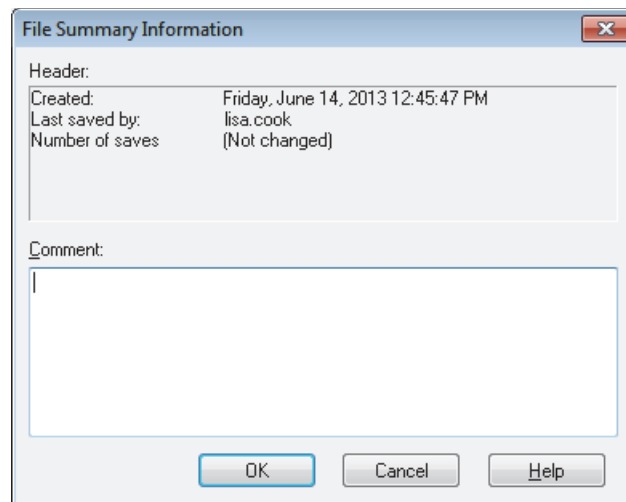
❖ To save the processing method

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

The File Summary Information dialog box opens.

2. Type **Processing method for drugx example** in the Comment box (Figure 29).

Figure 29. 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 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**.

Now that you have created a processing method, you are ready to batch reprocess the drugx data file set. Go to [Tutorial 2: Batch Reprocessing Data Files](#).

2 Tutorial 1: Creating a Processing Method

Saving the Processing Method

Tutorial 2: Batch Reprocessing 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 reprocesses the sequence with the processing method, the data system creates a result file for each raw data file.

Whether you are processing or reprocessing the data, the results are the same.

This tutorial describes how to add a processing method to a sequence and how to batch reprocess the sequence that contains the drugx raw data files.

Contents

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

Adding a Processing Method to a Sequence

An Xcalibur sequence is a list containing sample acquisition and processing information. Sequence files in the Xcalibur data system have an .sld file name extension.

Sequences use one or more instrument methods to acquire data and one or more processing methods to process the data. Instrument methods (METH files) contain the chromatographic and data acquisition parameters for an LC/MS or GC/MS instrument. The processing methods (PMD files) contain the sample processing parameters for a qualitative analysis, a quantitative analysis, or a combination of both analysis types. You must add an instrument method to the sequence list to run the sequence. You can add a processing method to the sequence before or after you run the sequence.

For both bracketed (open, non-overlapping, or overlapping) and unbracketed sequences, you can select a different instrument method for each injection. When you are working with a bracketed sequence, you can select only one processing method for the sequence.

The example sequence that you are working with in this tutorial is an open-bracketed sequence. All sequences that you create manually by entering the sample information in the sequence rows of the Sequence Setup view are open-bracketed sequences.

3 Tutorial 2: Batch Reprocessing Data Files

Adding a Processing Method to a Sequence

For information about using the New Sequence Template dialog box to create unbracketed sequences or sequences with non-overlapping or overlapping brackets, refer to the *Xcalibur Data Acquisition and Processing User Guide*.


To quantify the drugx target component in the example data files, add the drugx_example.pmd processing method to the existing drugx.sld sequence. You created this processing method by following [Tutorial 1: Creating a Processing Method](#).

❖ To add the processing method to the sequence

1. If you are working in the Processing Setup window, choose **GoTo > Xcalibur Home Page** from the menu bar.

The Xcalibur home page window opens.

2. To open the Sequence Setup view, do one of the following:

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

–or–

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

3. Choose **File > Open**.

The Open dialog box opens.

4. Browse to the following folder:

drive:\Xcalibur\examples\methods

5. Select **drugx.sld** and click **Open**.

The **drugx.sld** sequence opens in the Sequence Setup view (Figure 30).

Figure 30. Sequence Setup view, showing the sequence **drugx.sld**

	Sample Type	File Name	Path	Inst Meth	Proc Meth	Level
1	Std Bracket	drugx_01	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx	cal 1
2	Std Bracket	drugx_02	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx	cal 1
3	Std Bracket	drugx_03	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx	cal 1
4	Std Bracket	drugx_04	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx	cal 2
5	Std Bracket	drugx_05	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx	cal 3
6	Std Bracket	drugx_06	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx	cal 4
7	Std Bracket	drugx_07	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx	cal 5
8	Std Bracket	drugx_08	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx	cal 6
9	Std Bracket	drugx_09	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx	cal 7
10	Std Bracket	drugx_10	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx	cal 8
11	Std Bracket	drugx_11	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx	cal 9
12	Std Bracket	drugx_12	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx	cal 9
13	Std Bracket	drugx_13	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx	cal 9
14	QC	drugx_14	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx	QC 1
15	QC	drugx_15	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx	QC 1
16	QC	drugx_16	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx	QC 1
17	QC	drugx_17	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx	QC 1
18	QC	drugx_18	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx	QC 1
19	QC	drugx_19	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx	QC 1
20	QC	drugx_20	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx	QC 2
21	QC	drugx_21	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx	QC 2
22	QC	drugx_22	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx	QC 2
23	QC	drugx_23	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx	QC 2
24	QC	drugx_24	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx	QC 2
25	QC	drugx_25	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx	QC 2
26	QC	drugx_26	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx	QC 3
27	QC	drugx_27	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx	QC 3
28	QC	drugx_28	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx	QC 3
29	QC	drugx_29	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx	QC 3
30	QC	drugx_30	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx	QC 3
31	QC	drugx_31	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx	QC 3
*						

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6. To replace the processing method with your new processing method, do the following:

- a. Double-click any row in the Proc Meth column.

The Select Processing Method dialog box opens.

- b. Browse to the folder where you stored your new processing method.

drive:\Xcalibur\examples\methods

Note If you have not already created a new processing method, create one by following the procedures in [Tutorial 1: Creating a Processing Method](#).

3 Tutorial 2: Batch Reprocessing Data Files

Adding a Processing Method to a Sequence

- c. Select **drugx_example.pmd** and click **Open** to enter the new processing method in all the rows of the sequence.
7. Change some of the QC sample types to unknown sample types as follows:
 - a. In row 14, click the Sample Type column and select the **Unknown** sample type from the list.
 - b. Repeat this procedure to select the Unknown sample type for rows 15 to 18, 20 to 24, and 26 to 30.

Notice that the Level column lists the calibration level of each standard. When you add a quantitative processing method to a sequence and select a standard sample type in the Sample Type column (Std Bracket for an open-bracket sequence), the Level list appears in the Level column (Figure 31). To finish setting up the calibration information, you must select the appropriate calibration level for each standard sample.

Also notice that the Level column still lists the QC names for the QC samples you changed to the Unknown sample type. The data system updates the information in the Level column when you save the sequence file.

Figure 31. Level list for the drugx processing method

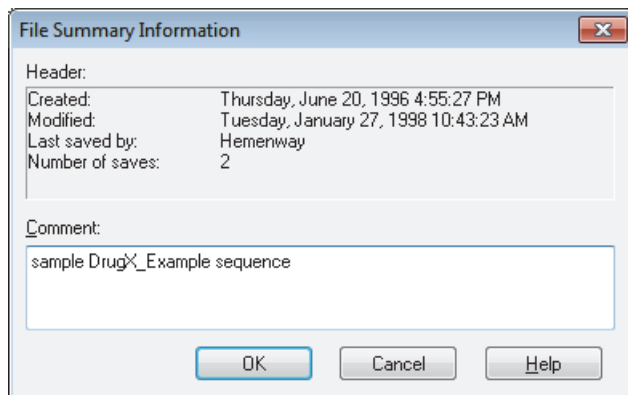
	Sample Type	File Name	Proc Meth	Level
1	Std Bracket	drugx_01	C:\Xcalibur\examples\methods\drugx	cal 1
2	Std Bracket	drugx_02	C:\Xcalibur\examples\methods\drugx	
3	Std Bracket	drugx_03	C:\Xcalibur\examples\methods\drugx	cal 1
4	Std Bracket	drugx_04	C:\Xcalibur\examples\methods\drugx	cal 2
5	Std Bracket	drugx_05	C:\Xcalibur\examples\methods\drugx	cal 3
6	Std Bracket	drugx_06	C:\Xcalibur\examples\methods\drugx	cal 4
7	Std Bracket	drugx_07	C:\Xcalibur\examples\methods\drugx	cal 5
8	Std Bracket	drugx_08	C:\Xcalibur\examples\methods\drugx	cal 6
9	Std Bracket	drugx_09	C:\Xcalibur\examples\methods\drugx	cal 7
10	Unknown	drugx_10	C:\Xcalibur\examples\methods\drugx	cal 8
11	Unknown	drugx_11	C:\Xcalibur\examples\methods\drugx	cal 9

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

The File Summary Information dialog box appears.

9. Type **sample Drugx_Example sequence** in the Comment box (Figure 32).

Figure 32. File Summary Information dialog box



10. Click **OK**.

The Save As dialog box opens.

11. Type **drugx_example** in the File Name box and click **Save**.

The sequence is saved as drugx_example.sld in the following folder:

drive:\Xcalibur\examples\methods

12. Verify that the sequence now looks like the one shown in Figure 33.
 - The ProcMeth column lists your new processing method, drugx_example.
 - In the Sample Type column, rows 14–18, 20–24, and 26–30 list the Unknown sample type.
 - In the Level column, rows 14–18, 20–24, and 26–30 are blank.

The information in the Instrument Method, Position, and Inj Vol columns is required for data acquisition, but this information is not used for data processing.

3 Tutorial 2: Batch Reprocessing Data Files

Adding a Processing Method to a Sequence

Figure 33. Drugx sequence, with drugx_example.pmd selected as the processing method

	Sample Type	File Name	Path	Inst Meth	Proc Meth	Level
1	Std Bracket	drugx_01	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx_example.pmd	cal 1
2	Std Bracket	drugx_02	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx_example.pmd	cal 1
3	Std Bracket	drugx_03	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx_example.pmd	cal 1
4	Std Bracket	drugx_04	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx_example.pmd	cal 2
5	Std Bracket	drugx_05	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx_example.pmd	cal 3
6	Std Bracket	drugx_06	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx_example.pmd	cal 4
7	Std Bracket	drugx_07	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx_example.pmd	cal 5
8	Std Bracket	drugx_08	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx_example.pmd	cal 6
9	Std Bracket	drugx_09	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx_example.pmd	cal 7
10	Std Bracket	drugx_10	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx_example.pmd	cal 8
11	Std Bracket	drugx_11	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx_example.pmd	cal 9
12	Std Bracket	drugx_12	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx_example.pmd	cal 9
13	Std Bracket	drugx_13	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx_example.pmd	cal 9
14	Unknown	drugx_14	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx_example.pmd	
15	Unknown	drugx_15	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx_example.pmd	
16	Unknown	drugx_16	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx_example.pmd	
17	Unknown	drugx_17	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx_example.pmd	
18	Unknown	drugx_18	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx_example.pmd	
19	QC	drugx_19	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx_example.pmd	QC 1
20	Unknown	drugx_20	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx_example.pmd	
21	Unknown	drugx_21	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx_example.pmd	
22	Unknown	drugx_22	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx_example.pmd	
23	Unknown	drugx_23	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx_example.pmd	
24	Unknown	drugx_24	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx_example.pmd	
25	QC	drugx_25	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx_example.pmd	QC 2
26	Unknown	drugx_26	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx_example.pmd	
27	Unknown	drugx_27	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx_example.pmd	
28	Unknown	drugx_28	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx_example.pmd	
29	Unknown	drugx_29	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx_example.pmd	
30	Unknown	drugx_30	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx_example.pmd	
31	QC	drugx_31	C:\Xcalibur\examples\data	C:\Xcalibur\examples\methods\drugx	C:\Xcalibur\examples\methods\drugx_example.pmd	QC 3
*						


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Batch Reprocessing the Sequence to Produce Result Files

After adding a processing method to the sequence, batch process data files to produce result files (RST) that you can view in the Quan Browser window.

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

1. Do one of the following:

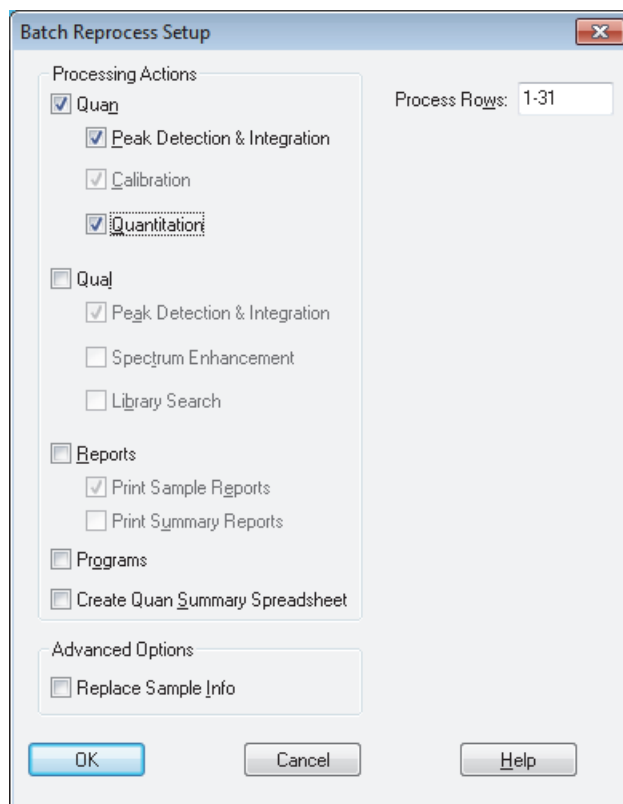
- Click the **Batch Reprocess** icon, , in the toolbar.

–or–

- Choose **Actions > Batch Reprocess**.

The Batch Reprocess Setup dialog box opens (Figure 34).

Figure 34. Batch Reprocess Setup dialog box



2. To set up the batch process options as shown in Figure 34, select the **Quan**, **Peak Detection & Integration**, and **Quantitation** check boxes.
3. Make sure that the Process Rows box displays **1–31**.

3 Tutorial 2: Batch Reprocessing Data Files

Batch Reprocessing the Sequence to Produce Result Files

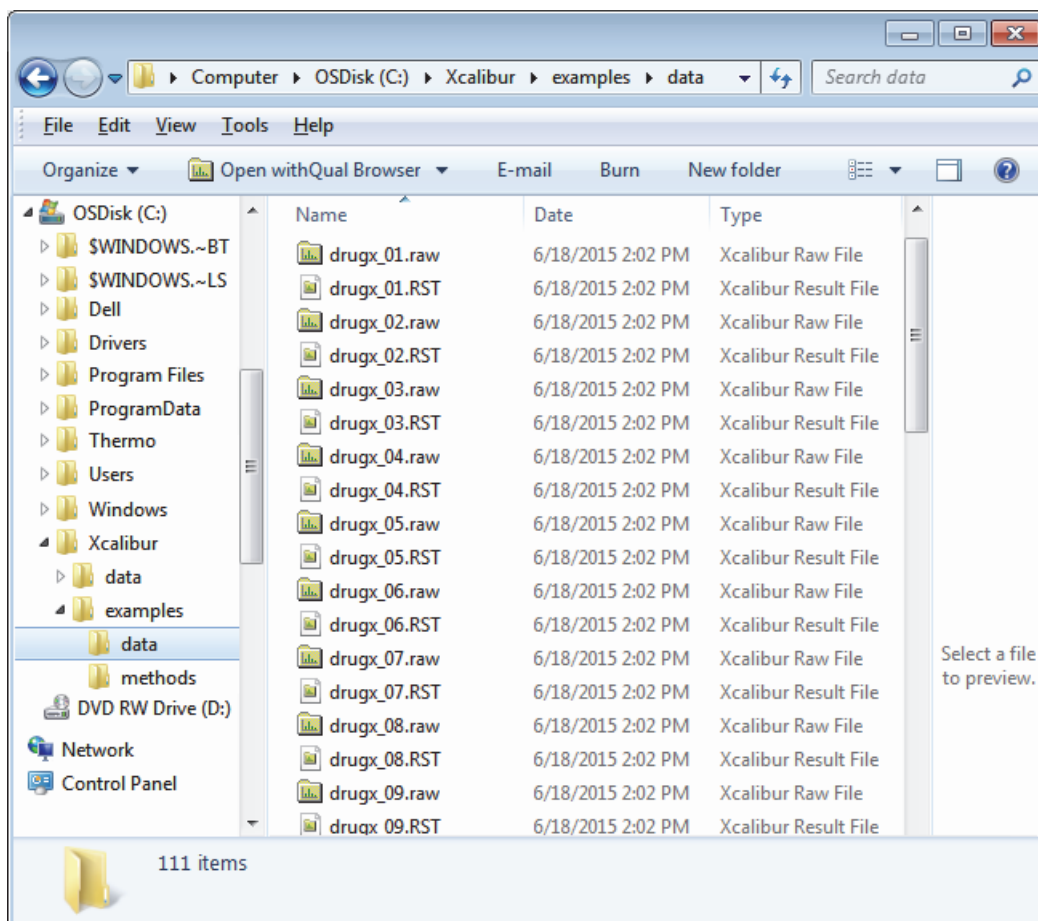
4. To start batch reprocessing, click **OK**.

For each raw data file, the data system creates a result file with the same name. The data system exports the result files to the folder where the raw data files are located.

In this example, the raw data files and result files are in the following folder (Figure 35):

drive:\Xcalibur\examples\data

Figure 35. Explore directory, showing the location of the raw data files (RAW) and the result files (RST)



Tutorial 3: Working with Result Files in Quan Browser

After adding a processing method to the sequence and then batch reprocessing the sequence, review the result files and the calibration curve for the drugx target component in the Quan Browser window. If necessary, 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 the Quan Browser window.

Contents

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

When the Xcalibur data system processes a bracketed sequence, it stores the calibration results for the quantified components in the result files (RST), bracket by bracket. When you open a processed sequence in the Quan Browser window, Quan Browser displays the list of associated result files by bracket.

The example drugx sequence is an open-bracketed sequence. This means that the entire sequence is treated as one bracket. When you open the processed sequence in the Quan Browser window and select the All tab to display all of the sample types, the Bracket in Use list displays Bracket 1. The Calibration File box lists the calibration in use as an Embedded Calibration (that is, the calibration information in use is embedded in the result files).

Reviewing a Sequence of Result Files in Quan Browser

In the Quan Browser window, review the quantitative analysis results of the processed drugx sample set. For additional information about using Quan Browser, refer to the *Xcalibur Quan Browser User Guide*.

❖ To review the results after you batch reprocess a sequence

1. To open the processed sequence for the drugx sample set in the Quan Browser window, do the following:

- a. From the Xcalibur Home Page, choose **GoTo > Quan Browser**.

The Quan Browser window opens.

- b. Choose **File > Open**.

The Open dialog box opens.

- c. In the File of Types list, select **Sequence List Files (SLD)**.

In the Quan Browser window, you can open a sequence list of result files (SLD), a single result file (RST), or a Quan Browser file (XQN).

When the Xcalibur data system processes a sequence of raw data files, it creates one result file for each raw data file, gives the result file the same file name as the raw data file, and stores the result files (RST) in the same directory as the raw data files.

If you delete the result files or move them to a different directory than the directory listed in the sequence file, Quan Browser will not be able to locate the files.

- d. In the Look In list, browse to the appropriate folder.

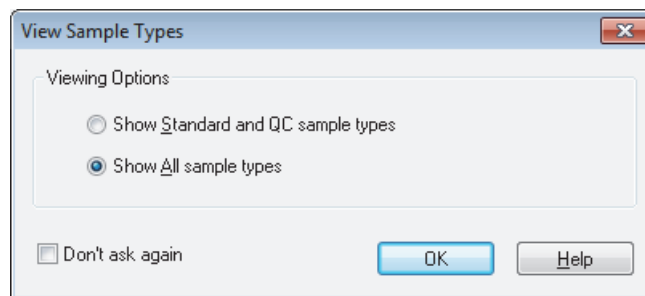
drive:\Xcalibur\examples\methods

Note If you have not already created a sequence with a processing method, create one by following the instructions in [Tutorial 1: Creating a Processing Method](#) and [Tutorial 2: Batch Reprocessing Data Files](#). Or, open the drugx.sld sequence.

- e. Select **drugx_example.sld** and click **Open**.

The View Sample Types dialog box opens ([Figure 36](#)).

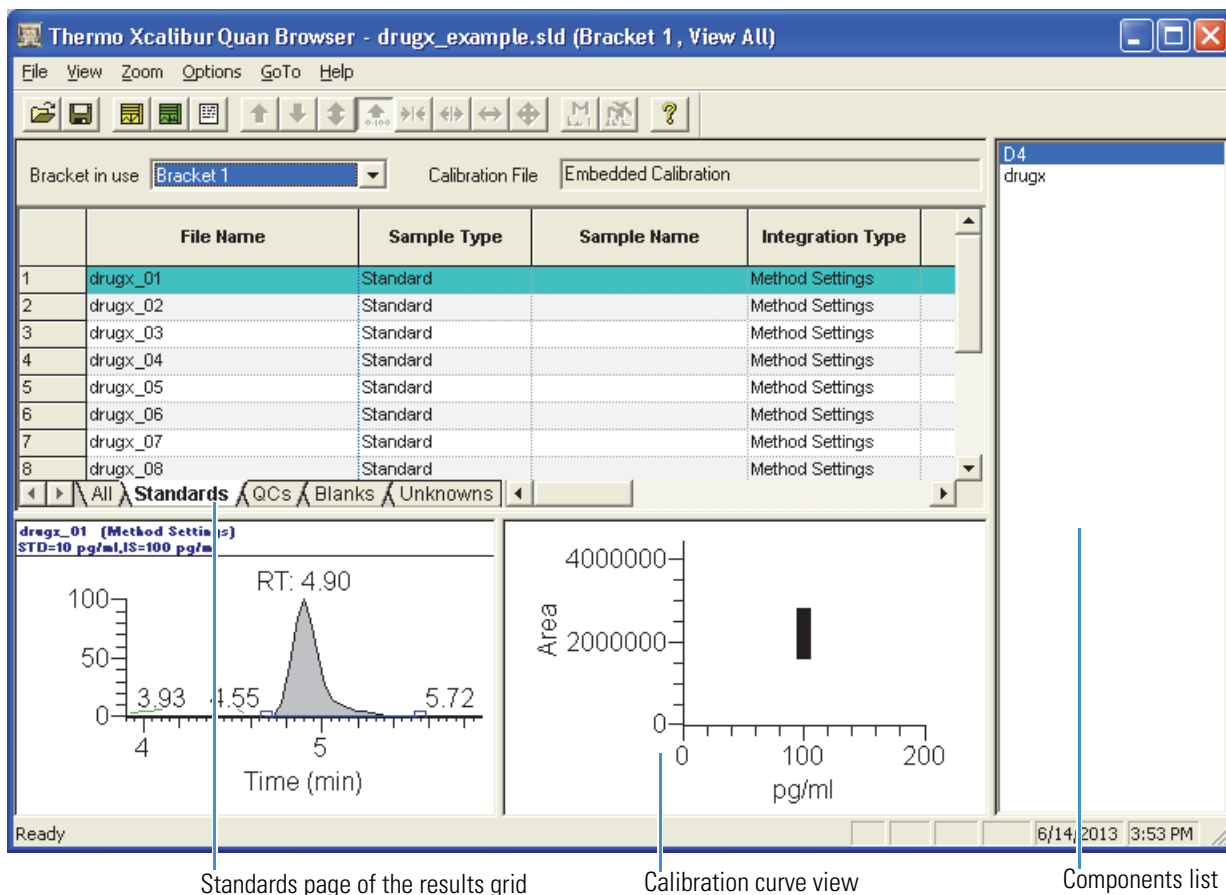
Figure 36. View Sample Types dialog box



- f. Select the **Show All Sample Type** option and click **OK**.

The drugx_example.sld sequence opens in the Quan Browser window. The results grid contains five tabbed pages: All, Standards, QCs, Blanks, and Unknowns. As shown in Figure 37, the Standards page is displayed in the results grid. The internal standard D4 is selected in the component list, and the calibration curve view is displayed in the companion view.

Figure 37. Quan Browser window with the internal standard D4 selected in the component list



2. To display all of the data files, click the **All** tab at the bottom of the results grid.
3. Scroll down the results grid and verify that the sample types and calibration levels are labeled correctly.
4. Select the first data file in the results grid.
5. Check each component in the data file for peak detection and integration problems as follows:
 - a. Select **D4** in the components list.

4 Tutorial 3: Working with Result Files in Quan Browser

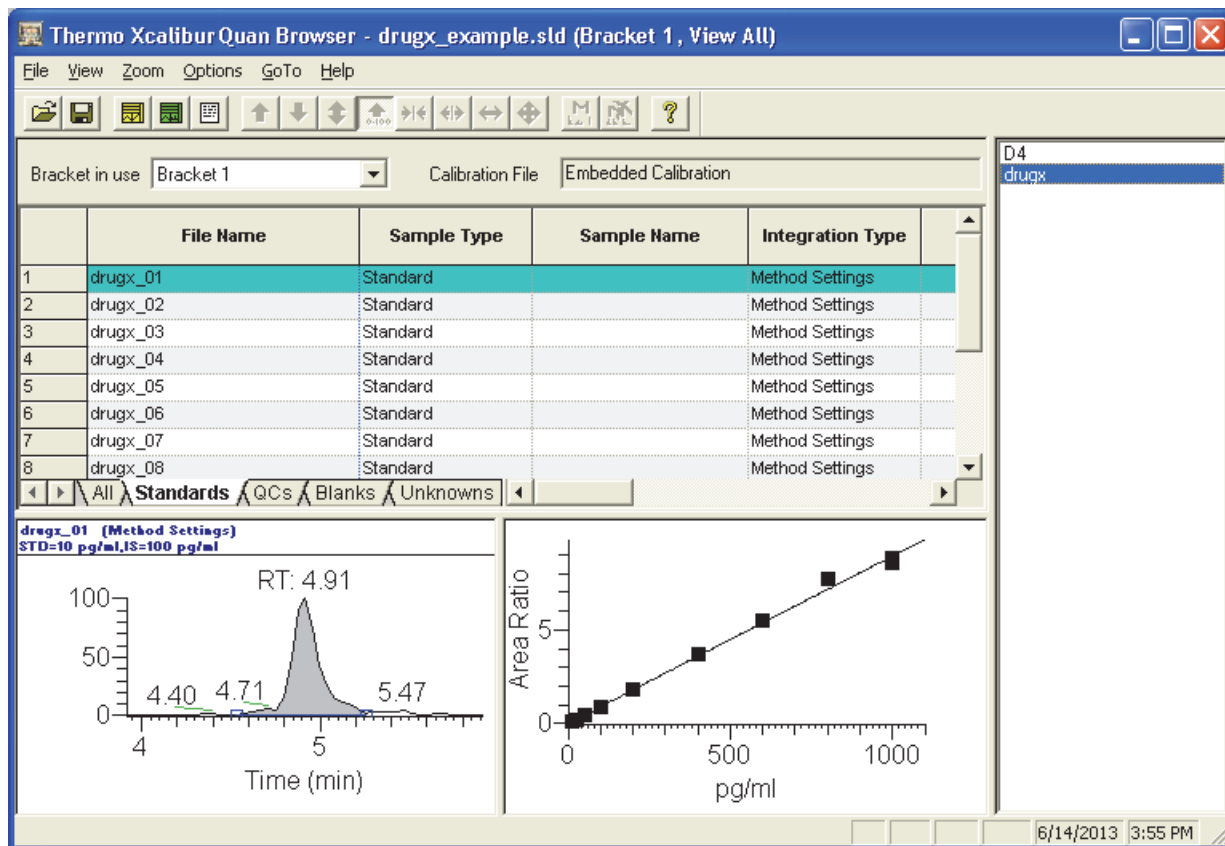
Reviewing a Sequence of Result Files in Quan Browser

- b. Inspect the component peak in the chromatogram view as follows:
 - i. Verify that the data system found the peak.

The data system shades found peaks gray and marks the starting and ending points with square integration markers.
 - ii. Make sure that the peak is integrated properly and that the shaded area accurately represents the contribution of the component to the chromatogram.
 - c. If necessary, modify the peak detection or integration parameters for D4.
 - d. Select **drugx** in the components list.
 - e. Inspect the component peak in the chromatogram view and verify that the data system found the peak and that the peak is integrated properly.
 - f. If necessary, modify the peak detection or integration parameters for drug x.
 - g. Click the next row in the results grid view to select the next data file.
6. Repeat [step 5](#) for each data file.
 7. Check the calibration curve for the target compound, drug x, as follows:
 - a. In the Components list, select **drugx** to display the results for the target compound.
 - b. Inspect the calibration curve in the calibration curve view ([Figure 38](#)).
 - c. If necessary, modify the processing method's calibration curve parameters.

For more information about modifying processing methods in the Quan Browser window, see [Modifying the Processing Method in Quan Browser](#).

Figure 38. 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. The sections that you can modify include the identification, detection, and integration parameters for the chromatographic peaks in the components list and several of the calibration curve parameters. You cannot modify the amounts for the calibration levels.

❖ To modify the processing method

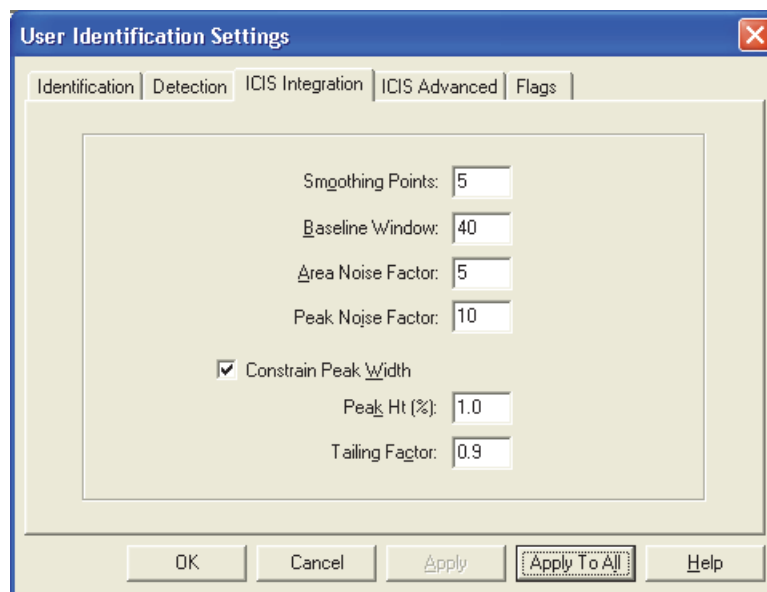
1. If the sequence for the drugx sample set is not open in the Quan Browser application, open this sequence as described in [step 1 of Reviewing a Sequence of Result Files in Quan Browser](#).
2. In the components list on the right side of the Quan Browser window, select **drugx**.

Note You can modify some of the settings for a processing method in the Quan Browser window:

- Use the User Peak Detection Settings dialog box to modify the component identification, detection, and integration settings.
 - Use the Calibration Options dialog box to modify some of the calibration curve parameters.
3. To modify an identification, a detection, or an integration parameter, such as Constrain Peak Width, do the following:
 - a. Right-click the chromatogram plot view and choose **User Peak Detection Settings** from the shortcut menu.

The User Identification Settings dialog box opens ([Figure 39](#)).

Figure 39. User Identification Settings dialog box



- b. Click the **ICIS Integration** tab.

The ICIS Integration page opens.

- c. Select the **Constrain Peak Width** check box.
- d. Type **1** in the Peak Ht[%] box.
- e. Type **0.9** in the Tailing Factor box.
- f. Click **Apply To All** to update the integration of the result files in the sequence.

The Processing dialog box opens and processes the result 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.

4. To modify the calibration curve, do the following:
 - a. Right-click the calibration curve plot view and choose **Calibration Settings** from the shortcut menu.

The Calibration Settings dialog box opens.

- b. Click the **Curve** tab.

The Curve page opens.
- c. Select **Linear** from the Calibration Curve Type list.
- d. To display the new curve fit in the calibration curve plot view, click **Apply**.
- e. Click **OK** to close the dialog box.

Note You cannot change the amount of the target component for each calibration level. But you can exclude calibration points from the calibration curve and save the new settings as an Xcalibur Quan file (XQN). The Xcalibur Quan file lists the excluded calibration points.

5. To save the modifications as a new processing method, do the following:
 - a. Choose **File > Export Method**.

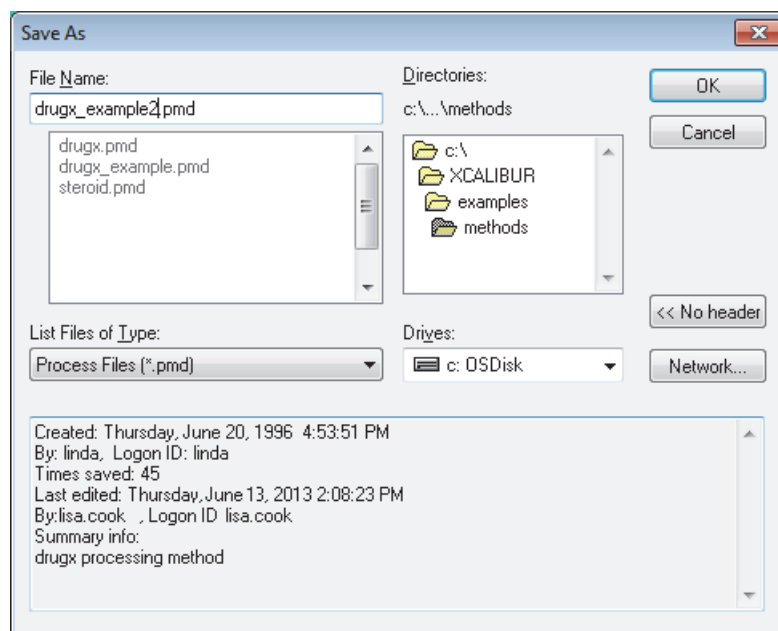
The Save As dialog box opens.
 - b. Type **drugx_example_2** in the File Name box.
 - c. In the Directories box, browse to the following folder (Figure 40):

drive:\Xcalibur\examples\methods

4 Tutorial 3: Working with Result Files in Quan Browser

Modifying the Processing Method in Quan Browser

Figure 40. Save As dialog box



- d. Click **OK** to export the processing method to the selected folder and close the dialog box.

Tutorial 4: Reviewing, Specifying, and Printing Reports

To print reports as you batch reprocess 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 During Batch Reprocessing](#)

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 reports helps you avoid printing reports with inadequate information or inefficient formatting.

❖ To preview a representative peak integration report and a representative calibration report

1. To start the XReport application, do one of the following:
 - On the computer desktop, double-click the **XReport** icon, .

–or–

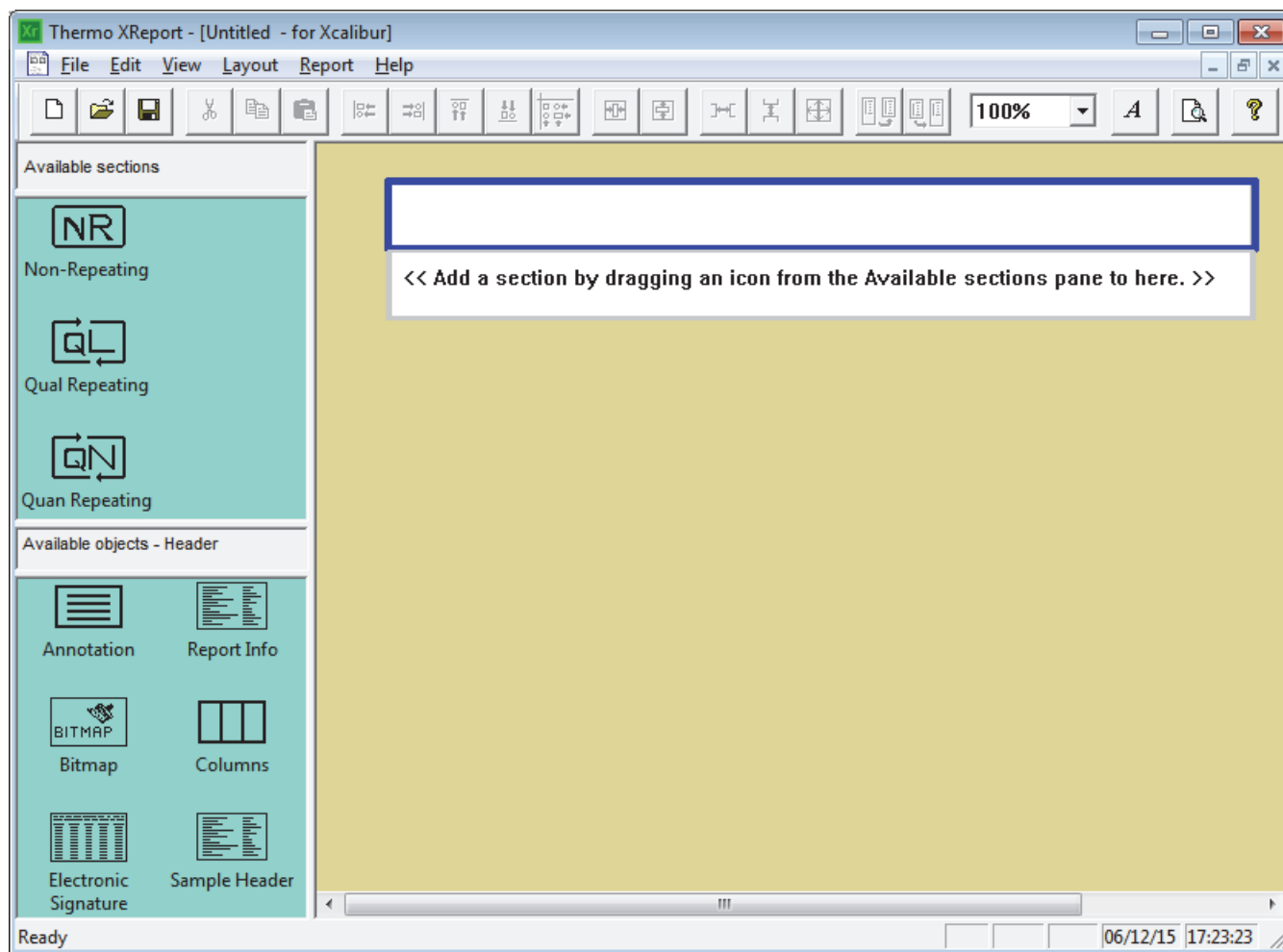
- From the taskbar, choose **Start > Thermo Scientific Xcalibur > XReport**.

XReport opens and creates a new template (Figure 41).

5 Tutorial 4: Reviewing, Specifying, and Printing Reports

Previewing Reports in XReport

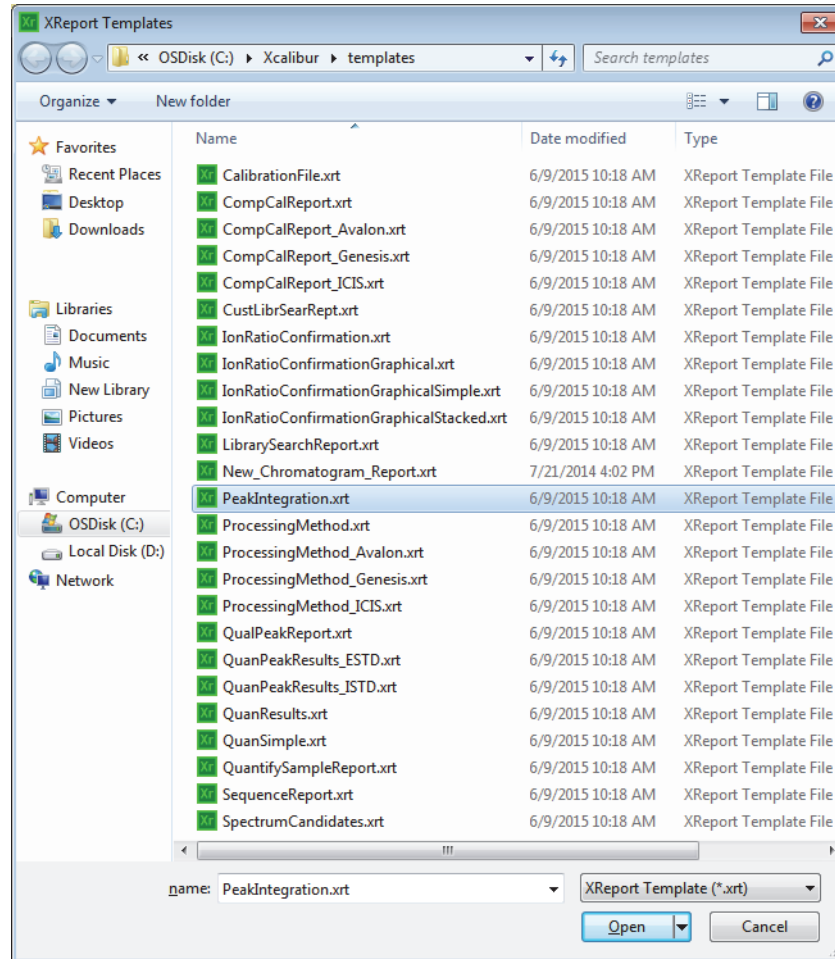
Figure 41. XReport window showing a new blank report template



2. Choose **File > Open**.

The XReport Templates dialog box opens (Figure 42).

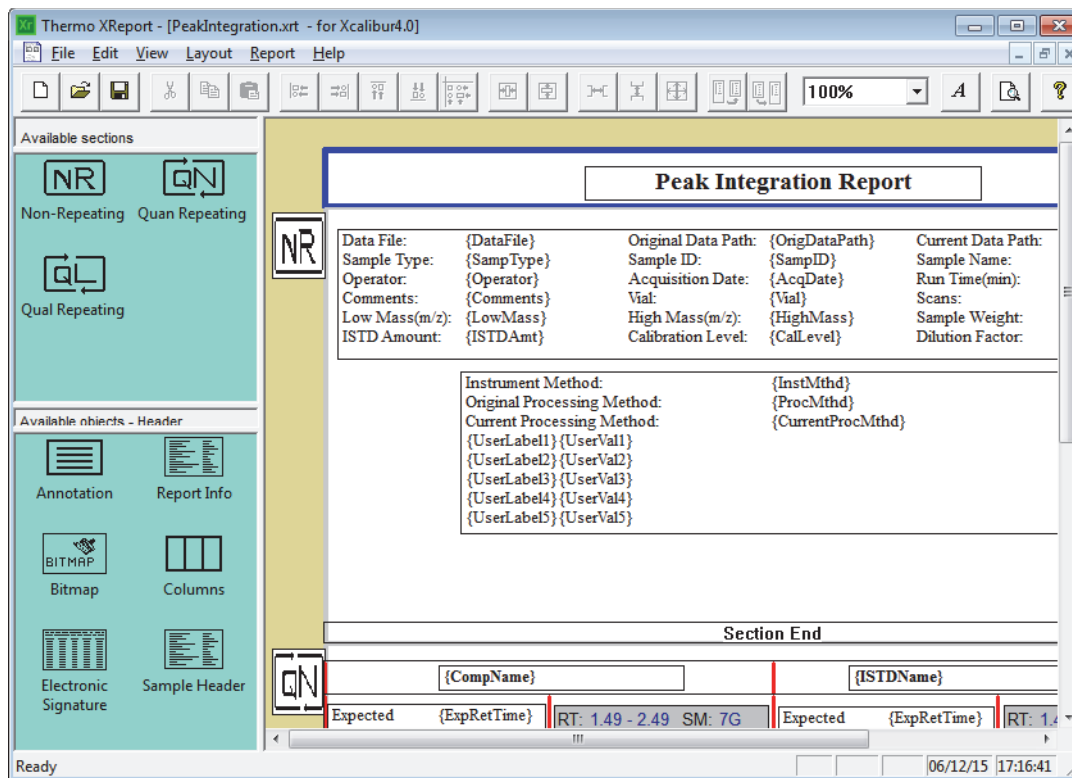
Figure 42. XReport Templates dialog box



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


The PeakIntegration.xrt report template opens in the XReport window (Figure 43).

Figure 43. 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. To test a sample report, you must open a representative processing method, raw data file, result data file, and sequence file.

5. Select the appropriate files:
 - Select the processing method as follows:
 - a. In the Processing Method File area, click .
 - The Select Processing File dialog box opens.
 - b. Browse to this folder: *drive:\Xcalibur\examples\methods*.
 - c. Select **drugx.pmd**.
 - d. Click **Open**.




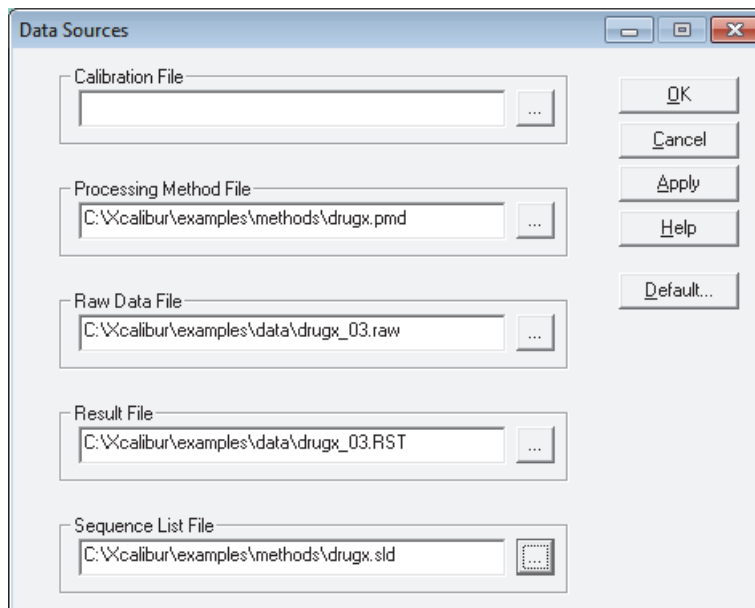
- Select the raw data file as follows:
 - a. In the Raw Data File area, click .
 - The Select Raw Data File dialog box opens.
 - b. Browse to this folder: *drive:\Xcalibur\examples\data*.
 - c. Select **drugx_03.raw**.
 - d. Click **Open**.
 - Select the result file as follows:
 - a. In the Raw Data File area, click .
 - The Select Result File dialog box opens.
 - b. Browse to this folder: *drive:\Xcalibur\examples\data*.
 - c. Select **drugx_03.rst**.
 - d. Click **Open**.
 - Select the sequence file as follows:
 - a. In the Sequence List File area, click .
 - The Select Sequence dialog box opens.
 - b. Browse to this folder: *drive:\Xcalibur\examples\methods*.
 - c. Select **drugx_x.sld**.
 - d. Click **Open**.
6. Verify that the selections in the Data Sources dialog box are the same as those in [Figure 44](#).

Figure 44. Data Sources dialog box



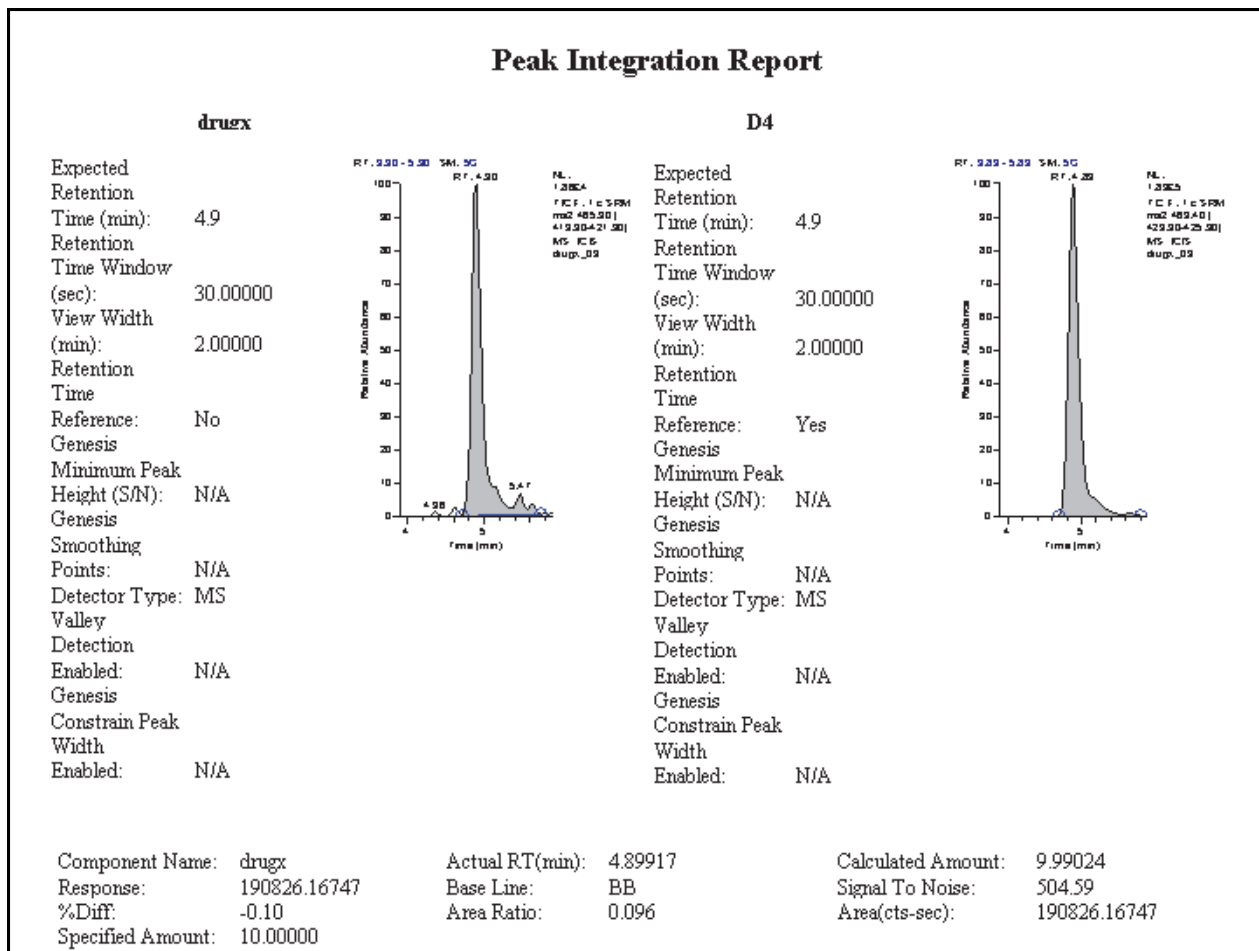
7. Click **OK** to accept the settings and close the dialog box.
8. Choose **Report > Resolve Report** from the XReport main window.

The peak integration report opens, displaying the data from the drugx.rst file. For this data file, the report is two pages. Figure 45 shows the first page and Figure 46 shows the second page.

Figure 45. Peak Integration Report, page 1

Peak Integration Report					
Data File:	drugx_03	Original Data Path:	C:\LCQ\Data\mrw_27	Current Data Path:	C:\Xcalibur\example
Sample Type:	Std Update	Sample ID:	04	Sample Name:	s\data
Operator:	linda	Acquisition Date:	05/04/96 10:31:23 PM	Run Time(min):	6.98
Comments:	STD=10 pg/ml,IS=100	Vial:	104	Scans:	314
Low Mass(m/z):	419.30	High Mass(m/z):	425.30	Sample Weight:	0.00
ISTD Amount:	0.000	Calibration Level:		Dilution Factor:	1.00
	Instrument Method:		C:\LCQ\Methods\		
	Original Processing Method:				
	Current Processing Method:		C:\Xcalibur\examples\methods\drugx_example		
	Study				
	Client				
	Laboratory				
	Company				
	Phone				

Figure 46. Peak Integration Report, page 2



9. Close the report, but do not close the XReport application.

10. Choose **File > Open**.

The XReport Templates dialog box opens.

11. Select **CompCalReport_ICIS.xrt** and click **Open**.

XReport opens the CompCalReport_ICIS.xrt report template.

12. To select a representative sequence file to test the component calibration report, do the following:

a. Choose **Report > Data Sources**.

The Data Sources dialog box opens (see [Figure 44](#) on [page 66](#)). The dialog box is populated with your previous selections.

b. Click **OK** to close the Data Sources dialog box.

13. Choose **Report > Resolve Report**.

The application combines the data with the report template and opens the component calibration report, displaying the data from the drugx.sld sequence file. The component calibration report for the drugx.sld sequence file is six pages long. Page 5, containing the calibration curve for drugx, is shown in Figure 47. Page 6, which shows the calculated amounts for drugx, is shown in Figure 48 on page 69.

Figure 47. Component calibration report, showing the calibration curve for drugx, the target compound

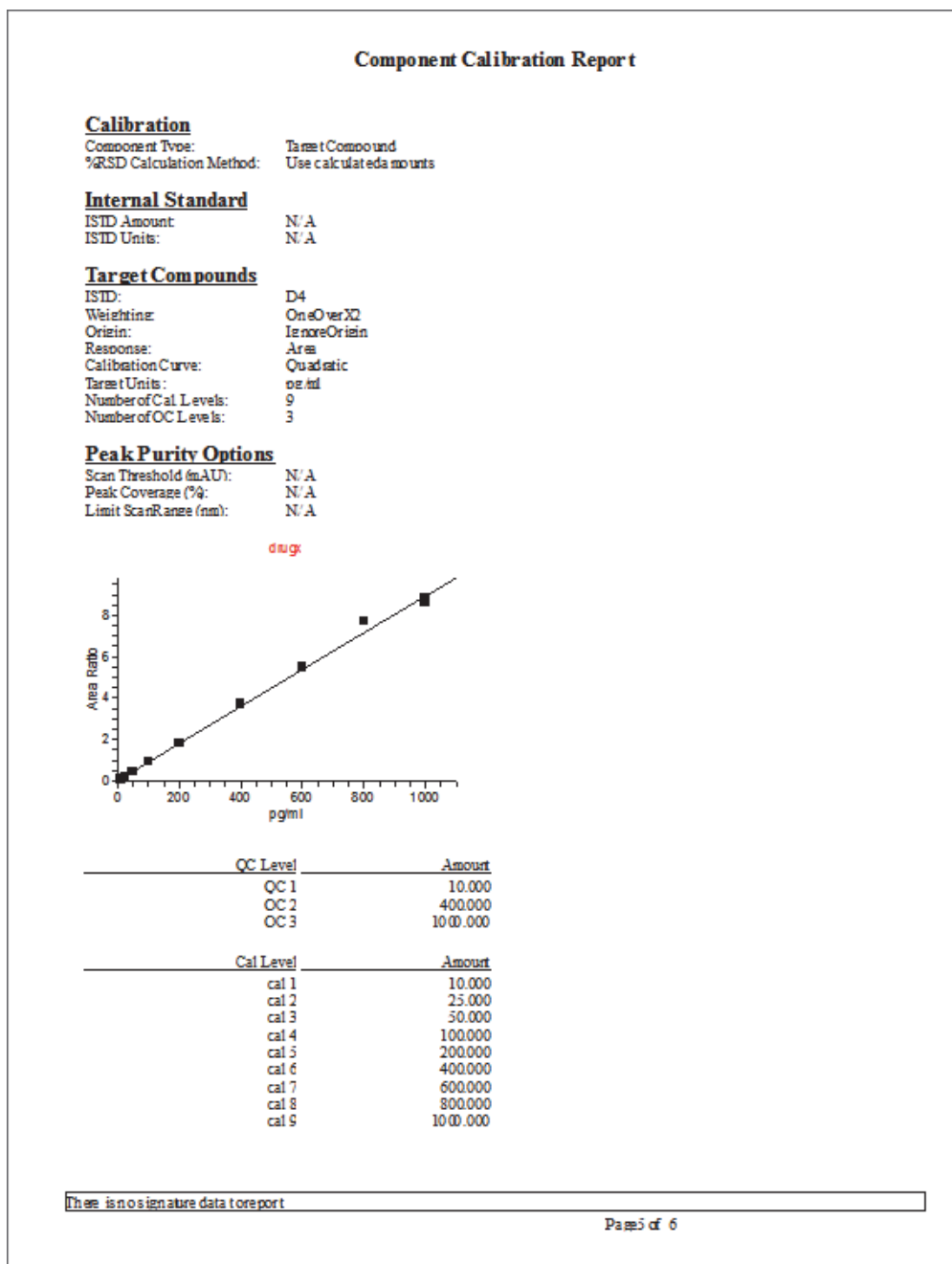


Figure 48. Component calibration report, showing the calculated amounts for drugx, the target compound

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	2576958.562	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\mrw_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 basic formats for reporting results. To change the layout of a report or to create a completely new template, use the XReport application. For instructions on creating custom reports, refer to the *XReport User Guide*.

After previewing the results of combining a sample data set with the report templates in the XReport application, follow this procedure to add the report templates to the processing method.

❖ To specify the report templates for a processing method

1. Open the Reports view of the Processing Setup window by doing one of the following:

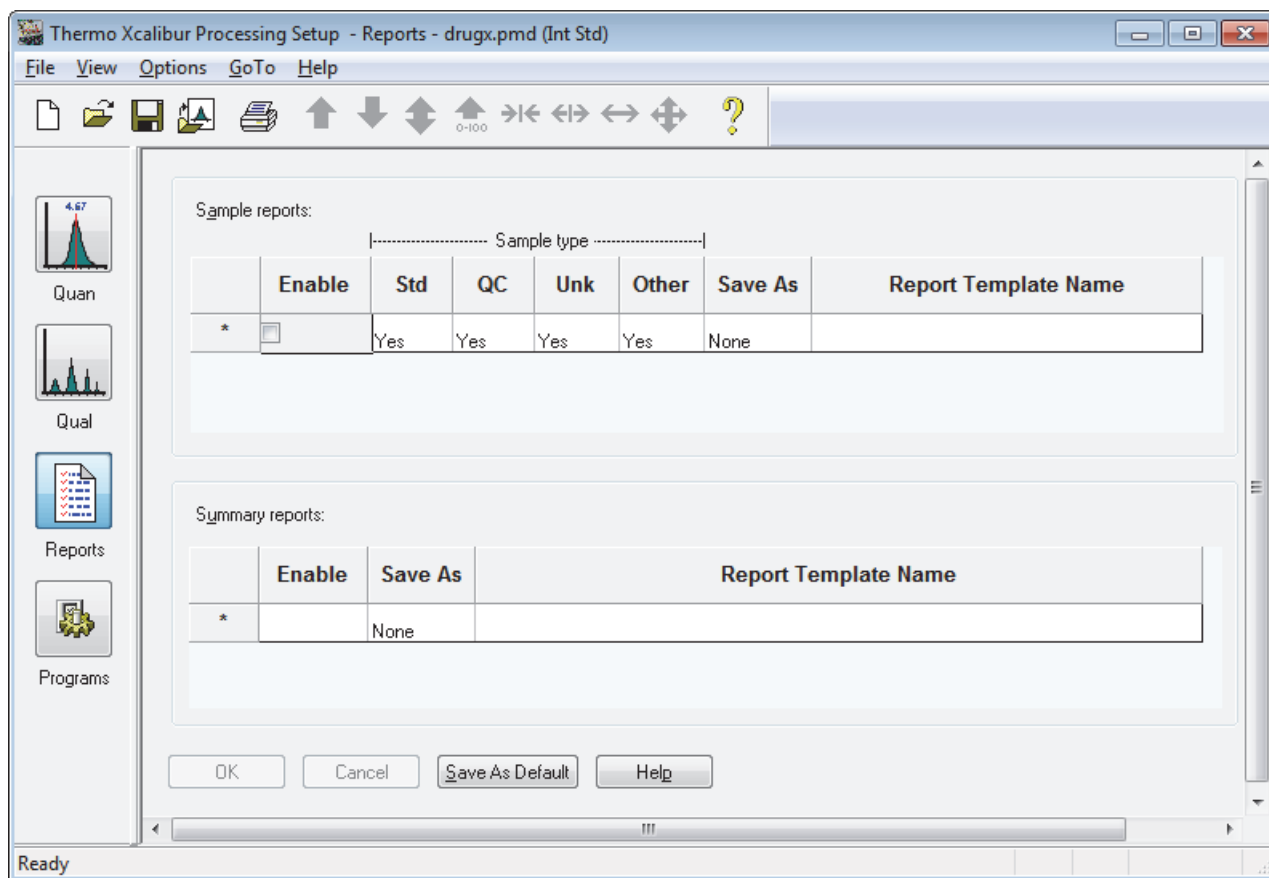
- On the View bar, click the **Reports** icon, .

–or–

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

The Reports view opens (Figure 49).

Figure 49. Reports view of the Processing Setup window



2. In the first row of the Sample Reports table, set up a sample report as follows:

a. Click the **Enable** column.

The data system selects the **Enable** check box. When you click anywhere else in the view, the text “Yes” replaces the check box.

b. In the Save As column of the same row, select **Doc** to save the report as a DOC file.

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, *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, XReport adds a date stamp before the suffix.

c. Select a sample report template as follows:

i. Double-click the **Report Template Name** column.

The Browse for Sample Report Template dialog box opens to the following folder:

drive:\Xcalibur\templates

ii. To choose the sample peak integration report template, select **PeakIntegration.xrt** and click **Open**.

3. In the second row of the Sample Reports table, set up a sample report as follows:

a. Double-click the **Enable** column.

The data system selects the **Enable** check box.

b. In the Save As column of the same row, select **Doc** to save the report as a DOC file.

c. Select a sample report template as follows:

i. Double-click the **Report Template Name** column.

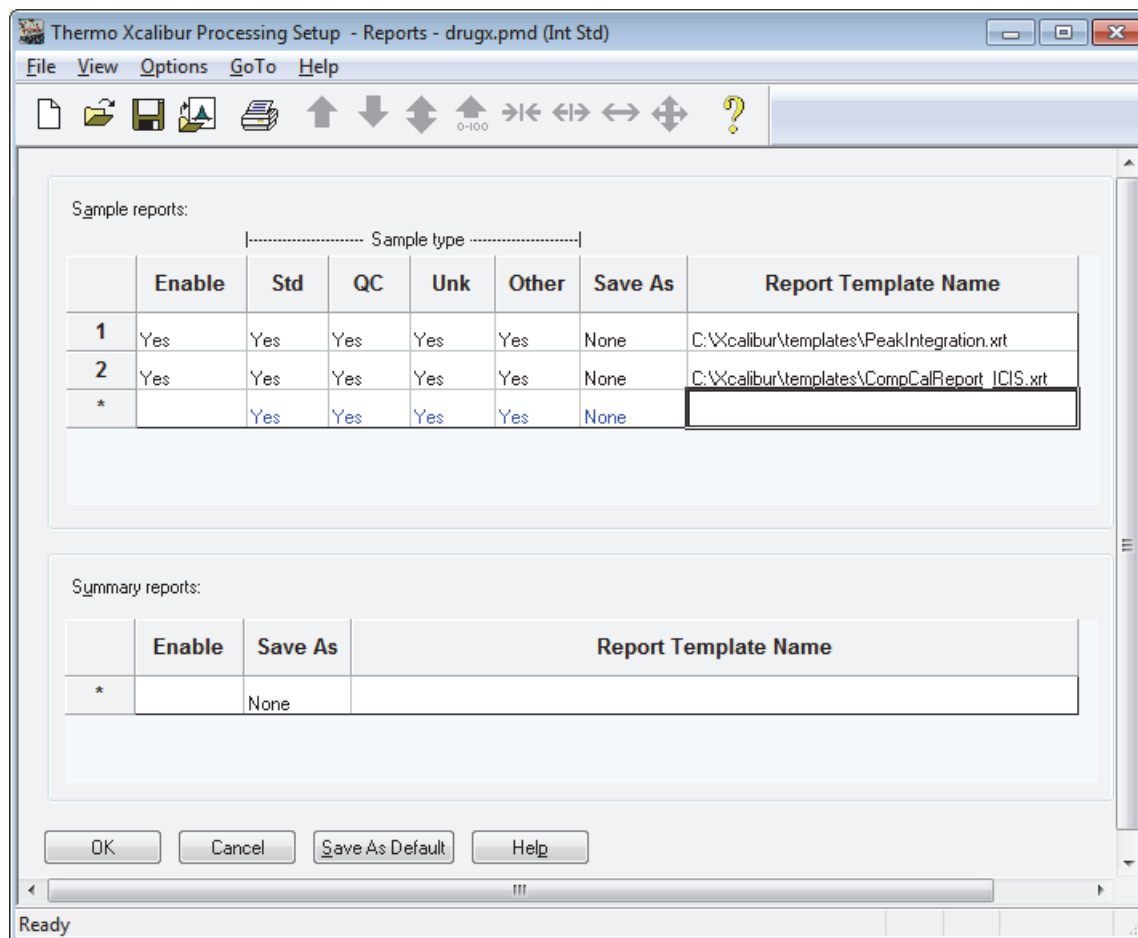
The Browse for Sample Report Template dialog box opens.

ii. To choose the sample component calibration report template, select **CompCalReport_ICIS.xrt** and click **Open**.

4. Click **OK** to save the settings.

5. Verify that the Report view matches [Figure 50](#).


Figure 50. Selecting peak integration report and component calibration report templates




Printing Reports During Batch Reprocessing

The data system uses the report templates that you specify in the processing method to print reports when you batch process (or reprocess) a sequence.

❖ To print reports while batch reprocessing a sequence


1. Return to the Xcalibur home page by choosing **GoTo > Xcalibur Home Page** from the menu bar.
2. Open the Sequence Setup view by doing one of the following:
 - On the View toolbar, click the **Sequence View** icon, .

–or–

 - On the menu bar, choose **View > Sequence Setup View**.
3. If the `drugx_example.sld` sequence is not already open, open it as follows:
 - a. Do one of the following:
 - On the Sequence Editor toolbar, click the **Open** icon, .

–or–

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

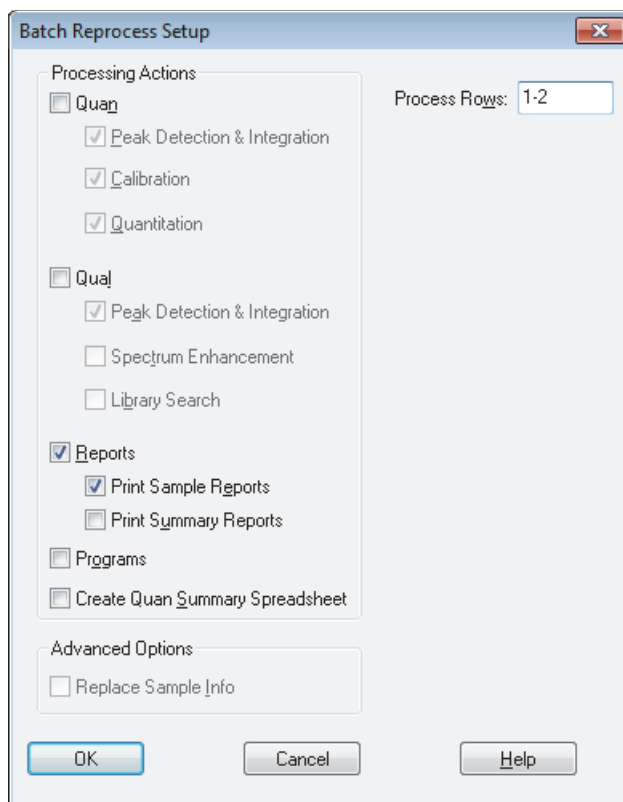
The Open dialog box opens.
 - b. Browse to the following folder:
`drive:\Xcalibur\examples\methods`
 - c. Select **drugx_example.sld** and click **Open**.
The `drugx_example.sld` sequence opens.
4. Open the Batch Reprocess dialog box by doing one of the following:
 - On the Sequence Editor toolbar, click the **Batch Reprocess** icon, .

–or–

 - On the menu bar, choose **Actions > Batch Reprocess**.

Figure 51 shows the Batch Reprocess Setup dialog box.

Figure 51. Batch Reprocess Setup dialog box showing selections for printing reports



5. Select the **Reports** check box, and then select the **Print Sample Reports** check box.
6. Type **1–2** in the Process Rows box.
7. 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 about acquiring and processing data, refer to the *Xcalibur Data Acquisition and Processing User Guide*.

For more information about reviewing quantification data, refer to the *Xcalibur Quan Browser User Guide*.

For more information about the XReport reporting tool, refer to the *XReport User Guide*.



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