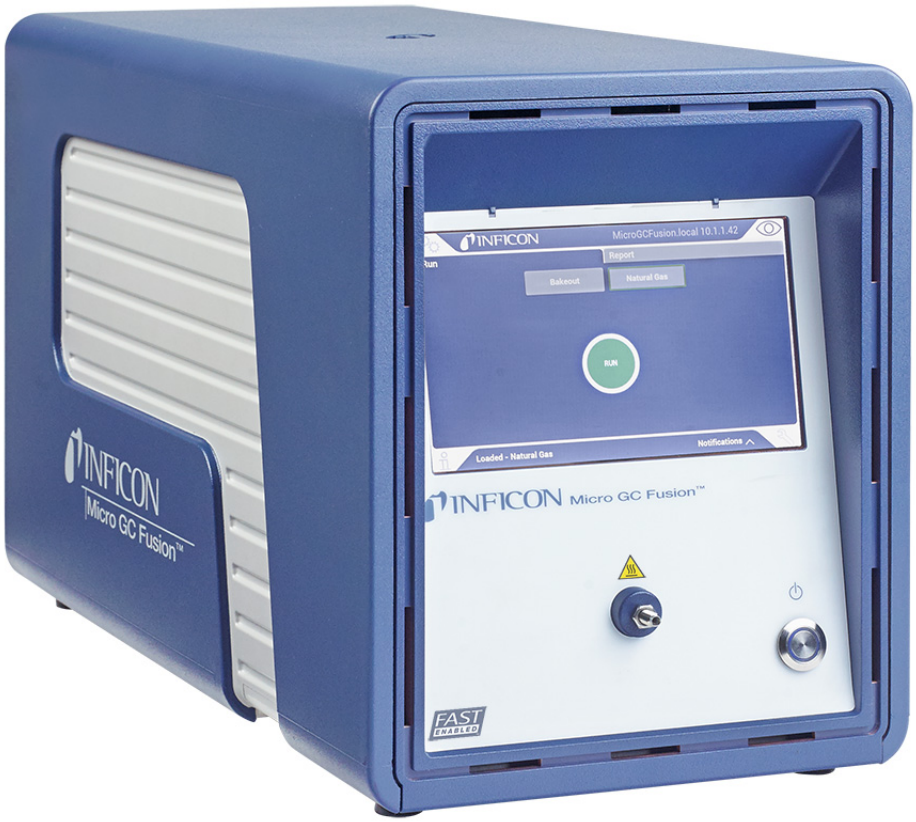
O P E R A T I N G M A N U A L



EZ IQ™

Chromatography Software

PN 074-659-P1A

INFICON

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Chapter 1
Using this Manual

1.1 Introduction

This operating manual provides a basic operating overview and tutorial for the INFICON EZ IQ data system.

This manual is designed to instruct new users on the acquisition of data and processing of results.

1.2 How to Contact INFICON

Worldwide support is available by contacting:

- Technical Support, to correspond with an applications engineer with questions regarding INFICON products and applications
- Sales Office, to correspond with the sales team for commercial inquiry
- Service Center, to correspond for repair services

When reporting an issue with Micro GC Fusion, please have the following information readily available:

- Micro GC Fusion part number and serial number
- A description of the problem
- An explanation of any corrective action that may have been attempted
- The exact wording of any error messages observed

To contact Customer Support, see the **Support** page at **www.INFICON.com**.

To submit a repair request in North America, fill out a Service Request Form at **http://service.inficon.com**.

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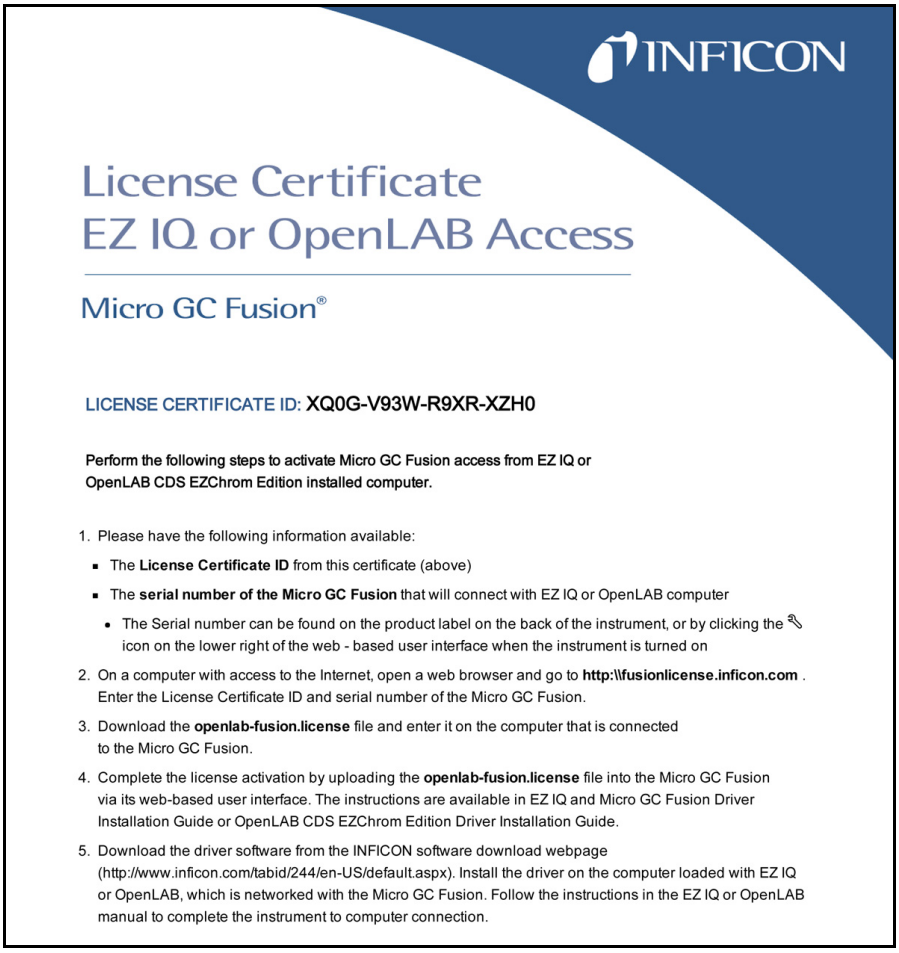
Chapter 2
Installation and Configuration

Micro GC Fusion is compatible with INFICON EZ IQ chromatography software. To connect and configure the Micro GC Fusion to EZ IQ, the Micro GC Fusion driver for EZ IQ must be installed on the computer and the License Certificate for EZ IQ or OpenLAB Access (PN 952-389-G1) must be purchased from INFICON and installed on the Micro GC Fusion.

- In addition to a License Certificate ID, the License Certificate for EZ IQ or OpenLAB Access (PN 952-389-G1) provides instructions to license a Micro GC Fusion for EZ IQ access (See Figure 2-1.)
- The instructions to install the EZ IQ driver and connect an EZ IQ computer with a Micro GC Fusion is available in the EZ IQ and Micro GC Fusion Driver Installation Guide (PN 074-663-P1)

Figure 2-1 An example of License Certificate for EZ IQ or OpenLAB Access (PN 952-389-G1)



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License Certificate
EZ IQ or OpenLAB Access

Micro GC Fusion®

LICENSE CERTIFICATE ID: XQ0G-V93W-R9XR-XZH0

Perform the following steps to activate Micro GC Fusion access from EZ IQ or OpenLAB CDS EZChrom Edition installed computer.

1. Please have the following information available:
   - The **License Certificate ID** from this certificate (above)
   - The **serial number of the Micro GC Fusion** that will connect with EZ IQ or OpenLAB computer
     - The Serial number can be found on the product label on the back of the instrument, or by clicking the icon on the lower right of the web - based user interface when the instrument is turned on
2. On a computer with access to the Internet, open a web browser and go to **http:\\fusionlicense.inficon.com** . Enter the License Certificate ID and serial number of the Micro GC Fusion.
3. Download the **openlab-fusion.license** file and enter it on the computer that is connected to the Micro GC Fusion.
4. Complete the license activation by uploading the **openlab-fusion.license** file into the Micro GC Fusion via its web-based user interface. The instructions are available in EZ IQ and Micro GC Fusion Driver Installation Guide or OpenLAB CDS EZChrom Edition Driver Installation Guide.
5. Download the driver software from the INFICON software download webpage (http://www.inficon.com/tabid/244/en-US/default.aspx). Install the driver on the computer loaded with EZ IQ or OpenLAB, which is networked with the Micro GC Fusion. Follow the instructions in the EZ IQ or OpenLAB manual to complete the instrument to computer connection.

The Micro GC Fusion EZ IQ driver is available for download from **http://www.inficon.com/tabid/244/en-US/default.aspx**.

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2.1 EZ IQ Hardware and Software Requirements

EZ IQ is validated on both the English and Western European Language versions of Windows.

2.1.1 Computer Minimum Requirements

Type	Microsoft® Operating System	CPU	RAM1	Disk Space	Network	Graphics
Minimum Configuration	XP Pro. SP3 with .Net 3.0 or Vista Business SP1 or Windows 7 Pro 32-bit	2 GHz	2 GB	10 GB	See instrument requirements	1024 x 768
Recommended Configuration	XP Pro. SP3 with .Net 3.0 or 3.5 SP1 or Vista Business SP1 or Windows 7 Pro 32-bit	Dual Core 2 GHz	2 GB	10 GB and >60% free HD space	100 Mbps or Higher	1280 x 1024 or higher
[1] RAM total available memory for EZ IQ including the operating system, but no other application.						

2.1.2 Important Notes

- Microsoft TCP/IP networking is required for all products. WAN's (wide area networks) are not supported.
- Disk Space requirements should be adjusted based on archival periodicity. INFICON recommends a minimum of one year of the expected disk usage on top of the recommendation of the operating system. For reference, each analysis will generate a data file of ~200Kb.

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Chapter 3
Instrument Wizard

When EZ IQ is opened for the first time, the **Instrument Wizard - Micro GC Fusion** window will display. The **Instrument Wizard** is designed to direct the user through the basic functions of the instrument window. (See Figure 3-1 and Table 3-1.)

Figure 3-1 Instrument Wizard - Micro GC Fusion

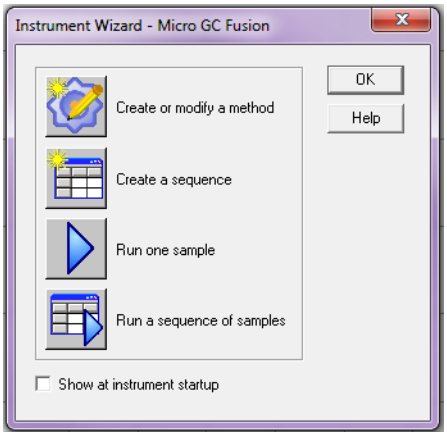

Table 3-1 Instrument Wizard parameters

Function	Description
Create or modify a method	This button steps the user through creating or modifying a method
Create a sequence	This button steps the user through creation of an acquisition or reprocessing sequence
Run one sample	This button begins data acquisition using a stored method
Run sequence of samples	This button begins data acquisition using a stored sequence
Show at instrument startup	If this box is selected, the **Instrument Wizard** will appear each time this instrument is started

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3.1 Offline Instrument Wizard

To use an instrument offline, open the EZ IQ Offline program. The **Instrument Wizard** will display. (See Figure 3-2.)

Figure 3-2 Instrument Wizard - Micro GC Fusion (Offline)

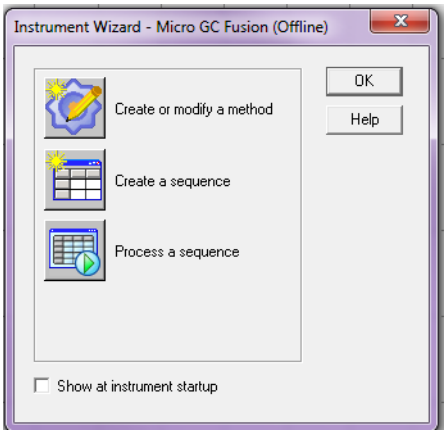

Table 3-2 Instrument Wizard parameters

Function	Description
Create or modify a method	This button steps the user through creating or modifying a method
Create a sequence	This button steps the user through creation of an acquisition or reprocessing sequence
Process a sequence	This button steps the user through reprocessing an existing sequence

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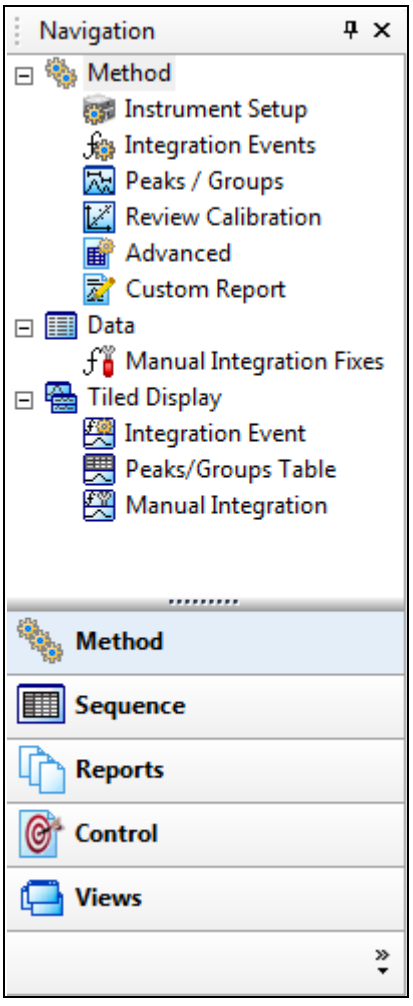
Chapter 4
Navigation Pane

4.1 Navigation Pane

Upon opening EZ IQ, a **Navigation** pane will display at the left side of the instrument window. (See Figure 4-1.) The **Navigation** pane enables the user to select functions of the instrument window.

Figure 4-1 Navigation pane



To turn the Navigation pane on

Click **View >> Navigation Pane**.

To turn the Navigation pane off

Click the **x** button at the top-right of the **Navigation** pane.

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To dock the Navigation pane

The **Navigation** pane can be docked at the left of the Instrument window to provide additional work space. To dock the **Navigation** pane, click at the top of the **Navigation** pane. (See Figure 4-1.)

Once the **Navigation** pane is docked, it can be viewed again by moving the cursor over the **Navigation** tab. The **Navigation** pane will disappear when the cursor is moved back into the work space.

The **Navigation** pane of the instrument window allows the user to access method, sequence, report, control, and viewing options. The **Navigation** function bars at the bottom of the **Navigation** pane open command trees that give access to commands that are also available from the menu bar of the instrument window. (See Table 4-1.)

Table 4-1 Navigation pane command trees

Navigation Function Bar	Displays
Method	Instrument Setup, Integration Events, Peaks/Groups, Review Calibration, Advanced, Custom Report, Manual Integration Fixes
Sequence	Edit
Reports	Reports, Report, Template Properties
Control	Instrument Setup, Run Queue, Instrument Status
Views	Data Display Options, Manual Integration Fixes, Baseline Check Status, Sample Entry

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Chapter 5
Method and Data File Structure

5.1 About Method Files

A method is used to acquire and/or reprocess a data file. A method contains:

- Data acquisition parameters (run time, sampling rate, etc.)
- Integration events
- Calibration and peak information
- Reports
- Optional functions such as data export and user programs

Each method is capable of acquiring multiple modules of data from Micro GC Fusion. Each module has its own complete independent parameters, including column temperature, ramp rate, run time, integration events, and calibration.

Although the method file is a separate file, the information contained in the method is saved in the raw data file at time of acquisition. This way, the original method can be reproduced, even if the method file was subsequently modified.

5.2 About Data File Structure

A data file is created whenever a sample is acquired. The data file contains the following information:

File Information Header. Contains information such as the date and time of acquisition.

Complete method parameters used to acquire and process the data.

NOTE: This is the original method saved only when the data is acquired.

Because multiple modules of data can be simultaneously acquired on Micro GC Fusion, the method section may contain complete parameters for more than one module.

Raw data points for the run saved. Multiple chromatograms may be present in a single data file, each of which represents a detector module acquired for the run. The raw data points are saved in binary format.

Results. The original integration results are saved in the file and can be viewed when the file is opened. In addition, the most recent analysis results and method are saved in the data file and updated whenever analysis occurs. The **Sample ID** for the results and manual integration fixes are also saved.

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File Description. If a description was entered for the file, this text information is stored with the file, and can be viewed under the **Data File Properties** or from the **Open Data File** window.

Instrument Configuration. The configuration of the instrument used to acquire the data file is saved.

Data File Audit Trail. An audit trail log is always saved in the data file that tracks analysis of the data. Data files are saved using the filename and extension specified when initiating the data acquisition. The limit on filename length is 255 characters, including path.

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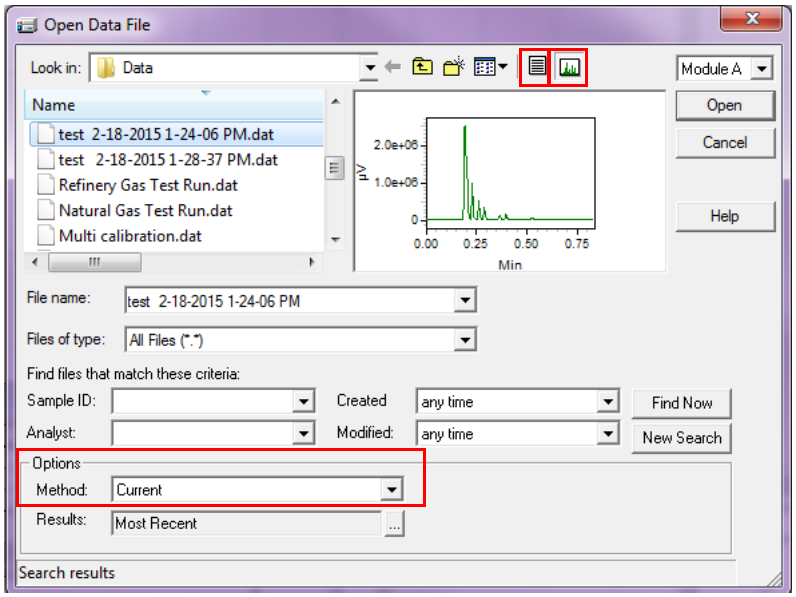
Chapter 6
Opening and Saving Files

6.1 Open Data Files

1. Click **File >> Data >> Open**.
2. The **Open Data File** window will display. (See Figure 6-1.)
3. The **Open Data File** window provides search options for data files. The list of files by type selected (**Files of type**) will display. The files can be viewed as a list and details can be shown by clicking the appropriate icon at the top of the window. In addition, the chromatogram in a data file can be previewed by selecting the icon, or the file description can be viewed by clicking the icon.

   NOTE: The * wildcard character can be used to view a list of certain file types. Files are stored in the current project folder. (See Figure 6-1.)

Figure 6-1 Open Data File window



6.1.1 Open Data File Options

The **Options** box allows the user to select additional information at the time the data file is opened. (See Figure 6-1.)

- If **Current** is selected, the current method will not change when the data file is opened. When one of the other **Method** options is selected, the method selected will be loaded at the time the data file is opened
- **From Results** loads the method used to create the selected results. When one of the **From Results** options is selected, the data file will be opened along with the selected results. When a data file is opened with results, the integration and baselines that generated those results will be displayed automatically when the chromatogram is drawn on the window. If **Most Recent** is selected, the data file will be opened with the results from the last time the chromatogram was analyzed
- **Original/Acquisition** loads the method used for the original acquisition of the data file. This method will replace the current active method

6.1.2 Searching for Data Files

In **Find files that match these criteria**, files containing certain information can be searched. All or part of a **Sample ID** can be specified. Files may be searched by designated **Analyst**, or by specific acquisition time frame such as **Yesterday**, **Last 7 Days**, **Today**. Files may also be searched by specific modification time frame. These criteria can be used one at a time or combined. (See Figure 6-1.)

Wildcards can be included as part of the file name searching. To perform a search, fill in the field of interest for the **Files of type** to search, then click **Find Now**. For example, by entering **Test*** in the **Sample ID** field and clicking **Find Now**, all the files where the **Sample ID** begins with **Test** will be displayed. Click the **New Search** button to clear the search settings to search using new criteria.

NOTE: When using the search feature, ensure the Windows **Hide File Extensions for Known File Types** option is turned **OFF**. To turn this off, click **My Computer >> Tools >> Folder Options...** and select the **View** tab.

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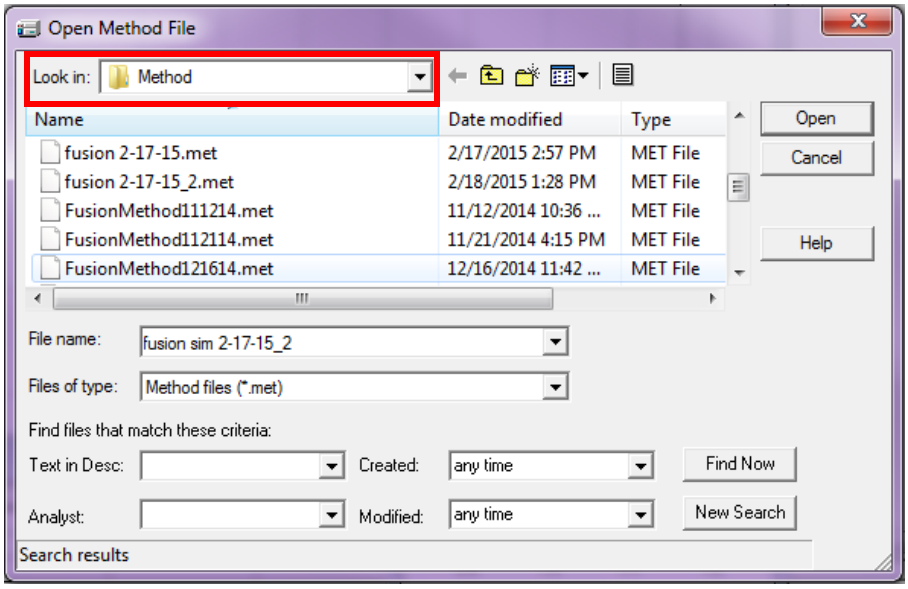
6.2 Open Method and Sequence Files

To open a method or sequence file:

1. Click **File >> Method** (or **Sequence) >> Open**.
2. The **Open Method File** or **Open Sequence File** window will display. Files are stored in the current project folder. A **Look in:** shortcut menu is included in the window to facilitate navigation. (See Figure 6-2.)

Figure 6-2 Open Method File window



6.2.1 Searching for Method and Sequence Files

The criteria used to search for specific method and sequence files in **Find files that match these criteria:** includes the selection of specific text found in the file description (**Text in Desc.**), **Analyst** name, and date **Created** or last **Modified**. (See Figure 6-2.)

NOTE: When using the search feature, ensure the Windows **Hide File Extensions for Known File Types** option is turned **OFF**. To turn this off, click **My Computer >> Tools >> Folder Options...** and select the **View** tab.

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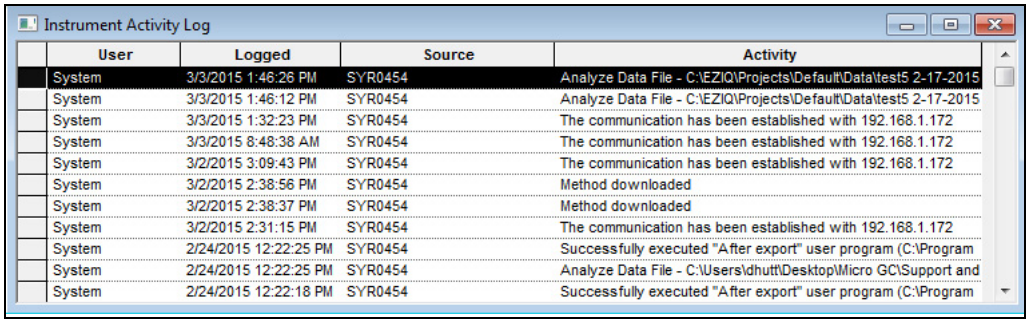
Chapter 7
The Instrument Window

7.1 View the Instrument Activity Log

1 To view the instrument activity log for the currently connected instrument, click **File >> Instrument Activity Log >> Display Log**. The **Instrument Activity Log** window will display. (See Figure 7-1.) The **Instrument Activity Log** window displays the **User**, the time the activity was **Logged**, the **Source**, and a description of the **Activity**.

Figure 7-1 Instrument Activity Log



2 To view details of any line in the **Instrument Activity Log**, click the line to highlight it, then right-click within the spreadsheet. From the shortcut menu, details of the highlighted line can be viewed or printed. (See and Table 7-1.)

Figure 7-2 Instrument Activity Log spreadsheet

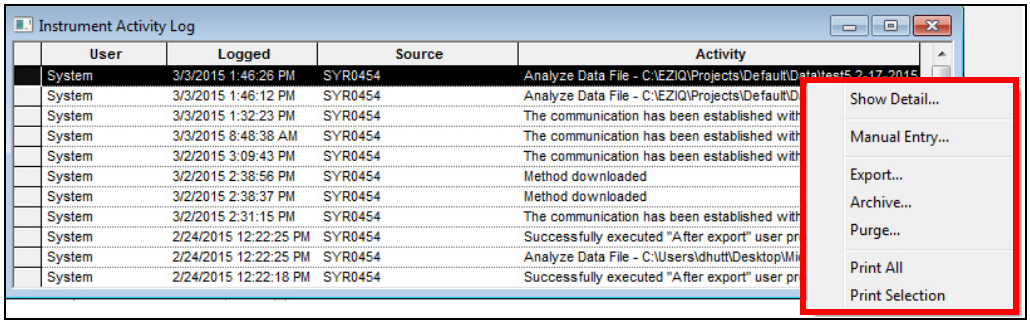


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Table 7-1 Instrument Activity Log parameters

Parameter	Description
Show Detail	Displays a pop up box with additional information
Manual Entry	Allows the user to add a log
Export	Exports the log as a .txt file
Archive	Saves the activity log to another location as a .logarc file
Purge	Clears the log of all activity
Print All	Prints the entire activity log
Print Selection	Prints only the selected logs

3 The **Instrument Activity Log** will record all activities. To free up memory space, select the **Purge** function to clear the log of all activities. The activity log can be saved to another location by selecting the **Archive** function.

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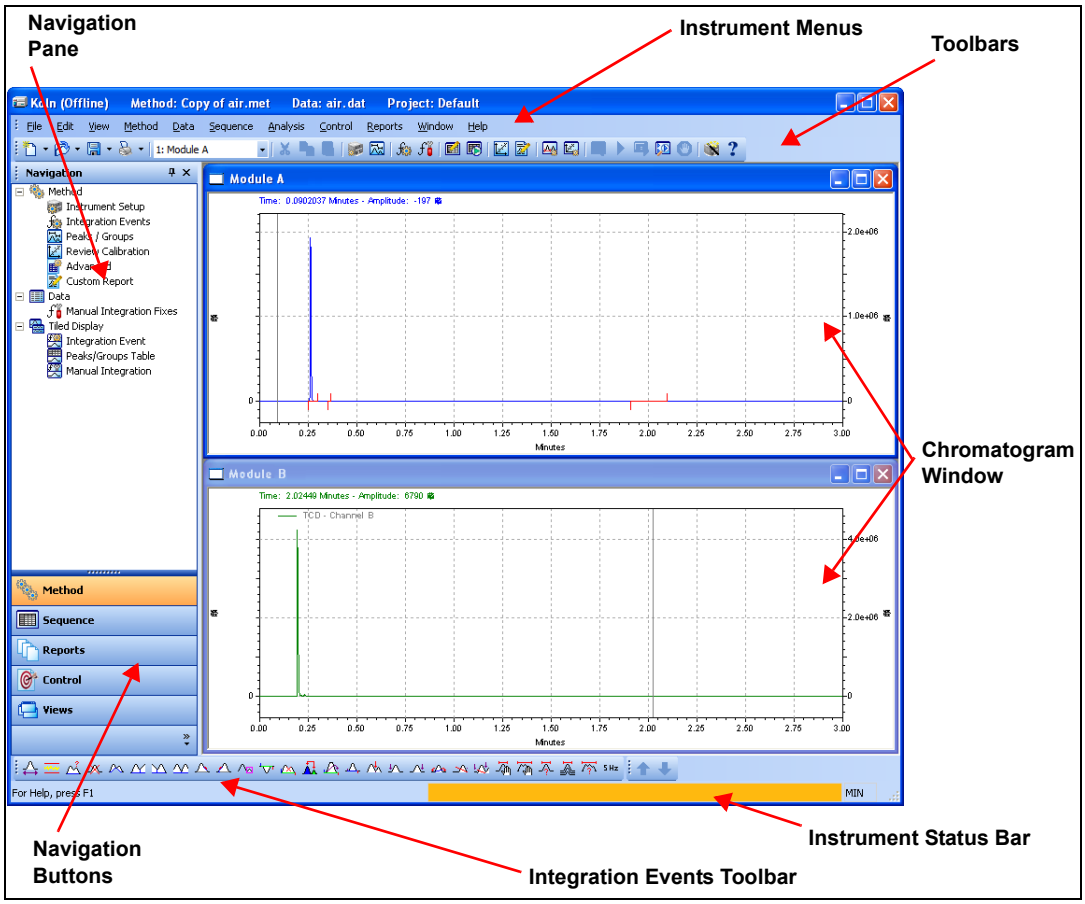
7.2 About the Instrument Window

When an instrument is connected and EZ IQ is opened, the **Instrument Window** will display. (See Figure 7-3.) From this window the following functions can be accessed:

- Method development
- Calibration
- Sequence development
- Instrument control and data acquisition
- Analysis and review of data
- Reporting
- Data export

The appearance of the **Instrument Window** can be customized by adding or removing the **Navigation** pane and toolbars.

Figure 7-3 Instrument window



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7.2.1 Change View Preferences

To change the appearance of the **Instrument Window**:

1. Click **View >> Preferences**.
2. Select the **General** tab. (See Figure 7-4 and Table 7-2.)

Figure 7-4 General tab

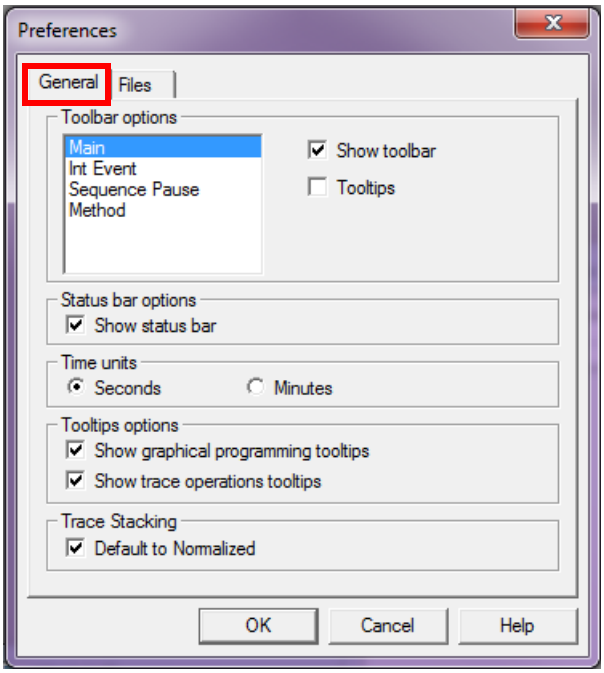

Table 7-2 Preferences parameters

Function	Description
General tab	Used to set up general preferences in the instrument window
Toolbar options	To enable toolbars and tooltips, select the desired **Toolbar** option and select the **Show toolbar** and **Tooltips** boxes
Status bar options	Select the **Show status bar** box to turn on the status bar
Time units	Select the time units for display of chromatographic information

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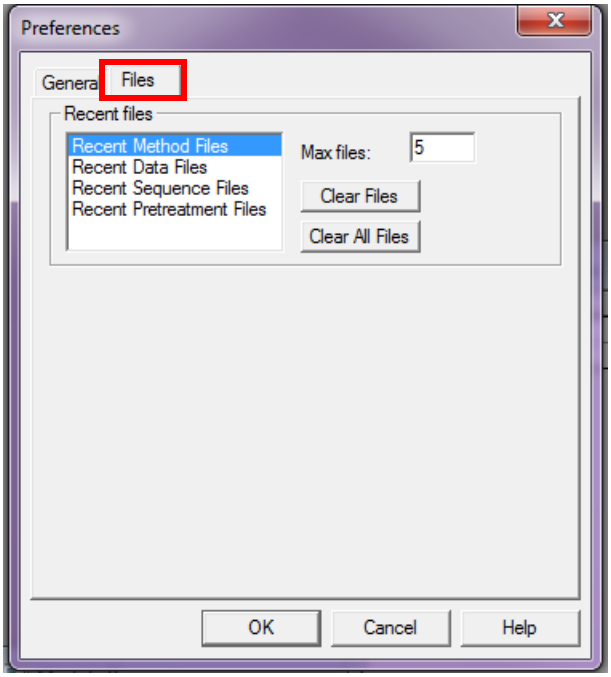
7.2.2 Change File View Preferences

To change the appearance of the **Instrument Window**:

1. Click **View >> Preferences**. The **Preferences** window will display. (See Figure 7-5.)
2. Select the **Files** tab.
3. Select the file type under **Recent files**, then enter the number of files to display in the **Max Files** box. This determines the number of selected files to be displayed in the **File** menu.
4. Click **Clear Files** to clear the current recent files list for the selected file type.
5. Click **Clear All Files** to clear the recent files for all the file types.

Figure 7-5 Preferences window



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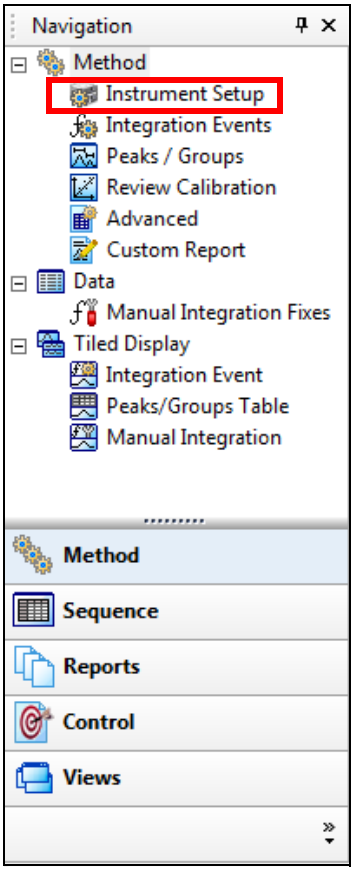
Chapter 8
Method Acquisition Parameter Setup

8.1 Method Acquisition Parameters

As part of a chromatographic method, method acquisition parameters can be defined in the **Instrument Setup** window **Navigation** pane. (See Figure 8-1.)

Figure 8-1 Navigation pane



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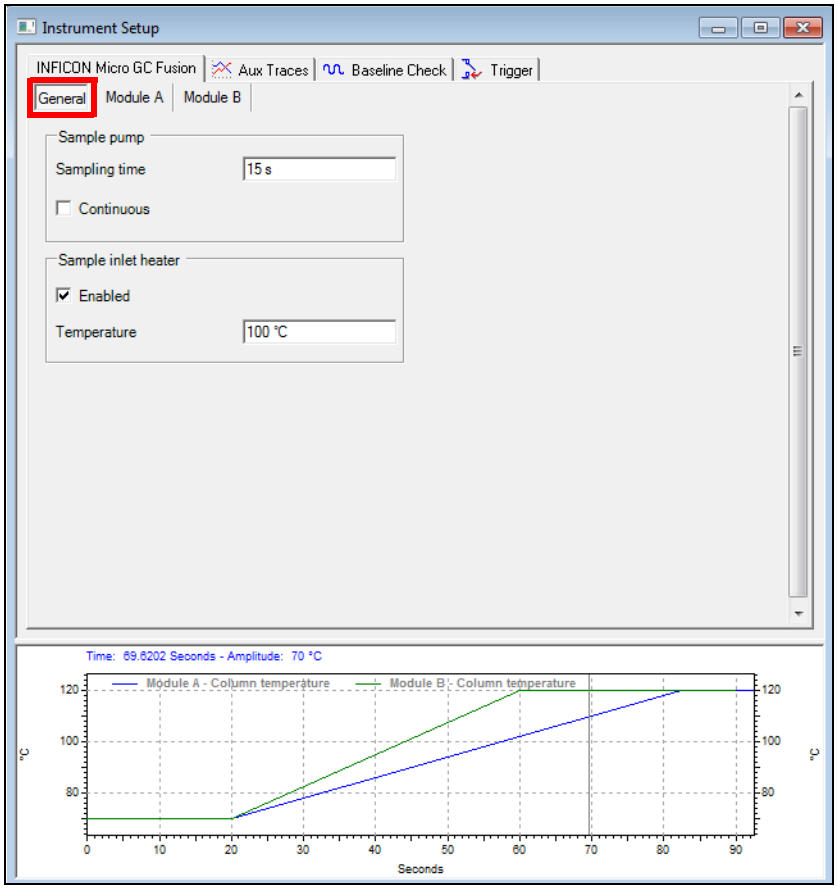
Double-click **Instrument Setup.** The **Instrument Setup** window will display. The **General** tab contains method parameters that are common to all modules. (See Figure 8-2.) A temperature graph will display at the bottom of the **Instrument Setup** window.

Figure 8-2 Instrument Setup General tab



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The **Module** tabs contain module specific method parameters. (See Figure 8-3 and Table 8-1.)

Figure 8-3 Instrument Setup Module tab

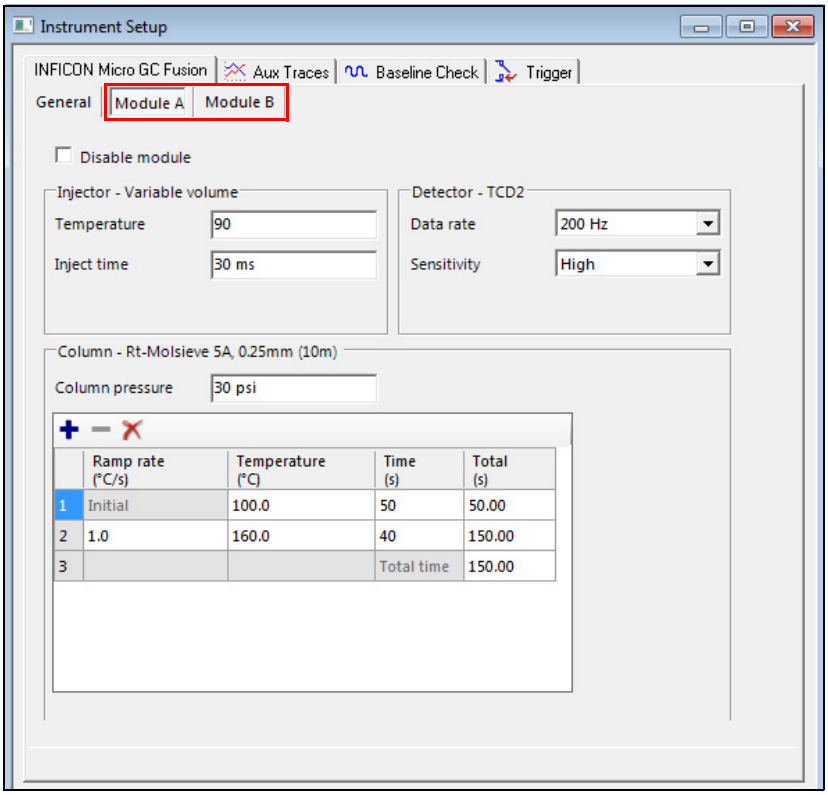

Table 8-1 Instrument Setup general method parameters

Method Parameter	Unit	Description
Sampling Time	s	Duration the sample pump pulls sample into the instrument
Continuous	N/A	Disables the sample pump and allows sample to continuously flow through the injector, assuming positive sample pressure
Sample Inlet Heater Enabled	N/A	Enables the sample inlet heater
Sample Inlet Heater Temperature	°C	Temperature set point of the sample inlet
Sample Conditioner Purge Time	s	Duration the sample conditioner is purged (if installed)
Sample Conditioner Flow Rate	N/A	Sets the sample conditioner flow rate to low or high (if installed)
Disabled	N/A	Disables the selected module
Injector Temperature	°C	Temperature of the injector
Inject time	ms	Duration the injector valve is open to allow sample to enter the column
Backflush Time (if configured)	s	Time between the sample injection and injector backflush action to allow undesired compounds from the pre-column to vent
Data Rate	Hz	Detector signal data points per second
Sensitivity	N/A	Can be set to high or standard; high sensitivity should only be used for low ppm trace analysis **NOTE:** There is no sensitivity setting for ***FAST Enabled*** Micro GC Fusion as it is dynamically adjusted during run time.
Column pressure	psi	Carrier gas pressure applied at the column head to direct sample gas into the analytical column
Ramp rate	°C/s	Temperature ramp rate of analytical column **CAUTION** **Do not exceed recommended maximum temperature ramp rate to avoid instrument damage. (See Table 8-2.)**
Temperature	°C	Temperature set point(s) of the analytical column
Time	s	Duration the column remains at the desired temperature
Sample Conditioner Enable Heater	N/A	Enables the sample conditioner (if installed)

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Table 8-2 Maximum column ramp rates by length

Column Length	Maximum Ramp Rate
8m	5°C/s
10m	4°C/s
>10m	2.5°C/s

8.1.1 Trigger Setup

The **Trigger** tab allows for the user to delay the start of a run until a **External** or **Manual** trigger is initiated.

1. From the **Navigation** pane, click **Method >> Instrument Setup**.
2. Select the **Trigger** tab.
3. From the shortcut menu, select a trigger **Type**. (See Figure 8-4 and Table 8-3.)
4. When the **Trigger** setup information is completed, close the window.

Figure 8-4 Trigger Type selection

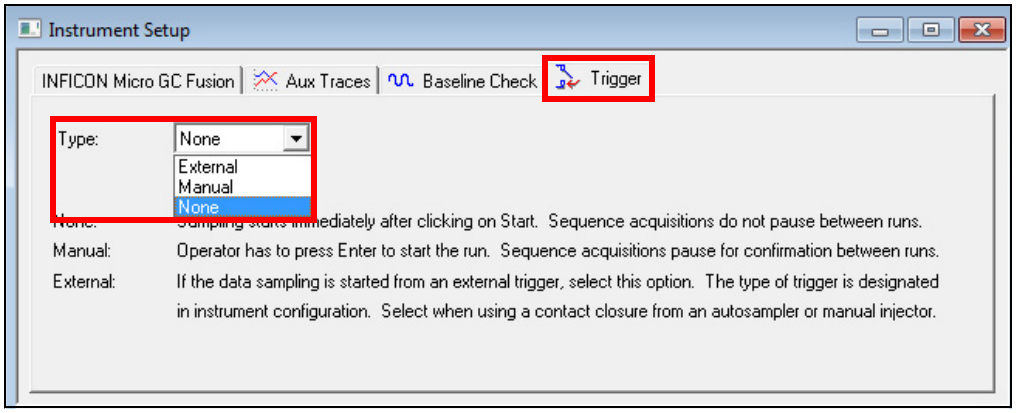

Table 8-3 Trigger Type selections

Navigation Function Bar	Displays
External	Data sampling starts when externally triggered
Manual	User must start the data sampling
None	Sampling of data starts immediately when **Start** is clicked in the **Single Run** window

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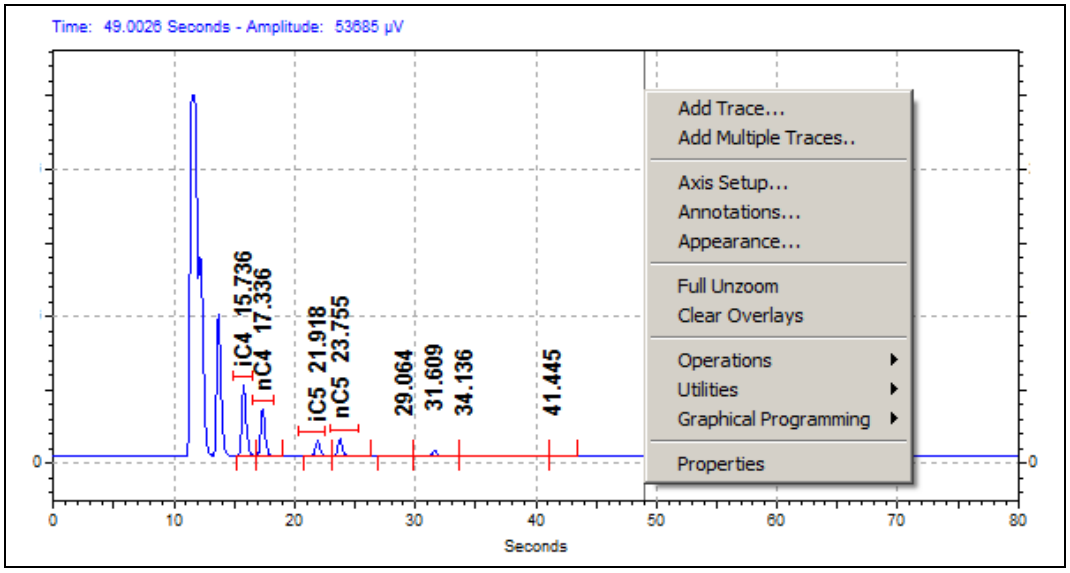
Chapter 9
The Chromatogram Window

9.1 About the Chromatogram Window

Each module will have its own chromatogram window to display data. It is possible to add multiple traces to a single chromatogram window to perform comparison and mathematical operations. To access specialized commands for the chromatogram window, right-click anywhere within the chromatogram window to display a list of commands. These commands allow for a wide range of functions, including: adding multiple traces to the window, changing the appearance of the chromatogram, adding annotations, adjusting X- and Y-axes, and performing mathematical operations. There is also an option to view or change the properties of the chromatogram. (See Figure 9-1.)

Figure 9-1 Chromatogram window



The chromatogram window will display data in real time. At the end of a run, the data becomes the current data. Annotations, fonts and labeling for the chromatogram can be customized. Right-click on the chromatogram and click **Annotations** to access this feature. In **Utilities**, the current window view can be printed, copied to a clipboard, or saved in a file.

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9.2 View Tiled or Overlay Data

By default, each module will have a chromatogram window. Chromatograms from different modules can be overlaid onto a single window by selecting **View >> Overlay Data**. (See Figure 9-2.) The chromatograms can be separated into multiple windows by selecting **View >> Tile Data**. (See Figure 9-3.) Individual modules may be zoomed in and their appearances may be changed as described below.

In **Tiled** mode, window tiling preference can be set by clicking **Window >> Cascade**, **Window >> Tile Horizontally**, or **Window >> Tile Vertically**.

Figure 9-2 Overlaid data

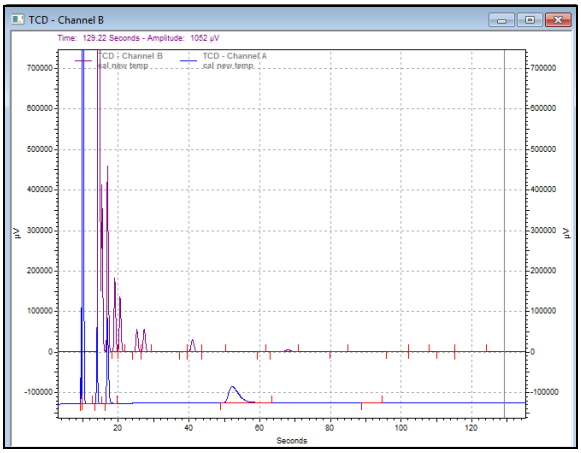
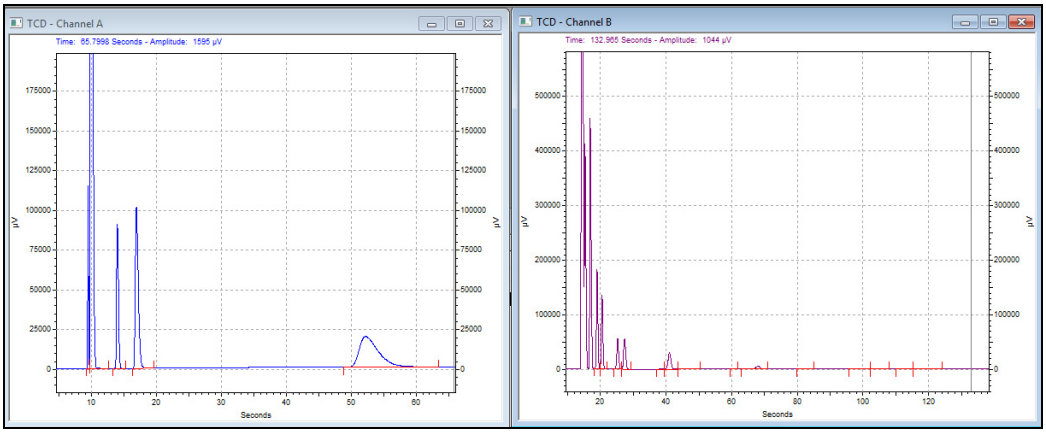


Figure 9-3 Tiled data, tiled vertically

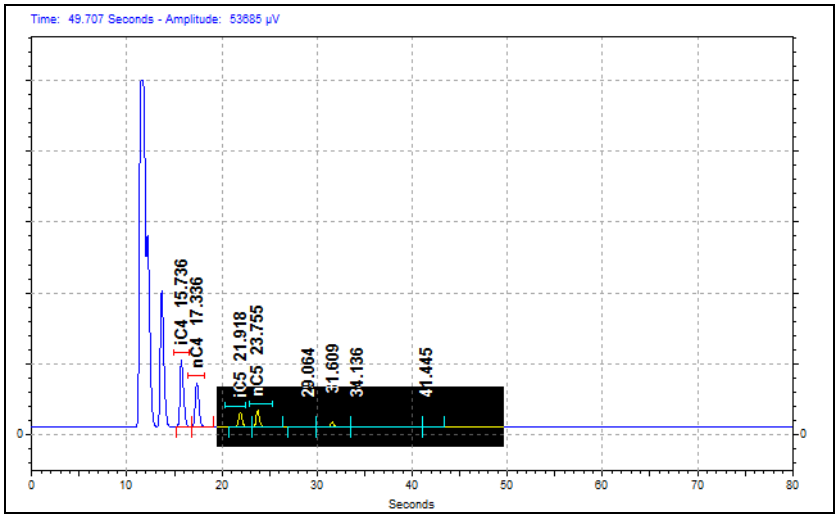


9.3 Zooming

It is possible to examine a chromatogram in more detail by zooming in on a portion of the chromatogram. Left-click and drag to open a box to highlight the area of interest. Release the mouse button to zoom. (See Figure 9-4.)

NOTE: The zoom function can be used multiple times to further define a region of the chromatogram.

Figure 9-4 Zooming



To return to the previous level of zoom, double-click the chromatogram. To restore the full chromatogram view, right-click anywhere in the chromatogram window, and click **Full Unzoom**. Alternately, **Ctrl-Z** or **shift-double-click** in the chromatogram window to return to the full chromatogram view. When the chromatogram is zoomed in, it can be scrolled. (See section 9.4, Scroll the Chromatogram, on page 9-4.)

Time and **Amplitude** are displayed at the top of the chromatogram window. These values change as the cursor is moved to reflect the time and amplitude of the trace at that location. To display an alternate trace, click on the other trace. If the traces are displayed in different colors, the color of the **Time** and **Amplitude** display will reflect the color of the trace displayed.

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9.4 Scroll the Chromatogram

A zoomed chromatogram can be scrolled to the right or left while maintaining the zoom. Press the **CTRL+SHIFT** keys and move the mouse until the cursor changes to a hand. Left-click and drag the cursor to the left or right.

The X- or Y- axis can be scrolled to access features which may be out of view. Press **CRTL+SHIFT** while the cursor is outside the graph area, yet near the axis of interest. The cursor will change to an up/down arrow near the Y-Axis, or a left/right arrow near the X-Axis. Move the cursor to scroll the graph up/down or left/right on the axis.

To restore the full chromatogram view, right-click anywhere in the chromatogram and click **Full Unzoom**.

9.5 Add a Trace (Add a Single Chromatogram)

The chromatogram window is used to view current data (real-time) in the instrument window, or saved data. Multiple chromatograms can be viewed in a single chromatogram window. This is convenient to compare a past run with current data, or to overlay a temperature profile.

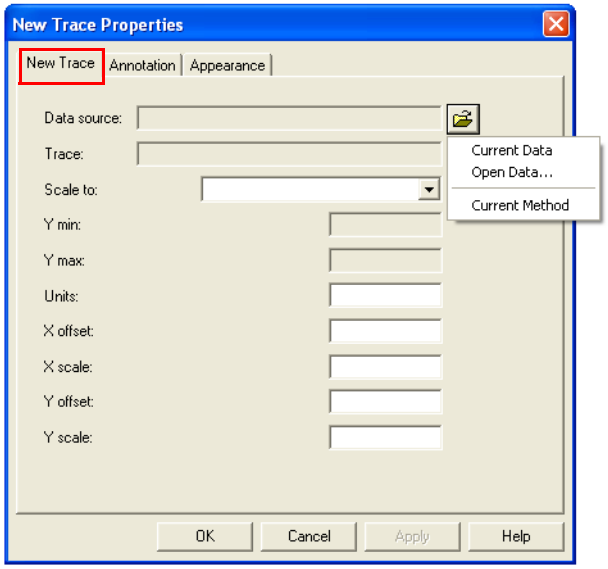
To add a new trace to the chromatogram window:

1 Right-click anywhere in the chromatogram. A menu will appear. (See Figure 9-5.)

Figure 9-5 Chromatogram window options

2 Click **Add Trace…**. The **New Trace Properties** window will display. (See Figure 9-6.)

Figure 9-6 New Trace Properties window



3 Select the **New Trace** tab. Populate the fields to add a trace and its desired properties to the chromatogram window.

NOTE: These properties apply only to the trace selected and are not saved as part of the method. When a new trace is opened, the properties will be set to default values. Added traces are normalized by default.

Table 9-1 New Trace tab parameters

Navigation Function Bar	Displays
Data Source	Enter the name of the file from which to get the trace. Or, click the **File** icon adjacent to the field and select a data source
Current Data	Selects a trace from the current chromatography data
Open Data	Selects from stored data files in which a trace can be selected for display
Current Method	Selects a trace from the current method (if available)
Trace	Select the trace to be displayed. Click the icon to display available traces

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Table 9-1 New Trace tab parameters (continued)

Navigation Function Bar	Displays
Scale to	Select one of the scaling options:
Trace x	Scales to another trace in the window
Autoscale to largest peak	Scales such that the largest peak is on scale
Autoscale to 2nd largest peak	Scales such that the second largest peak is on scale
Autoscale to 3rd largest peak	Scales such that the third largest peak is on scale
User Defined	Allows entering a value for Y max and Y min
Normalized	Allows normalization of one trace to fit on the graph
Y Min	If **User Defined** scale is selected, enter a minimum value for the Y-Axis
Y Max	If **User Defined** scale is selected, enter a maximum value for the Y-Axis
Units	Select the units for display
X Offset	Enter a value in units for offset of the X-Axis
Y Offset	Enter a value in units for offset of the Y-Axis
X Scale	Enter a multiplier that will be applied to the entire trace
Y Scale	Enter a multiplier that will be applied to the entire trace

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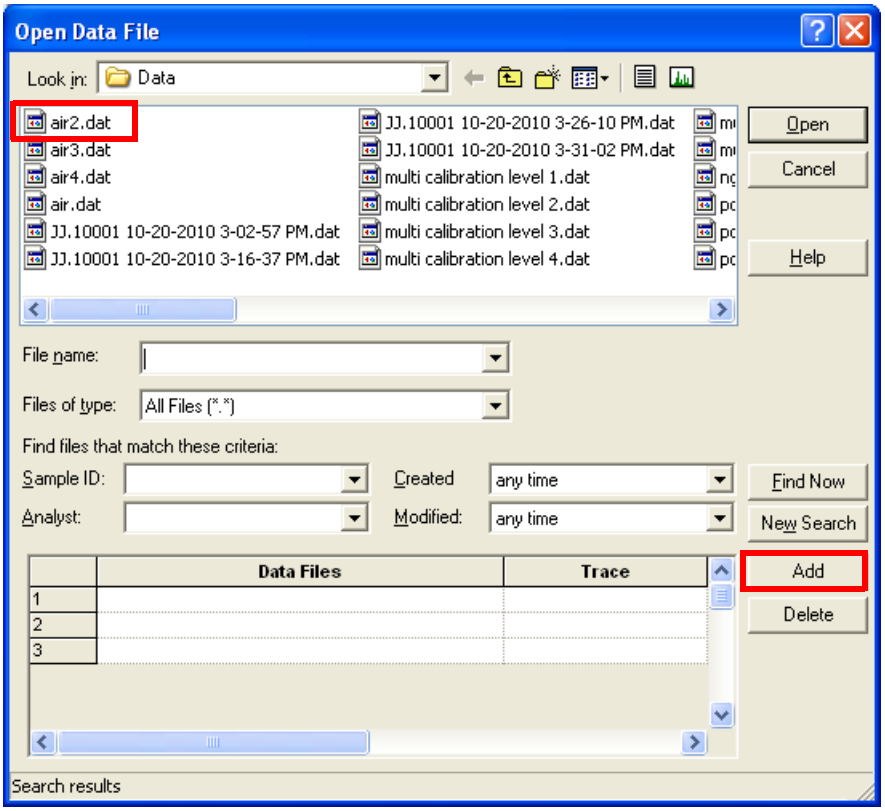
9.6 Add Multiple Traces to a Chromatogram Window

To add more than one chromatogram to the view:

1. Right-click in the chromatogram window, then click **Add Multiple Traces…**. The **Open Data File** window will display. (See Figure 9-7.)
2. To add a file, click the filename, then click **Add**. Alternately, double-click the filename from the list.

Figure 9-7 Open Data File window



3. Once a data file is added to the list, select the module by clicking in the **Trace** field, then click the down-arrow button. If multiple modules for that file are available, select the desired module.
4. To delete a trace from the **Data Files** list, click its name or number, then click **Delete**.

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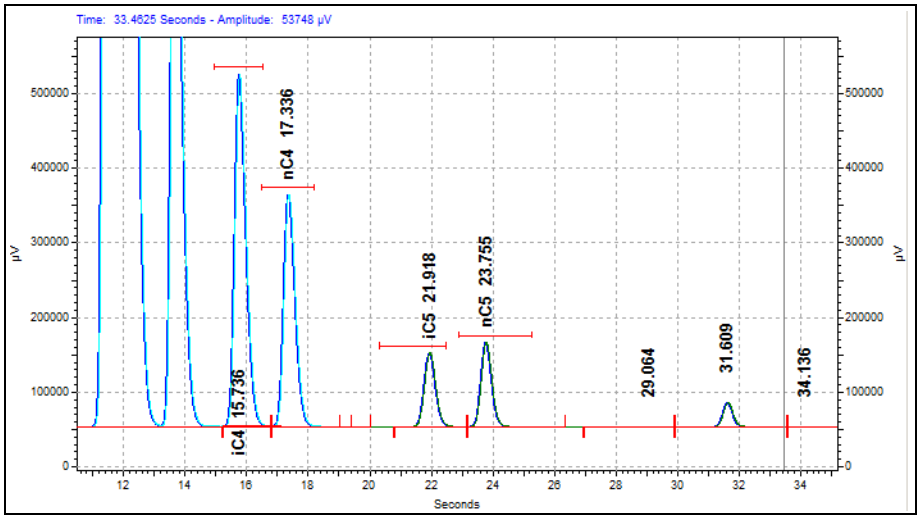
5 Click **Open**. The files under **Data Files** will appear in the chromatogram window. (See Figure 9-8.)

Figure 9-8 Selected files overlaid

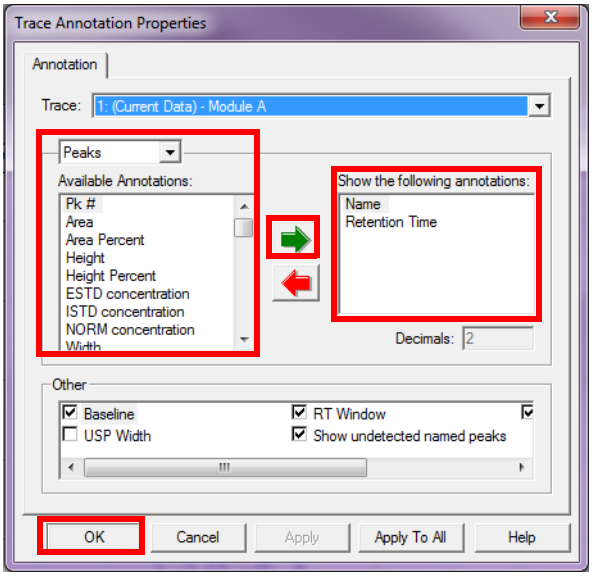


9.7 Annotate a Chromatogram

To change the annotations on the chromatogram:

1 Right-click in the chromatogram window and select **Annotations** to open the **Trace Annotation Properties** window. (See Figure 9-9.)

Figure 9-9 Trace Annotation Properties window



2 Select the desired trace from the shortcut menu.

3 For the selected trace, select **Peaks** or **Groups** from the shortcut menu to select the type of annotation to use.

4 Click the desired annotation to highlight it. Click the green arrow to add the annotation to the trace. Alternately, double-click the desired annotation to add it to the trace.

5 For certain annotations, the number of places to be displayed to the right of the decimal point can be designated. Enter this value in the **Decimals** box for the highlighted item.

6 In **Other**, select the check boxes to display desired parameters such as **Baseline**, **USP Width**, or **Retention Time Windows**, **Show Undetected Named Peaks**, and **Group Ranges** on the trace.

NOTE: The **Retention Time** window annotation displays the window set in the **Peak Table**. This window is not adjusted for relative retention time.

7 When finished adding annotations, click **OK** or **Apply**.

8 Select or change annotation for an existing trace by a right-click in the chromatogram window, then clicking the **Annotation**. The selections made will apply to all traces open for this module or until they are changed (via the **OK** or **Apply** button). Alternately, to apply the annotation changes to all open modules, click **Apply to All**.

NOTE: Annotations are not saved as part of the method and are considered a function of the instrument application. If the method is closed then opened, the current settings will apply.

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9.8 Change the Chromatogram Appearance

To change the appearance of a chromatogram or trace:

1 In the Chromatogram Window, right-click and select **Appearance**. The **Appearance Properties** window will display. (See Figure 9-10, Table 9-2, and Figure 9-11.)

Figure 9-10 Appearance Properties window

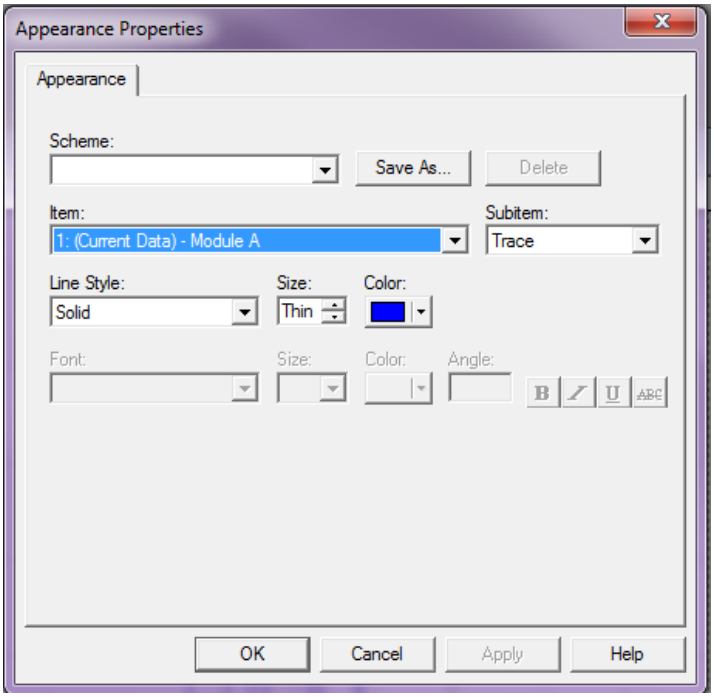


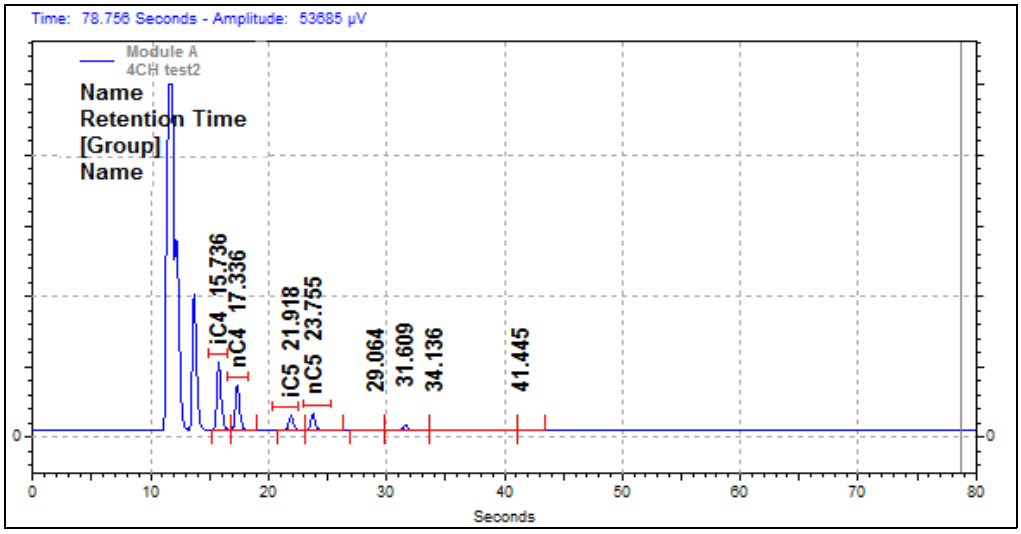
Table 9-2 Appearance parameters

Parameter	Displays
Scheme	If an appearance scheme has been previously saved, select it from this box. **Save As…** saves the existing appearance scheme with a user defined name. **Delete** deletes the scheme
Item	Use this shortcut menu to select the part of the chromatogram to modify. The choices include the graph itself (including background and legends) and the available traces

Table 9-2 Appearance parameters (continued)

Parameter	Displays
Sub-item	Use the shortcut menu to select the sub-item to modify. The choices will change based on the item selected. For example, if the item selected is the **graph**, setting up appearances of sub-items including the **background**, **axes** and **labels** for the graph are available. If the item selected is a **chromatogram data module**, access to setting appearances of sub-items such as **baselines**, **start and stop tick marks**, and **annotation** are available. If the item selected is **text**, access to the font formatting commands is available. When a sub-item is selected, access to fields appropriate to that item are available. For example, if **Baseline** is selected, the **Line Style**, **Size** and **Color** can be chosen. If **Annotation** is selected, the **Font**, **Size**, **Color** and **Angle** can be chosen

Figure 9-11 Module A chromatogram with new appearance parameters



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Sub-items available in the **Appearance** tab are shown in Table 9-3.

Table 9-3 Sub-items available in the Appearance tab

Item	Sub-Item	Description
Graph	Background	Select the color of the graph background. Default is black
Graph	Title	Select a color and/or font for the **Title** of the graph. There must be a Graph Title defined in the **Axis Setup** tab in order for it to appear in the window
Graph	Left Y-Axis	Select a color for the left **Y-Axis**
Graph	Left Y-Axis Major Ticks	Select a color for display of left **Y-Axis** major ticks
Graph	Left Y-Axis Minor Ticks	Select a color for display of left **Y-Axis** minor ticks
Graph	Left Y-Axis On/Off	Turns On or Off the left **Y-Axis**
Graph	Right Y-Axis	Select a color for display of a right **Y-Axis**
Graph	Right Y-Axis Major Ticks	Select a color for display of right **Y-Axis** major ticks
Graph	Right Y-Axis Minor Ticks	Select a color for display of right **Y-Axis** minor ticks
Graph	Right Y-Axis On/Off	Turns On or Off the right **Y-Axis**
Graph	X-Axis	Select a color for the **X-Axis**
Graph	X-Axis Major Ticks	Select a color for display of **X-Axis** major ticks
Graph	X-Axis Minor Ticks	Select a color for display of **X-Axis** minor ticks
Graph	X-Axis On/Off	Turns On or Off the **X-Axis**
Graph	Legend	Select a color and/or font for display of the graph legend. The legend indicates what traces are currently displayed in the window. The Legend is turned On or Off from the **Axis Setup** tab
Graph	Grid	Select a color for display of the grid lines. Grid lines are turned On and Off from the **Axis Setup** tab
Data	Trace	Select a color and/or line type for display of the selected **Trace**
Data	Annotation	Select a color and/or font for display of the trace **Annotation**(s). The items to be annotated for a trace are selected in the **Annotations** tab
Data	Baseline	Select a color and/or line type for display of the **Baseline**
Data	Baseline Start Tick	Select a color and/or line type for display of **Baseline Start Ticks**

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Table 9-3 Sub-items available in the Appearance tab (continued)

Item	Sub-Item	Description
Data	Baseline Stop Tick	Select a color and/or line type for display of **Baseline Stop Ticks**
Data	USP Width	Select a color and/or line type for display of the **USP Width**, if calculated
Data	RT Window	Select a color and/or line type for display of expected retention time windows for named peaks
Data	RT Window (undet.)	Select a color for display of **RT Window** for expected peaks that were not detected

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9.9 Change the Axis Properties

To change the properties of the axis of a chromatogram or trace:

1 In the Chromatogram, right-click and select **Axis Setup**. The **Axis Properties** window will display. (See Figure 9-12 and Table 9-4.)

Figure 9-12 Axis Properties window

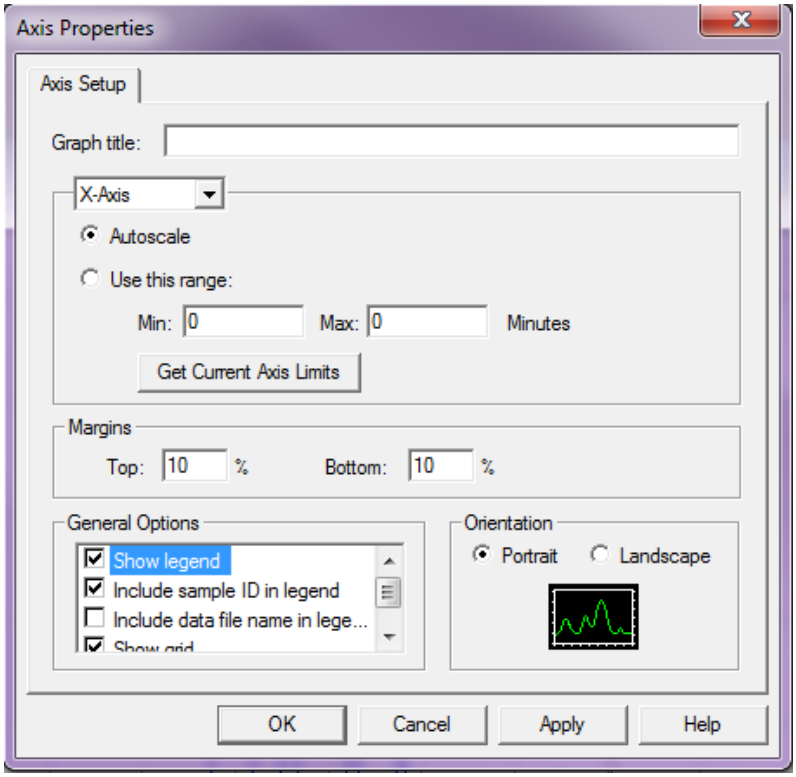

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Table 9-4 Axis Properties parameters

Navigational Function Bar	Displays
Graph Title	Enter a title for the graph, if desired. This appears at the top of the graph
Axis	From the shortcut menu, select the axis of interest: **Left Y-Axis**, **Right Y-Axis**, or **X-Axis**. Then choose the limits for the axis For **Y-Axis** selections, **Use Limits of Trace** will use the limits from one of the traces in the window. **Manually Set Trace's Limits** will box and set the Y-Axis limits to a user defined range. If **None**, no Y-Axis values will be displayed For the X-Axis, either choose to **Autoscale**, where the X-Axis is set to the longest trace, or, set an absolute range for the X-Axis by clicking **Use This Range**, then enter a minimum and maximum X-Axis value for the trace. Click **Get Limits** to retrieve the X-Axis range from the current trace
Margins	Enter a value for the trace margins, in percent, for top and bottom of the graph

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Table 9-4 Axis Properties parameters (continued)

Navigational Function Bar	Displays
General Options	Select the check boxes to turn graph annotations on and off. If the legend box is selected, the legend for a trace can be turned on or off from the **Trace Properties** spreadsheet (See Figure 9-13 and Figure 9-14.)

Figure 9-13 Chromatogram window with legend and grid displayed

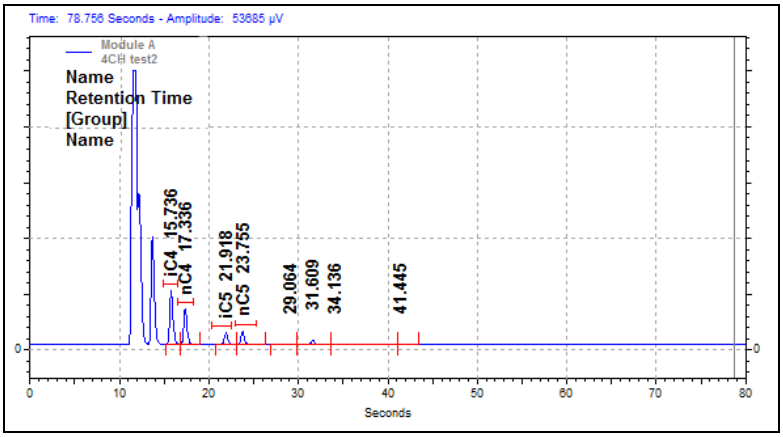
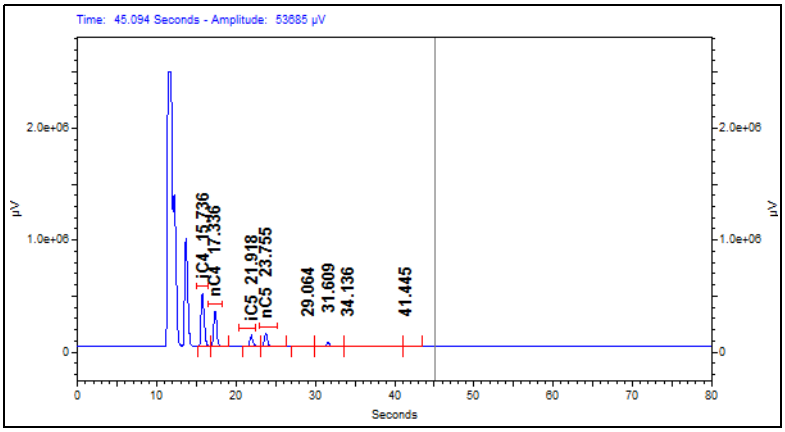


Figure 9-14 Chromatogram window with no legend or grid displayed



Orientation	Select portrait or landscape orientation for the graph by clicking the appropriate option button

9.10 Change Data Graph Properties

Whenever a trace is displayed in the chromatogram window, it uses the display settings contained in the **Data Graph Properties**.

To change the **Data Graph Properties**:

1. In the chromatogram window, right-click and select **Properties**.
2. Select the tab for the properties to view or change, as shown in Table 9-5.

Table 9-5 Properties tab parameters

Navigational Function Bar	Displays
Trace Setup	Add or remove traces, set legends, set scaling
Axis Setup	Add a graph title, change data range, set margins and orientation, turn on and off legends
Appearance	Set color schemes, line styles, and fonts

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9.11 Set Up a Trace

The **Trace Setup** tab allows for the addition and removal of traces as well as setting scaling options for the traces. (See Figure 9-15.) Each row in the spreadsheet represents one of the traces currently in the chromatogram window. The details of the highlighted trace appear in the trace properties boxes in the bottom of the window where they can be viewed or changed. See Table 9-6 for **Trace Setup** parameters and descriptions.

Figure 9-15 Trace Setup tab

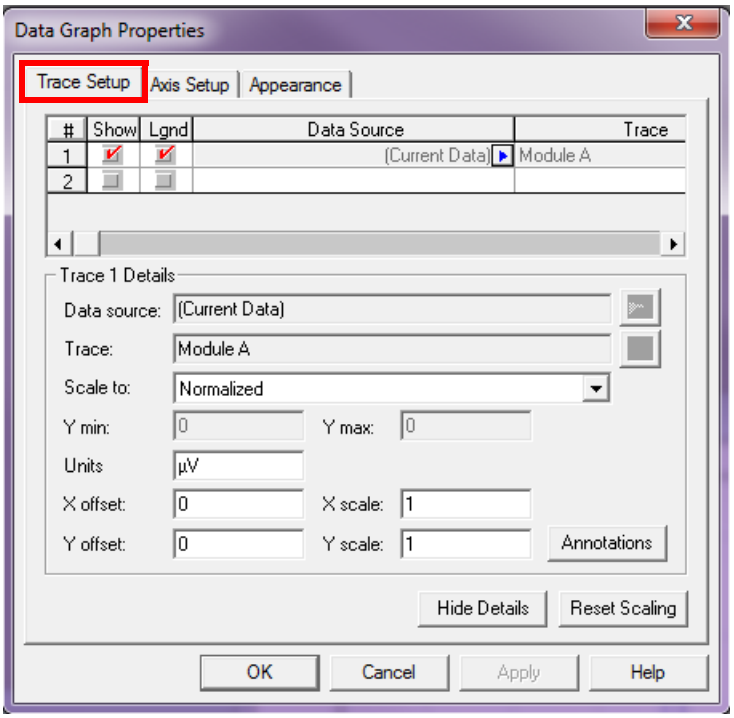

Table 9-6 Trace Setup parameters

Navigational Function Bar	Displays
Show	Select this box to display the trace in the chromatogram window. Clear this box to remove the trace from the chromatogram window
Lgnd	**NOTE:** If the **Legend** in the **Axis Setup** window is not turned on, then this box will have no effect. Select this box to show the **Legend** for the trace. The legend appears in the upper right corner of the window and displays the name of the trace. Clear this box to remove the legend for this trace from the chromatogram window. Setup for the appearance of the legend (color, etc.) can be accessed in the **Appearance** tab for the graph item

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Table 9-6 Trace Setup parameters (continued)

Navigational Function Bar	Displays
Data Source	Enter the name of the file from which to get the trace. Or, click the **File** icon adjacent to the field and select a data source. The **Data Source** can be a chromatogram or it can be a stored profile such as temperature or flow program
Current Data	Selects a trace from the current chromatography data
Open Data	Selects a stored data file from which a trace to be displayed can be selected
Current Method	Selects a trace from the **Current Method** (if available). For example, temperature profiles for instrument control
Trace	Select the module to be displayed
Scale to	Select one of the following scaling options
Trace x	Scales to another trace in the window
Autoscale to largest peak	Scales such that the largest peak is on scale
Autoscale to 2nd largest peak	Scales such that the second largest peak is on scale
Autoscale to 3rd largest peak	Scales such that the third largest peak is on scale
User Defined	Allows entering a value for Y maximum and minimum
Normalized	Allows normalization of one trace to fit on the graph
Y Min	If **User Defined** scale is selected, enter a minimum value for the Y-Axis
Y Max	If **User Defined** scale is selected, enter a maximum value for the Y-Axis
Units	Select the units for display
X Offset	Enter a value in units for offset of the X-Axis
Y Offset	Enter a value in units for offset of the Y-Axis
Y Scale	Enter a multiplier that will be applied to the entire trace **NOTE:** Set the X-Axis range by a right-click then selecting **Axis Setup**.

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Table 9-6 Trace Setup parameters (continued)

Navigational Function Bar	Displays
Annotations	Click to display the trace annotations window
Hide Details	Click to hide the current trace details and display only the spreadsheet
Reset Scaling	Click to reset the scaling values to their original values

9.12 Remove a Trace

If there are multiple traces in the chromatogram window, the user can remove one or more of them by right-clicking anywhere within the window and selecting **Properties…**. A spreadsheet will appear with the currently displayed traces listed.

To completely remove a trace from the chromatogram window, highlight the row by clicking on the number, then press **Delete**, or click **Edit/Delete**. To temporarily remove the trace from the window, clear the check box in the **Show** column. Click **OK** to return to the chromatogram window.

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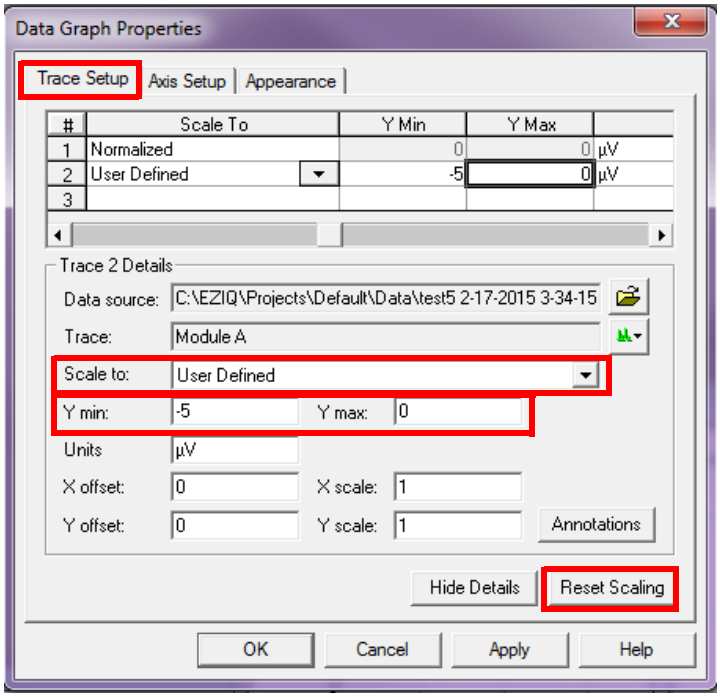
9.13 Set Limits for X-Axis and Y-Axis

Occasionally, an absolute range for either the X-Axis or Y-Axis, or both may be desired. To set limits for the X-Axis and Y-Axis:

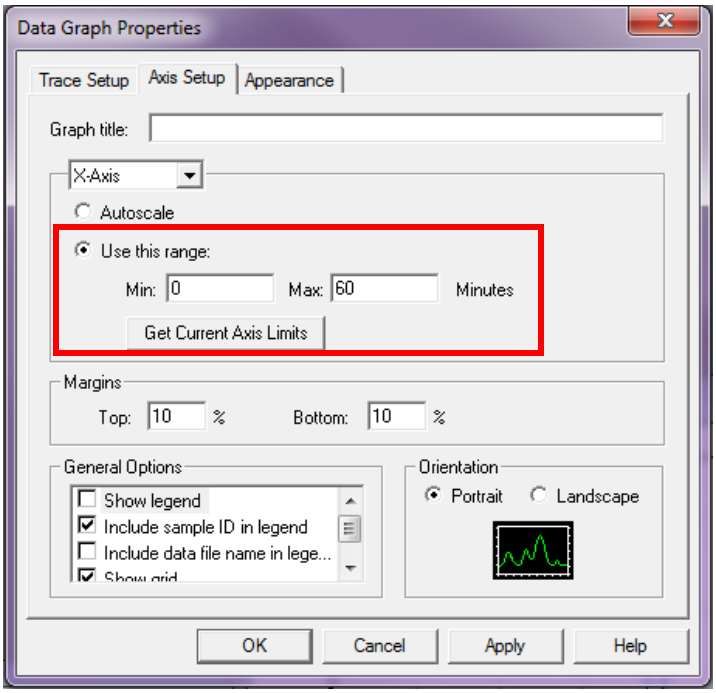
1. In the chromatogram window, right-click and select **Properties**. The **Data Graph Properties** window is displayed. (See Figure 9-16.)
2. To set Y-Axis minimum and maximum values, select the **Trace Setup** tab. To set an absolute voltage range for all chromatograms, use the **User-Defined** option from the shortcut menu for the **Scale To** field. Then, enter a **Y-Min** (minimum Y-Axis value) and **Y-Max** (maximum Y-Axis value) for each chromatogram. To display all chromatograms using the same voltage scale, enter the same values for all chromatograms. (See Figure 9-16.)

Figure 9-16 Trace Setup tab



3 To set absolute ranges for the trace, select the **Axis Setup** tab. (See Figure 9-17.) Click **X-Axis**, to set the range for the X-Axis. Click **Autoscale** to set the X-Axis range automatically to the range of the longest chromatogram (the default selection), or select **Use this range** to enter an absolute range in minutes. The **Get Current Axis Limits** button brings in the X-Axis range from the current chromatogram window. This is useful because it allows the use of the zoom function to identify the desired region of the chromatogram and automatically enter the range values.

Figure 9-17 Data Graph Properties Axis Setup tab



4 Once an absolute range for one or both of these axes is set, the designated chromatogram(s) will always be displayed in the chromatogram window using these ranges until they are changed or reset.

5 To reset the scaling of all chromatograms to default values, click **Reset Scaling** in the **Trace Setup** tab. (See Figure 9-16.)

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Chapter 10
Chromatogram Operations

10.1 About Chromatogram Operations

Chromatogram comparisons and mathematical operations are accessible from the chromatogram window. Right-click in the chromatogram window and select **Operations**. (See Figure 10-1 and Table 10-1.)

Figure 10-1 Operations

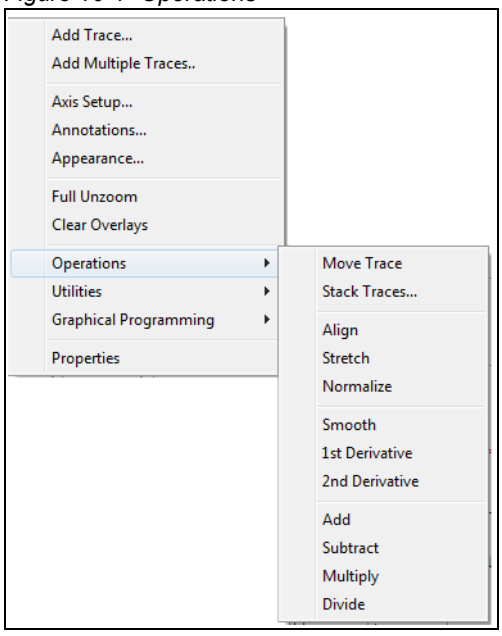

Table 10-1 Operation actions

Operation	Action
Move Trace	Click and move a trace within the chromatogram window
Stack Traces	Positions multiple traces with an offset
Align	Adjusts a second chromatogram such that a peak (or point) on one chromatogram will be aligned with a peak (or point) on the first chromatogram
Stretch	Performs a two-point contraction or expansion of chromatogram relative to another
Normalize	Normalizes one or more chromatograms to the first chromatogram, adjusting the heights such that the apex height of a selected peak matches that of the peak selected on the first trace

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Table 10-1 Operation actions (continued)

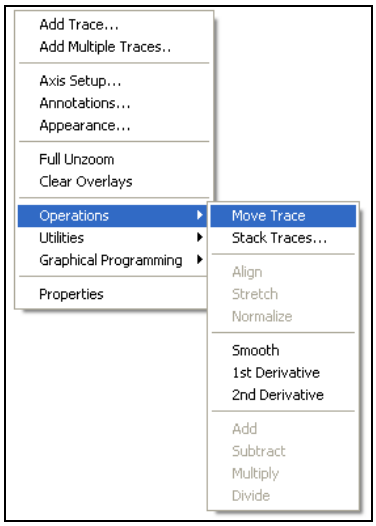
Operation	Action
Smooth	Performs a 9-point Savitzky-Golay smoothing operation on a selected trace
1st Derivative	Calculates and displays a 1st derivative of a selected trace
2nd Derivative	Calculates and displays a 2nd derivative of a selected trace
Add	Adds two traces and displays the result
Subtract	Subtracts two traces and displays the result
Multiply	Multiplies one trace by another and displays the result
Divide	Divides one trace by another and displays the result

10.1.1 Move a Trace

To move a trace:

1 In the chromatogram window, right-click and select **Operations >> Move Trace**. (See Figure 10-2.)

Figure 10-2 Operations: Move Trace



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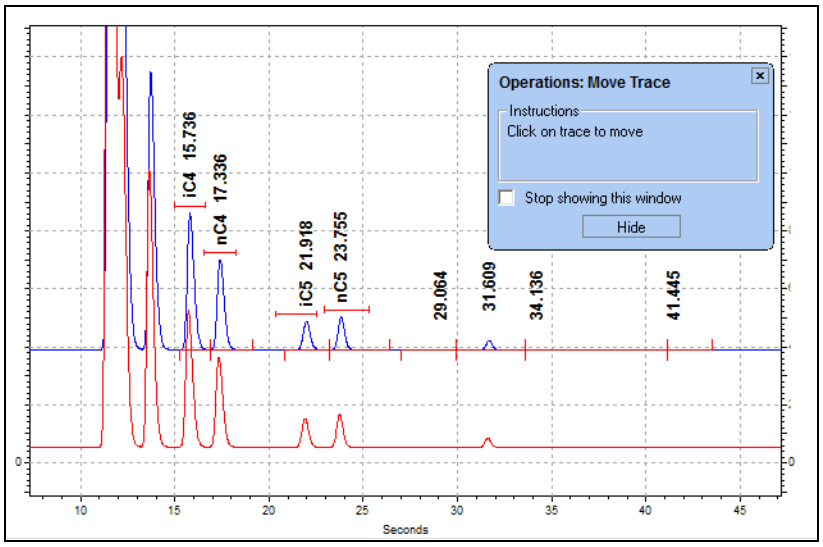
2 The **Operations: Move Trace** window will display. Move the cursor over a trace until it changes to a cross with arrows at the end.

3 Left-click and drag to move a trace to a new location. When the mouse button is released, the trace will be placed at the desired location. (See Figure 10-3.)

Figure 10-3 Operations: Move Trace



4 The **Operations**: **Move Trace** window will appear at the upper right corner of the chromatogram. Additional traces can be moved. When finished, right-click and select **Operations >> Move Trace** to turn off the move trace function.

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10.1.2 Stack Traces

Stack traces by changing the X-Axis and Y-Axis offsets:

1. In the chromatogram window, right-click and select **Operations >> Stack Traces...**.
2. Enter a new X-Axis and Y-Axis offset, and click **OK**. The offset will be applied to additional traces displayed in the chromatogram window. (See Figure 10-4 and Figure 10-5.)

Figure 10-4 Chromatograms before stacking

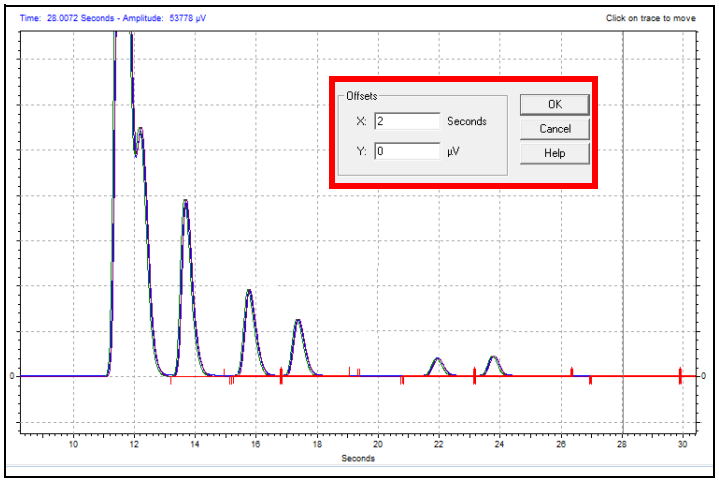
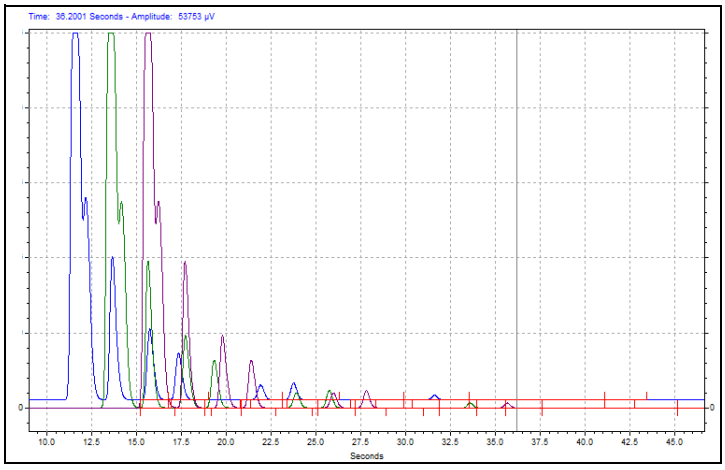


Figure 10-5 Chromatograms after stacking

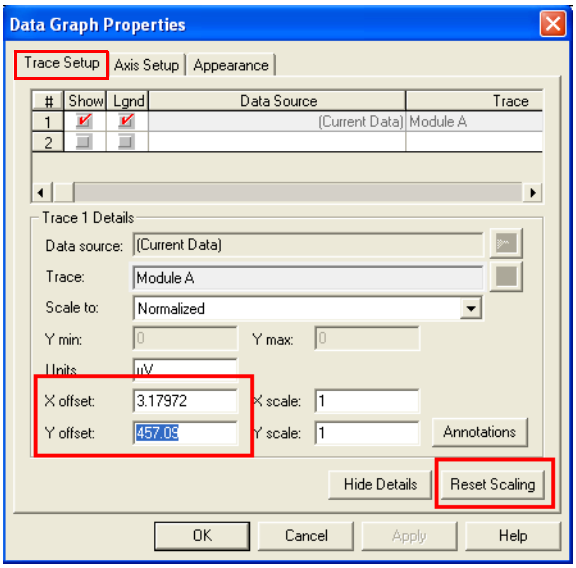


10.1.2.1 To Remove Offsets

To return a trace to the original X-Axis and Y-Axis offsets:

1. In the chromatogram window, right-click and select **Properties**.
2. The **Data Graph Properties** window will display. Select the **Trace Setup** tab. (See Figure 10-6.)

Figure 10-6 Remove offsets



3. Click **Reset Scaling** to restore all settings to their original values. (See Figure 10-6.)

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10.1.3 To Align Two Traces

To align one trace to another:

1. In the chromatogram window, right-click and select **Operations >> Align**. A **Operation: Align Trace** window will display. (See Figure 10-7.)
2. Click the desired peak on the first chromatogram, then click the desired peak on the second chromatogram to align it to the first peak. The selected peak in the second chromatogram will be adjusted such that it will be aligned with the selected peak in the first chromatogram.

Figure 10-7 Chromatograms before alignment

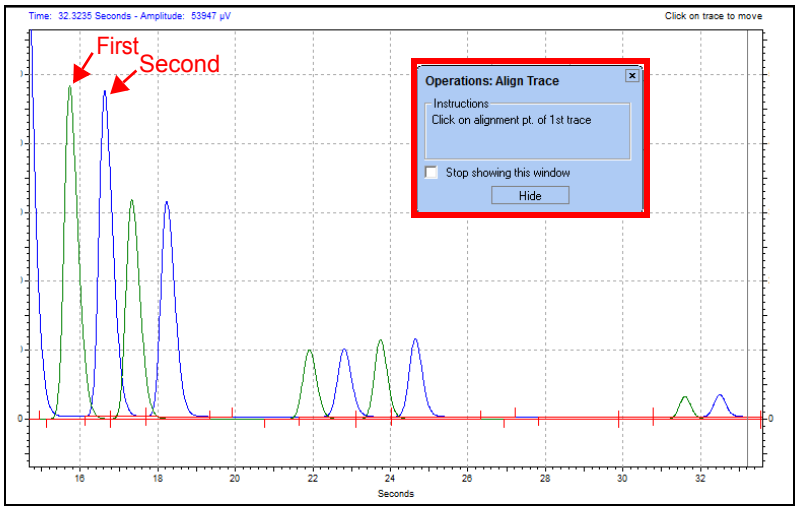
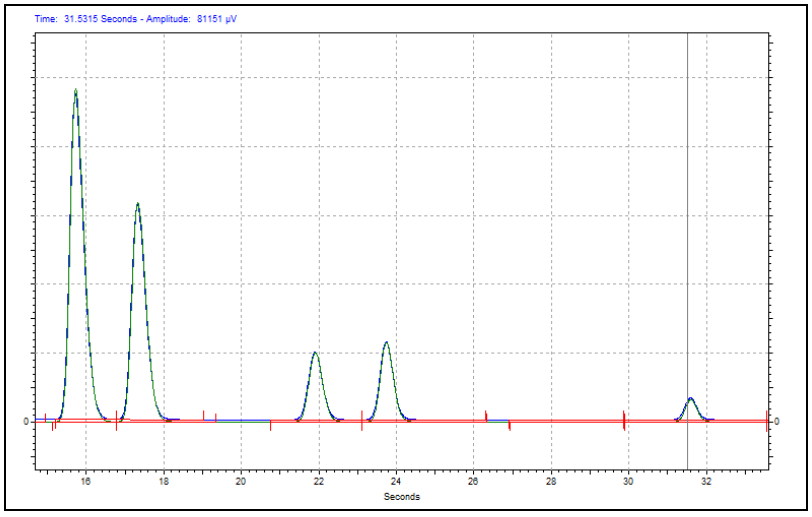


Figure 10-8 First peak of top chromatogram aligned to first peak on bottom chromatogram



3. To remove the alignment, right-click and select **Properties** to view the trace spreadsheet. Select the **Trace Setup** tab, then scroll to the right to access the **X-Axis** and **Y-Axis** offset columns to delete or change these settings. Click **Reset Scaling** to restore the original settings. (See Figure 10-6.)

10.1.4 Stretch a Chromatogram

Stretch allows a two-point contraction or expansion of chromatograms relative to another. To stretch a chromatogram:

1. In the chromatogram window, right-click and select **Operations >> Stretch**. The **Operations: Stretch** window will display. (See Figure 10-9.)
2. On the first chromatogram, click a starting peak, followed by a second peak. This provides the reference for the next chromatogram to stretch (or contract) to.
3. On the second chromatogram, click a starting peak, followed by a second peak. The chromatogram between these two peaks will be stretched or contracted to fit the two peaks specified on the first chromatogram. (See Figure 10-10.)

Figure 10-9 Chromatograms before stretching

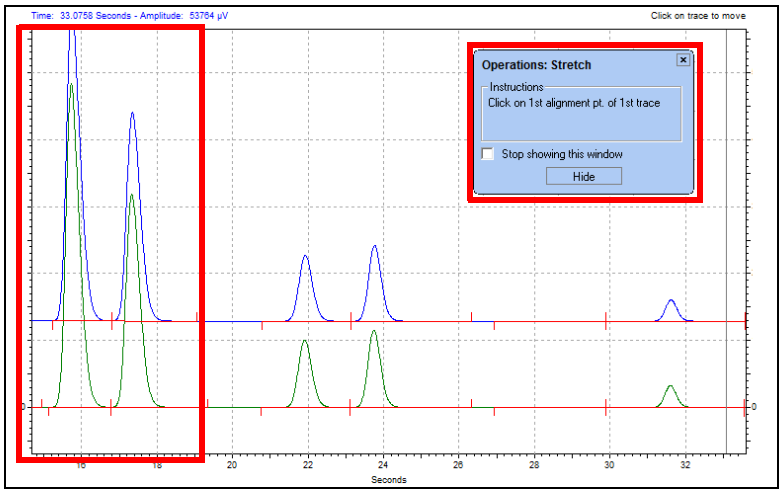
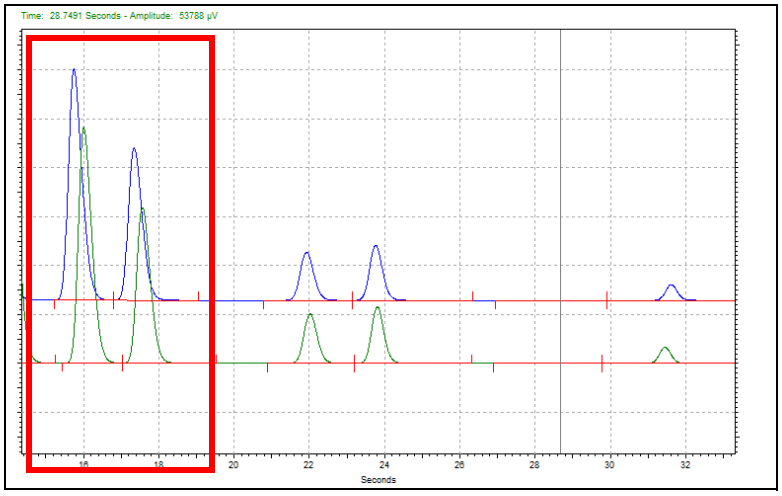


Figure 10-10 Bottom chromatogram stretched relative to top chromatogram



4. To undo the stretch, right-click and select **Properties** in the chromatogram window. Select the **Trace Setup** tab, then scroll to the right to access the X-Axis and Y-Axis offset columns where the stretched or contracted settings can be modified or deleted. Click **Reset Scaling** to restore the original settings. (See Figure 10-6.)

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10.1.5 Normalize Traces

Normalize Traces will normalize one or more chromatograms to the first chromatogram, adjusting the heights such that the apex of a selected peak matches that of the peak selected on the first trace.

1. In the chromatogram window, right-click and select **Operations >> Normalize**. The **Operations: Normalize** window will display. (See Figure 10-11.)
2. A window will prompt the user to click on the starting point of the desired peak. Once clicked, the window will prompt the user to click on the apex of the same peak.
3. The window will prompt the user to click on the starting point of the second peak. Once clicked, the window will prompt the user to click on the apex of the second peak. Once the apex is clicked, the chromatogram will normalize. (See Figure 10-12.)

Figure 10-11 Chromatograms before normalization

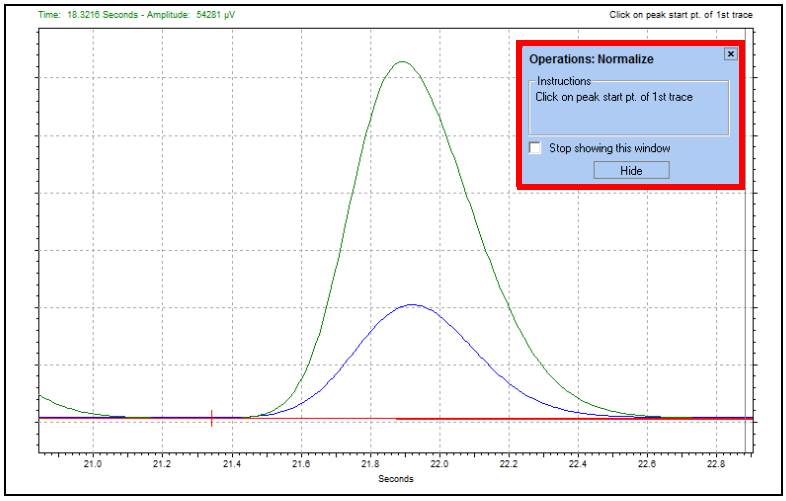
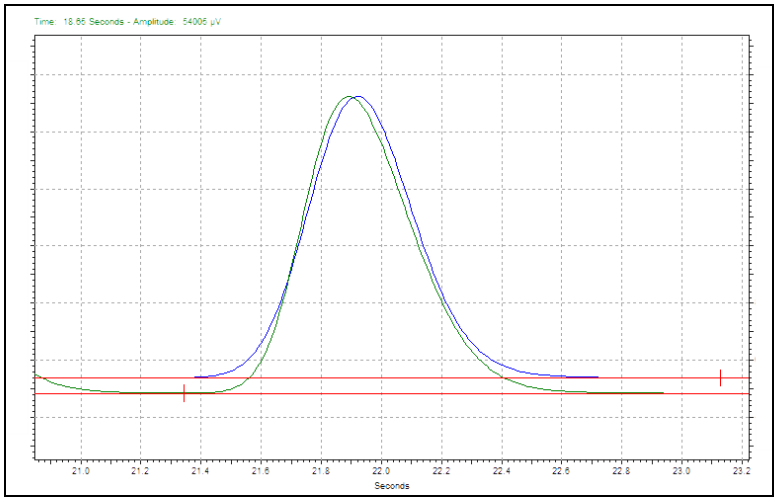


Figure 10-12 After normalization



4 To undo the normalization, right-click and select **Properties** in the chromatogram window. Select the **Trace Setup** tab, then scroll to access the right to access the **X-Axis** and **Y-Axis** offset columns where these settings can be modified or deleted. Click **Reset Scaling** to restore the original settings. (See Figure 10-6.)

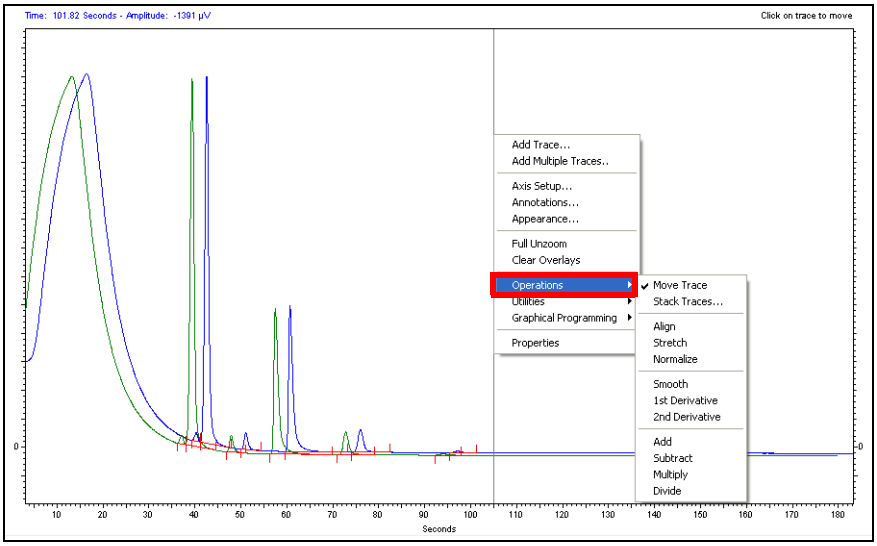
10.2 Perform Mathematical Operations on Traces

Mathematical operations on traces can be performed within the chromatogram window. To perform a mathematical operation on a trace:

1 In the chromatogram window, right-click and select **Operations**, then select the operation to perform. (See Figure 10-13.)

2 Follow the instructions displayed to perform the operation. The result of the operation will appear in the window.

Figure 10-13 Mathematical Operations



10.2.1 Smoothing

To perform a 9-point Savitzky-Golay smoothing operation on a selected data file:

1 In the chromatogram window, right-click and select **Operations >> Smooth**. The **Operations: Smooth** window will display.

2 Click the chromatogram to be smoothed. The resulting trace will display in the chromatogram window.

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10.2.2 Calculate Derivatives

To calculate and display the 1st or 2nd derivative of a chromatogram:

1. In the chromatogram, right-click and select **Operations >> 1st Derivative** or **Operations >> 2nd Derivative**. The **Operations:** window will display. (See Figure 10-14.)
2. Click the chromatogram to perform the operation. The resulting trace will display in the chromatogram window. (See Figure 10-15 and Figure 10-16.)

Figure 10-14 Trace before first derivative

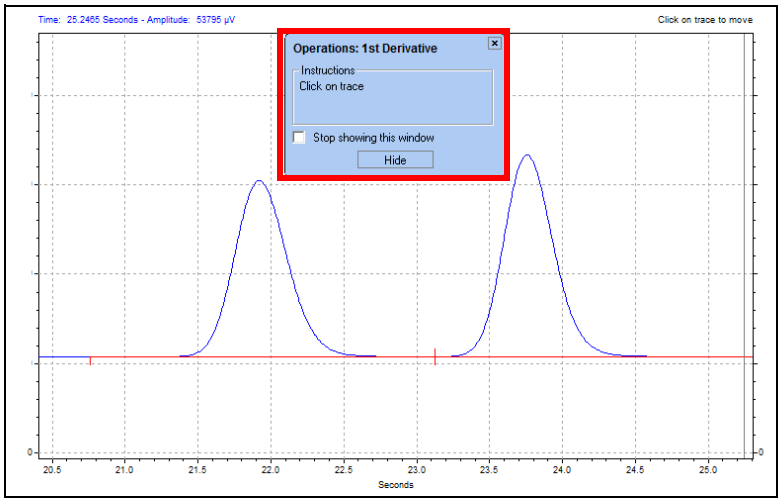


Figure 10-15 First derivative trace (red) displayed with original trace (blue)

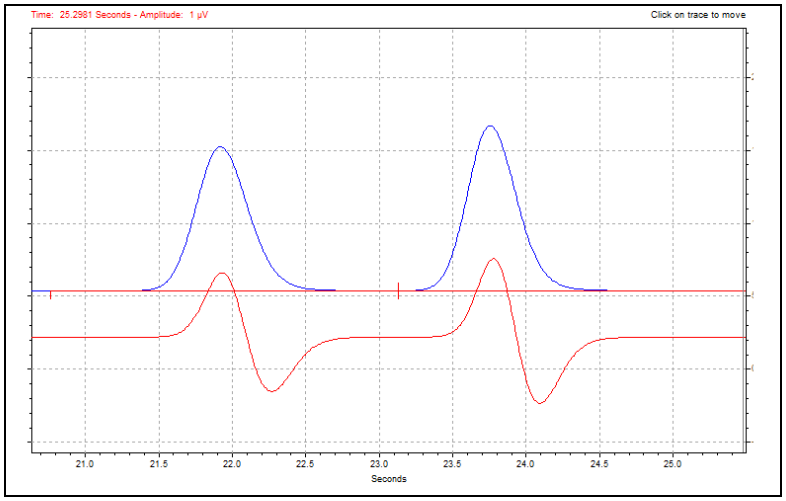
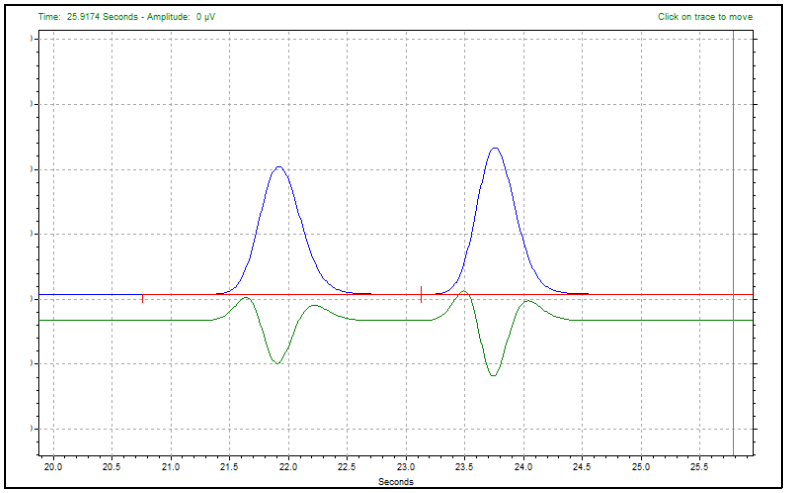


Figure 10-16 Second derivative trace (green) displayed with original trace (blue)



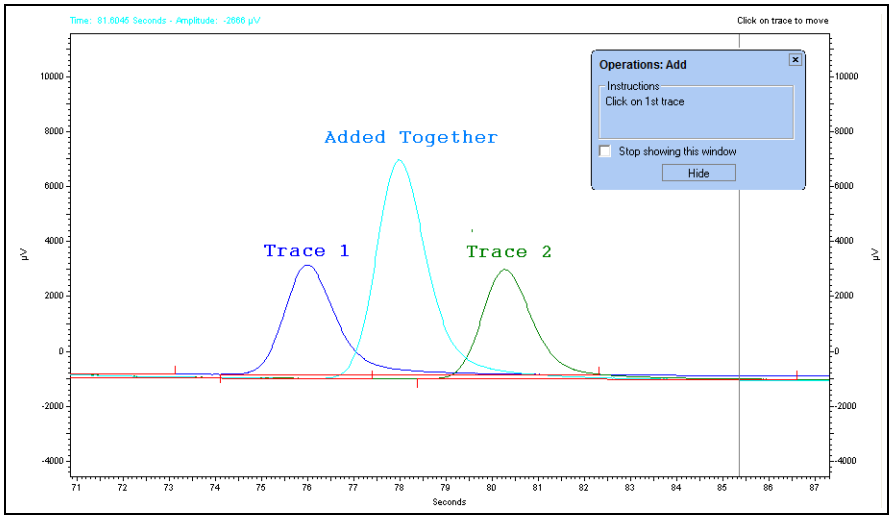
10.2.3 Add Two Traces

The **Add** operation adds together the area of two peaks from different traces to generate a third trace. To add two traces in a chromatogram window:

1. In the chromatogram window, right-click and select **Operations >> Add**.
2. Click the first trace to select it.
3. Click the second trace, which will be added to the first trace. The resulting trace will display in the chromagram window. (See Figure 10-17.)

   NOTE: For this operation to be valid, both traces must have the same sampling frequency.

Figure 10-17 Adding two traces



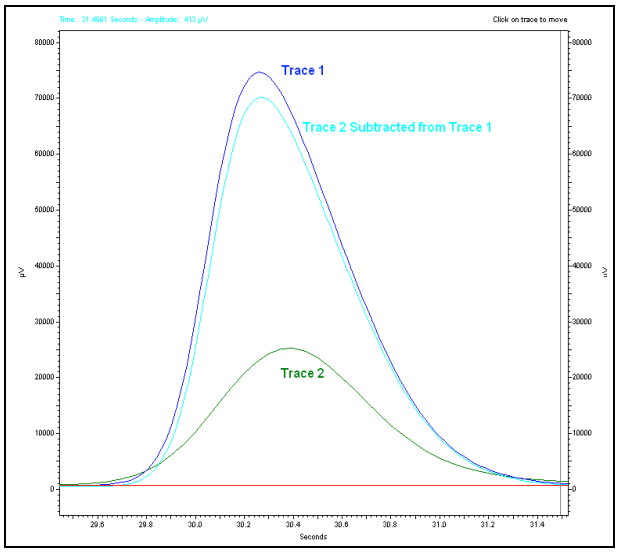
10.2.4 Subtract Two Traces

The **Subtract** operation subtracts the area of two peaks from different traces to generate a third trace. To subtract two traces:

1. In the chromatogram window, right-click and select **Operations >> Subtract**.
2. Click the first trace to select it.
3. Click the second trace, which will be subtracted from the first trace. The resulting trace will display in the chromatogram window. (See Figure 10-18.)

NOTE: For this operation to be valid, both chromatograms must have the same sampling frequency.

Figure 10-18 Subtract two chromatograms



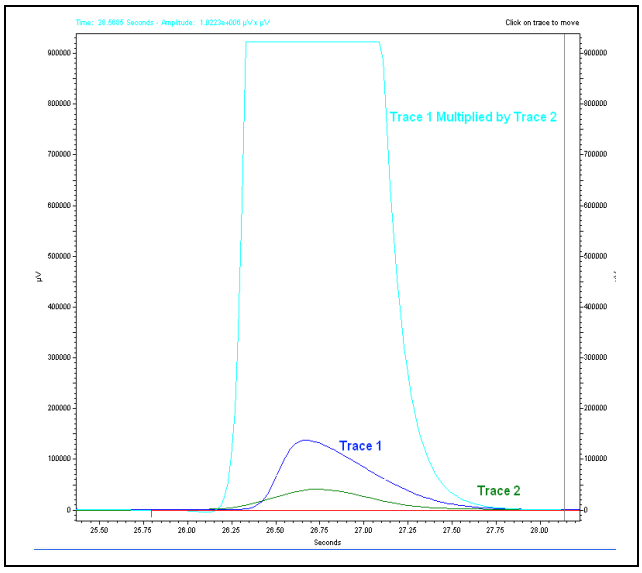
10.2.5 Multiply Two Traces

To multiply two traces:

1. In the chromatogram window, right-click and select **Operation >> Multiply**.
2. Click the first trace to select it.
3. Click the second trace, which will be multiplied by the first trace. The resulting trace will display in the chromatogram window.

NOTE: For the multiply operation, the units of the resultant trace are <chromatogram 1 units> x <chromatogram 2 units>. (See Figure 10-19.)

Figure 10-19 Multiply two chromatograms



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10.3 Utilities

The **Utilities** menu in the chromatogram window provides access to commands for saving, copying, or printing the current chromatogram window. To access the **Utilities** menu, right-click in the chromatogram window and select **Utilities**. (See Figure 10-20 and Table 10-2.)

Figure 10-20 Utilities

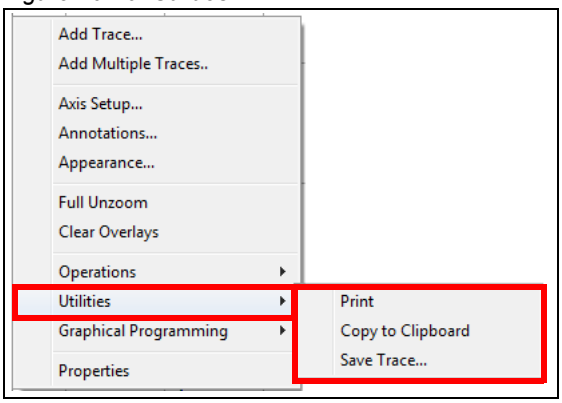

Table 10-2 Utilities

Utility	Action
Print	Sends the current chromatogram view to the printer
Copy to Clipboard	Copies the contents of the chromatogram window to the clipboard
Save Trace...	Prompts to click a trace then opens the save data file window

10.3.1 Print

To print a trace, right-click and select **Utilities >> Print**. (See Figure 10-20.)

10.3.2 Copy to Clipboard

To copy the contents of the chromatogram window to the clipboard, right-click and select **Utilities >> Copy to Clipboard**. (See Figure 10-20.)

This command copies the current chromatogram window to the clipboard as a metafile. The chromatogram can then be pasted into a word processing document or other application that supports the clipboard.

NOTE: To paste into Microsoft® Word, click **Edit >> Paste >> Special >> Picture**.

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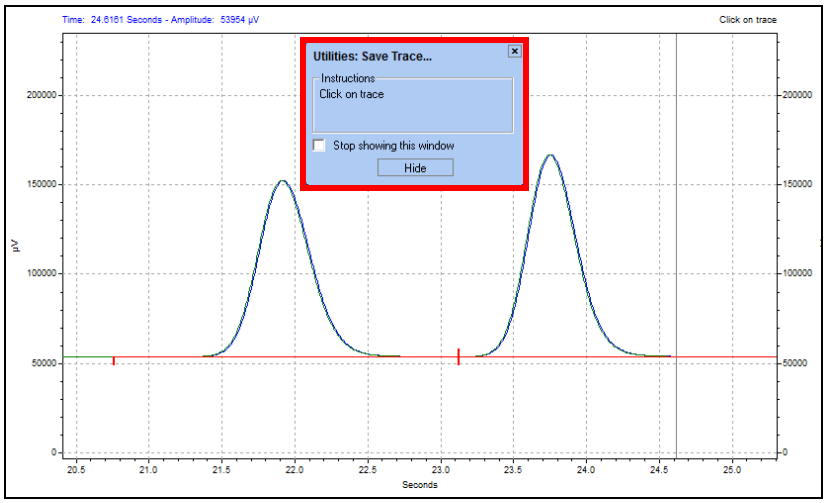
10.3.3 Save Trace

Use this utility to save a trace as a data file.

1 In the chromatogram window, select **Utilities >> Save Trace**. The **Utilities: Save trace...** window will display. (See Figure 10-21.)

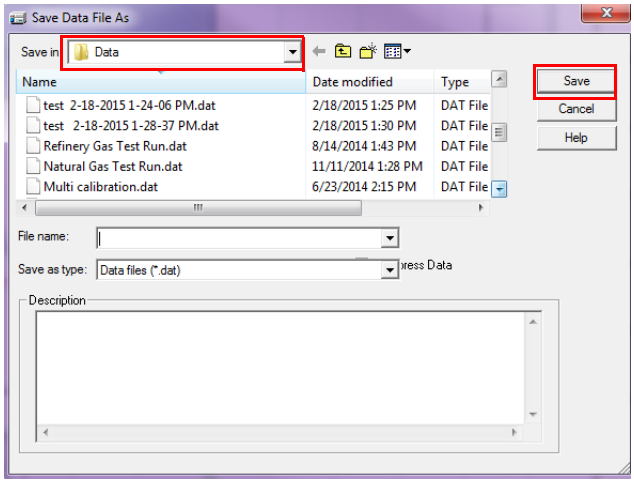
Figure 10-21 Save trace



2 Click the trace to select it.

3 In the **Save Data File As** window, browse to the desired location and enter a name for the file to be saved. (See Figure 10-22.) Click **Save**.

Figure 10-22 Save Data File As window



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Chapter 11
Graphical Programming

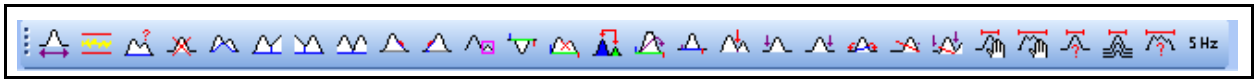
11.1 About Graphical Programming

The **Graphical Programming** menu is used to add timed integration events and set up other method parameters graphically by clicking on the displayed chromatogram. These commands are also available from the Graphical Programming Toolbar, which is displayed by default at the bottom of the Instrument Window. (See Figure 11-1 and Table 11-1.)

To turn on the Graphical Programming Toolbar

1. Click **View >> Preferences**.
2. Click **Int Events** and then click **Show toolbar**.

Figure 11-1 Graphical Programming toolbar



Parameters that can be set using graphical programming include:

Table 11-1 Graphical Programming parameters

Parameter	Icon	Action
Width		Insert a **Width** event at a point on the chromatogram
Threshold		Insert a **Threshold** event at a point on the chromatogram
Shoulder Sensitivity		Insert a **Shoulder Sensitivity** event at a point on the chromatogram
Integration Off		Turn off integration at a point on the chromatogram
Valley to Valley		Turn on **Valley to Valley** baseline detection
Horizontal Baseline		Force a **Horizontal Baseline** from a point on the chromatogram
Backward Horizontal Baseline		Force a **Backward Horizontal Baseline** from a point on the chromatogram
Lowest Point Horizontal Baseline		Force a horizontal baseline at the next lowest point
Tangent Skim		Force a **Tangent Skim**

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Table 11-1 Graphical Programming parameters (continued)

Parameter	Icon	Action
Front Tangent Skim		Force a **Front Tangent Skim**
Minimum Area		Set a **Minimum Area** for peak detection
Negative Peak		Turn on **Negative Peak** detection
Disable Peak End Detection		Disable the end of peak detection
Reassign Peak		Designate a different peak as the calibrated peak
Manual Baseline		Manually define a baseline
Manual Peak		Manually define the beginning and end of a peak
Split Peak		Force a perpendicular to split a peak
Force Peak Start		Force the start of a peak
Force Peak Stop		Force the end of a peak
Move Baseline		Manually move a baseline
Reset Baseline		Force a baseline to the point
Reset Baseline at Valley		Reset the baseline to the next valley
Adjust Retention Time Window		Adjust the retention time window
Adjust Group Range		Adjust the group range
Define Single Peak		Define a single peak and add it to the peak calibration table
Define Peaks		Define multiple peaks and add them to the peak calibration table
Define Groups		Define groups and add them to the group calibration table
Suggest Sampling Frequency		Suggest a sampling frequency for the chromatogram

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Chapter 12
Data Acquisition and Control

12.1 Data Acquisition and Control

Commands that are available from the **Control** menu are related to data acquisition and control of the instrument. In general, there are two ways to acquire data:

- Single run acquisition, where data is acquired for a single injection
- Sequence acquisition, where data is acquired automatically for a series of runs using a pre-programmed sequence that defines the number of injections, methods, file names, and calibration

Additional control menu items will appear depending on the features supported by the instrument configured.

12.2 Single Run Acquisition

1 To make a single run, click the **Single Run** icon or click **Control >> Single Run**. The **Single Run Acquisition** window will display. (See Figure 12-1 and Table 12-1.)

Figure 12-1 Single Run Acquisition window

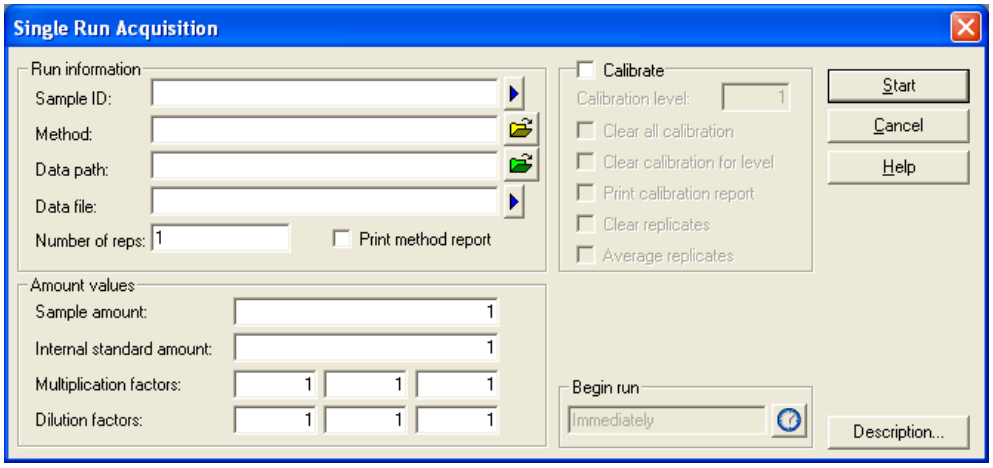

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Table 12-1 Single Run Acquisition parameters

Navigation Function Bar	Displays
Run information	Used to specify various files for the run
Sample ID	Type a **Sample ID** for the run. This can contain text and numbers, and is saved with the data file. Click the arrow to select from a number of predefined IDs
Method	Select the **Method** from a list of available methods by clicking the file icon adjacent to the field
Data path	Type a **Data path** name where the data acquired for this run will be stored. Click the file icon to select an available path
Data file	Type a **Data file** name for the data to be saved on disk. Click the arrow to select from a number of predefined names. It is not possible to use an existing filename, unless the file exists in located in a directory whose path contains the term “public”. For example, if the data files are saved in a directory entitled **C:\Public\Data**, the files saved in this directory can be overwritten. The software automatically appends a **.dat** file extension
Number of reps	Type the number of runs to conduct. The runs will automatically proceed without review until completed, incrementing each filename if designated in the **Data file** field. If the sequence of single runs is aborted, and the single acquisition is repeated without changing any parameter, the run number will start with the next number as if the sequence was not aborted. For example, if setting 4 runs with starting run number of 101, then aborting during run 102, upon restarting the next run number will be 103. If the **Sample ID** is also incremented, it will increment in parallel
Print Method Report	When this box is selected, the method report (or reports) will be printed at the end of the run

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Table 12-1 Single Run Acquisition parameters (continued)

Navigation Function Bar	Displays
Amount Values	**NOTE:** When making a single data acquisition prior to calibrating the method, leave these values at their default
Sample amount	The **Sample amount** value is used as a divisor during calculation of concentrations. It is intended to compensate for differences between samples due to weight and when percentages of the total sample are being calculated rather than the amount detected in an injection
Internal standard amount	For calibration runs, the **Internal standard amount** is acquired from the method Peak Table. For unknown runs, enter the amount of the Internal Standard in an unknown sample
Multiplication factors	Enter one to three multiplication factors to be used for this run. All quantitated peaks will be multiplied by these factors
Dilution factors	Enter one to three dilution factors to be used for this run. All quantitated peaks will be divided by these factors
Calibrate	Select this box if the sample is a calibration sample. Once this box is selected, the following fields and options will be available
Calibration level	Type the number of the calibration level represented by the calibration standard. If this is a single level calibration, type 1
Clear all calibration	Select this box to clear all existing calibration information from the method before running the sample
Clear calibration for level	Select this box to clear the existing calibration information for a specific level before running the sample
Print calibration report	Select this box to print a calibration report after running the sample
Clear replicates	Select this box to clear all existing replicates from the existing calibration level before running the sample
Average replicates	Select this box to average the replicates for this calibration level

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Table 12-1 Single Run Acquisition parameters (continued)

Navigation Function Bar	Displays
Begin run	By default, a run will start immediately. Click  to open the **Schedule Run** window to enter or select the time to start the sequence When the **Single Acquisition Run** window is completed, click **Start** to begin the acquisition. The current data will appear in the chromatogram window as it is acquired and will be stored on disk. At the end of the run, the chromatogram will be analyzed according to the method parameters, and, if specified, a report will be generated. If the sample analysis is not displayed at the end of the acquisition, click **Analysis >> Analyze** to view the results

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12.3 Run a Sequence

Once a sequence has been created and saved, it can be used to acquire and process data. To start a sequence acquisition:

1 From the Instrument Window, click the **Sequence Run** icon . Alternately, click **Control >> Sequence Run...**. The **Run Sequence** window will display. (See Figure 12-2 and Table 12-2.)

2 Type or select a sequence to use, set a run range, mode, printing options and review options, then click **Start**.

Figure 12-2 Run Sequence window

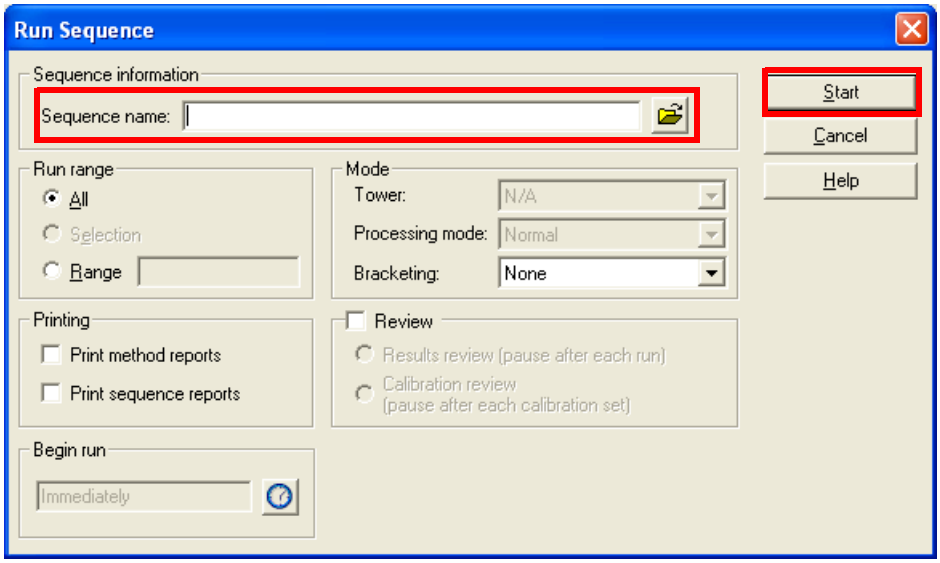

Table 12-2 Run Sequence parameters

Parameter	Description
Sequence information	Type the **Sequence name** to be used, or select the sequence file from a list of available sequence files by clicking the file icon
Run range	Select the range of the sequence to be run
All	Click **All** to execute all runs in the sequence
Selection	If a series of runs in the sequence spreadsheet has been selected (highlighted), click **Selection** to run only the highlighted runs
Range	Enter a range of runs to be executed. For example, an entry of 4 - 6 will execute runs 4, 5, and 6 of the sequence. An entry of 4 executes the fourth run through to the end of the sequence

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Table 12-2 Run Sequence parameters (continued)

Parameter	Description
Mode	Select the manner by which to handle autosampler dual towers (if any), processing mode, and bracketed calibration (if used)
Tower	If the instrument is configured for Dual Tower, select the tower mode to be used for the sequence run. Selections include **Dual**, **Front**, and **Rear**
Processing mode	Select a mode for reprocessing the data. Options will vary depending on the instrument configuration. If the instrument does not support this feature, **Processing mode** will be grayed out. For certain instruments, **Overlap Sample Prep** mode will be available. See **About Overlap Sample Prep** for information and restrictions for using this mode
Bracketing	Select the type of bracketing to perform (See **Bracketed Calibrations** for details.)
None	Select to NOT bracket calibrations
Standard	Select to perform the standard mode of bracketing calibrations
Std. w/Clear Calib	Select to perform the standard mode of bracketing calibrations, clearing the calibration before the start of each calibration set
Sequence	Select to perform the sequence mode of bracketing calibrations
Seq. w/ Back Calc	Select to perform the sequence mode of bracketing calibrations and back-calculate calibration runs
Review	
Results review	Select this box to pause the sequence between runs to review results
Calibration review	Select this box to pause the sequence after each calibration set, where a calibration set is defined as one or more calibration runs that occur in a sequence

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Table 12-2 Run Sequence parameters (continued)

Parameter	Description
Printing	
Print method reports	Select this box to print a custom report, defined in the method, for each run of the sequence
Print sequence reports	Select this box to print sequence reports
Begin run	**NOTE:** By default, a run will start immediately. To schedule the start of the sequence for a later time or date, click the  icon to open the **Schedule Run** window to enter or select the time to start the sequence

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12.4 Stop a Run in Progress

To stop data acquisition during a run:

1. Click the icon, on the command toolbar, when the run is in progress. Alternately, click **Control >> Stop Run**. The **Stop Run** window will display. (See Figure 12-3 and Table 12-3.)
2. Select the desired manner to stop the run.

Figure 12-3 Stop Run window

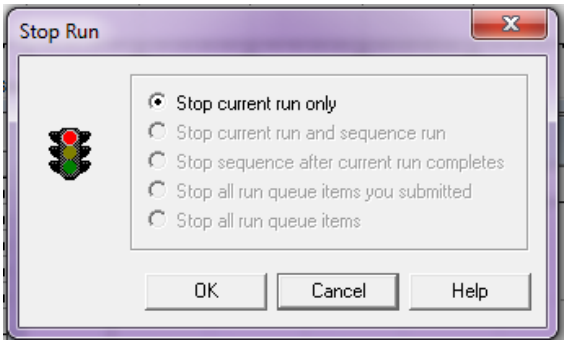

Table 12-3 Stop Run parameters

Parameter	Description
Stop current run only	Select this to end the run currently in progress. If the run is a part of a currently queued sequence, the sequence will continue with the next run
Stop current run and sequence run	Stops the run currently in progress, and terminates its sequence. Other queued items will proceed
Stop sequence after current run completes	Aborts the sequence after the current run is completed
Stop all run queue items you submitted	Stops the run currently in progress, and terminates all the items in the queue that were submitted by the current user. Queue items submitted by other users will be unaffected
Stop all run queue items	This selection stops the run currently in progress, and terminates all items in the run queue

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Chapter 13
Tutorial

This chapter guides the user through the basics of using EZ IQ. Follow the steps to set up a method and acquire a data file, then optimize the method for integration and set up calibration. Use the Tutorial files provided with the software to learn the software and become comfortable with its use. Details on data file structure, application window features, how to open and save files are located in Chapter 5, Method and Data File Structure, and Chapter 6, Opening and Saving Files.

NOTE: This tutorial assumes:

- That EZ IQ is installed on the computer. Refer to section 2.2, Install EZ IQ, on page 2-2
- The computer running EZ IQ is connected to Micro GC Fusion instrument via the TCP/IP connection
- EZ IQ is configured for Micro GC Fusion. Refer to section 2.4, Install EZ IQ Driver for Micro GC Fusion, on page 2-8

13.1 Tutorial Overview

The following is a quick overview of the tutorial contents. For best results, follow all steps in the Tutorial, in the order presented.

1 Create a Data Acquisition Method
- Set up acquisition run time and sampling rate
- Save the method
- Run a preliminary sample
- Set integration parameters graphically

2 Create a Single Level Calibration
- Name calibrated peaks
- Run a single level calibration

3 Create and Run a Sample Sequence

4 Using Tutorial Files
- Review a multi-level calibration
- Explore a peak table
- Examine a custom report
- Change integration parameters

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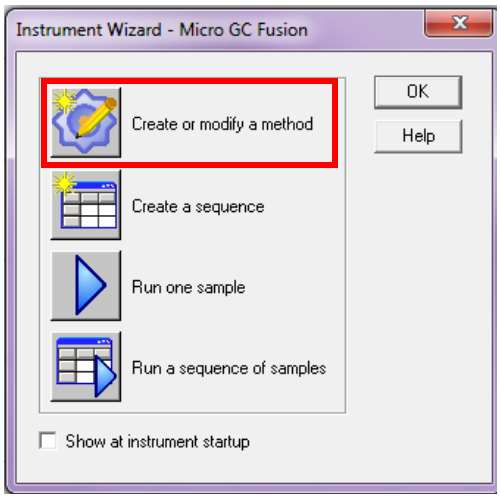
13.2 Instrument and Method Wizards

The **Instrument Wizard** and **Method Wizard** make it easy to locate and step through the windows necessary to create or modify methods. To create Tutorial methods, use the wizard buttons to display the window associated with a Tutorial step.

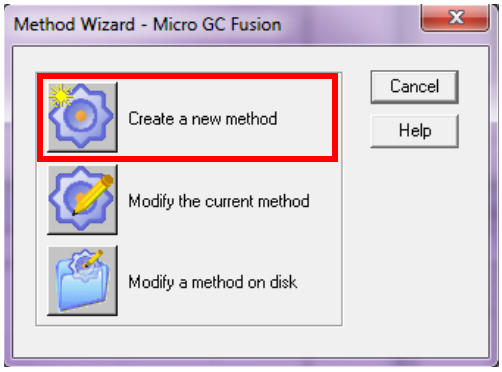
1 When EZ IQ is opened, the Instrument Wizard will display. Click **Create or Modify a Method** to start the **Method Wizard**. (See Figure 13-1.)

Figure 13-1 Instrument Wizard



2 The **Method Window** will display. Click **Create a New Method** to create the tutorial method. (See Figure 13-2.)

Figure 13-2 Method Wizard



When **Create a New Method** is selected, the **Method Wizard** sets up icons in the application window that allow the user to step through all windows of method generation. A **Save** icon is also provided. (See Figure 13-3.)

Figure 13-3 Step and Save icons

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13.3 Create a Data Acquisition Method

The first step toward acquiring a data file is to create a data acquisition method. Ensure that the method has a long enough run time for the last peak to elute, using the default data acquisition sampling rate.

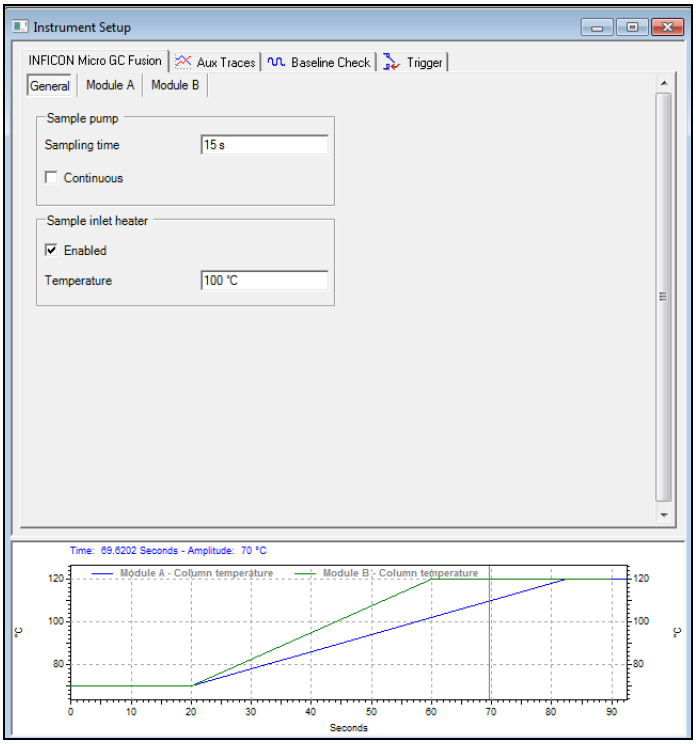
NOTE: Skip this step and use data and method files provided if there is no access to an instrument.

13.3.1 Instrument Setup

After clicking **Create a new method** from the **Method Wizard**, the **Instrument Setup** window will display. Alternately, click **Method >> Instrument Setup.** (See Figure 13-4.)

Edit acquisition parameters in the **General** and **Module** tabs. Refer to section 8.1, Method Acquisition Parameters, on page 8-1.

Figure 13-4 Instrument Setup window



Select the **Trigger** tab and select the **Type** for the type of remote start (if any) installed on the instrument. The trigger type for each instrument is set up during configuration. If no trigger is being used, select **None** for **Type**. (See Figure 13-5 and Table 13-1.)

Figure 13-5 Trigger tab

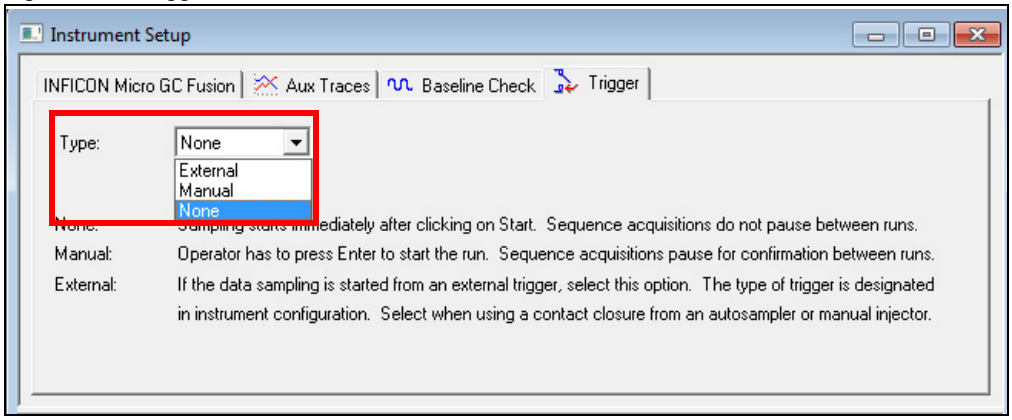


Table 13-1 Trigger tab parameters

Navigation Function Bar	Displays
External	Data sampling starts when externally triggered
Manual	User must start the data sampling
None	Sampling of data starts immediately when **Start** is clicked

When the acquisition setup information is complete, close the window.

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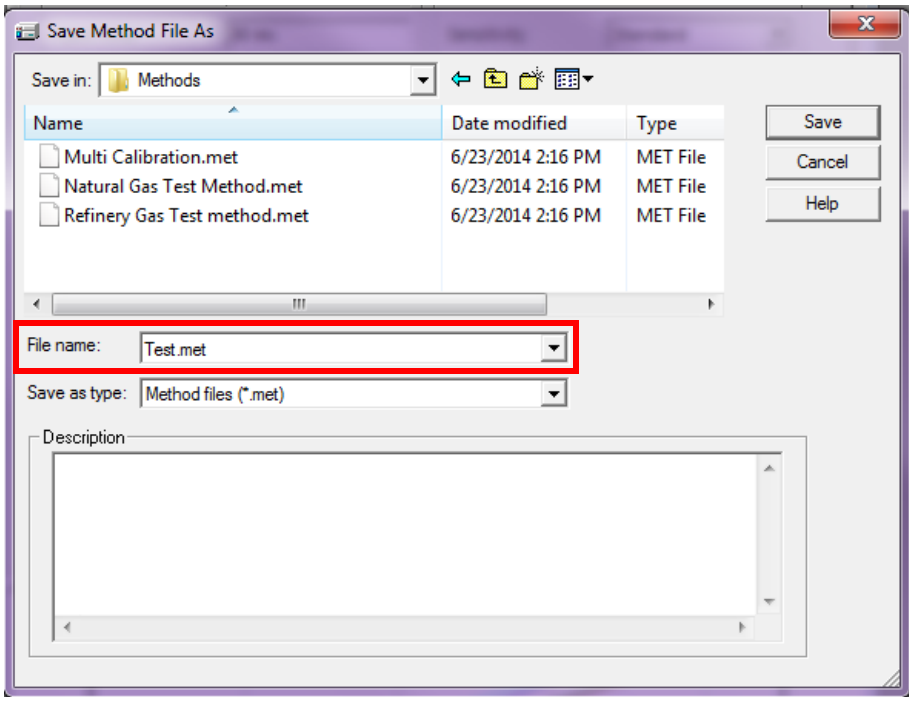
13.3.2 Save the Method

1 Once the acquisition parameters are set, save the method. Click **File >> Method >> Save As…**. The **Save Method File As** window will display. (See Figure 13-6.)

Figure 13-6 Save Method File As window



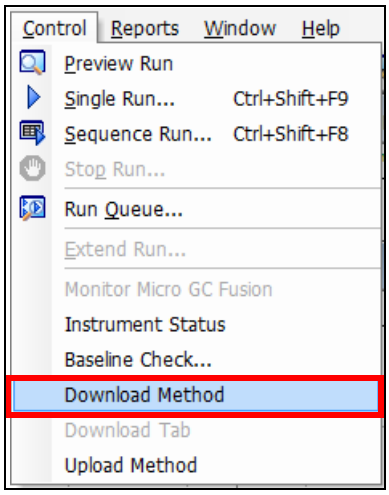
2 Select a desired folder to save the method file. In the **File name** field, enter **Test.met** as the filename. Click **Save**.

13.3.3 Downloading a Method

When a new method is created, or when a method is opened, it must be downloaded to Micro GC Fusion to make it available on the instrument.

Click **Control >> Download Method**. (See Figure 13-7.)

Figure 13-7 Download Method



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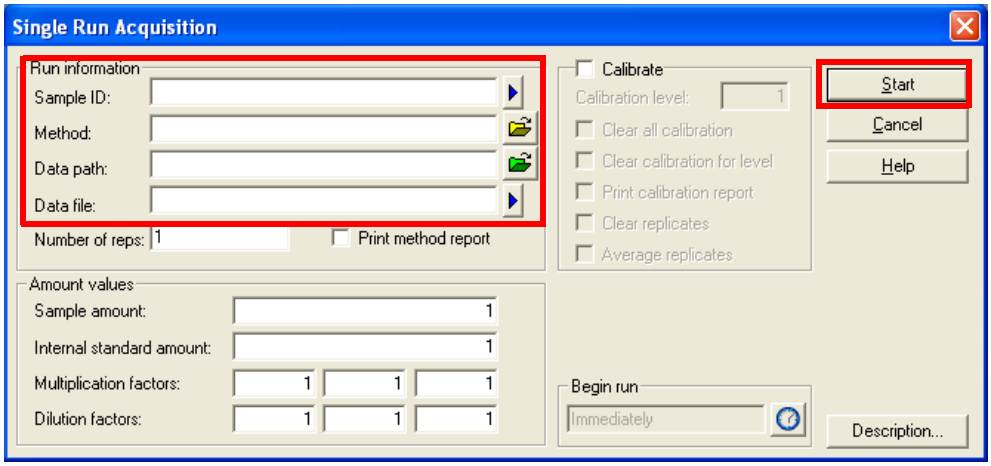
13.3.4 Run a Preliminary Sample

The data acquisition method (**Test.met**) will be used to make the first data acquisition run. To aid in later steps of the tutorial, run a calibration gas sample for the first acquisition run.

1 Click **Control >> Single Run**. (See Figure 13-7.) The **Single Run Acquisition** window will display. (See Figure 13-8.)

Figure 13-8 Single Run Acquisition window



2 Type **Test** in the **Sample ID** field.

3 In the **Method** field, select the **Test.met** file from a file list by clicking the file icon adjacent to the field.

4 Enter a path for storage of data files in the **Data path** field, or select a path from a list presented by clicking the file icon adjacent to the field.

5 Enter **Test.dat** as the name for storing data in the **Data file** field. A unique file name must be entered in this field. If this tutorial has been performed previously, any saved files will need to be deleted or moved to a different directory.

6 Click **Start** and inject the standard sample. As it is acquired, data will be displayed in the chromatogram window.

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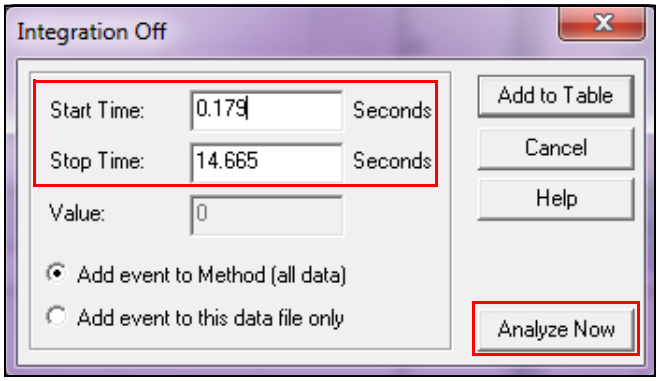
13.3.5 Set Integration Parameters Graphically

EZ IQ uses default integration parameters that are appropriate for most simple chromatography. However, certain peaks may require special integration treatment. Such special integration treatments are entered into the method as **Integration Events**. These events can be placed at the beginning of the run to apply to all peaks, or they can be inserted at a certain place in the chromatogram such that only some peaks are affected. Follow the steps below to add the timed event to turn off integration to the method.

NOTE: This step can be performed using a stock data file provided with the software.

1. At this point, the recently acquired chromatogram will be displayed in the chromatogram window. If it is not, click **File** >> **Data** >> **Open...** and then select the data file from the list displayed.
2. Click **Analysis >> Analyze** to integrate the chromatogram and display the baselines.
3. To add the **Integration Off** timed event, click the **Int Off** button on the **Int. Event** Toolbar. Click a part of the chromatogram to turn integration off at that point. This is the **Start Time**. Click the chromatogram again at the point where integration will be turned on again. This is the **Stop Time**. An **Integration Off** window will display. (See Figure 13-9.)

Figure 13-9 Example Integration Off



4. The integration will be turned off between the **Start Time** and the **Stop Time**. The **Value** is set at zero, as no numeric value is required for this event.
5. Select **Add event to Method (all data)** to add event to the **Integration Events** table (where it will be used on all chromatograms analyzed using this method). To view the table, click **Method >> Integration Events**. (See Figure 13-9.)

   NOTE: Select **Add event to this data file only** to add the event to the **Manual Integration Fixes** table of the present chromatogram (where it will be applied only to this chromatogram). (See Figure 13-9.)

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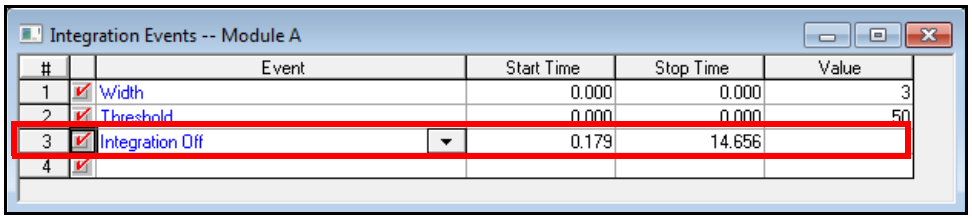
6 Click **Analyze Now** to add the event to the method and re-integrate the chromatogram. (See Figure 13-9.)

NOTE: Click **Add to Table** to add the event to the integration timed events table without re-integration.

The chromatogram will be re-drawn using the new integration event. Note that the selected area (between that **Start Time** and **Stop Time**) has no baselines drawn because the integration has been turned off for these peaks.

7 To remove the **Integration Off** event from the method, click **Method >> Integration Events**. Click the **Integration Off** event name or the row number, then press the **Delete** key on the keyboard. The event can also be deleted using the **Edit >> Cut** command. The event can be re-inserted using the **Edit >> Paste** command. To temporarily view the effect of removing an event without actually removing it from the table, select the check box adjacent to the event to clear it. To re-select the event, select the check box once again. (See Figure 13-10.)

Figure 13-10 Integration Events



8 When finished with the **Integration Events** table, close the window to return to the chromatogram.

13.3.6 Create a Calibration

For peak quantitation (calculation of results based on the running of standards), the method for must be calibrated. For further details on how to set up multiple level calibrations, refer to **Calibration** in the embedded help file by clicking **Help >> Contents**. For this tutorial, the user will set up a single level calibration.

NOTE: Pressing F1 in the EZ IQ software window will trigger the online help file.

Calibration involves the following steps.

- Identify the calibrated peaks and enter known standard amounts in the method
- Run the standard sample(s)
- Review the calibration curve

The easiest way to enter calibration peak data is to run the calibration gas sample first, then use the stored data file to graphically define the calibration peaks. If the user has been following this tutorial, there should already be a calibration gas sample saved. If not, the user can either run a calibration gas sample using the steps shown in section 13.3.4, Run a Preliminary Sample, on page 13-7, or the user may select one of the data files provided.

1. Open the stored data file by clicking **File >> Data >> Open...** Select the calibration gas sample data file from the list, or select one of the supplied data files. Once the file is displayed in the current data chromatogram window, click **Analyze** to integrate the chromatogram and show the baselines.
2. Click the **Define Single Peak** button from the **Int Event** toolbar. The **Define Single Peak** window will display for the first detected peak in the chromatogram. (See Figure 13-11 and Table 13-2.)

Figure 13-11 Example Define Single Peak window

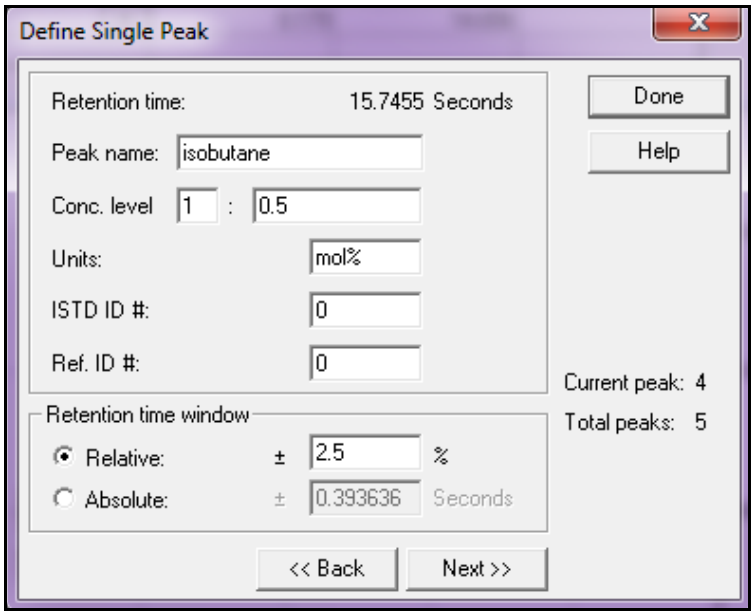


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Table 13-2 Define Single Peak Window Parameters

Parameter	Description
Retention time	The retention time of the first detected peak will display. To add this peak to the peak table, populate the window for this peak. To skip this peak, click **Next**. To move to a specific peak in the chromatogram, click the specific peak. The retention time shown in the window will change to reflect the selected peak
Peak name	Type the name of the compound in this field
Conc level	Concentration Level 1 is shown. Enter the concentration of this component in the field to the right of the **Conc. Level** **NOTE:** The concentrations of calibration gas components are normally provided by the gas supplier on the label attached to the gas cylinder. **NOTE:** For setting up more than one level for this compound, enter 2 for the **Conc. Level** and enter the concentration for that level. Continue to enter concentration levels until all desired number of calibration levels are completed.
Units	Enter the units to be used when displaying the results
ISTD ID #	If performing an internal standard calibration, enter the ID # for the internal standard peak for this compound. This is the peak ID number from the peak table. If the **ISTD ID #** is unknown, it can be added in the peak table later
Ref ID #	The **Ref ID #** corresponds to the peak ID # in the peak table. Enter the peak ID # in the **Ref ID #** field. If the peak ID # is unknown, it can be added in the peak table later. Reference peaks are used to locate calibrated peaks when chromatographic conditions change such that retention times shift

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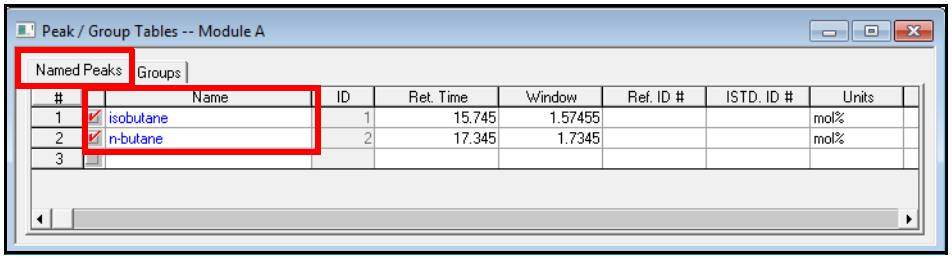
Table 13-2 Define Single Peak Window Parameters (continued)

Parameter	Description
Retention time window	Select the parameter to enter the retention time window for this peak. The window is used for peak identification in case of slight deviations from the expected retention time
Relative	Click **Relative** to calculate the retention time window based on a % of the expected retention time of the peak. Enter the % to use to calculate the retention time window
Absolute	Click **Absolute** to enter an absolute retention time window for the peak. Enter the value for the retention time, in minutes

3 Click **Next** to move to the next detected peak. Click **Back** to move to the previous detected peak in the chromatogram. The current peak and total peaks in the chromatogram are displayed on the right of the window. When finished adding peaks to the peak table, click **Done**. Each defined peak will become a row in the peak table. If peaks are already in the peak table, the recently defined peaks will be added to those already present.

4 Once peaks have been defined, click **Method >> Peaks/Groups...**. The **Peak/Group Tables** window will display. (See Figure 13-12.) Select the **Named Peaks** tab. Each peak defined will appear as a row in the peak table spreadsheet, along with its retention time and the other parameters entered.

Figure 13-12 Peak/Group Tables - Module A



Information in the table can be edited or changed by scrolling through the rows and columns. Details on contents of the peak table are described in the **Calibration** chapter of the online help file.

5 Do not enter information in the other columns at this time. Close the **Peak/Group Tables**.

The method is now ready to be calibrated. Before calibrating, save the method. Click **File >> Method >> Save**. (To save the method using a different name, click **File >> Method >> Save As**.)

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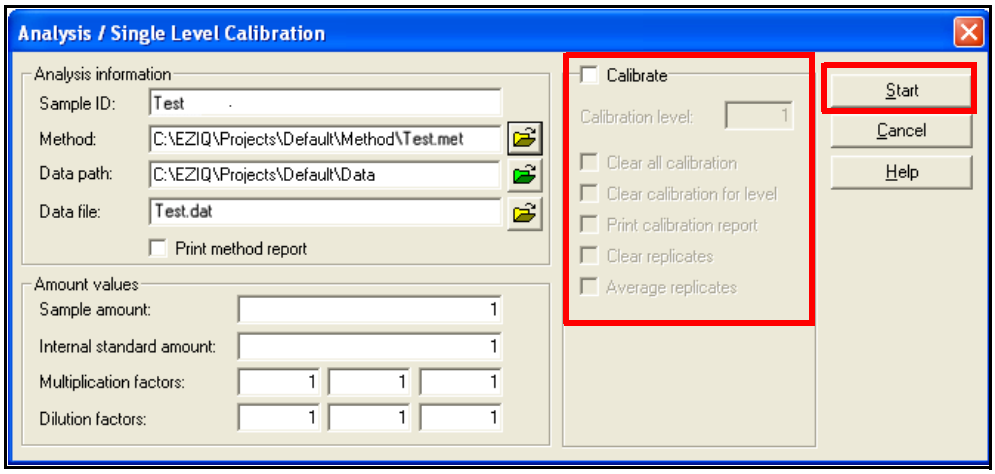
13.3.7 Calibrate Using a Stored Data File

In order for the software to calculate concentrations for unknown samples, the method must contain the peak areas generated for each component in the calibration gas sample. To store these areas into the method, either run the calibration gas sample again, designated as a calibration run, or calibrate the method using the stored data file created earlier in this tutorial.

To use the stored data file to calibrate the method:

1. Click **Analysis >> Analysis Single Level Calibration**. An **Analysis/Single Level Calibration** window will display. (See Figure 13-13.)
2. In the **Sample ID** field, enter sample identification information, if not present. If following this tutorial, enter **Test**.

Figure 13-13 Analysis/Single Level Calibration window



3. In the **Method** field, click the file icon and select the method file from the list. The tutorial method is **Test.met**.
4. In the **Data path** field, type the data path name, or select it from the list using the file icon.
5. Type the name of the calibration data file in the **Data file** field. Click the file icon and select a saved filename.

   NOTE: The name used in this tutorial is **Test.dat**.
6. Leave the **Amount values** set to **1**. For details on how these values are used, refer to the **Calibration** chapter in the online help file.
7. Select the **Calibrate** box.
8. Type **1** for **Calibration level**. Since this method is currently uncalibrated, it is unnecessary to select any of the check boxes dealing with calibrations or replicates. However, if unsure of the method contents, select **Clear all calibration** before starting.

9 Click **Start**. When the analysis is complete, the chromatogram will be integrated, and the areas for the peaks identified as calibration compounds will be entered into the method. Enter the concentration of the calibration gas into corresponding Level field in the **Peak / Group Tables** if not already populated.The calibration curves will be generated using these areas. At this point, the method is calibrated for a single level, and it can now be used to run and analyze samples with the calibration compounds in unknown amounts.

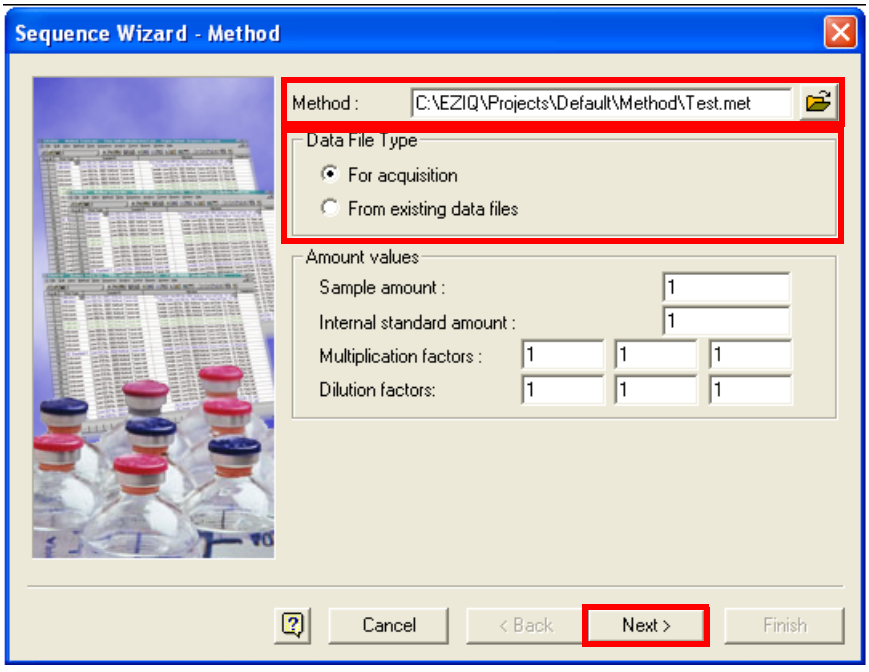
13.3.8 Create and Run a Sample Sequence

If using an automatic stream selection valve to inject samples, the user must define the samples to be injected and how they will be acquired and analyzed. This is performed using a sample **Sequence**. A sample sequence can be used to acquire both calibration and unknown samples. It can also be used to automatically re-analyze stored data files. Details on creating and using a sequence can be found in the **Sequence** chapter of the online help file. In this part of the tutorial a simple sequence will be created and used to acquire a calibration sample and two or three unknown samples.

NOTE: The procedure related to stream selection valve described in this section is applicable when the stream selection valve is connected to the EZ IQ computer.

1 Click **File >> Sequence >> Sequence Wizard**. A **Sequence Wizard** window will display. (See Figure 13-14.)

Figure 13-14 Sequence Wizard - Method window



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2 Select the **Method** to be used for the acquisition by clicking the file icon.If the user is following this Tutorial, select **Test.met** as the method name.

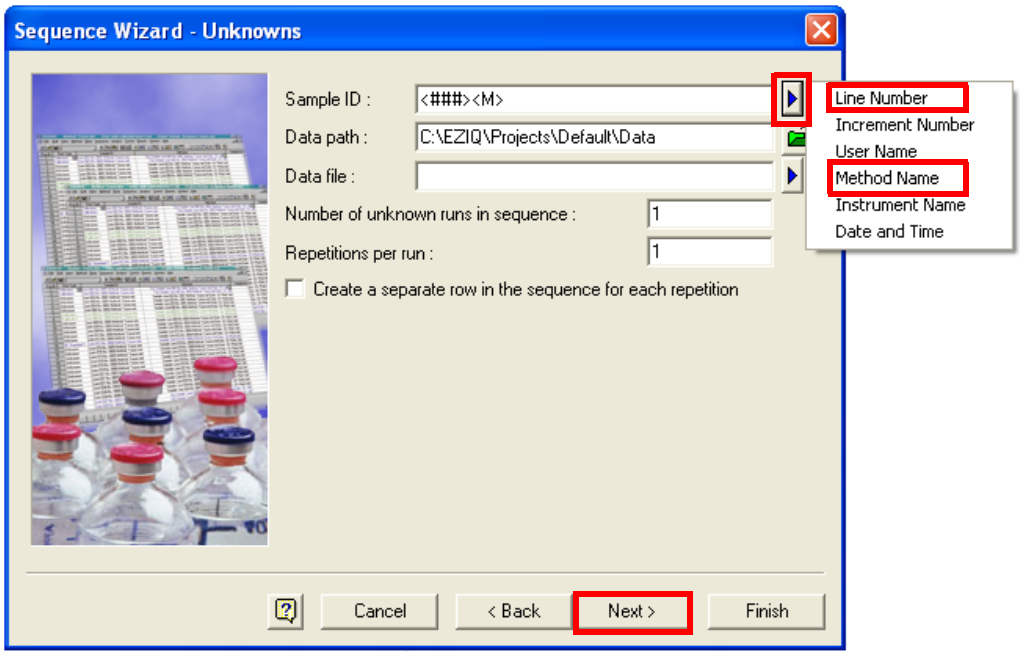
3 Select **For acquisition**.

4 Leave the **Amount values** at their default values.

5 Click **Next**. The **Sequence Wizard - Unknowns** window will display. (See Figure 13-15.)

6 The **Sample ID** field is used to identify the samples. Click the blue arrow and select **Line Number** and **Method Name**. Each **Sample ID** will contain the sequence line number and the current method name. (See Figure 13-15.)

Figure 13-15 Sequence Wizard - Unknowns window

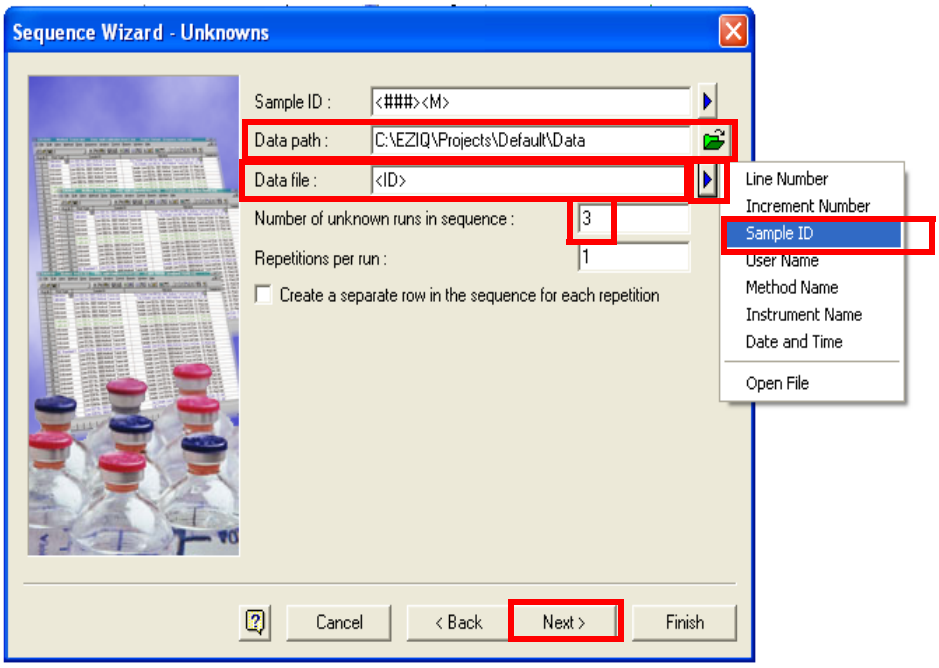


7 In the **Data path** field, type the path to where the data will be stored, or select an existing path by clicking the file icon. (See Figure 13-16.)

8 For **Data file**, click the blue arrow and select **Sample ID**. The data files will be named using the **Sample ID** selected above. Using numbered identification ensures the data filename for each run is unique, preventing errors that will occur when trying to acquire data using an existing data filename. (See Figure 13-16.)

9 For **Number of unknown runs in sequence,** enter **3**. Leave the other fields with their default values. (See Figure 13-16.)

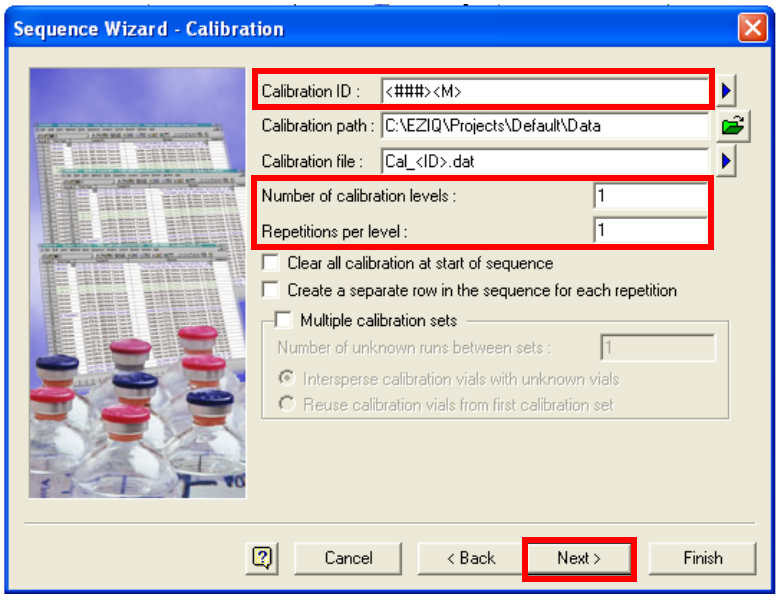
Figure 13-16 Sequence Wizard - Unknowns window



10 Click **Next** to continue. (See Figure 13-16.) The **Sequence Wizard - Calibration** window will display. (See Figure 13-17.)

11 The **Calibration ID** is automatically set to the identification from the previous window. Set the **Number of calibration levels** to **1**, and leave the calibration **Repetitions per level** at **1**. Leave all other boxes cleared.

Figure 13-17 Sequence Wizard - Calibration window



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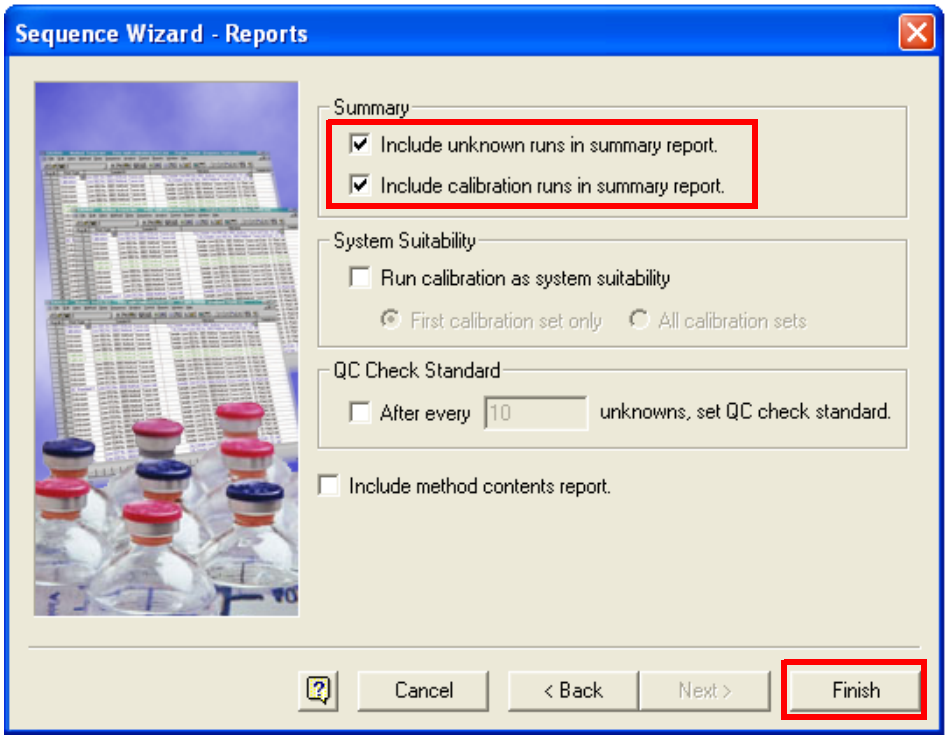
12 Click **Next**. (See Figure 13-17.) The **Sequence Wizard - Reports** window will display. (See Figure 13-18.)

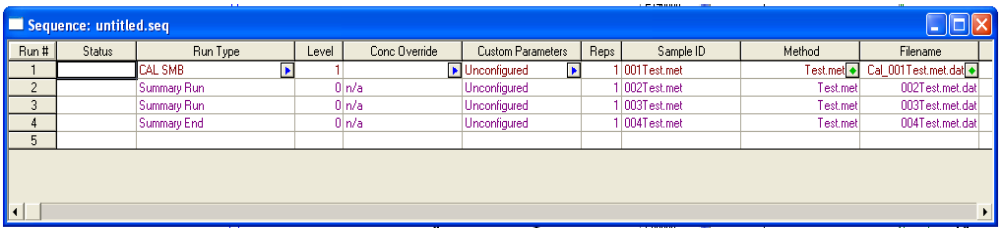
13 Select **Include unknown runs in summary report** and **Include calibration runs in summary report**. Do not select the other boxes. (See Figure 13-18.)

Figure 13-18 Sequence Wizard - Reports window



14 Click **Finish**. (See Figure 13-18.) A **Sequence:** table will appear, with the file and method names specified. (See Figure 13-19.)

Figure 13-19 Sequence table



15 At this point, the sequence is set up to run one calibration sample and three unknown runs. Notice the **Sample ID**s and **Filename**s are numbered automatically to prevent duplication. In order to run a calibration standard as the first run, the run must be designated as a calibration run. This was performed automatically by the **Sequence Wizard**. Unknown runs always have a **Level** of **0**. The information in the **Run Type** field may be abbreviated if there is more than one run type designation. To view the possible **Run Types**, click the arrow next to the run type. For details on each of these run types, refer to

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the **Sequence** chapter in the online help file. Since the method created in this Tutorial is a single level calibration, only one calibration standard run is necessary.

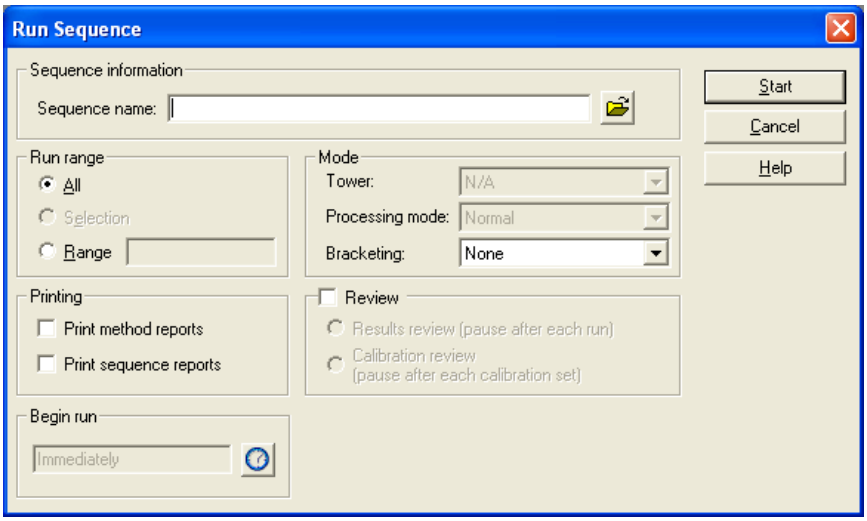
16 To save the sample sequence file, click **File >> Sequence >> Save As**. Select the **C:\EZIQ\Sequence** folder. Type the name **Test** or **Test.seq** for the sequence file name.

NOTE: By default, sequence files are saved with the **.seq** extension.

13.3.9 Run a Sequence

1 To acquire data using the sequence file just created, click **Control >> Sequence Run**, or right-click in the **Sequence** table and select **Run Sequence**. A **Run Sequence** window will display. (See Figure 13-20.)

Figure 13-20 Run Sequence window



2 Enter the name of the sequence file by typing the name, along with path, in the **Sequence name** field. Alternatively, select it from a list of sequence files by clicking the **Open File** icon to the right of the **Sequence name** field. Leave the other parameters as their defaults.

3 Prepare the automatic stream selection valve to inject a standard sample, followed by three unknown samples. When ready to inject the first sample, click **Start**. When the sequence is completed, data files are acquired and saved for one standard and three unknown runs, and a simple result report for each unknown sample and a summary report for the sequence are generated.

NOTE: Because a sequence summary report has not yet been defined, do not select the **Print sequence reports** box.

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13.4 Review Multi-level Calibration Curves

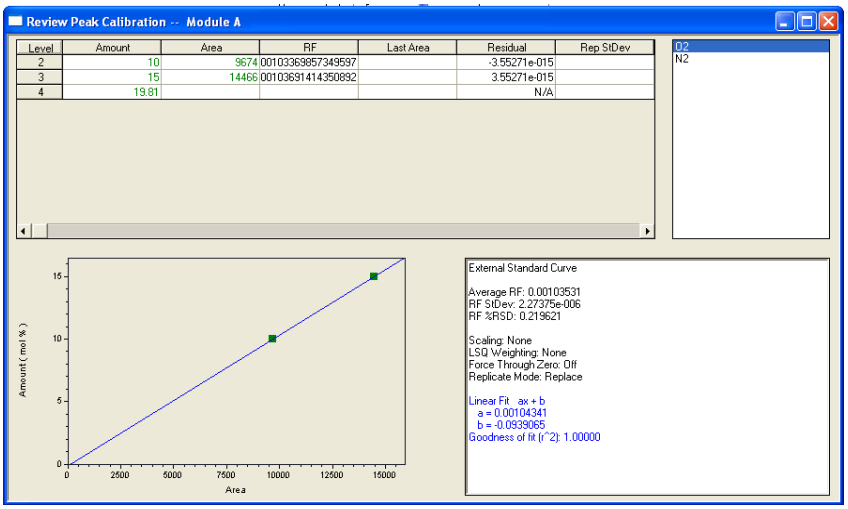
Once a method is calibrated, the calibration curves and associated data can be viewed using **Review Calibration**. To see a fully calibrated multilevel calibration, use the **Multi Calibration.met** file provided with the software.

NOTE: The **Multi Calibration.met** method file was developed with another instrument and will not work when downloading to the Micro GC Fusion. However, the steps outlined in this section remain valid.

1. Open the **Multi Calibration.met** method file by clicking **Open >> Open Method**. Select the **Multi Calibration.met** file. It will be located in the **\EZIQ\Projects\Default\Method** folder.

2. Click **Method >> Review Calibration**. The **Review Peak Calibration** window will display. (See Figure 13-21.)

Figure 13-21 Example Review Peak Calibration



The calibrated peaks in the method are listed in the peak list at the top right corner of the window. The calibration curve shown is for the highlighted peak. View the other curves by highlighting their peak name. The top left portion of the window contains a table that displays all the calibration information, including areas used to create the current calibration curve.

3. The calibration curve fit type by default is **Point-to-Point**. To overlay a different fit type, right-click anywhere in the white calibration curve box and select **Fit Type >> Linear**. The new linear calibration curve will overlay on the Point-to-Point curve. In the box at the right, the equations for the different fit types displayed are shown, along with the goodness of fit calculation.

   NOTE: The r^2 value is not calculated for the Point-to-Point curve since it is by definition a perfect fit to the data.

For additional details on using **Review Calibration**, refer to the **Calibration** chapter in the online help file.

13.5 Explore a Peak Table

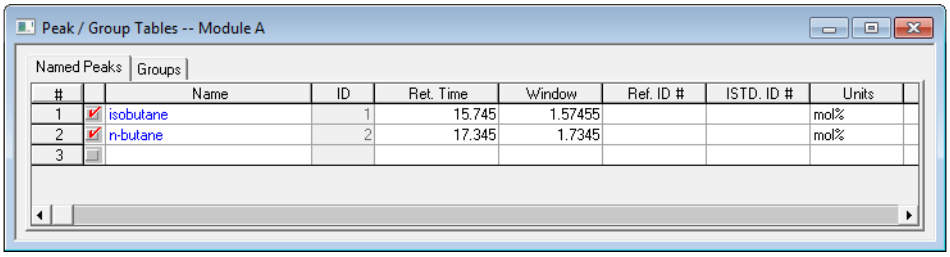
Method calibration information is located in the **Peak / Group Tables**. In this section, the user will use the method provided with the software to examine and become familiar with a completed peak table.

1 Open the **Multi Calibration.met** method which is located in **\EZIQ\Projects\Default\Method** by clicking **File** >> **Method**. Select the **Multi Calibration.met** method from the list.

NOTE: The **Multi Calibration.met** method file was developed with another instrument and will not work when downloading to the Micro GC Fusion. However, the steps outlined in this section remain valid.

2 Click **Method >> Peak/Groups**. The **Peak / Group Tables** window will display. (See Figure 13-22.)

Figure 13-22 Peak / Groups Tables - Module A



3 In the **Named Peaks** tab, a table containing all of the calibration information for the calibrated peaks in this method is displayed. By scrolling to the right, many different columns appear, each of which represent a parameter for the calibration, such as **Levels**, which contain the calibration amounts for each compound at each level of calibration. Note that it is possible to customize the peak table such that only parameters needed for a given calibration are displayed. Details on what each column represents, along with how to customize the peak table, are available in the **Calibration** chapter in the online help file.

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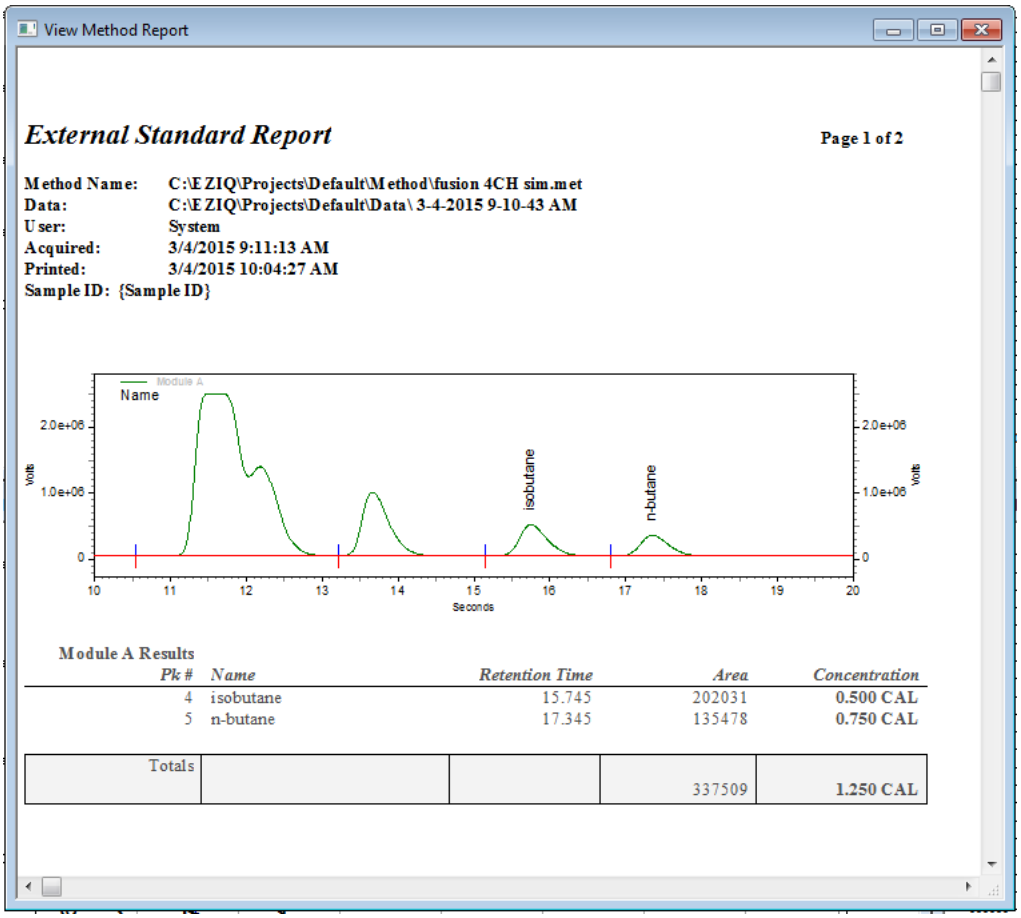
13.6 Examine a Custom Report

A variety of report templates are provided with the software that can be used without modification to generate reports.

To see an example of one of these reports

Click **Reports >> View >> External Standard**. (Make sure the current chromatogram has been analyzed first.) The **External Standard Report** will display. (See Figure 13-23.)

Figure 13-23 View Method Report window



If the method contains no defined custom report, the system will use the standard report formats to print reports.

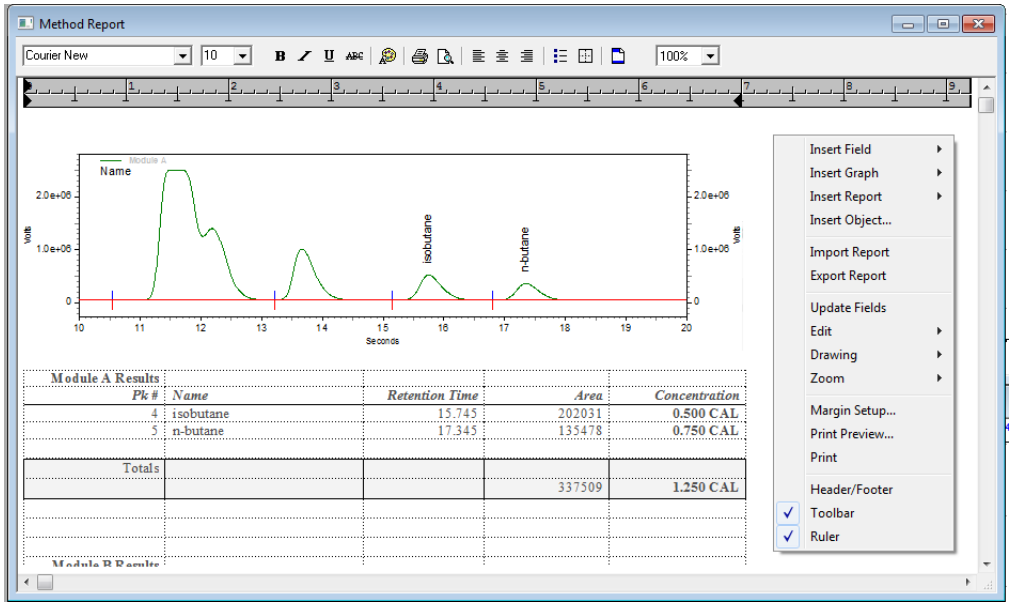
The standard report templates can be modified, or entirely new reports can be created using **Custom Report**. Both custom method reports and custom Sequence reports can be created. These are described in detail in the **Custom Reporting** chapter in the online help file.

To view the custom report in the **Multi Calibration.met** file

1 Click **File >> Method >> Open**, and select **Multi Calibration.met** from the file list, if not already open.

2 Click **Method >> Custom Report** to access the **Method Report** window. The current method custom report will display. (See Figure 13-24.)

Figure 13-24 Method Report window



3 Examine the custom report template by scrolling through it using the scroll bars. Before attempting to edit or create a custom report, thoroughly review **Custom Reporting** chapter in the online help file.

4 To return to the method, close the **Method Report** window.

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