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

EZ IQ™

3000 Micro GC Chromatography Software

IPN 074-537-P1A

INFICON

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EZ IQ

3000 Micro GC Chromatography Software

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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 information regarding:

- Technical Support, to contact an applications engineer with questions regarding INFICON products and applications, or
- Sales and Customer Service, to contact the INFICON Sales office, or
- Repair Service, to contact the INFICON Service Center

is available at www.inficon.com.

If you are experiencing a problem with your instrument or software, please have the following information readily available before contacting INFICON:

- the serial number for the instrument,
- a description of the problem,
- an explanation of any corrective action that was already attempted,
- and the exact wording of any error messages that may have been received.

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Chapter 2
Instrument Wizard

Each time an instrument application is initiated (by double-clicking the instrument icon from the Main window), an **Instrument Wizard** will appear. This wizard is designed to direct the user through the basic functions of the instrument window. See Figure 2-1.

Figure 2-1 Instrument Wizard

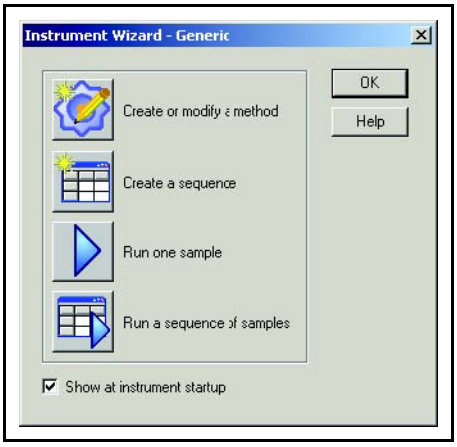

Table 2-1 Instrument Wizard Parameters

Create or modify a method	The **Method Wizard** steps the user through creating or modifying a method.
Create a sequence	The **Sequence Wizard** steps the user through creation of an acquisition or reprocessing sequence.
Run one sample	This button opens a window to use a stored method to run a single sample.
Run sequence of samples	The Run Sequence window starts 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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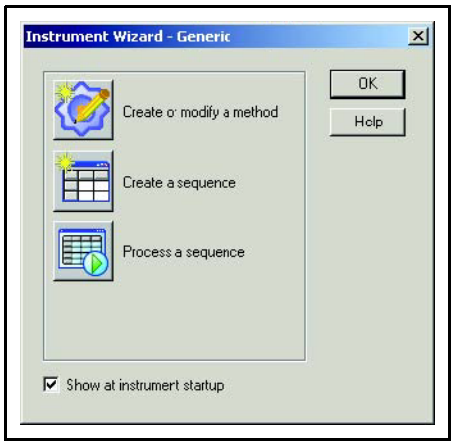
2.1 Offline Instrument Wizard

To use an instrument offline, open the EZ IQ Offline program. The **Instrument Wizard** will display the buttons shown in Figure 2-2 for creating methods, sequences, or processing a stored sequence.

Figure 2-2 Instrument Wizard Offline



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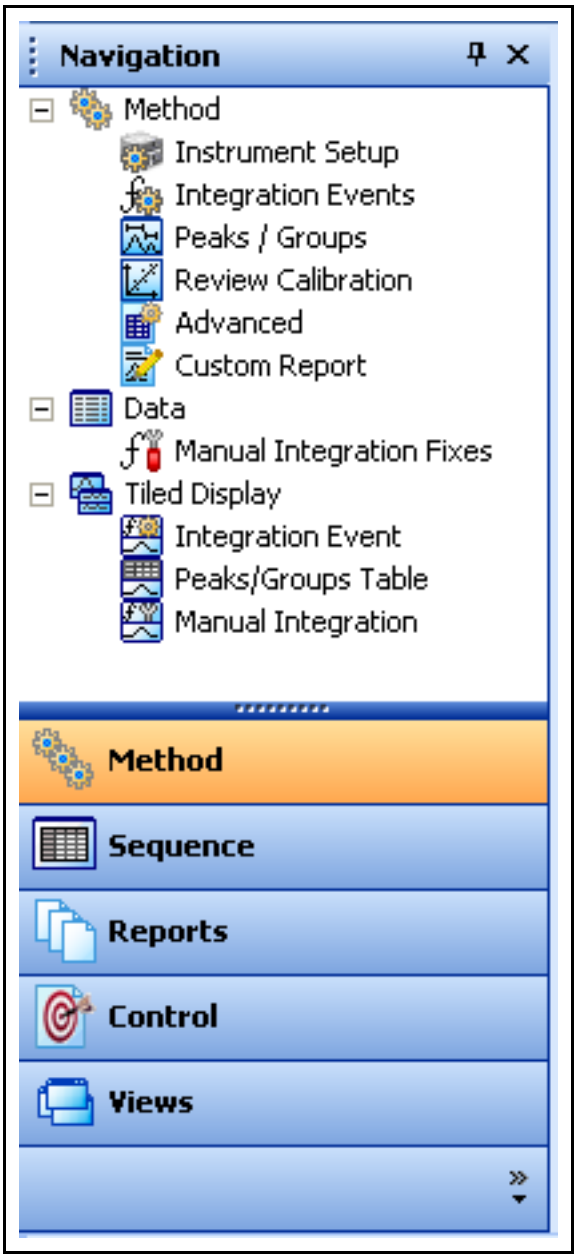
Chapter 3
Navigation Pane

A **Navigation** pane is displayed at the left side of the instrument window. See Figure 3-1. The Navigation pane enables the user to quickly switch between the major functions of the instrument window. A functional area can also be accessed by clicking on one of the function bars located at the bottom of the **Navigation** pane.

Figure 3-1 Navigation Pane



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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.

To "park" the Navigation pane

The **Navigation** pane can be "parked" at the left of the Instrument window to provide additional work space.

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

To "park" the **Navigation** pane, click the push-pin button at the top of the **Navigation** pane.

The **Navigation** pane of the instrument window gives single-click access to 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. These commands are explained in Table 3-1.

Table 3-1 Navigation Pane Parameters

Navigation Function Bar	Displays
Method	Method commands, Data manual integration fixes, and Tiled Display to display current data tiled with selected Integration or Calibration (Peak Table) information.
Sequence	Edit.
Reports	Reports, Report template properties.
Control	Instrument Setup, Run Queue, Instrument Status.
Views	Data Display options. Manual Integration Fixes, Baseline Check Status.

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Chapter 4
Program Architecture and Data Structure

4.1 About Method Files

A method is used to acquire and/or reprocess a data file. A method contains instructions for data acquisition (run time, sampling rate, etc.), integration, calibration and peak information, reports, as well as optional functions such as data export and user programs. Each method is capable of acquiring multiple independent channels of data from a single chromatograph. Each channel can have its own complete independent parameters, including sampling rate, run time, integration events, external events, calibration, and reporting.

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.

4.2 About Data File Structure

A data file is created whenever a sample is acquired, or when a data file is saved, using **Save As 32-bit…**. 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 (this is the "original" method saved only when the data is acquired). Because multiple channels of data can be simultaneously acquired on a given chromatogram, the method section may contain complete parameters for more than one channel.

Raw data points for the run saved. Multiple chromatograms may be present in a single data file, each of which represents a detector channel 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 recalled later when the file is opened. In addition, the most recent analysis results and method are also saved in the data file and updated whenever analysis occurs. The Sample ID for the results is also saved, as are manual integration fixes.

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.

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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 5
Opening and Saving Files

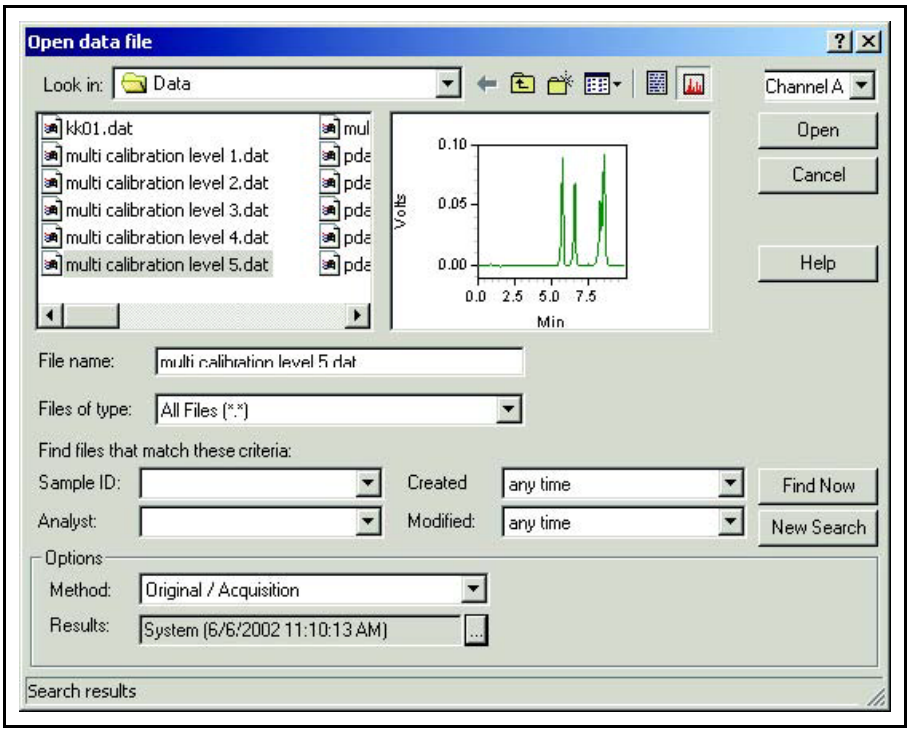
5.1 Open Data Files

The **Open File** icon on the command toolbar will open the **Open File** menu.

Whenever a file is opened using the data system, an **Open data file** window is displayed that allows opening the file and specifying parameters for searching, as well as previewing, file contents. See Figure 5-1.

The **Open data file** window provides options for how to open and search for files. The list of files of the type selected (**Files of type**) are shown. The files can be viewed as a list and their 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 **Preview Chromatogram** icon, or the file description can be viewed by clicking the **Description icon**. The * wildcard character can be used to view a list of certain file types. Files are stored in the current project folder. A folder bar is included in the window to facilitate navigation.

Figure 5-1 Open Data File Window



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5.1.1 Open Data File Options

The **Options** region allows loading additional information at the time the data file is opened.

5.1.1.1 Method

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. **Original/Acquisition** loads the method used for the original acquisition of the data file. This method will replace the current active method.

5.1.1.2 Results

When one of the **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.

5.1.1.3 Searching for Data Files

There are options that allow display of only files of interest. Using **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**, 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.

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** is **Test** followed by anything will be displayed. Click the **New Search** button to clear the search settings and use new criteria for searching.

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

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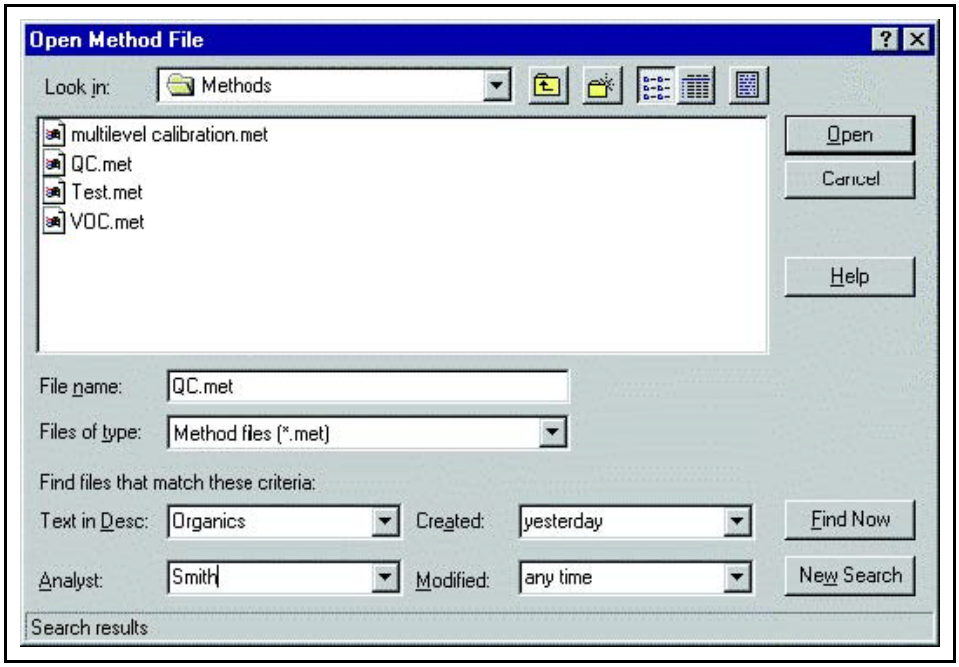
5.2 Open Method and Sequence Files

To open a method or sequence file,

1. From the **File** menu, click **Method** or **Sequence**, followed by **Open**.
2. **Open Method File** and **Open Sequence File** windows are identical. Files are stored in the current project folder. A drop-down menu is included in the window to facilitate navigation. See Figure 5-2.

Figure 5-2 Open Method File Window



5.2.1 Searching for Method and Sequence Files

The criteria used to search for specific method and sequence files includes the selection of specific text found in the file description (**Text in Desc.**), **Analyst** name, and date **Created** or last **Modified**.

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

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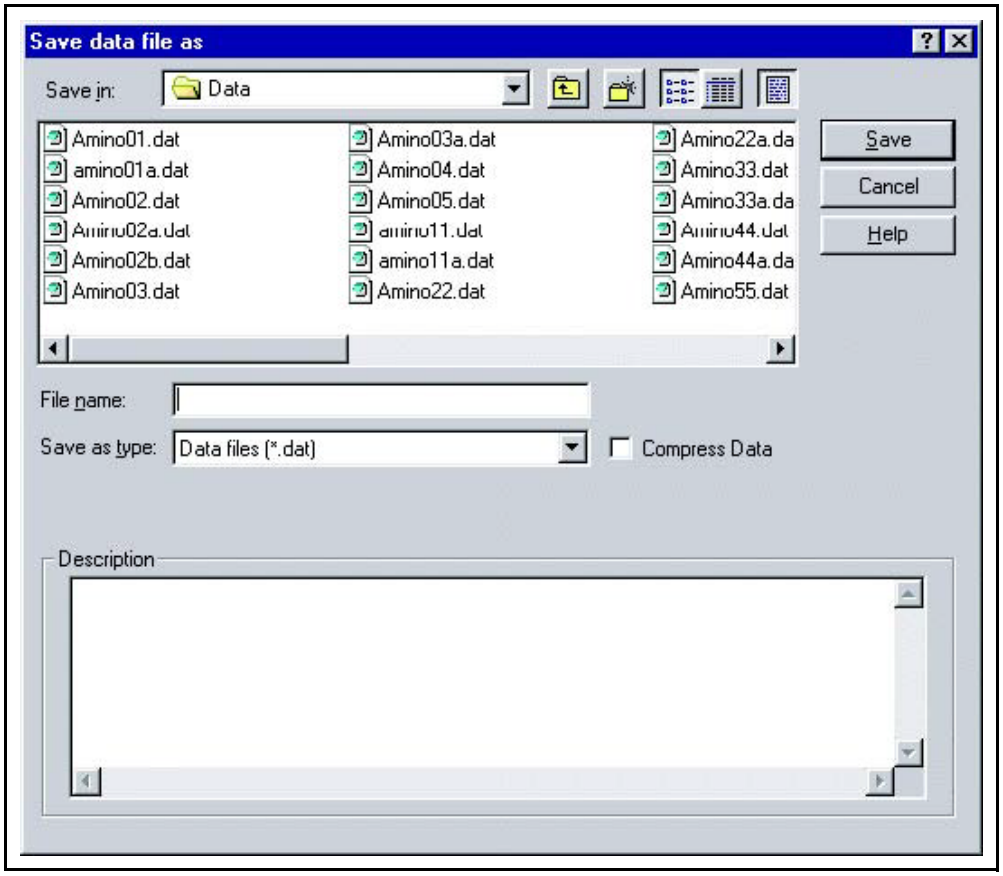
5.2.1.1 Save Data Files

To save a data file,

1. Click **File >> Data >> Save as 32-bit...**.
2. A **Save data file as** window opens to allow the user to browse to a location and the the filename to be used to save the file. See Figure 5-3.

This command will save the current data file along with the current method in a single file. This command is only enabled when the current data file is not in 32-bit EZ IQ data format (such as 16-bit or converted files). In order to comply with good laboratory practices, the **Save as 32-bit…**command does not allow using same name as an existing data file, unless the file is located in a public directory. A public folder is a folder where the path contains the term **public**. Data files in all other data system folders are protected from being overwritten and are stored within the current project folder. A drop-down menu is included in the window to facilitate navigation.

Figure 5-3 Save Data File As Window



To save current data in a new data file, enter the name of the new data file in the **File name** field, then click **Save**. Use the icons at the upper right of the window to view **details** of a highlighted file, or to view the **description** of a highlighted file. An entry **Saved from <FILENAME>** will be logged into the saved file as the first entry.

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If the **Compress Data** box is selected, the file will be saved in a compressed format. Once saved in compressed format, it will automatically be decompressed whenever the file is opened. However, once a file is saved in compressed format, **Save as** must be used to save the compressed file back into its decompressed format.

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Chapter 6
Reading CDF Files

When opening a CDF file, the software searches for one of the following Y-axis labels:

- microvolts, uvolts, uv, uau
- millivolts, mvolts, mv, mau

If one of these labels is not found, the software will try to read it from an **`AIA.ini`** file, which is used to get multipliers for non-standard file types. If there is no **`AIA.ini`** file available, the software will try to make an estimate of the multipliers based on the range of values. The data system determines the multiplier by picking the largest number that will not overflow a 22-bit floating point number. It does this by taking the largest value in the data stream and multiplying it by 1000000, 1000, 1 and picking the largest multiplier that does not overflow the 22-bit float.

If the CDF file being read is non-standard, the user will have to make an **`AIA.ini`** file and put it in the data system program folder. The file should contain the Y-axis label and multiplier and its format is as follows:

[YLabelSection]

YLabelCount=<number of labels>

YLabelString1=<y axis label name 1>

YLabelValue1=<multiplier 1>

YLabelString2=<y axis label name 2>

YLabelValue2=<multiplier 2>

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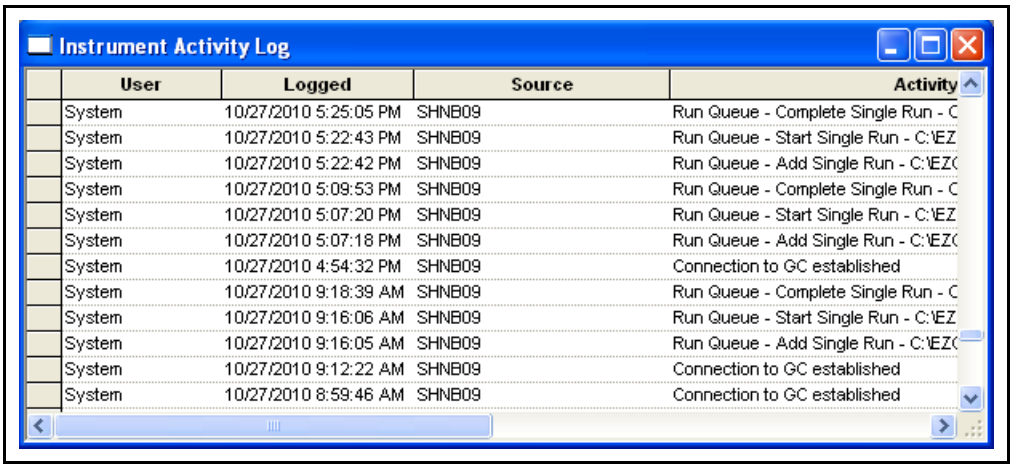
Chapter 7
The Instrument Window

7.1 View the Instrument Activity Log

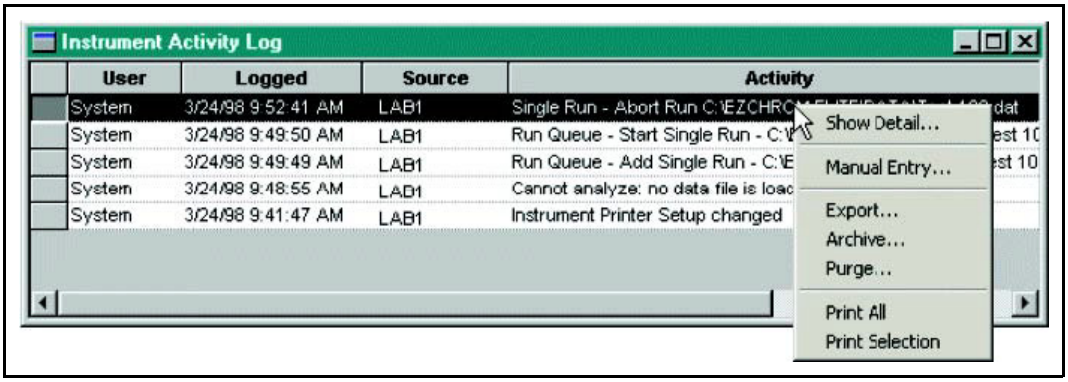
A log of activity from the current instrument is generated upon user operation. To view this log, click **File >> Instrument Activity Log >> Display Log**. The **Instrument Activity Log** window is displayed. See Figure 7-1. The **Instrument Activity Log** window displays the instrument operator, the time the activity was logged, and a description of the activity.

Figure 7-1 Instrument Activity Log



To view details of any line in the Instrument Activity Log, click on the line to highlight it, then right-click within the spreadsheet. From the drop-down menu, details of the highlighted line can be viewed or printed. Select **Print All** to print the entire Instrument Activity Log. In addition, the activity log can be exported, archived, or purged. See Figure 7-2.

Figure 7-2 Instrument Activity Log Spreadsheet



NOTE: The Instrument Activity Log will record all activities. Over time, the size of the file containing the log will increase. To save space, the user may chose to 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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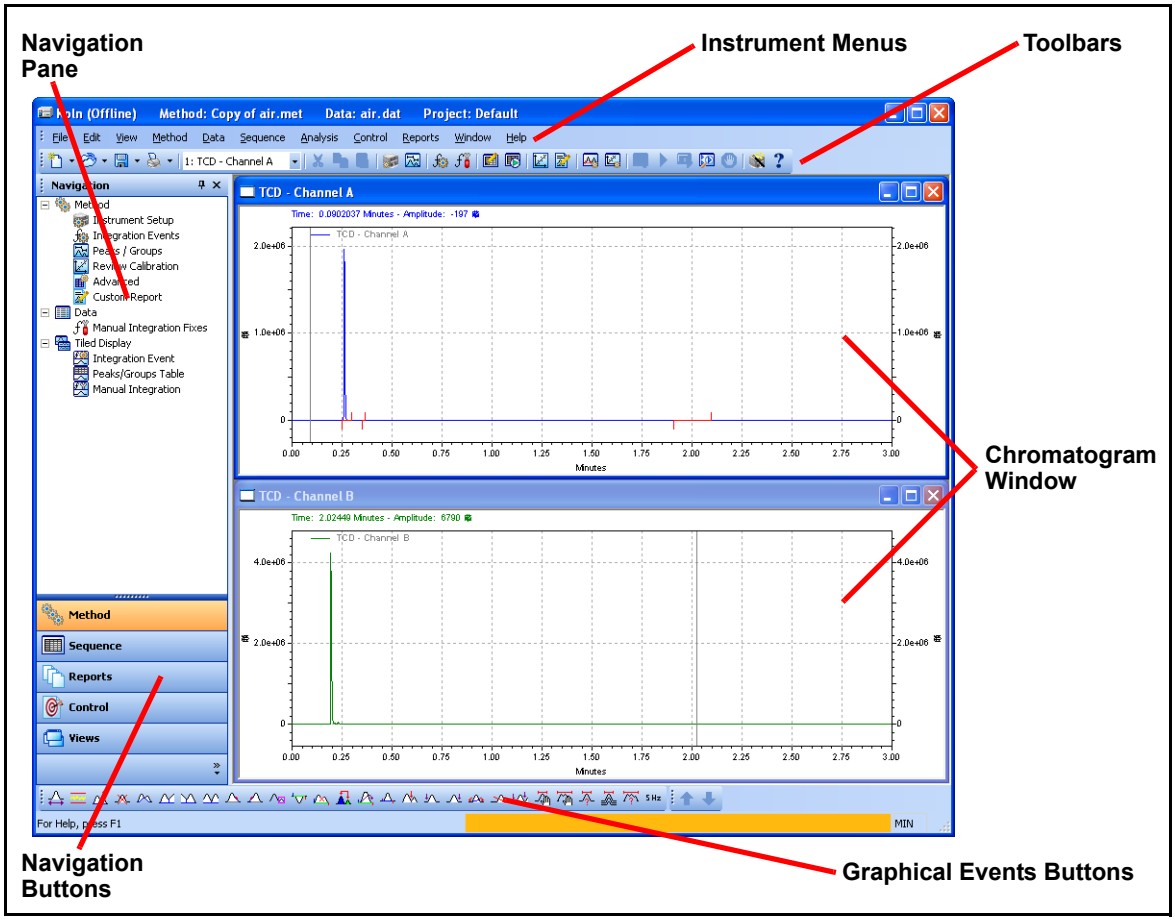
7.2 About the Instrument Window

When an instrument is connected and EZ IQ is opened, the **Instrument Window** will display. See Figure 7-3. From this window, all aspects of using the instrument are accessible, including

- 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, adding or removing Toolbars and Status information. These features are designed to make the system easier to use, and most users prefer to have them displayed.

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 to change the general view preferences for the instrument window. See Figure 7-4.

Figure 7-4 General Tab

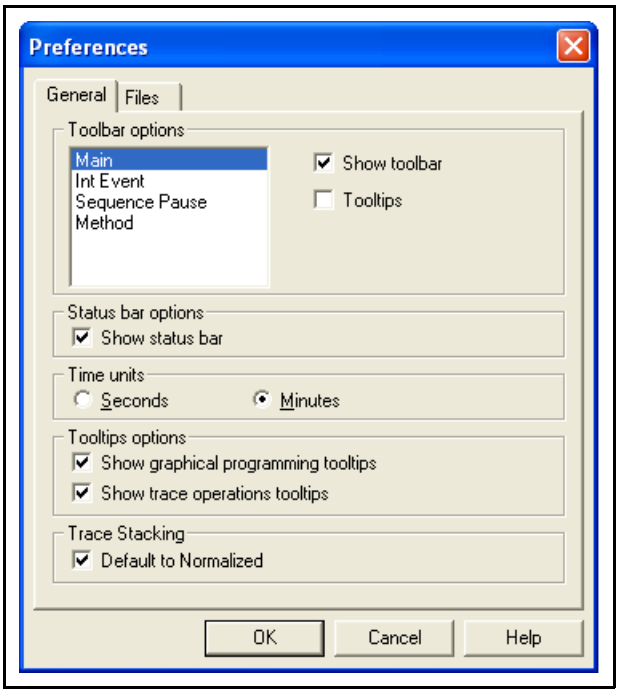


Table 7-1 Preferences Parameters

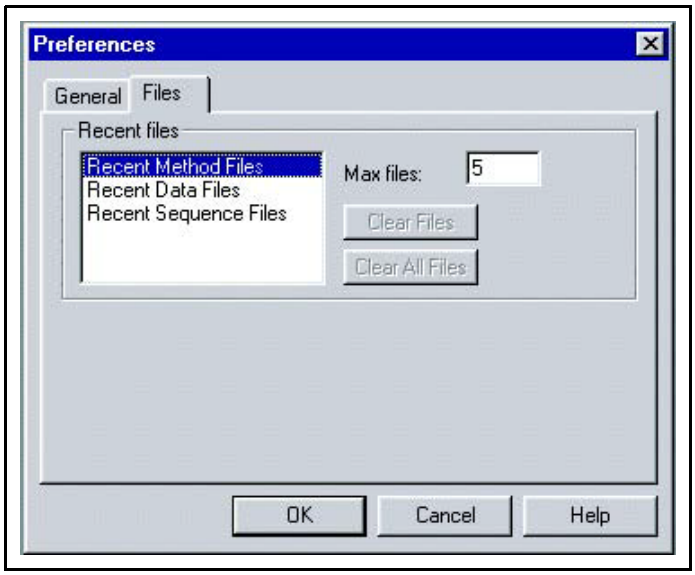
General tab	Used to set up general preferences in the instrument window.
Toolbar options	For each area of the window listed, Toolbar and Tooltips (if available) can be turned off or on. Click on the toolbar area, then select the **Show toolbar** and **Tooltips** boxes to enable them.
Status bar options	Select the checkbox to turn on the status bar. The status bar provides brief information at the bottom of the instrument window.
Time units	Select the time units for display of chromatographic information.

7.2.2 Change File View Preferences

To change the appearance of the instrument window,

1. Click **View >> Preferences**. The window shown in Figure 7-5 is displayed.
2. Select the **Files** tab to change the file view preferences for the instrument window.
3. Select the file type, then enter the number of files to display in the **Max Files** box. This determines the number of recent files 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
Acquisition Parameter Setup

8.1 Introduction

EZ IQ is equipped with two 3000 Micro GC drivers. Both provide full control of the instrument and differ mainly in the acquisition parameter setup.

3000 Micro GC Classic Driver

The Classic Driver was released when the 3000 Micro GC was introduced to the instrument market. Support is provided for backward compatibility.

3000 Micro GC Enhanced Driver

The Enhanced Driver was developed later to provide significant improvement in software efficiency and graphical interface improvement. If a new 3000 Micro GC is installed, it is highly recommended to adopt the Enhanced Driver.

Highlights on Enhanced Driver Update over Classic Driver

- Significant reduction in prerun and postrun time required by the software
- Introduced intuitive graphics for the "Instrument Status" window
- The area count of the Classic driver is 100x times larger than Enhanced driver. The Classic driver conducst a software multiplication on the area count while the Enhanced driver does not implement this multiplier.

8.1.1 Configure the 3000 Micro GC Using the Classic Driver

Configuration of the 3000 Micro GC is required in order for EZ IQ to control the instrument. Proceed as follows to configure a 3000 Micro GC.

1. Start the **EZ IQ Config** application (**EZStartConfig.exe**) from the Windows **Start** menu
2. On the **EZ IQ Configuration** window, click **Instrument Configuration** …
3. On the **Instrument Configuration** window, enter the **Instrument Name**, click **Instrument Type**, and then click **Configure**.
4. Click the **INFICON 3000 Micro GC Classic** icon to highlight it and then click the green arrow to move the **INFICON 3000 Micro GC Classic** icon from **Available Modules** to **Configured Modules**.
5. Double-click the **INFICON 3000 Micro GC Classic** icon in the **Configured Modules** pane to open the configuration window.
6. Select the **General** tab.

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7 Enter information regarding the instrument configuration into the **General** tab, see Figure 8-1. For the system to automatically retrieve the configuration settings, enter the **Host Name** or the **IP Address** and click **Auto Configure**.

Figure 8-1 General Settings Tab

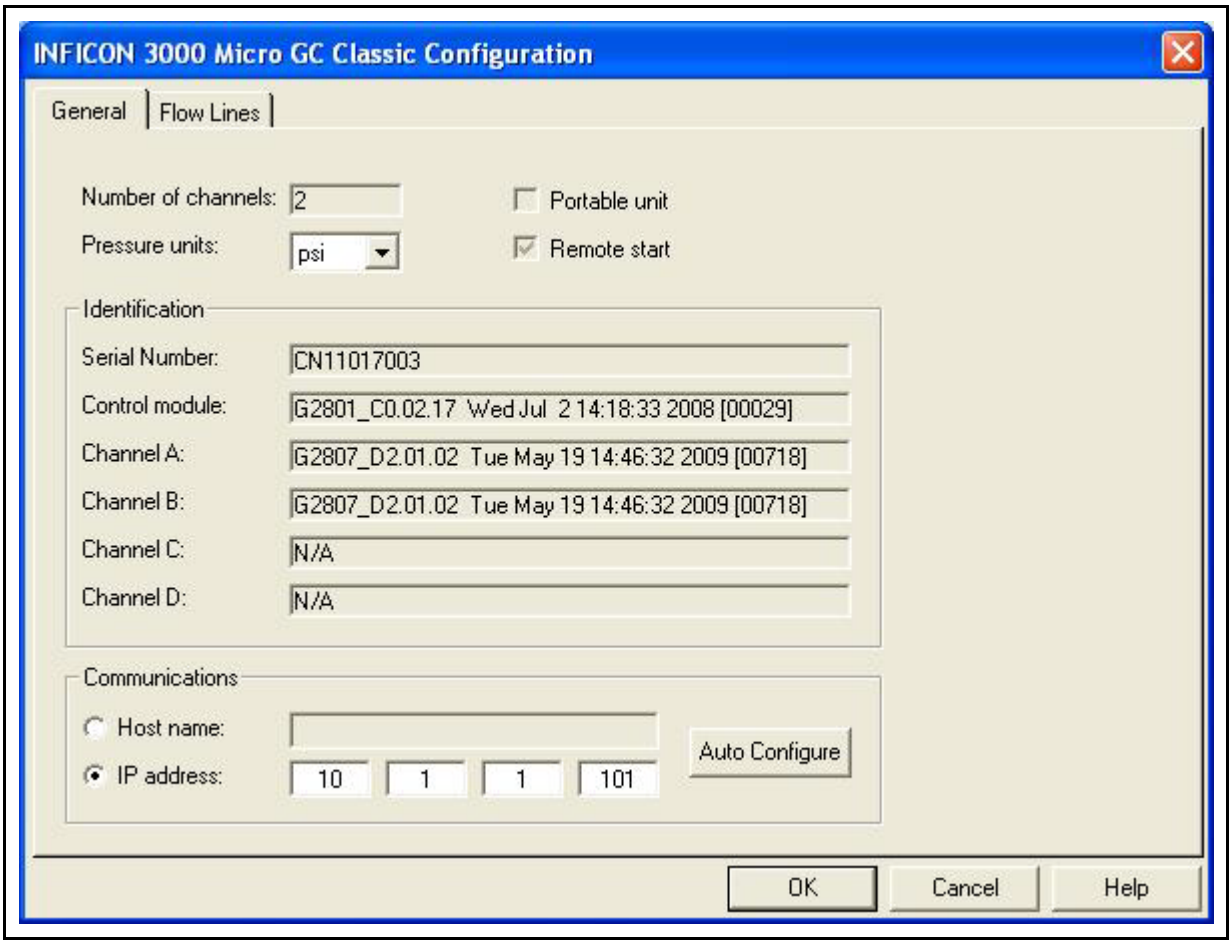

Table 8-1 General Settings Parameters

Portable unit	Select when using a 3000 Micro GC portable unit with a battery power source.
Remote Start	Select when an external start module has been installed in the 3000 Micro GC.
Pressure units	Use the drop-down list to select the desired units to be displayed for pressure.
Serial Number, Control module, Channel A - B- C- D	These read-only fields display information as obtained from auto-configuration.

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Table 8-1 General Settings Parameters (continued)

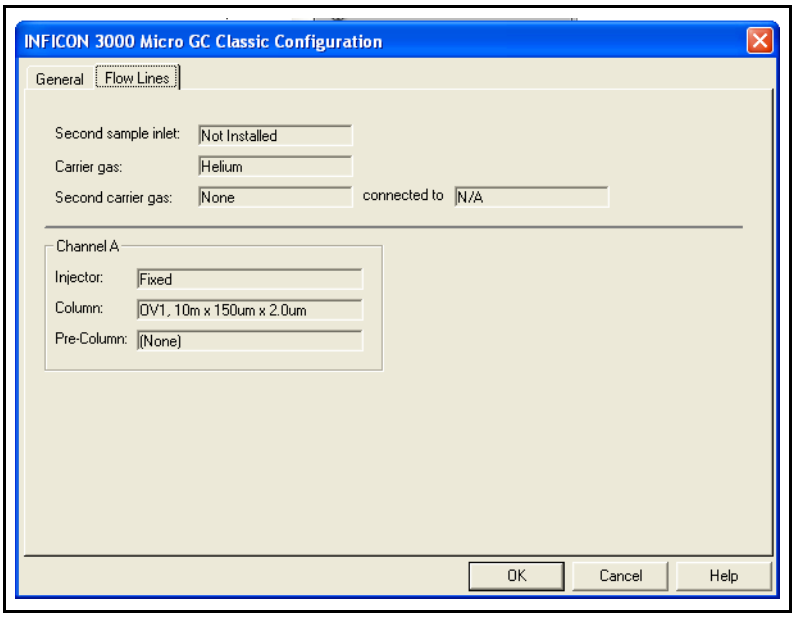
Auto Configure	Click to establish communications with the 3000 Micro GC using the user specified communications parameters. When successful, the Serial number and Firmware part numbers will be populated.
Communications	Specifies the addressing mode for TCP/IP communications with the 3000 Micro GC.

8.1.2 Classic Driver Provision Flow Lines

Proceed as follows to configure information about the carrier gas flow lines for the 3000 Micro GC.

1. Start the **EZ IQ Config** application (**EZStartConfig.exe**) from the Windows **Start** menu.
2. From **Instrument Configuration** click **Configure**.
3. Click the **INFICON 3000 Micro GC Classic** icon to highlight it and then click the green arrow to move the **INFICON 3000 Micro GC** icon from **Available Modules** to **Configured modules**.
4. Double-click the **INFICON 3000 Micro GC Classic** icon in the **Configured Modules** pane to open the Configuration window.
5. Select the **Flow Lines** tab and populate the fields. See Figure 8-2.

Figure 8-2 Flow Lines



The following describes terms used in this window.

Table 8-2 Flow Lines Parameters

Second sample inlet	Specifies if a second sample inlet port is installed, which will allow a second independent sample to be injected.
Carrier gas	Use to specify the type of carrier gas to be used for analysis. This gas will be used for all channels, unless the second carrier gas is enabled.
Second carrier gas	Used to specify if a second carrier gas line has been installed. **NOTE:** This field is disabled if the number of channels is less than 2.
Connected to	Use to specifty the channel to which the second carrier gas is connected. This field is disabled if the second carrier gas control is set to None.
Channel A/B/C/D	Use to specify the details of the input streams for each 3000 Micro GC channel. Depending on the **Number of Channels** selection on the **General** Tab, some of these groups may be hidden.
Injector	Use to select the injector type—fixed or variable.
Column	Use to select the column installed for the channel from the drop-down list. Available column selections will depend on the type of injector installed.

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8.1.3 Classic Driver Method Control Parameters

Proceed as follows to set the method control parameters for the 3000 Micro GC.

1. Click **Method >> Instrument Setup**. See Figure 8-3.
2. Select the **INFICON 3000 Micro GC** tab.
3. Select the **GC** tab and populate the fields.

Figure 8-3 GC Tab

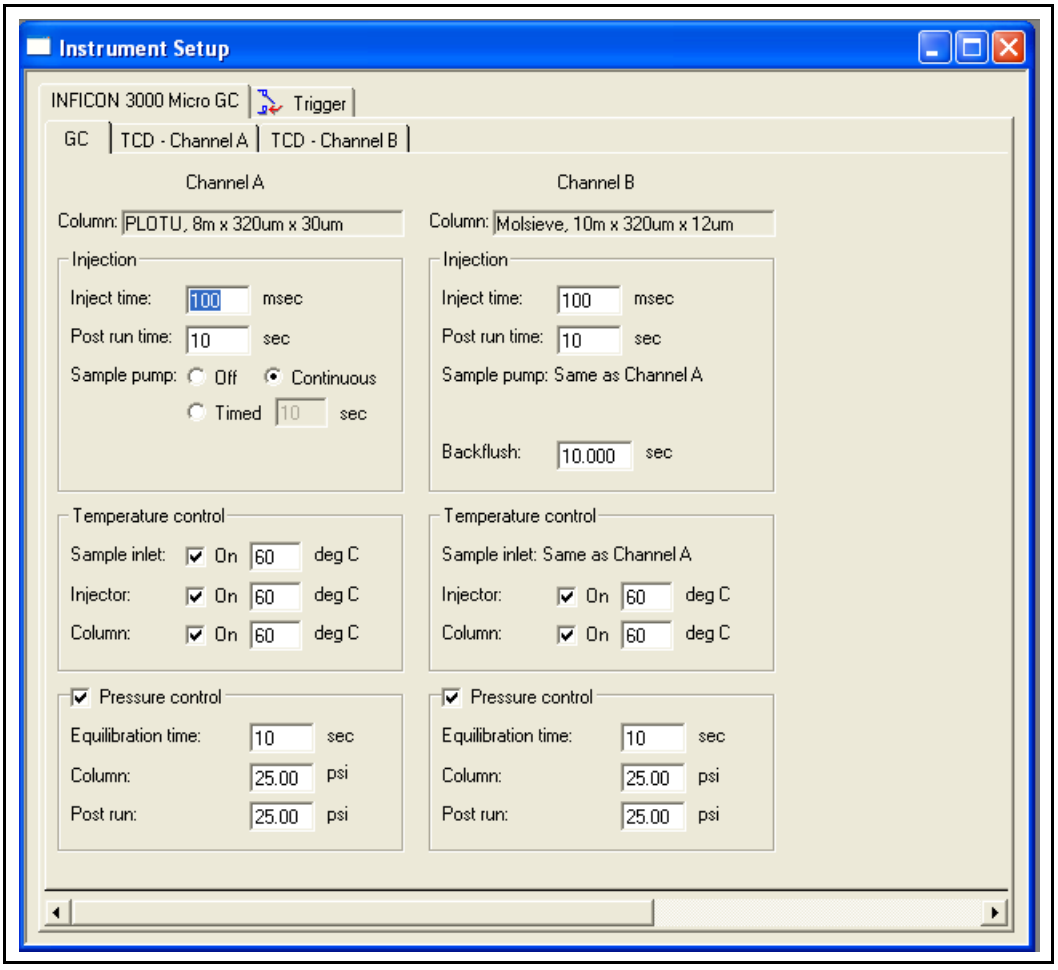

Table 8-3 GC Tab Parameters

Inject time	Used to specify the duration of the injection.
Post run time	Used to specify the duration of the post run pressure after analysis time.
Sample pump	Used to specify the manner in which the sample pump flushes the injection line.
Backflush	When applicable, used to specify time after the injection that the injector should be cleaned by backflushing.

Table 8-3 GC Tab Parameters (continued)

Temperature control	Used to establish temperature set points for the 3000 Micro GC heated zones. Select the checkbox adjacent to the zone to enable the temperature control and enter a value.
Pressure control	Used to set target pressures to be maintained by the EPC (Electronic Pressure Controller). Select the checkbox to enable the pressure control and then enter the desired values. When the box is selected, the run will not begin until the flow line has reached the target pressure specified by the **Column** field and has maintained it for the time specified by the **Equilibration Time** field. After the run is complete, the flow line pressure will be set to the value specified by the **Post run** field. **NOTE:** The instrument will not run if the filament is ON and the column pressure is below 5 psi (34.5 kPa, 0.35 bar) in a method.
Equilibrium time	Specifies the time to wait to perform an injection once the flow line has reached the target column pressure
Column	Used to specify the target pressure for the flow line.
Post run	Specifies the target pressure for the flow line after the run has completed.

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8.1.4 Classic Driver TCD Parameters

To set the method control parameters for the 3000 Micro GC.

1. Click **Method >> Instrument Setup**.
2. Select the **INFICON 3000 Micro GC** tab.
3. Select the **TCD** tab for the desired channel.
4. Select **Acquisition Channel On** and populate the fields. See Figure 8-4 for an example of a 2-channel 3000 Micro GC.

Figure 8-4 TCD - Channel A Tab

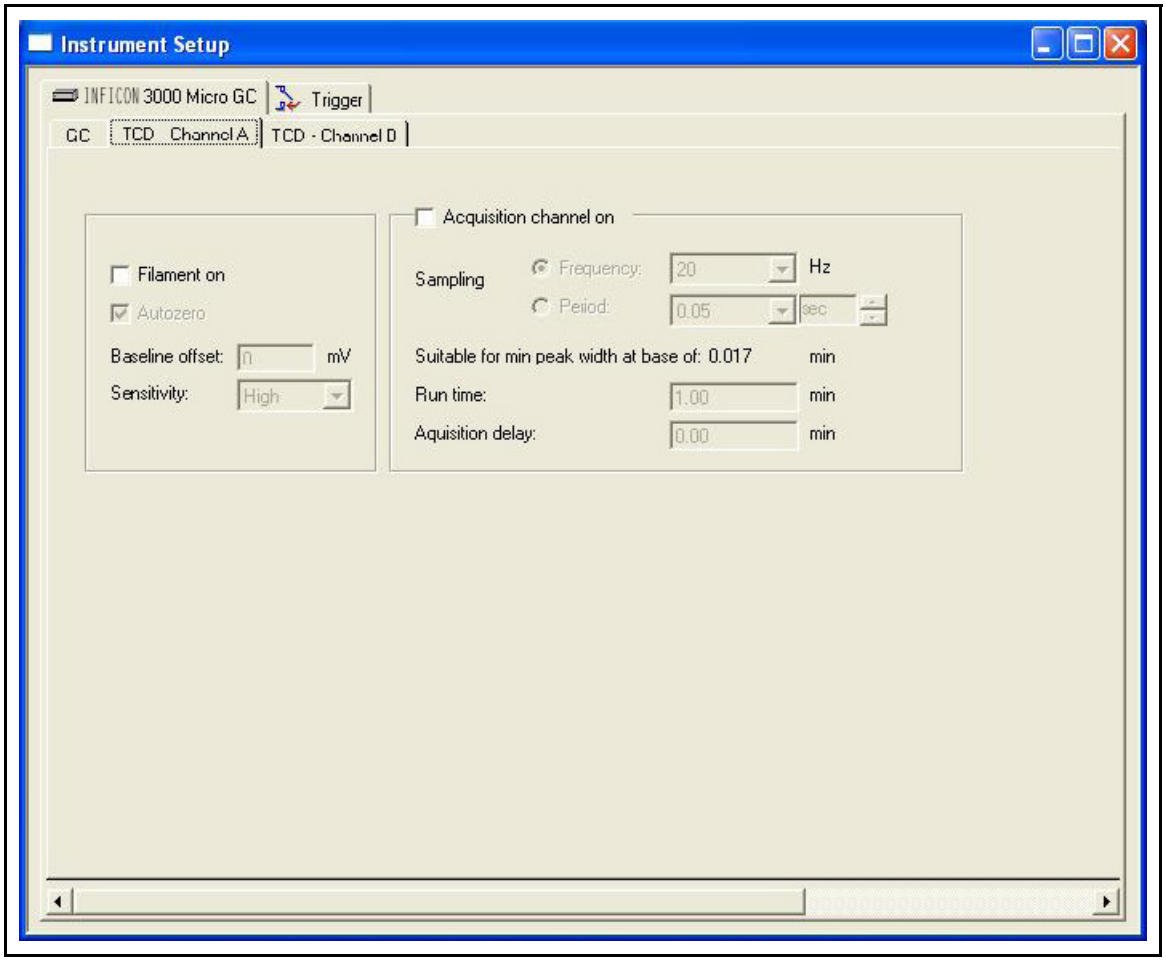

Table 8-4 Channel A Tab Parameters

Acquisition channel on	When selected, it will enable data acquisition using the detector. When cleared, fields except **Filament on** will be disabled.
Filament on	When selected, the detector filament will be turned on prior to acquisition. When cleared, it will be turned off.
Autozero	When selected, the detector output will be adjusted to zero prior to data acquisition.
Baseline Offset	Specifies a fixed offset that will be applied to the signal being returned by the detector. This offset is applied prior to the start of the run. This field will be disabled if the **Autozero** box is selected.
Sensitivity	Used to set the detector signal response sensitivity.
Sampling	This is the rate at which data points are collected and stored in the data file. When a sampling rate is selected, text appears below this field indicating the narrowest peak width for which this sampling rate is adequate. The sampling rate may be specified in terms of sampling frequency or sampling period.
Sampling Frequency	Sampling Frequency is the rate at which chromatographic data points are collected from the Thermal Conductivity Detector (TCD) expressed in Hz. 20, 50, 100, 200 Hz may be selected. This field is enabled when the **Sampling Frequency** option is selected. When cleared, it is disabled.

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Table 8-4 Channel A Tab Parameters (continued)

Sampling Period	Sampling Period is the rate at which chromatographic data points are collected from the Thermal Conductivity Detector (TCD) expressed in seconds. 0.005, 0.05, 0.02, 0.01 sec may be selected. This field is enabled when the **Sampling Period** option is selected. Otherwise, it is disabled.
Run Time	Determines the length of the analysis for this channel.
Acquisition Delay	Use to enter the interval between the start of the run (**Trigger**) and the time when sampling starts for this channel.

8.1.5 Classic Driver Trigger Parameters

The **Instrument Setup** window also provides a **Trigger** tab with a trigger **Type** selection. See Figure 8-5.

Figure 8-5 Trigger Tab

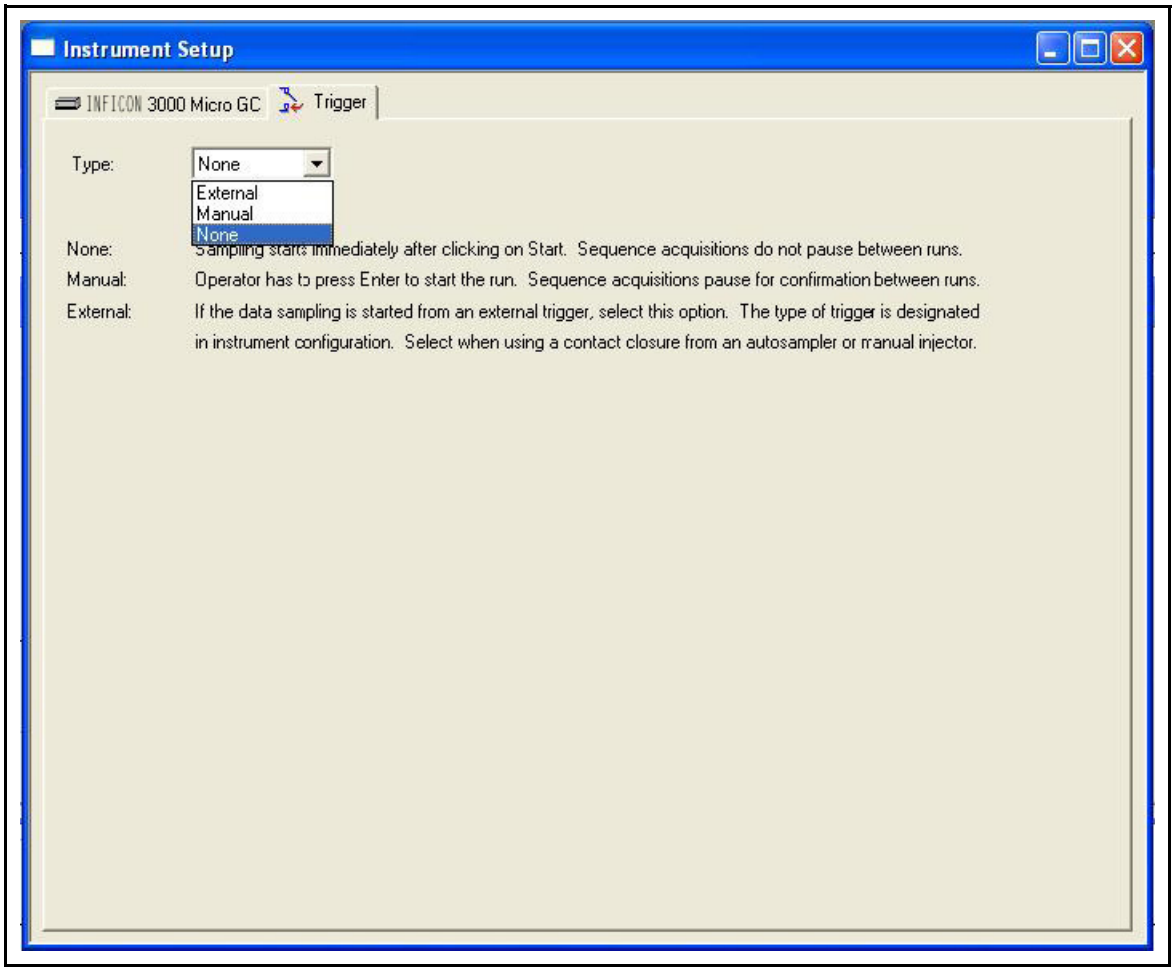

Table 8-5 Trigger Tab Parameters

External	Data sampling starts when externally triggered.
Manual	User inititated data sampling.
None	Sampling of data starts immediately when **Start** is clicked. Normally, select **None** for 3000 Micro GC. When completed with the acquisition setup information, click the X box in the upper right hand corner of the tab window to exit the window.

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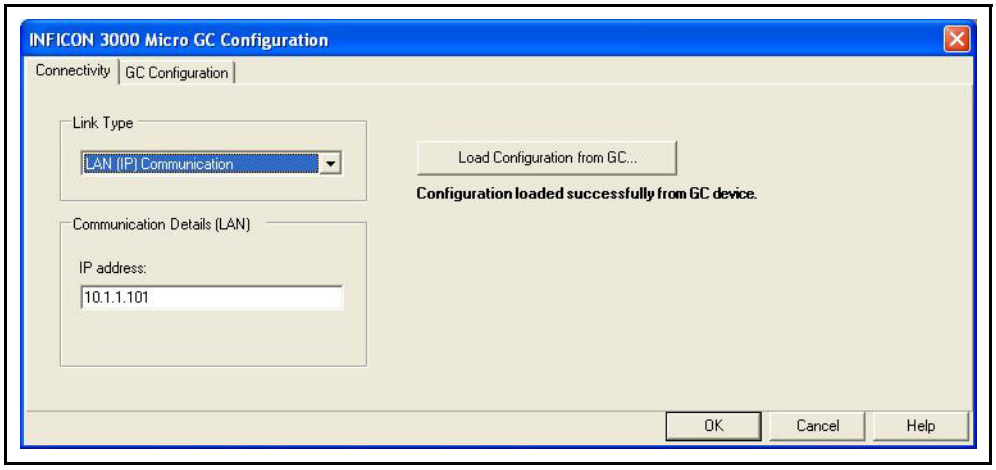
8.2 Acquisition Parameter Setup with Enhanced Driver

8.2.1 Configure the 3000 Micro GC Using the Enhanced Driver

Configuration of the 3000 Micro GC is required in order for EZ IQ to control the instrument. Proceed as follows to configure a 3000 Micro GC.

1. From the Windows **Start** menu, click the **Chromatography** folder. Open the program **EZ IQ Config** (**EZStartConfig.exe**).
2. On the **EZ IQ Configuration** window, click **Instrument Configuration …**
3. On the **Instrument Configuration** window, enter the **Instrument Name**, click **Instrument Type**, and then click **Configure.**
4. Click the **INFICON 3000 Micro GC** icon to highlight it and then click the Green arrow to move the **INFICON 3000 Micro GC** icon from **Available Modules** to **Configured Modules.**
5. Double-click the **INFICON 3000 Micro GC** icon in the **Configured Modules** pane to open the configuration window.
6. In **INFICON 3000 Micro GC Configuration** window, see Figure 8-6, select the **Connectivity** tab, enter the **IP Address** of the instrument, and then click **Load Configuration from GC**. The 3000 Micro GC configuration will load into EZ IQ.

Figure 8-6 Enhanced Driver - Load Configuration



7. Click **OK** to exit **INFICON 3000 Micro GC Configuration** window.
8. Click **OK** to exit **INFICON 3000 Micro GC** window.
9. Click **OK** to exit **Instrument Configuration** window.
10. Click **Close** to exit **EZ IQ Configuration** window.

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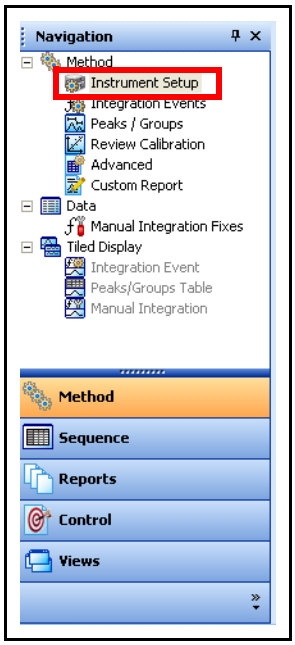
8.2.2 Enhanced Driver Acquisition Parameters

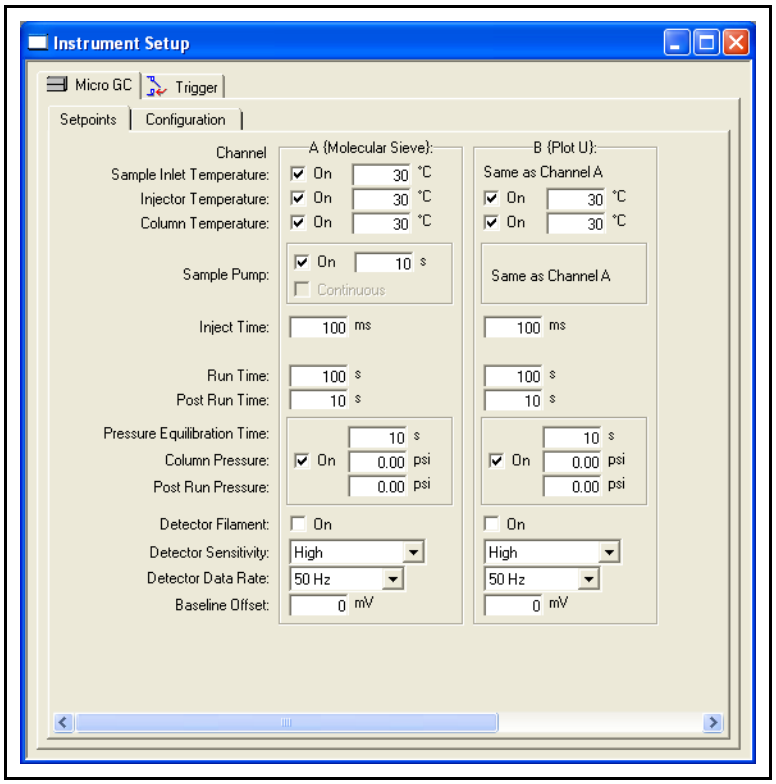
As part of a chromatographic method, acquisition parameters can be defined in the **Instrument Setup** window **Navigation** pane. See Figure 8-7.

Figure 8-7 Navigation Pane



Double-click **Instrument Setup** to obtain the **Instrument Setup** window. See Figure 8-8 as an example for a 2-channel 3000 Micro GC.

Figure 8-8 Instrument Setup Screen



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The following are acquisition setpoints for the 3000 Micro GC (window tool tips will provide valid data ranges).

Table 8-6 Acquisition Setpoints Parameters

NOTE: Regarding Sample Inlet, Injector and Column Temperature—Each heated zone has an associated checkbox; if selected, the zone is enabled (heating), if cleared, the zone is disabled (not heating). The setpoint value is preserved if the zone is disabled. This capability is especially useful with a 3000 Micro GC Portable to reduce battery drain.	
Sample Inlet Temperature	The temperature range of the sample gas as it flows though the inlet. If two or more GC modules share an inlet, only one temperature field is displayed.
Injector Temperature	The temperature range of the sample gas as it flows through the injector.
Column Temperature	The temperature range of the sample gas as it flows through the column.
Sample Pump (On/Off)	Selecting this checkbox enables the sample pump to run for a specified number of seconds. Clearing **Sample Pump** disables the pump, a capability which is especially useful with a Portable 3000 Micro GC to reduce battery drain.
Sampling Time	The length of time (in seconds) allowed for the sample gas to flow through the injector before the start of the run. If two or more 3000 Micro GC modules share a sampling pump, only one sampling time field will be available.
Continuous Sampling (On/Off)	Selecting this checkbox allows sample to continuously flow through the sample loop before an injection is made. When **Continuous Sampling** is selected, **Sampling Pump** will be off and **Sampling Time** will not be available.
Inject Time	The length of time (in milliseconds) allowed for the sample gas to flow into the column before the flow is stopped.
Run Time	The length of time (in seconds) allowed for the detector to collect data and send it to the PC.

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Table 8-6 Acquisition Setpoints Parameters (continued)

Post Run Time and Post Run Pressure	A step-increased (not a ramp) pressure push for a length of time (in seconds) to remove the remaining sample gas from the column.
Pressure Equilibration Time	Length of time (in seconds) the channel will need to stabilize at the pressure setpoint before the system is ready for a run. **Pressure Equilibration Time** begins when the actual column pressure stays within 0.5 psi (3.4 kPa) of the column pressure setting. **Pressure Equilibration Time** is not part of the run time.
Column Pressure	The pressure of the gas flowing through the column. **NOTE:** Each column has an associated checkbox; if selected, the gas is enabled (flowing), and if cleared, the gas is disabled (not flowing). The setpoint value is preserved if the gas flow is disabled. This capability is useful for conserving gas supplies when the column is not in use.
Detector Filament (On/Off)	Select the check box to turn the **Detector Filament** On, or clear it to turn the **Detector Filament** off. When the Filament is off, no data is collected for the selected signal. Turn the filament off before servicing the instrument or changing carrier gas.
Detector Sensitivity	The sample concentration ranges are **Standard** and **High**. Standard—Used to detect a wider range of responses. This setting sets the data acquisition to detect the widest range possible without over-ranging. High—Used to detect very small responses. This setting sets the data acquisition to allow detection of lower concentrations of sample components.
Detector Data Rate	The number of data points the 3000 Micro GC detector will collect every second. The Default Data Rate setting is 50 Hz.

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Table 8-6 Acquisition Setpoints Parameters (continued)

Baseline Offset	Sets the starting point for chromatographic data within a range from -50 to 500 mV. The default is zero.
Backflush Time	The time (in seconds from the beginning of the run), when the injector will backflush the sample gas in pre-column to vent. **NOTE:** This setpoint is provided only for an instrument channel with a backflush injector. **NOTE:** The time entered may be equal to or less than the **Run Time**, up to the maximum permitted run time for the given instrument (2400 seconds for a 2-Channel instrument or 1200 seconds for a 4-Channel instrument).

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8.2.3 Enhance Driver Trigger Parameters

The **Instrument Setup** window also provides **Trigger Type** selection. See Figure 8-9.

Figure 8-9 Trigger Type Selection

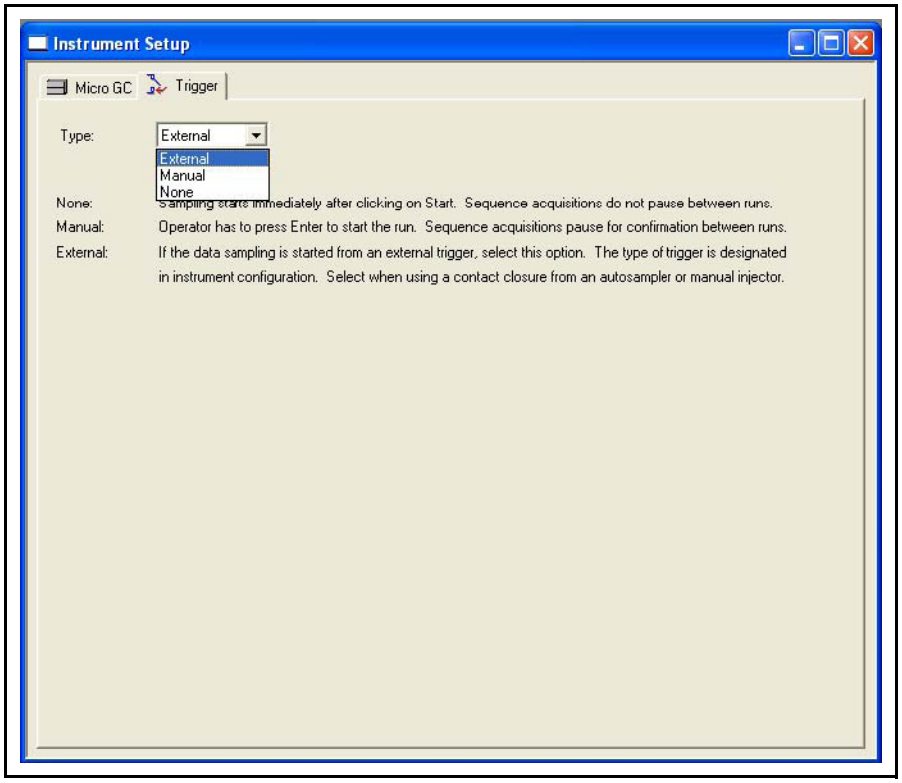

Table 8-7 Trigger Type Selection Parameters

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. When the acquisition setup information is completed, click the X box in the upper right hand corner of the tab window to exit the window.

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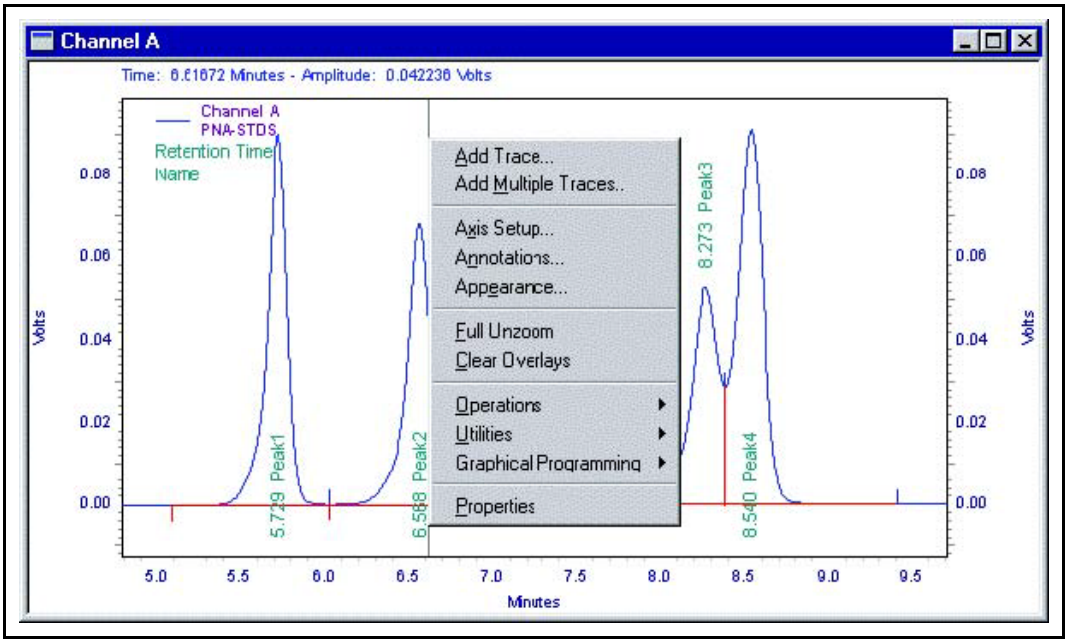
Chapter 9
The Chromatogram Window

9.1 About the Chromatogram Window

Data is displayed in the chromatogram window. Each channel will have its own chromatogram window. It is possible to add multiple traces to a single chromatogram window and perform comparison and mathematical operations on them. To access specialized commands for the chromatogram window, right-click anywhere within the chromatogram window area to display a list of commands. These commands allow for a wide range of functions, including: adding multiple chromatograms 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 as a sample is running. At the end of a run the data becomes the "current data". The appearance of the chromatogram can be changed by selecting annotations, fonts, and labeling. These features can be accessed by right-clicking on the chromatogram and clicking **Annotations**. In the **Utilities** menu, 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

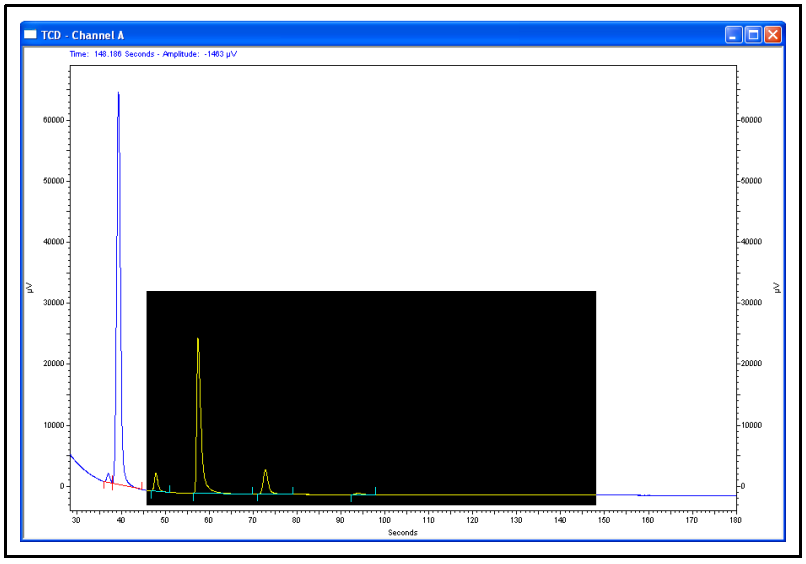
By default, each channel will have a chromatogram window. Chromatograms from different channels can be overlaid onto a single window by selecting **View**, then **Overlay Data**. The chromatograms can be separated into multiple windows by selecting **View**, then **Tile Data**. Individual channels may 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**.

9.3 Zooming

It is possible to examine a chromatogram in more detail by zooming in on a portion of the chromatogram. Press and hold the left mouse button and drag open the box so that it highlights the area of interest. Then release the mouse button. See Figure 9-2.

Figure 9-2 Zooming



To return to the previous level of zoom, double-click on the chromatogram. To zoom to the full chromatogram again after multiple zooming operations, right-click anywhere in the chromatogram window, then click **Full Unzoom** from the menu displayed. Or **Ctrl-Z** or **shift-double-click** in the chromatogram window. Once the chromatogram is in a "zoomed" view, it can be scrolled. See section 9.4.

Time and **Amplitude** are displayed at the top of the chromatogram window. These values change as the pointer is moved and reflect the time and amplitude of the trace where the pointer is located. If there is more than one trace, the display can be changed to another trace by clicking 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

Once zoomed in on a chromatogram, the chromatogram can be scrolled to the right or left without losing the zoom. Press the **CTRL+SHIFT** keys and move the mouse until the pointer changes to a hand. Press the left mouse button and drag the mouse to the left or right.

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

To restore the original view in the chromatogram window, right-click then click **Full Unzoom**.

9.5 Add a Trace (Add a Single Chromatogram)

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

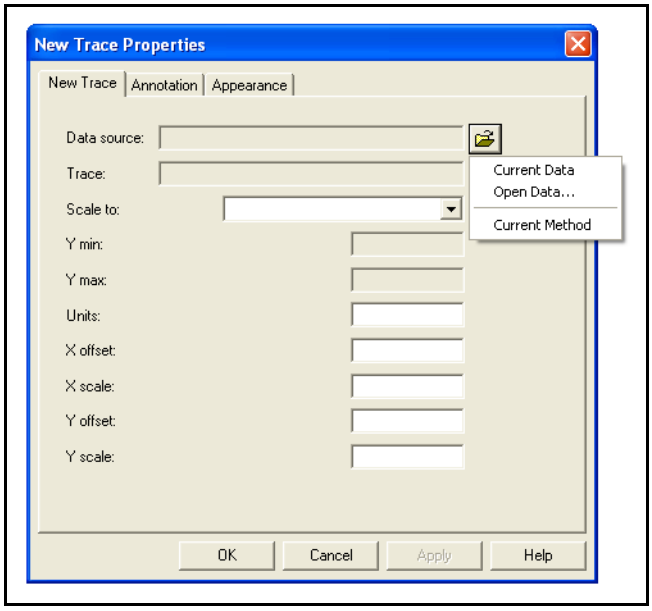
To add a new trace to the chromatogram window,

1 Right-click anywhere in the chromatogram window. A menu will appear. See Figure 9-3.

Figure 9-3 Chromatogram Window Options

2 Click **Add Trace…**. The **New Trace Properties** window will display. See Figure 9-4.

Figure 9-4 New Trace Properties Window



3 Select the **New Trace** tab. Fill in the fields to add a trace to the chromatogram window and set its properties. 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

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.
Current Method	Selects a trace from the current method (if available).
Open Data	Selects from stored data files in which a trace can be selected for display.
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)

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.
Y Scale	Enter a multiplier that will be applied to the entire trace.

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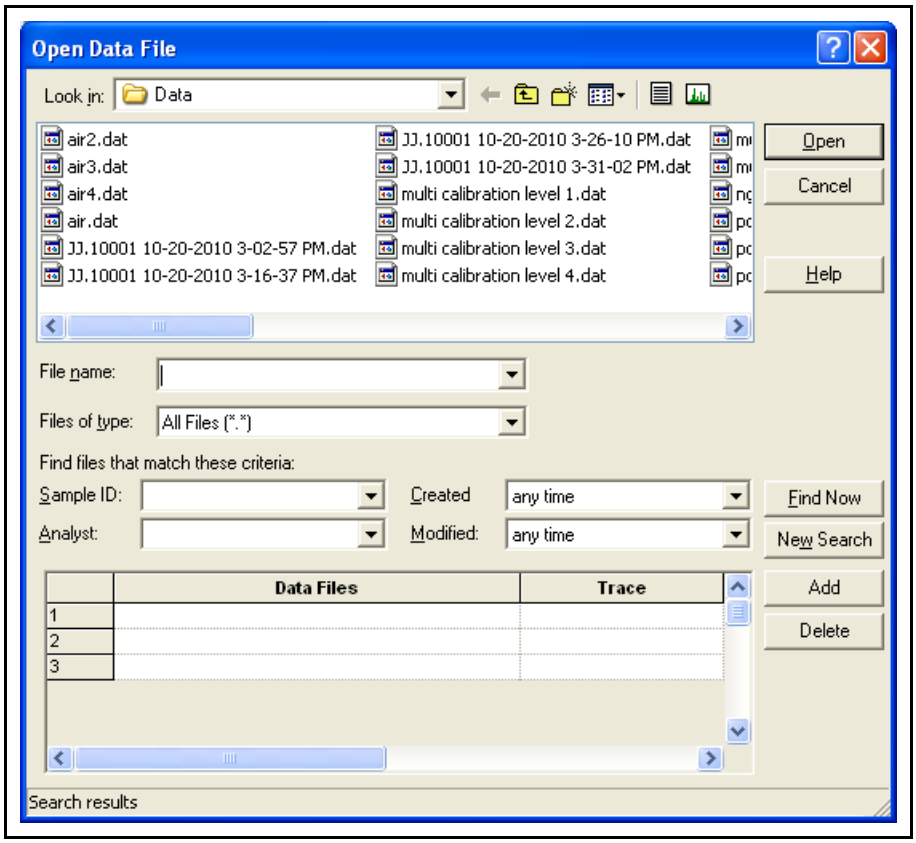
9.6 Add Multiple Traces to a Chromatogram Window

To add more than one chromatogram to the view,

1. In the chromatogram window right-click, then click **Add Multiple Traces…**. The **Open Data File** window will display the traces that can be selected from the file list. See Figure 9-5.

2. To add a file, either click on the filename, then click **Add**, or double-click on the filename from the list.

Figure 9-5 Open Data File Window



3. Once a data file is added to the list, select the channel by clicking on the **Trace** field, then click the down-arrow button. If multiple channels for that file are available, select the desired channel.

4. To delete a trace from the display list, click on its name or number, then click **Delete**.

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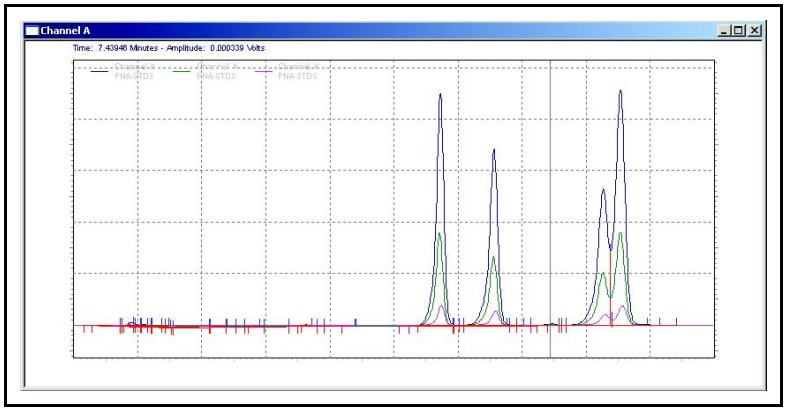
5 To open multiple traces, click **Open**. The selected files/channels will appear in the chromatogram window. See Figure 9-6.

Figure 9-6 Selected Files/Channels

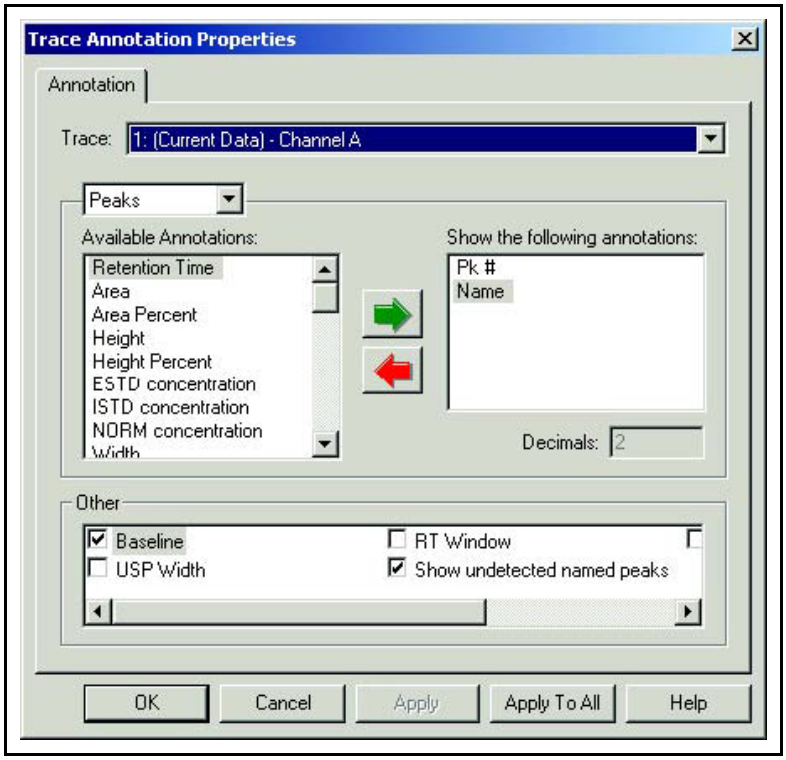


9.7 Annotate a Chromatogram

To change the annotations on the chromatogram,

1 To view trace annotations, right-click in the chromatogram window and select **Annotations** to open the **Trace Annotation Properties** window. See Figure 9-7.

Figure 9-7 Trace Annotation Properties Window



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2 Select the trace from the drop-down list.

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

4 Click on an **Available Annotation**. When an annotation is highlighted, add it to the annotations to be displayed by clicking the green arrow key (pointing to the right). This can also be achieved by double-clicking the selection.

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 Select the check box(s) to display **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 Continue to select as many annotations as desired for this trace. When finished, click **OK**.

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 channel or until they are changed (via the **OK** or **Apply** button). To apply the annotation changes to all open channels, click **Apply to All**. 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

The appearance of the trace (line type, color, etc.) can be changed in the **Appearance** tab in the **Data Graph Properties** window.

To change the appearance of a chromatogram or trace,

1. In the Chromatogram Window, right-click and select **Properties**. **The Data Graph Properties** window is displayed. See Figure 9-8.
2. Select the **Appearance** tab.

Figure 9-8 Data Graph Properties - Appearance Tab

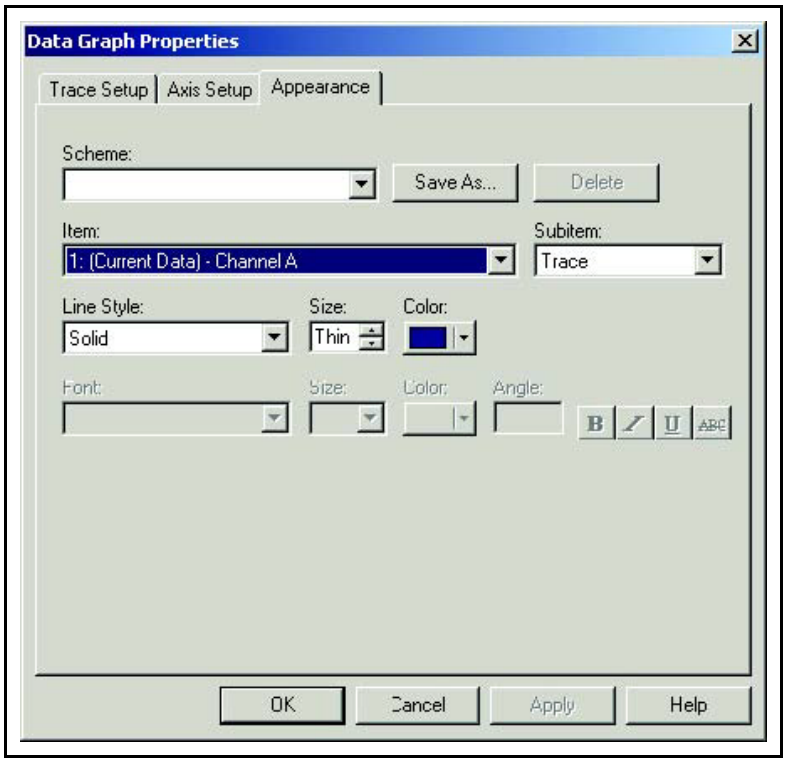

Table 9-2 Appearance Parameters

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	This drop-down menu provides options of which part of the chromatogram window to change . The choices include the graph itself (including background and legends) and the available traces.

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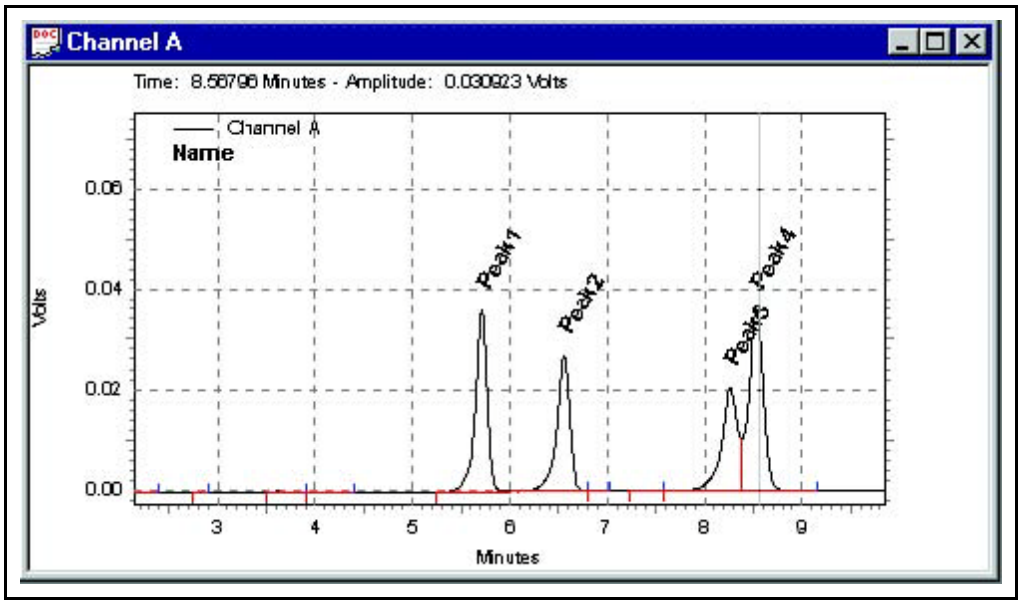
Table 9-2 Appearance Parameters (continued)

Sub-item	Use the drop-down 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 channel, access to setting appearances of sub-items such as baselines, start and stop tic 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 color and line type can be chosen. If **Annotation** is selected, the font appearance and color can be chosen.

Figure 9-9 Channel A Appearance



The appearance of any trace can be changed by right-clicking in the chromatogram window, then clicking **Appearance…**. A window identical to the one shown above for the **Appearance** tab will be displayed.

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

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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 major unit marks on the left Y-Axis.
Graph	Left Y-Axis Minor Ticks	Select a color for display of minor unit marks on the left Y-Axis.
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 major unit marks on the X-Axis.
Graph	X-Axis Minor Ticks	Select a color for display of minor unit marks on the X-Axis.
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.

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Table 9-3 Sub-items Available in the Appearance Tab (continued)

Item	Sub-Item	Description
Data	Baseline Start Tick	Select a color and/or line type for display of baseline start ticks.
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

The **Axis Setup** tab allows configuration of the appearance of the axis on the chromatogram. These settings apply to active traces. To change the Axis properties,

1 In the Chromatogram window, right-click and select **Axis Setup**. The **Axis Properties** window is displayed. See Figure 9-10.

Figure 9-10 Axis Properties Window

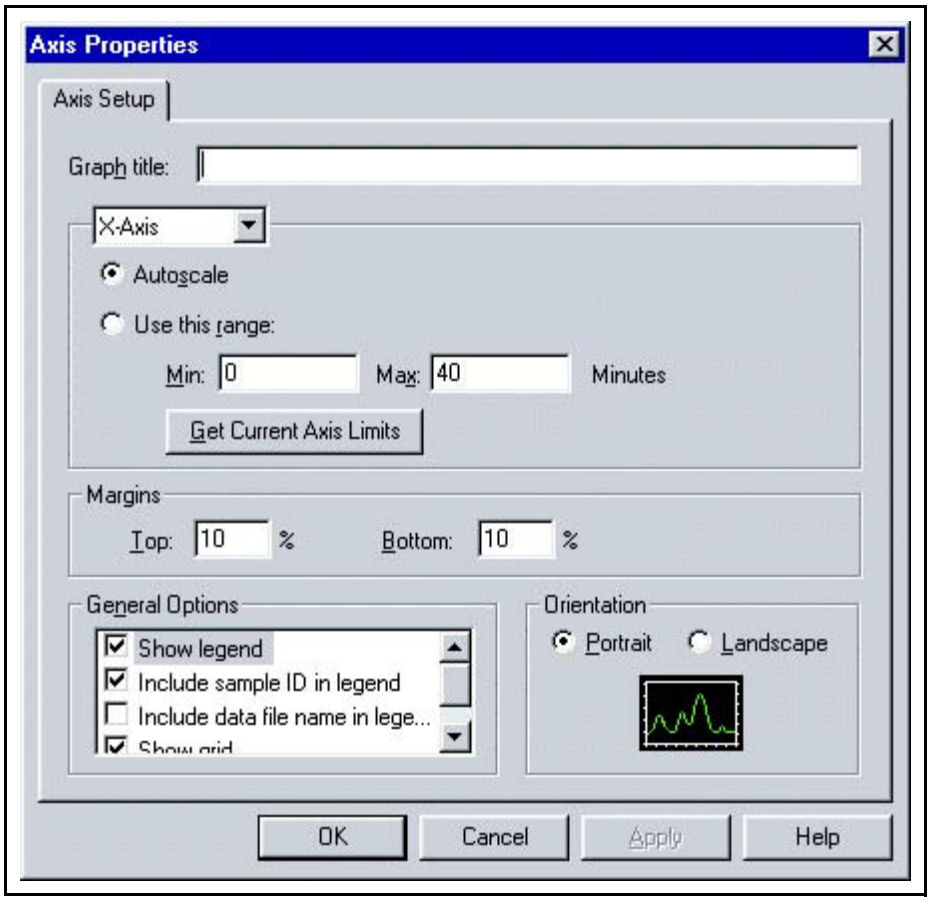

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Table 9-4 Axis Properties Parameters

Graph Title	Enter a title for the graph, if desired. This appears at the top of the graph.
Axis	From the drop-down list, 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 get 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)

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.

Figure 9-11 Chromatogram Window with Legend and Grid Displayed

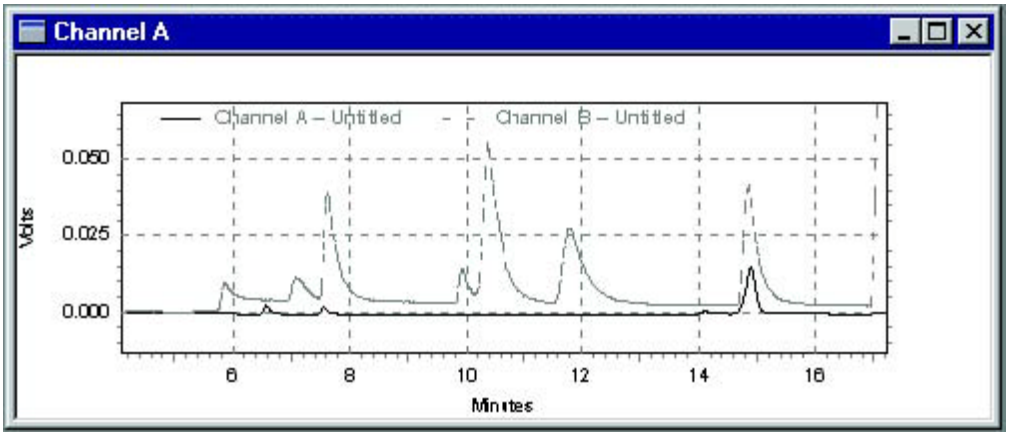
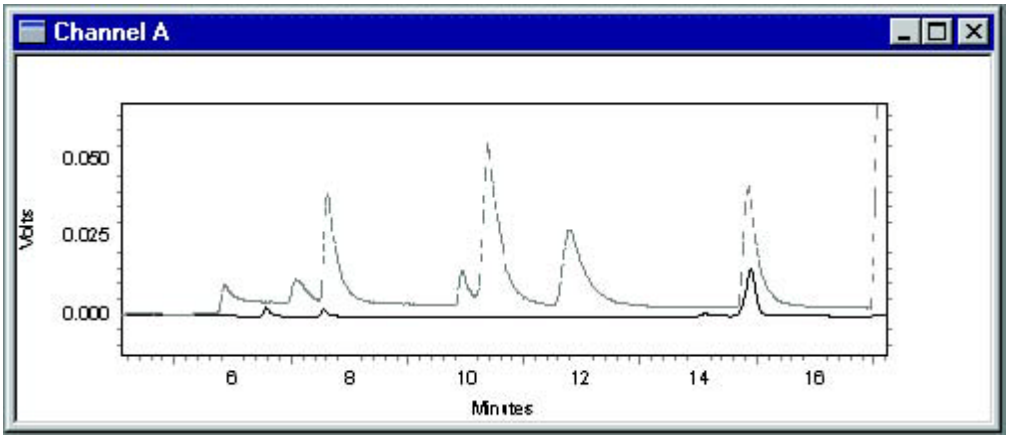


Figure 9-12 Chromatogram Window with No Legend or Grid Displayed



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

9.10 Change Data Graph Properties

Whenever a chromatogram or 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

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.

9.11 Set Up a Trace

The **Trace Setup** tab, see Figure 9-13, allows the addition and removal of traces as well as setting scaling options for the traces. 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.

Figure 9-13 Trace Setup Tab

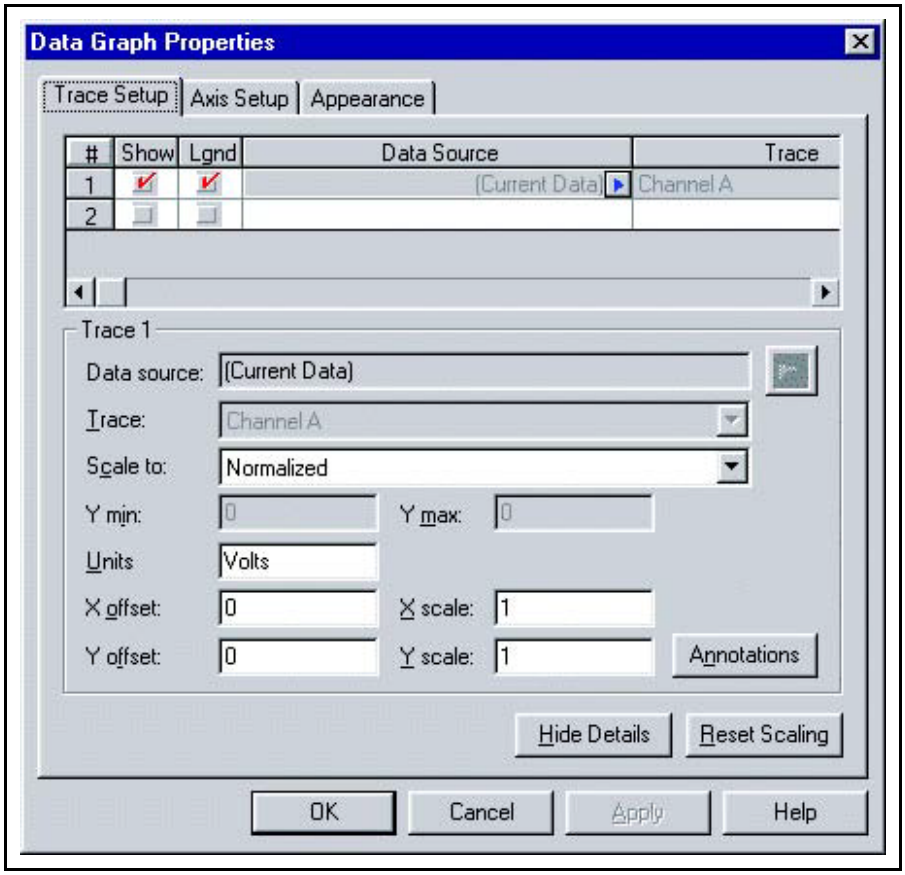


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Table 9-6 Trace Setup Parameters

Show	Select this box to display the trace in the chromatogram window. Clear this box to remove the trace from the chromatogram window. This is a convenient way to temporarily remove a trace from the viewing 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.
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 for display can be selected.
Current Method	Selects a trace from the current method (if available). For example, temperature profiles for instrument control.
Trace	Select the channel to be displayed.

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Table 9-6 Trace Setup Parameters (continued)

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**.
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.

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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.

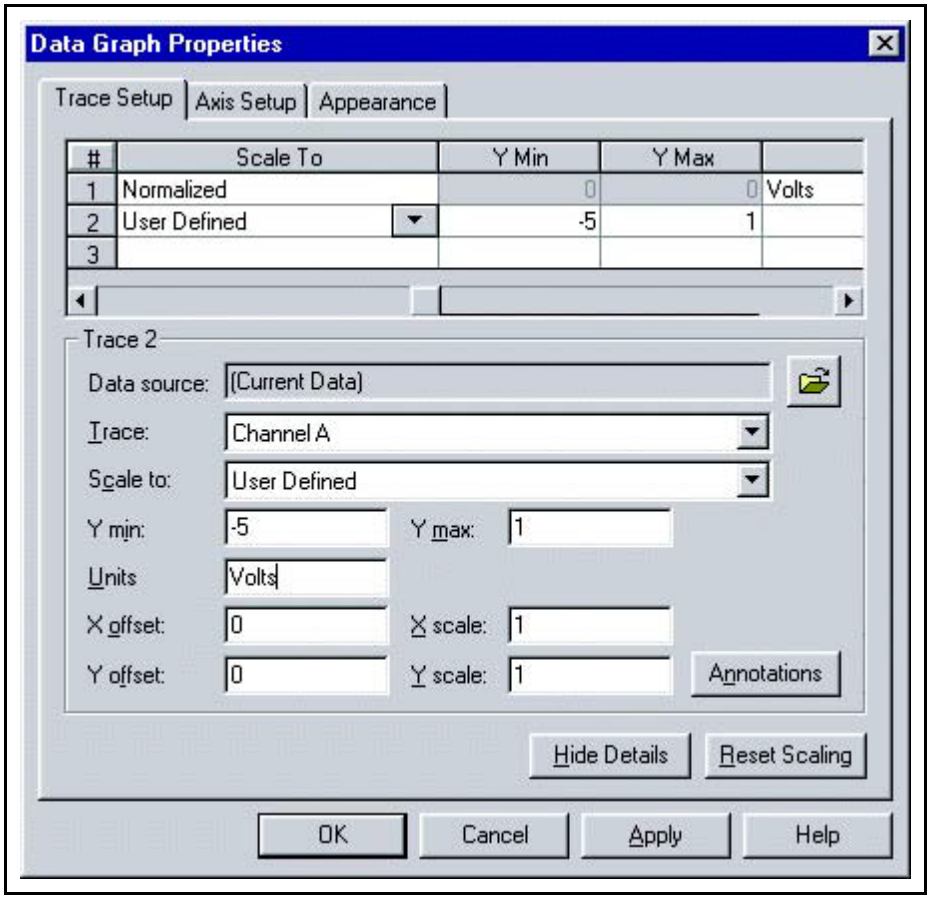
To completely remove a trace from the chromatogram window, select the row by clicking on the number, then press the **Delete** key, or click **Edit/Delete**. To temporarily remove the trace from the window, clear the checkbox in the **Show** column. Click **OK** to return to the chromatogram window.

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 9-14.
2. To set Y-Axis minimun and maximum values, select the **Trace Setup** tab. To set an absolute voltage range for all chromatograms, use the **User-Defined** option 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 this same voltage scale, enter the same values for all chromatograms.

Figure 9-14 Data Graph Properties Trace Setup Tab



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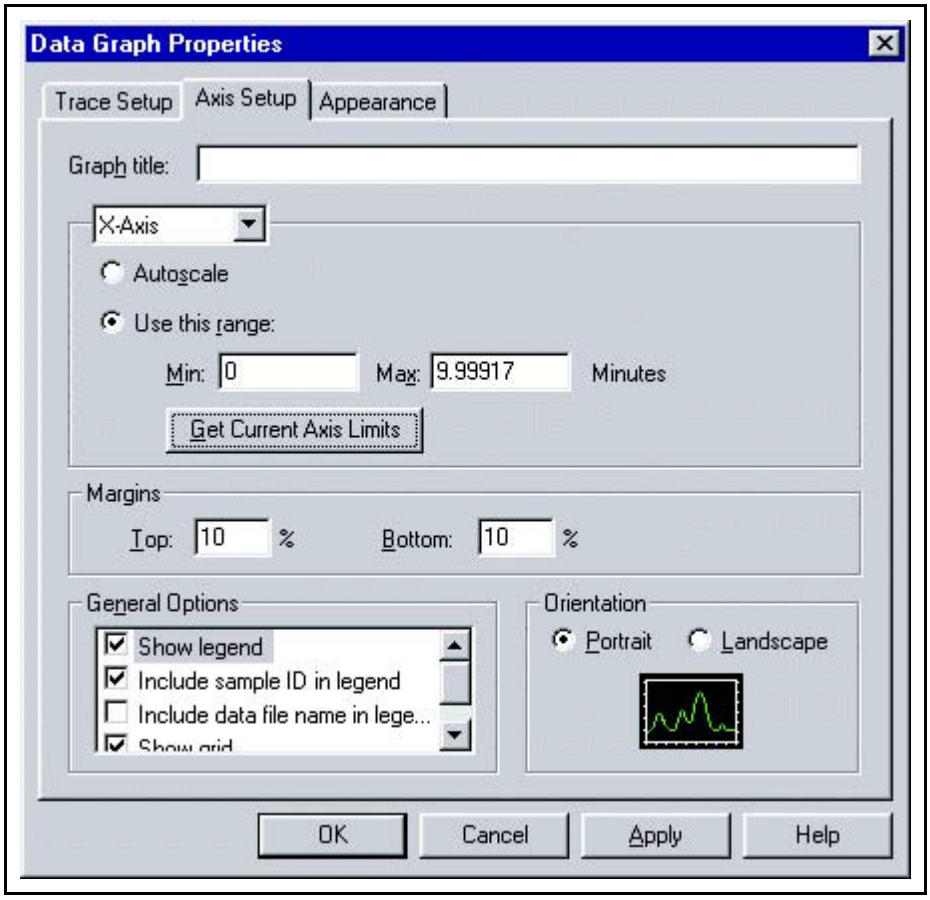
3 To set absolute ranges for the trace, select the **Axis Setup** tab, see Figure 9-15. Click **X-Axis**, to set the range for the X-Axis. Click **Autoscale** to set the X-Axis range automatically to the range of the longest chromatogram (the default selection), or click **Use this range** to enter an 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 9-15 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. Refer to Figure 9-14.

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Chapter 10
Chromatogram Operations

10.1 About Chromatogram Operations

Chromatogram comparison 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

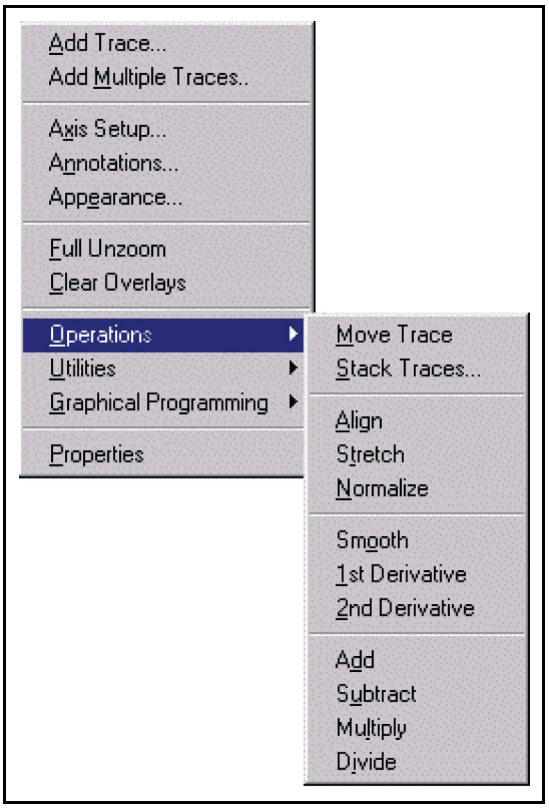

Table 10-1 Operation Actions

Operation	Action
Move Trace	"Grab" 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.

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Table 10-1 Operation Actions (continued)

Operation	Action
Nomalize	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.
Smooth	Performs a 9-point Savitsky-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.

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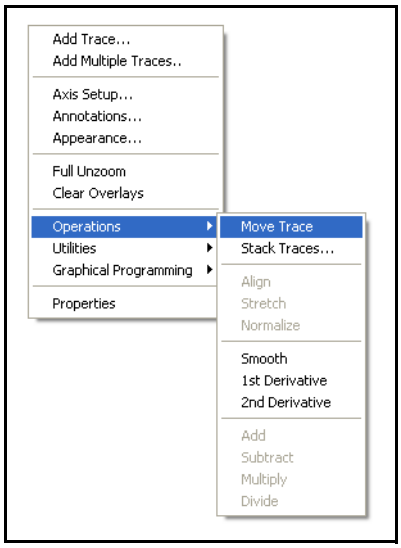
10.1.1 Move a Trace

To "grab" a trace and move it:

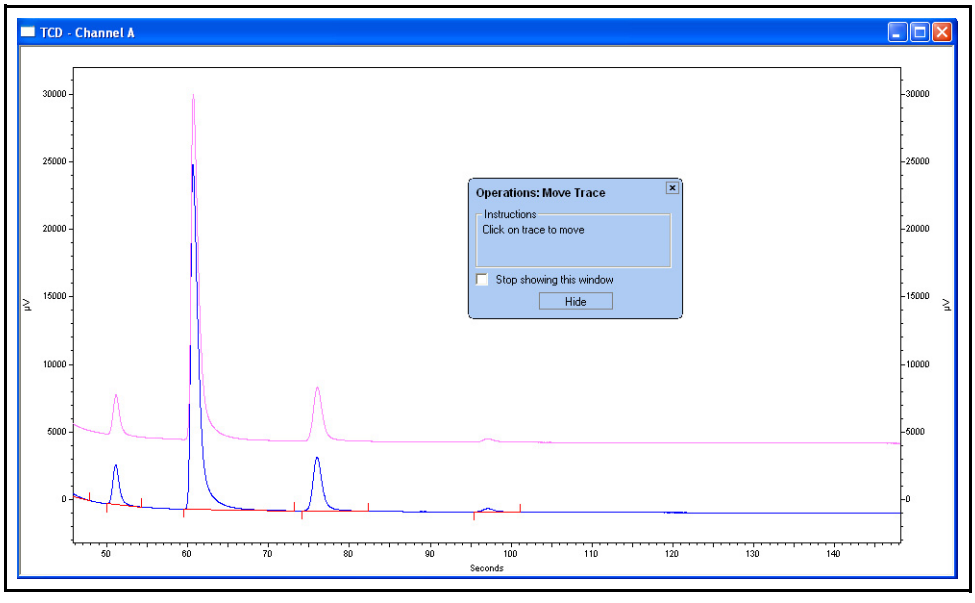
1 In the chromatogram window, right-click and select **Operations >> Move Trace**. See Figure 10-2.

Figure 10-2 Move Trace Utility



2 The **Operations: Move Trace** window will appear in the the upper right corner of the chromatogram window. Move the pointer over a trace until the pointer changes to a pointer with a cross with arrows at the end. See Figure 10-3.

Figure 10-3 Move Trace



3 Grab the trace by pressing the left mouse button and dragging the trace to a new location. When the mouse button is released, the trace will be placed at the pointer location.

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

10.1.2 Stack Traces

To change the X-axis and Y-Axis offset for a trace:

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

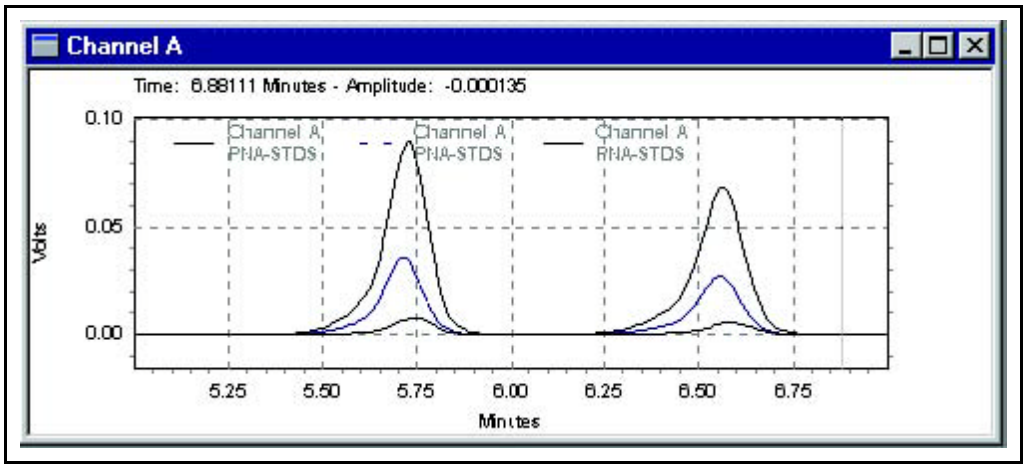
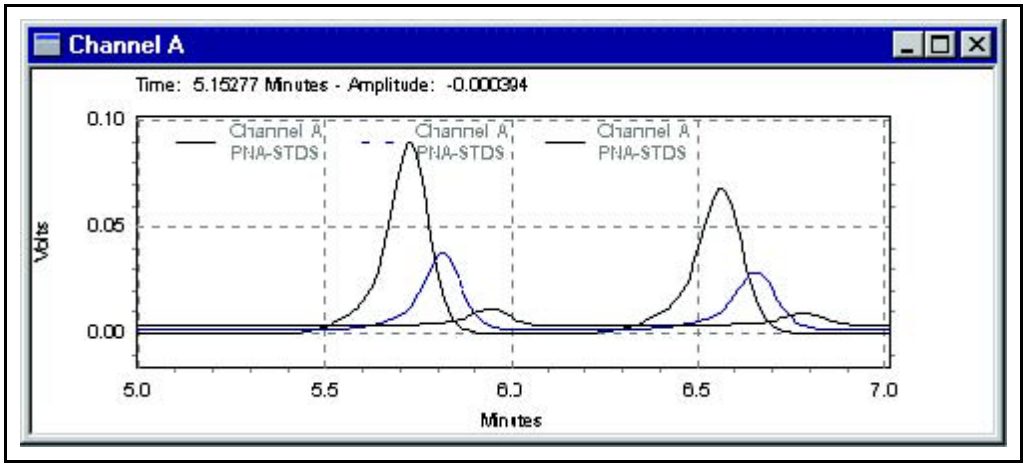


Figure 10-5 Chromatograms After Stacking



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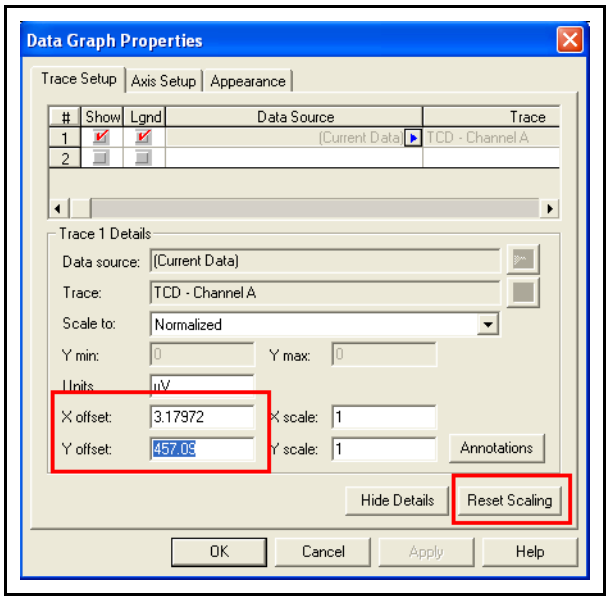
10.1.2.1 To Remove Offsets

1. In the chromatogram window, right-click and select **Properties**.
2. Select the **Trace Setup** tab, then scroll to the right to the X-Axis and Y-Axis offset columns when the settings can be modified or deleted. See Figure 10-6.

Figure 10-6 Remove Offsets



3. Click **Reset Scaling** to restore all settings to their original values. Or, the **Stack** command can be used again by entering "0" for both stack parameters.

10.1.3 To Align Two Traces

To align one chromatogram to another:

1. In the chromatogram window, right-click and select **Operations >> Align**. Click a peak on the first chromatogram to align to, then click on a 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.
2. 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 the X-Axis and Y-Axis offset columns to delete or change these settings. Click **Reset Scaling** to restore the original settings. See Figure 10-7 and Figure 10-8.

Figure 10-7 Chromatograms Before Alignment

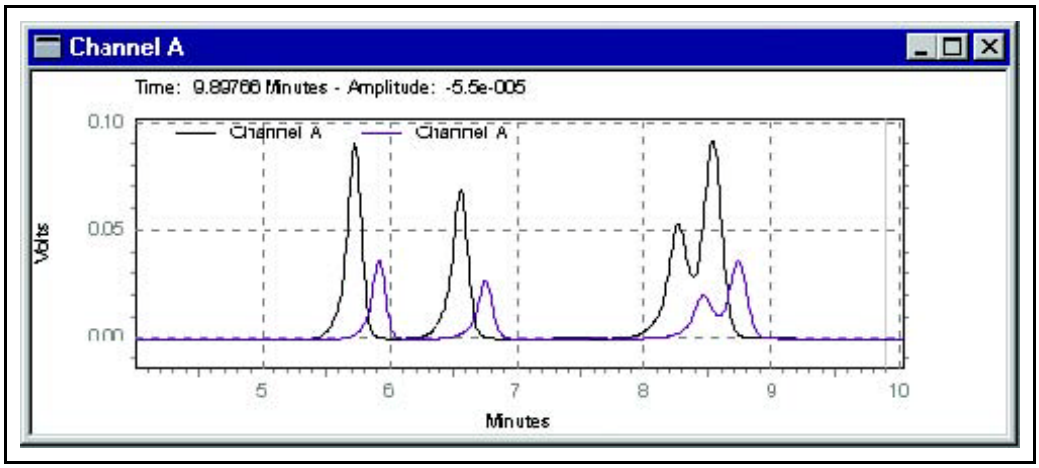
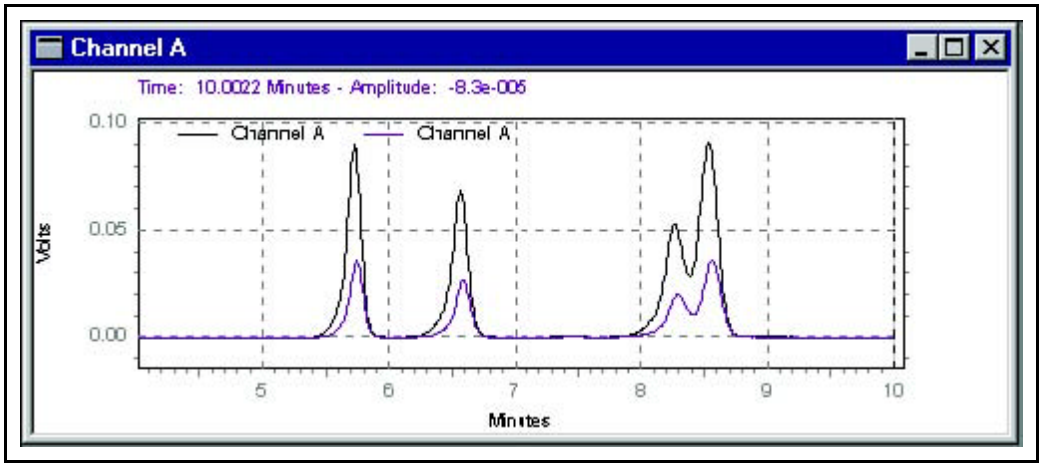


Figure 10-8 First Peak of Top Chromatogram Aligned to First Peak on Bottom Chromatogram



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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**.
2. Select peaks on the first chromatogram to which the second will be stretched (or contracted).
3. Select two peaks on the second chromatogram. The chromatogram between these two peaks will be stretched or contracted to fit the two peaks specified on the original chromatogram.

10.1.4.1 To Undo the Stretch,

1. In the chromatogram window, right-click and select **Properties**. Select the **Trace Setup** tab, then scroll to the right to the X-axis and Y-axis offset columns where the stretched or contracted settings can be changed or deleted. Click the **Reset Scaling** button to restore all settings to their original values. See Figure 10-9 and Figure 10-10.

Figure 10-9 Chromatograms Before Stretching

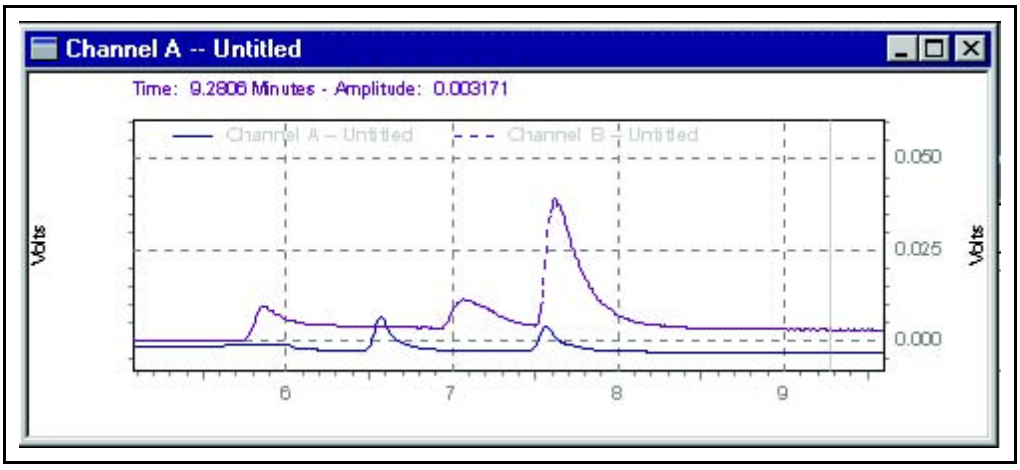
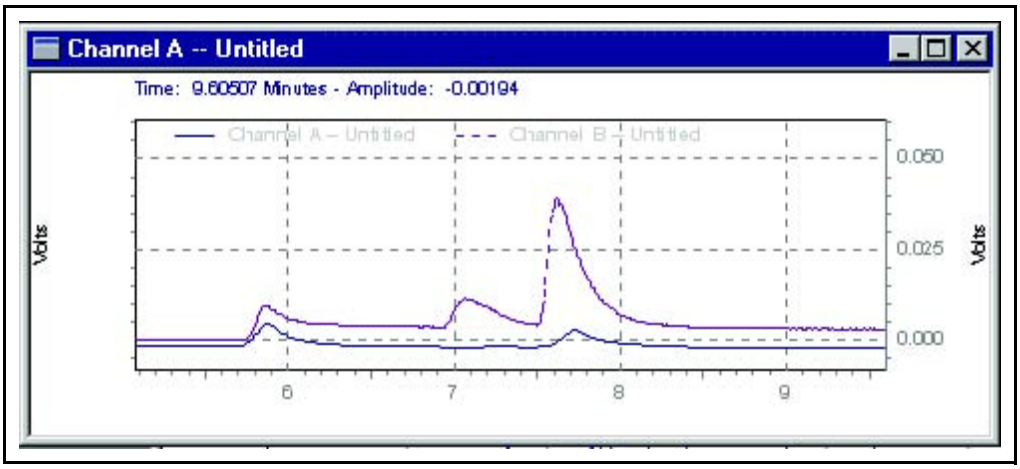


Figure 10-10 Bottom Chromatogram Stretched Relative to Top Chromatogram



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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 height of a selected peak matches that of the peak selected on the first trace. Once **Normalize Traces** is selected, the user will be prompted to select the start and the apex of a peak in the first trace. Then a prompt will appear to click on the start and apex of a peak in the second trace for normalization.

To undo the normalization, right-click and select **Properties** to view the trace spreadsheet. Select the **Trace Setup** tab, then scroll to the right to the X-Axis and Y-Axis offset columns where these settings can be deleted or changed. Click **Reset Scaling** to restore all settings to their original values. See .Figure 10-11 and Figure 10-12

Figure 10-11 Chromatograms Before Normalization

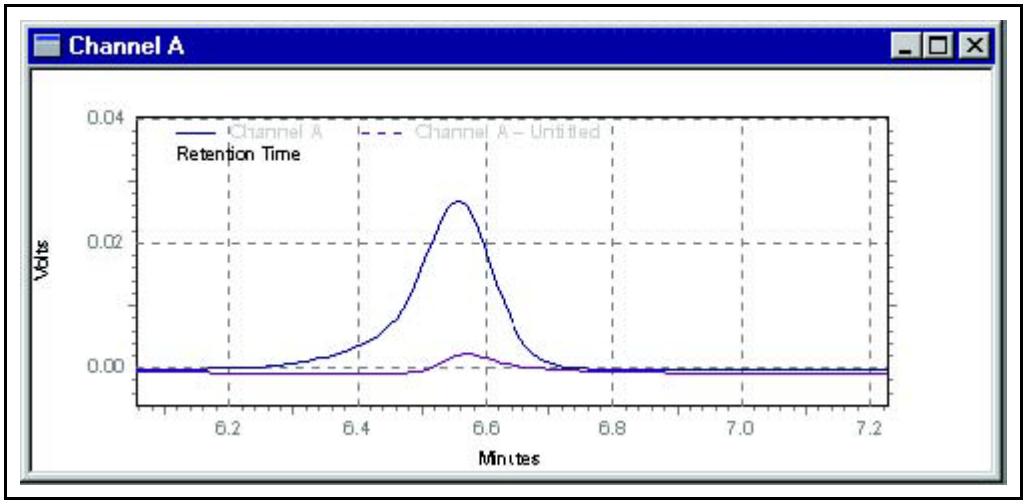
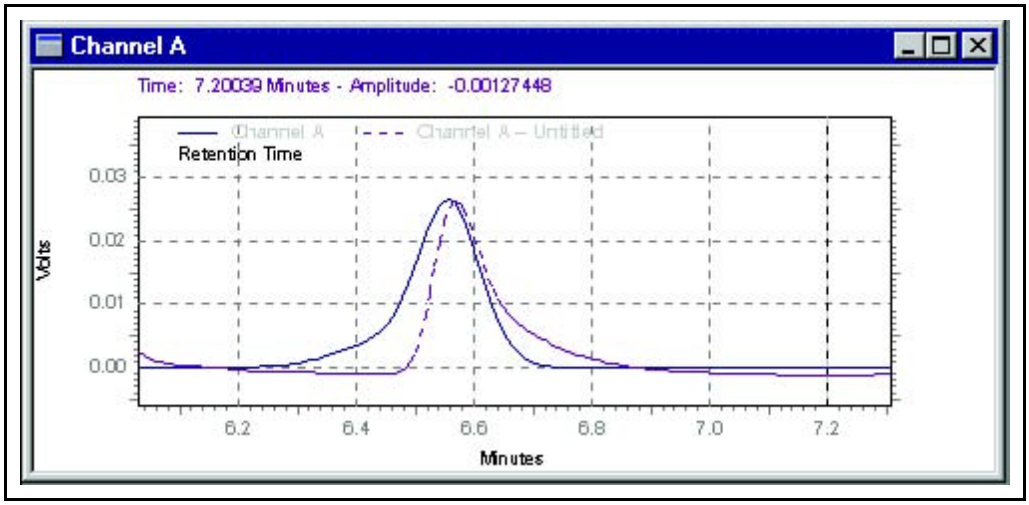


Figure 10-12 After Normalization



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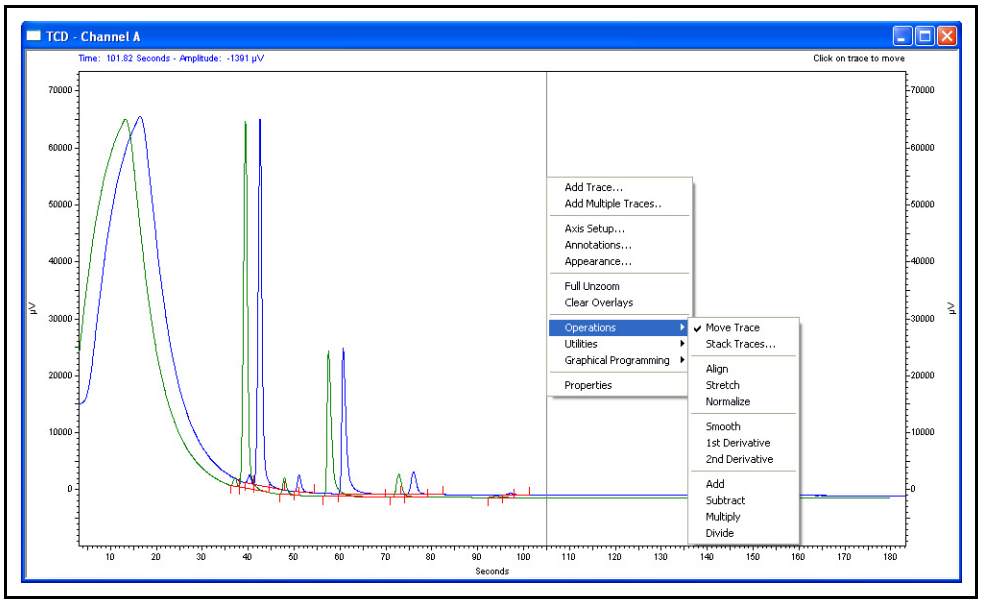
10.2 Perform Mathematical Operations on Traces

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 Savitsky-Golay smoothing operation on a selected data file:

1. In the chromatogram window, right-click and select **Operations >> Smooth**. A **Click on trace** prompt will be displayed
2. Click on the chromatogram to be smoothed. The resultant trace will appear in the window. See Figure 10-14 and Figure 10-15.

Figure 10-14 Chromatogram Before Smoothing

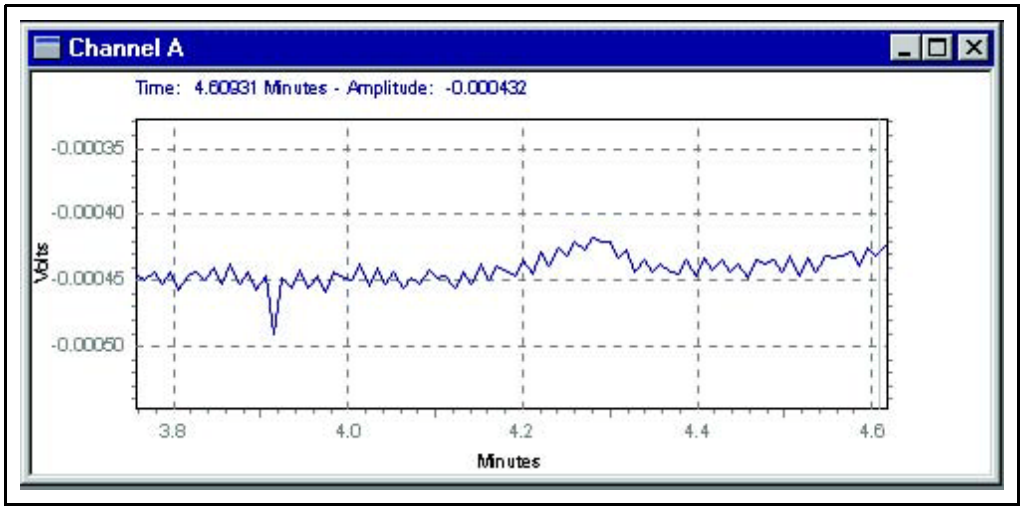
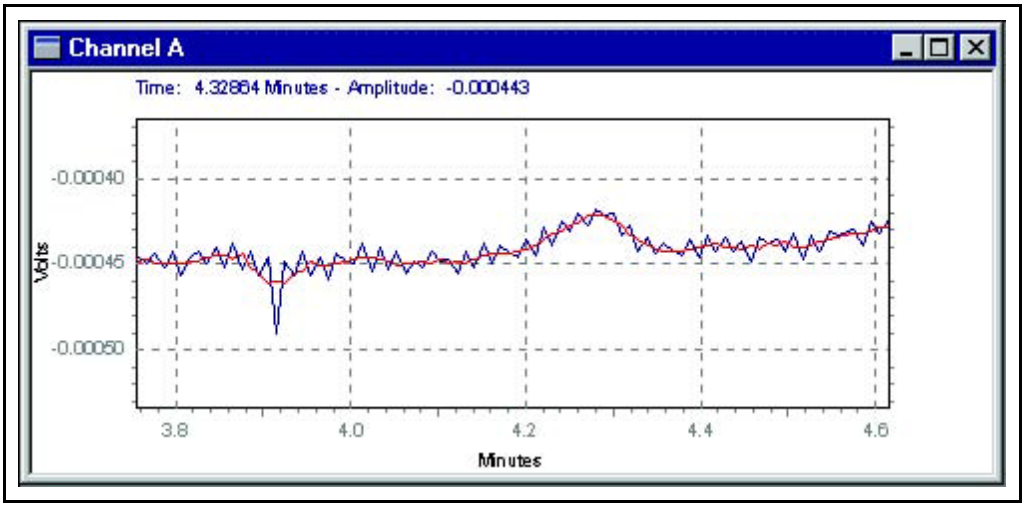


Figure 10-15 Smoothed Result Trace is Displayed with Original Trace



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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**. A **Click on trace** window will be displayed.
2. Click on the chromatogram to perform the operation. The resultant trace will appear in the window. See Figure 10-16, Figure 10-17 and Figure 10-18.

Figure 10-16 Trace Before 1st Derivative

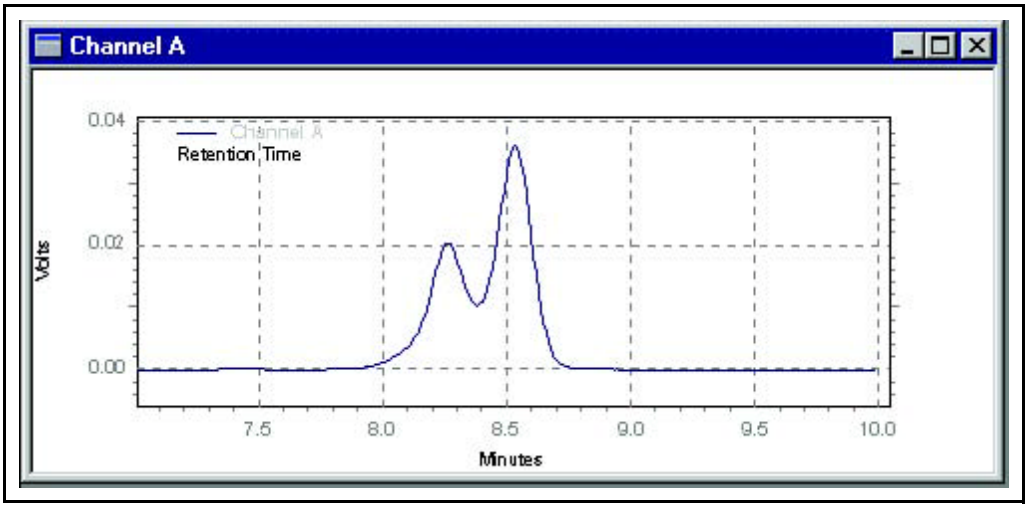


Figure 10-17 1st Derivative Trace Displayed with Original Trace

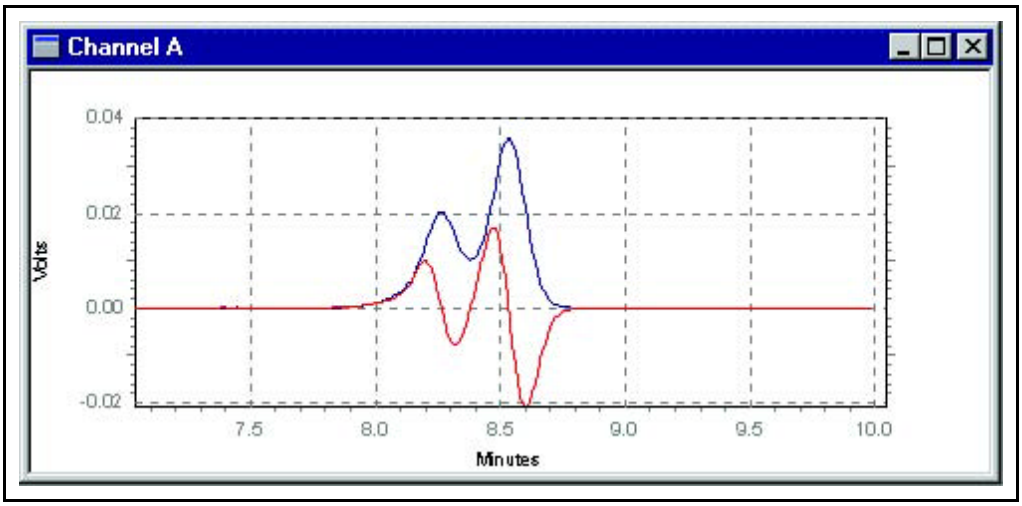
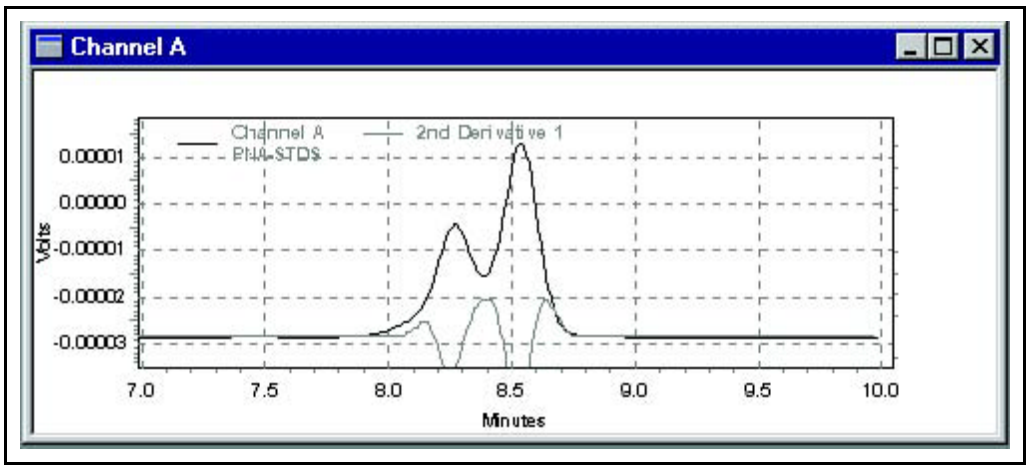


Figure 10-18 2nd Derivative Displayed with Original Trace



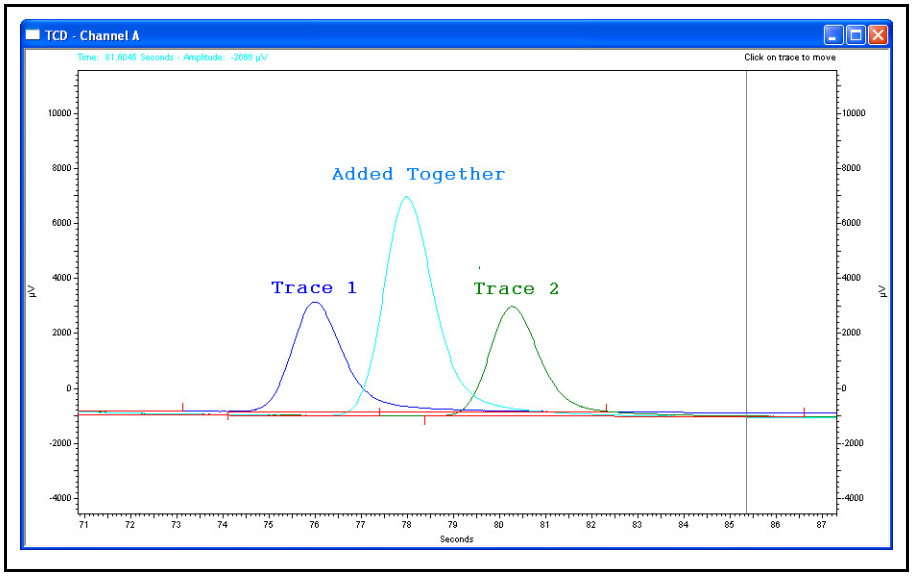
10.2.3 Add Two Traces

To add two traces to a chromatogram window:

1. In the chromatogram window, right-click and select **Operations >> Add**.
2. Click on first trace to select it.
3. Click on the second trace, which will be added to the first trace. The resulting trace will appear in the window. See Figure 10-19.

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

Figure 10-19 Adding Two Traces



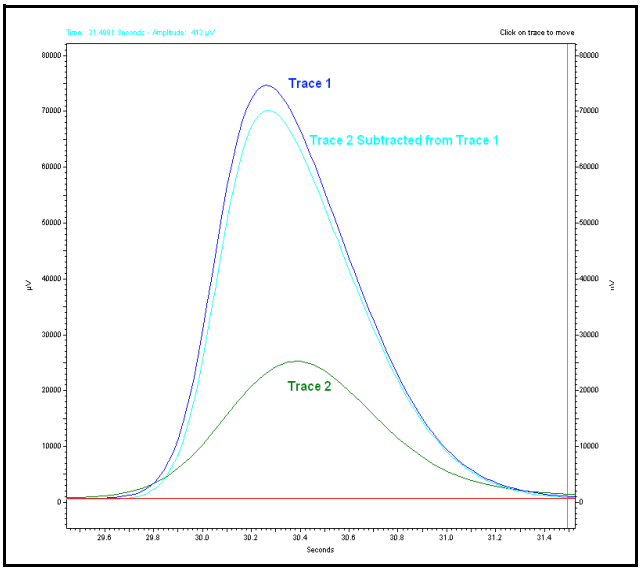
10.2.4 Subtract Two Traces

To subtract two traces:

1. In the chromatogram window, right-click and select **Operations >> Subtract**.
2. Click on the first trace to select it.
3. Click on the second trace, which will be subtracted from the first trace. The resultant trace will appear in the window. See Figure 10-20.

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

Figure 10-20 Subtract Two Chromatograms



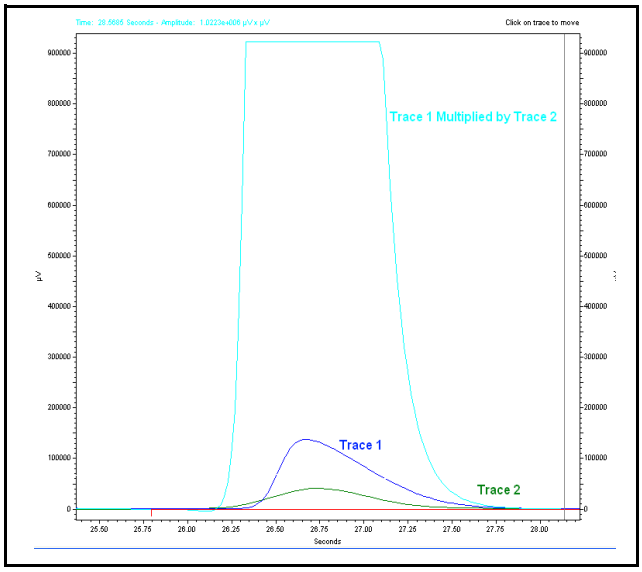
10.2.5 Multiply Two Chromatograms

To multiply two chromatograms:

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

   NOTE: For the multiply operation, the units of the resultant chromatogram are <chromatogram1 units> x <chromatogram 2 units>. See Figure 10-21.

Figure 10-21 Multiple 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 10-22 and Table 10-2.

Figure 10-22 Utilties Parameters

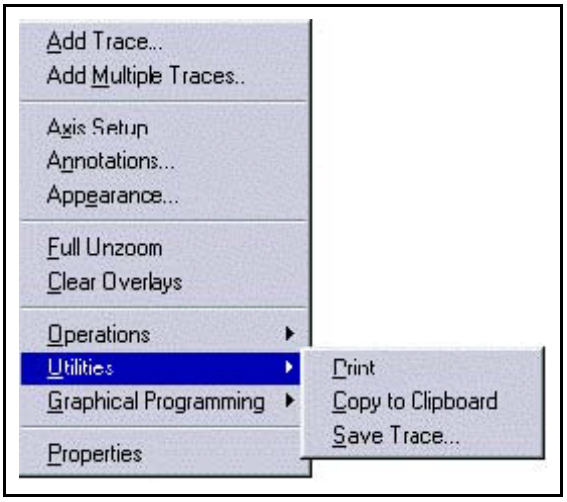

Table 10-2 Utilities

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 on a trace then opens the save data file window.

10.3.1 Print

This command sends the current chromatogram window view to the printer.

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**.

This command copies the current chromatogram window to the clipboard as a metafile. From here, view can 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**.

10.3.3 Save Trace

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

1. From the **Utilities** menu, click **Save Trace**.
2. Click on the trace to save.
3. In the **Save Data File As** window, browse to the location for saving the file and enter a name for the file.

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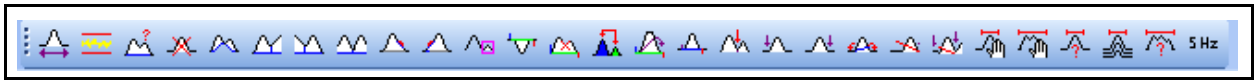
Chapter 11
Graphical Programming

11.1 About Graphical Method Programming

The **Graphical Programming** menu is used to add timed 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. To turn on the Graphical Programming Toolbar,

1. From the menu, click **View >> Preferences**.
2. Click **Int Events** and then click **Toolbar**. See Figure 11-1 and Table 11-1.

Figure 11-1 Int Events Tool Bar



Parameters that can be set using graphical programming include:

Table 11-1 Graphical Programming Parameters

Command	Action
Width	Inserts a Width event at the point on the chromatogram.
Threshold	Inserts a Threshold event at the point on the chromatogram.
Shoulder Sensitivity	Inserts a Shoulder Sensitivity event at the point on the chromatogram.
Integration Off	Turns off integration at the point on the chromatogram.
Valley to Valley	Turns on valley to valley baseline detection.
Horizontal Baseline	Forces a horizontal baseline from the point on the chromatogram.
Backward Horizontal Baseline	Forces a backward horizontal baseline from the point on the chromatogram.
Lowest Point Horizontal Baseline	Forces a horizontal baseline at the next lowest point.
Tangent Skim	Forces a tangent skim.
Front Tangent Skim	Forces a front tangent skim.
Minimum Area	Set a minimum area for peak detection.
Negative Peak	Turn on negative peak detection.

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Table 11-1 Graphical Programming Parameters (continued)

Command	Action
Disable Peak End Detection	Disables the end of peak detection.
Reassign Peak	Designates 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	Adjusts 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

There are two ways to acquire data. One way is with a sequence (for multiple runs), and the other way is to make a single run. To make a single data acquisition run, specify the method to be used for analysis, and a filename for data storage.

NOTE: In order to use a method for data acquisition, its **Instrument Setup** should have the acquisition channel turned **On**, and a sampling rate and run time designated.

To make a single run, click the **Single Run** icon  or click **Control >> Single Run**. The **Single Run Acquisition** window is displayed, see Figure 12-1 and Table 12-1.

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Figure 12-1 Single Run Acquisition Window

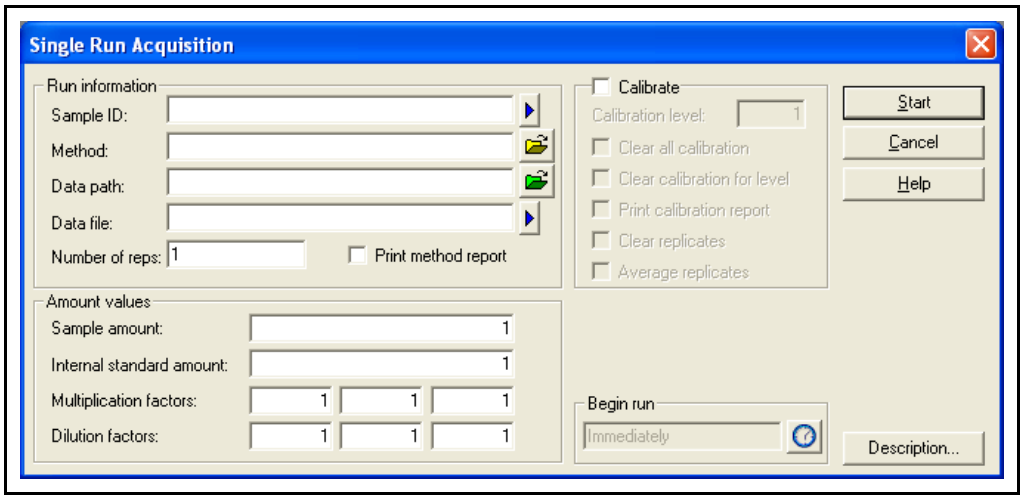

Table 12-1 Single Run Acquisition Parameters

Run information	Used to specify various files for the run.
Sample ID	Enter 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 ID's.
Method	Enter the name of the method to be used for data acquisition and processing. Include the entire path name if the method is not in the default method directory. Select the method from a list of available methods by clicking the **File** icon adjacent to the field.
Data Path	Enter a path name where the data acquired for this run will be stored. Click the **File** icon to select a path from a listing of available paths.
Data File	Enter a filename for the data to be saved on disk. Select from one of the predefined names by clicking the arrow button adjacent to the field. 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.

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Table 12-1 Single Run Acquisition Parameters (continued)

Number of reps	Enter the number of runs to conduct. The runs will automatically proceed without review until completed, incrementing each filename as designated. 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, setting 4 runs with starting run number of 101, then aborting during run 102, upon restarting the next run number will be 105. 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.
Amount Values	Enter values that affect how the concentrations are calculated. 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.

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Table 12-1 Single Run Acquisition Parameters (continued)

Calibrate	Select this box if the sample is to be a calibration sample. Once this box is selected, the following fields and options will be available.
Calibration level	Enter the number of the calibration levels represented by this calibration standard. If this is a single level calibration, enter 1.
Clear all calibration	Select this box to clear all existing calibration factors from the method before running the sample.
Clear calibration for level	Select this box to clear the existing response factors 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.
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 **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 or from the **Control** menu, click **Sequence Run...**. The **Run Sequence** window is displayed. See Figure 12-2 and Table 12-2.
2. Enter 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

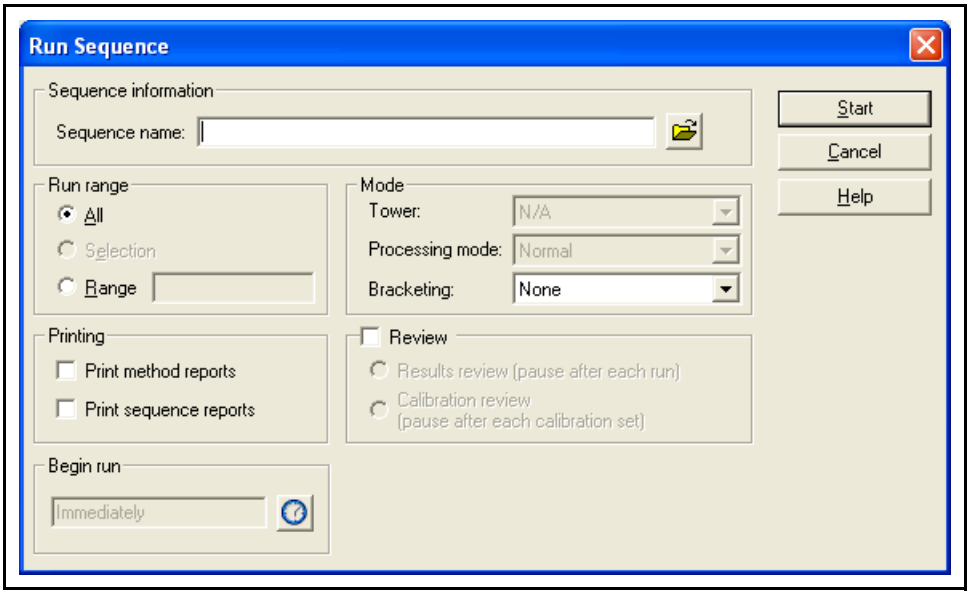

Table 12-2 Run Sequence Parameters

Sequence information	Enter 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)

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 this to NOT bracket calibrations.
Standard	Select this to perform the standard mode of bracketing calibrations.
Std. w/Clear Calib	Select this to perform the standard mode of bracketing calibrations, clearing the calibration before the start of each calibration set.
Sequence	Select this to perform the sequence mode of bracketing calibrations.
Seq. w/ Back Calc	Select this 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 in order 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)

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 where the time to start the sequence can be entered or selected.
Email Recipient(s)	Use this field to enable e-mail notification to be sent to a designated address (entered in the To: field). Select the **On Start** box to send e-mail notification when the sequence starts. Select the **On Stop or Error** box to send e-mail notification when the sequence stops or if an error occurs. When the window is completed, click **Start** to initiate the sequence acquisition. The data is displayed in real time in the chromatogram window(s), if the current data is selected for viewing.

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12.4 Stop a Run in Progress

NOTE: STOP cannot be accessed by anyone other than the instrument controller.

To stop data acquisition during a run:

1. Click the **STOP** icon, on the command toolbar, when the run is in progress, or click **Control >> Stop Run**. The **Stop Run** window is displayed. See Figure 12-3 and Table 12-3.

   NOTE: When using the **STOP** icon, press the left mouse button down until the **STOP** icon changes appearance before releasing the mouse button.

2. Select the desired manner to stop the run.

Figure 12-3 Stop Run Window

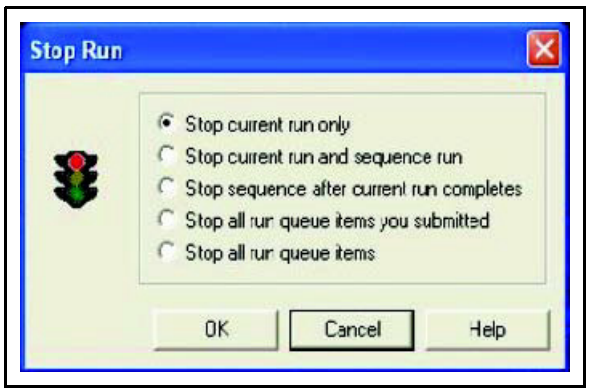

Table 12-3 Stop Run Parameters

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 it's 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 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.

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Table 12-3 Stop Run Parameters (continued)

Stop all run queue items	This selection stops the run currently in progress, and terminates all items in the run queue. **NOTE:** When a run is stopped, the data up to that point is saved in the data file. However, no analysis of the data will be performed. To produce a report or view results from a run that was stopped, Analyze the data file.

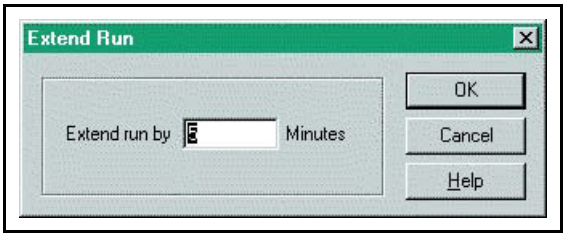
12.5 Extend Run

NOTE: If the current user is not the instrument controller, or the current user is using an instrument offline, the current user does not have access to **Extend Run**.

While a run is in progress, data acquisition can be extended beyond the designated run time by:

1. Click **Control >> Extend Run**.
2. The **Extend Run** window is displayed. See Figure 12-4.
3. Enter the number of minutes to extend the run, then click **OK**.

Figure 12-4 Extend Run Window



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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 4, Program Architecture and Data Structure, and Chapter 5, Opening and Saving Files.

NOTE: This Tutorial assumes:

- That EZ IQ is installed with all instruments installed and properly configured
- The PC running EZ IQ is connected to a 3000 Micro GC instrument via the TCP/IP connection
- The 3000 Micro GC enhanced driver is loaded for the EZ IQ configuration. See Chapter 8, Acquisition Parameter Setup, for the procedure to load a 3000 Micro GC configuration using EZ IQ.

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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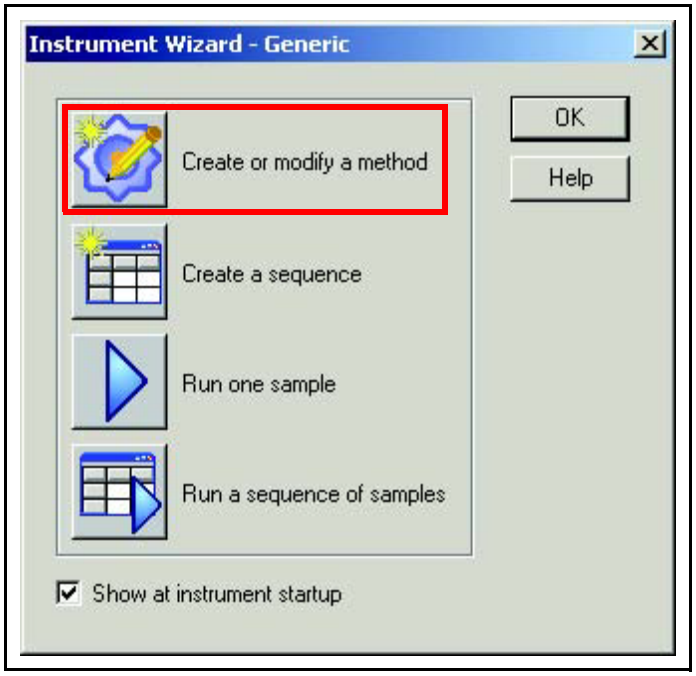
13.2 Instrument and Method Wizards

Instrument and Method Wizards 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.

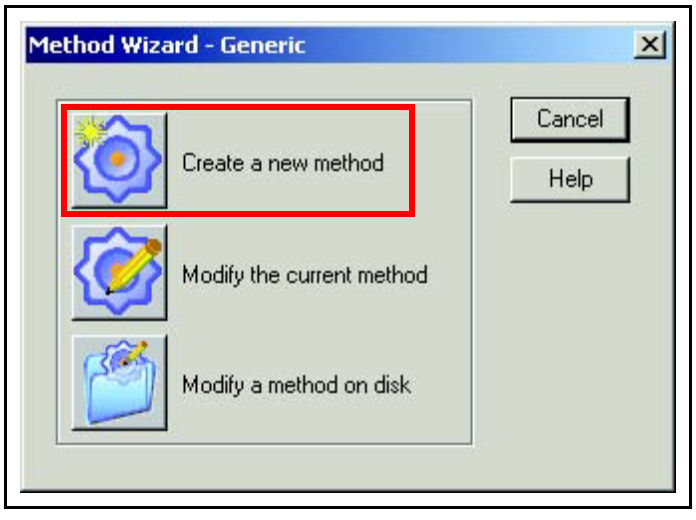
The **Method Wizard** is started from the **Instrument Wizard** by clicking **Create or Modify a Method**. See Figure 13-1.

Figure 13-1 Instrument Wizard



The **Method Wizard** window will display. See Figure 13-2.

Figure 13-2 Method Wizard



Click **Create a New Method** to start creating the tutorial method.

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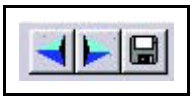
When **Create a New Method** is selected, the Method Wizard sets up icons in the application window that allow the user to "step" through all windows of method generation. A **Save** icon is also provided. See Figure 13-3.

Figure 13-3 Step and Save Icons



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 will acquire data with a long enough run time for the last peak to elute, using the default data acquisition sampling rate (which is adequate for most samples except for fast capillary runs).

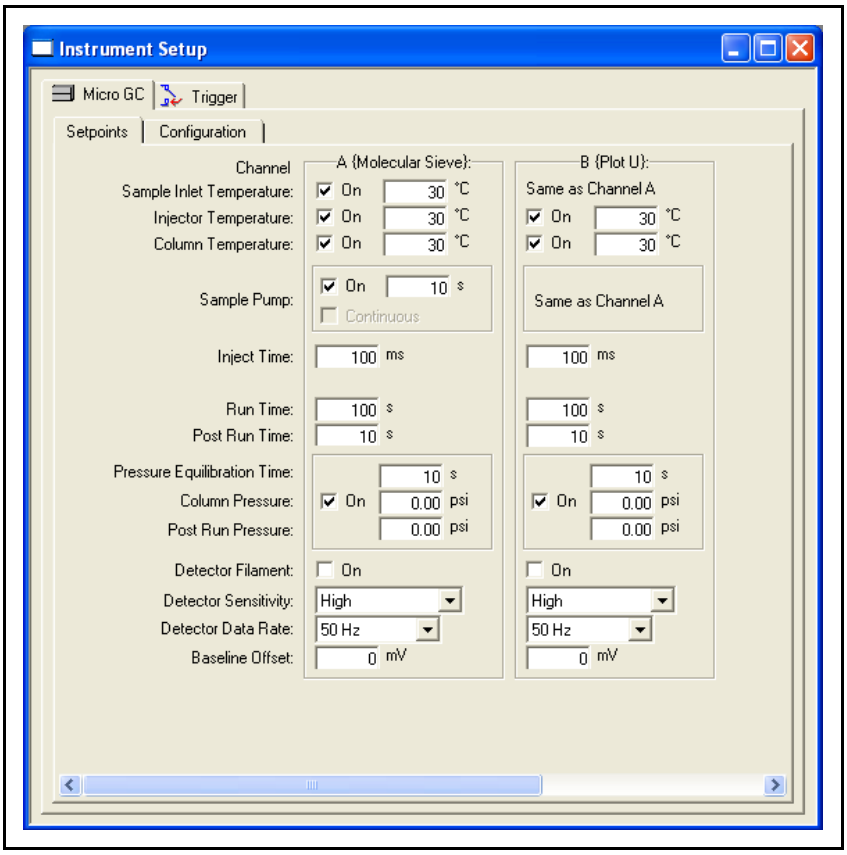
NOTE: Skip this step and use data and method files provided if there is no access to an instrument.

13.3.1 Acquisition Setup

To set acquisition run time and sampling rate, go to the **Instrument Setup** window. See Figure 13-4. This is the first window displayed when using the **Method Wizard**. Or, click **Method >> Instrument Setup**, or click the **Instrument Setup** icon.

NOTE: The tabs and contents of the **Instrument Setup** area will vary depending on the type of instrument and its configured modules.

Figure 13-4 Instrument Setup Window



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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

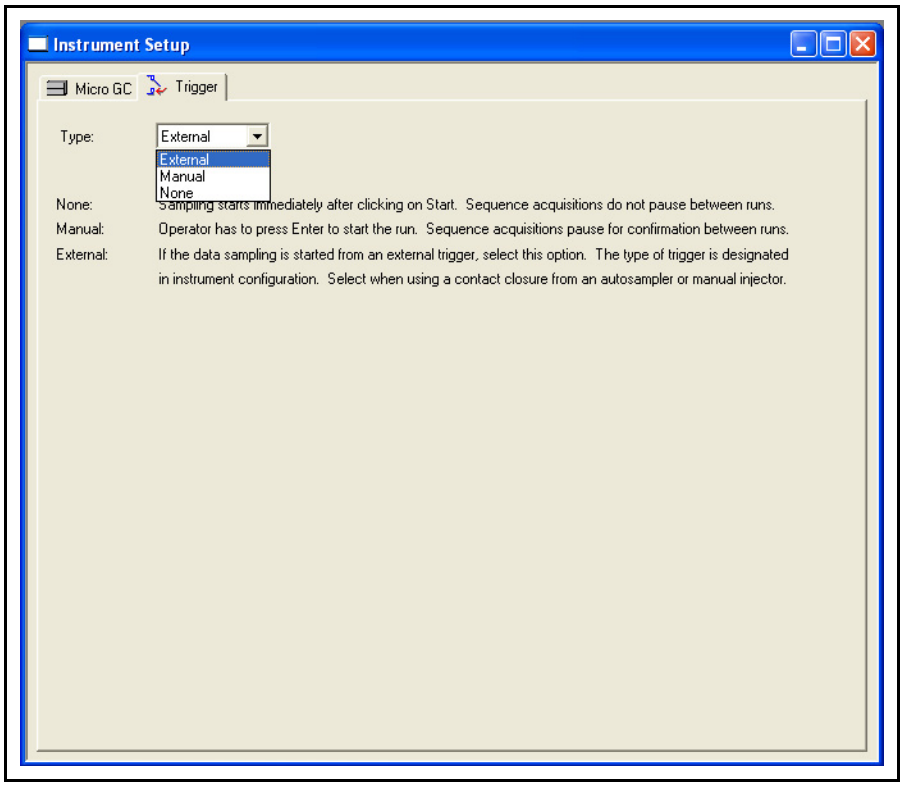

Table 13-1 Trigger Tab Parameters

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, click the **X** box in the upper right hand corner of the tab window to exit the window.

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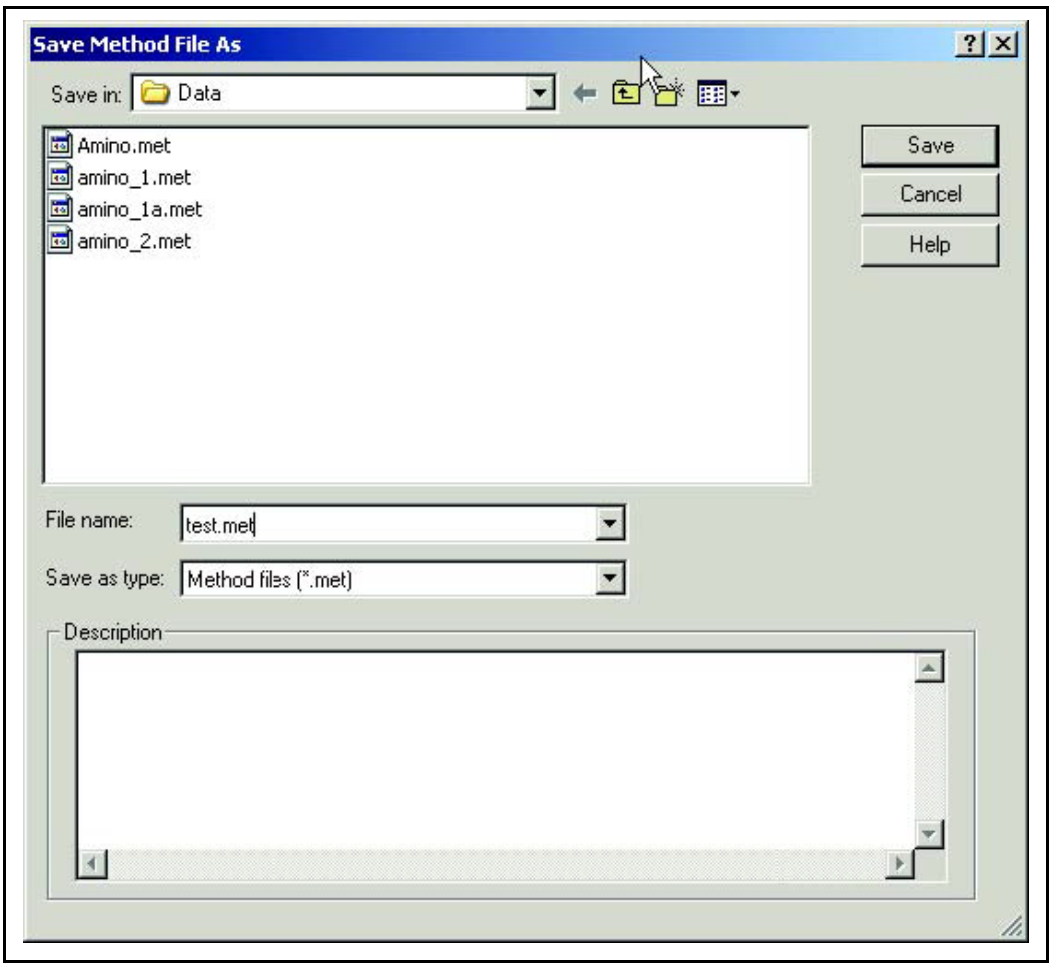
13.3.2 Save the Method

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

Figure 13-6 Save Method File As Window



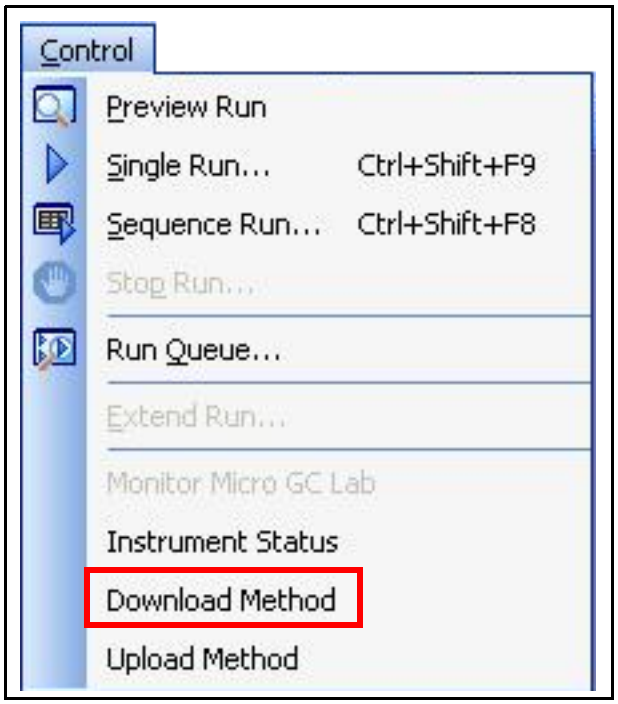
Select the folder in which to save the method file. In the **File name** field, enter **Test.met** as the filename for saving the method.

13.3.3 Downloading a Method

When a new method is created, or when a method is opened, it must be downloaded to the 3000 Micro GC to make it available on the instrument.

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

Figure 13-7 Downloading a Method



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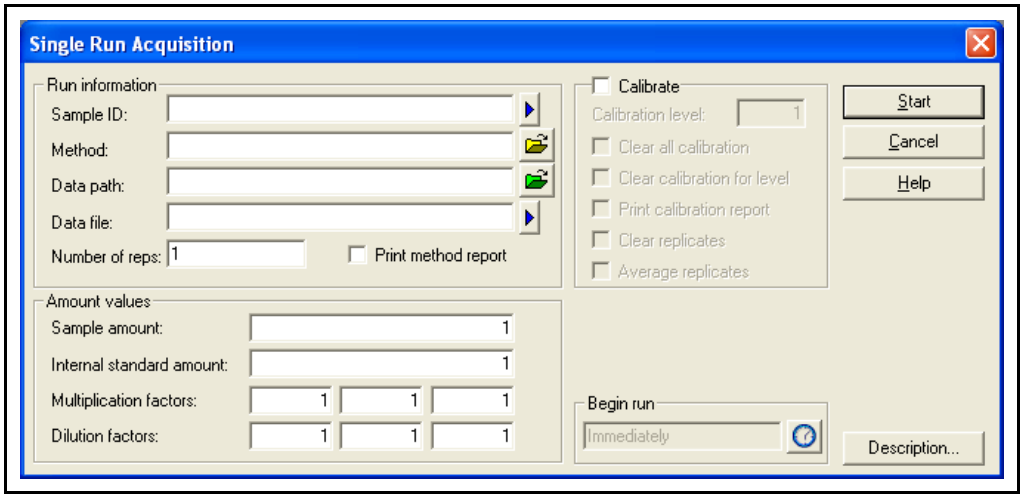
13.3.4 Run a Preliminary Sample

The data acquisition method (**Test.met**) will be used to make the first data acquisition run. To aid in later steps of the Tutorial, it is best to run a standard sample for the first acquisition run.

1 To start the run, click **Control >> Single Run**. Refer to Figure 13-7. The **Single Run Acquisition** window is displayed. See Figure 13-8.

Figure 13-8 Single Run Acquisition Window



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

3 In the **Method** field, either enter **Test.met**, along with its path, or select the **Test.met** file from a file list by clicking the **Open 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 **Open 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.

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 Timed 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 the **Multi calibration.dat** file provided with the software.

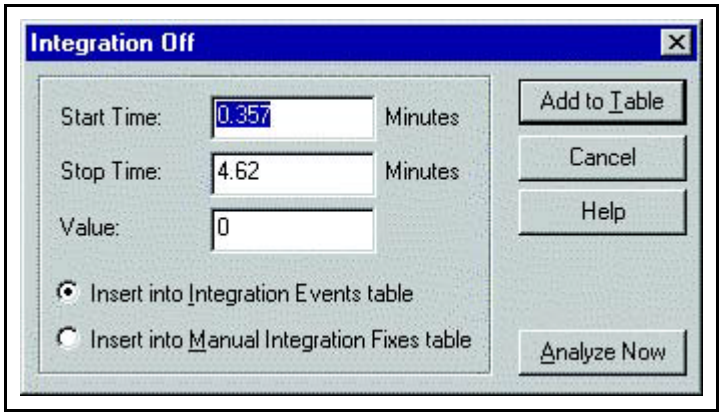
1. At this point, the recently acquired chromatogram will be displayed in the chromatogram window. If it is not, click **File** >> **Data** >> **Open...** and then select the data file from the list displayed. Alternatively, one of the files supplied with EZ IQ can be selected.

2. Click **Analyze** to integrate the chromatogram and display the baselines.

   NOTE: If an icon's function is unknown, hover the pointer over the button and a Tooltip will display showing the icon's name or function.

3. To add the **Integration Off** timed event, click the **Int Off** button on the **Int. Event** Toolbar. Click on a part of the chromatogram to turn integration off at that point. This is the **Start Time**. Click on the chromatogram again at the point where integration will be turned on again. This is the **Stop Time**. An **Integration Off** window will appear. See Figure 13-9.

Figure 13-9 Integration Off



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. Click **Analyze Now** to add the event to the method and re-integrate the chromatogram. (Clicking **Add to Table** will add the event to the integration timed events table without re-integration.)

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Select **Insert into Integration Events Table** and the event will be added to the Integration Events Table of the method (where it will be used on all chromatograms analyzed using this method). Select **Insert into Manual Integration Fixes Table** and the event will be added to the Manual Integration Fixes Table of the present chromatogram (where it will be applied only to this chromatogram).

The chromatogram will be re-drawn using the new integration event. Notice that the selected area has no baselines drawn because the integration has been turned off for these peaks.

4 The integration event is put into the Integration Timed Events table. To view this table, click **Integration Events** from the **Navigation** panel or click **Method >> Integration Events...**. The integration timed events table will appear. Notice the **Integration Off** timed event has been added to the table.

5 To remove the **Integration Off** event from the method, 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.

6 When finished with the **Integration Events** table, close it to return to the chromatogram.

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13.3.6 Create a Calibration

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

Setting up 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 standard 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 standard sample saved. If not, the user can either run a standard 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 standard 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 13-10 and Table 13-2.

Figure 13-10 Define Single Peak Window

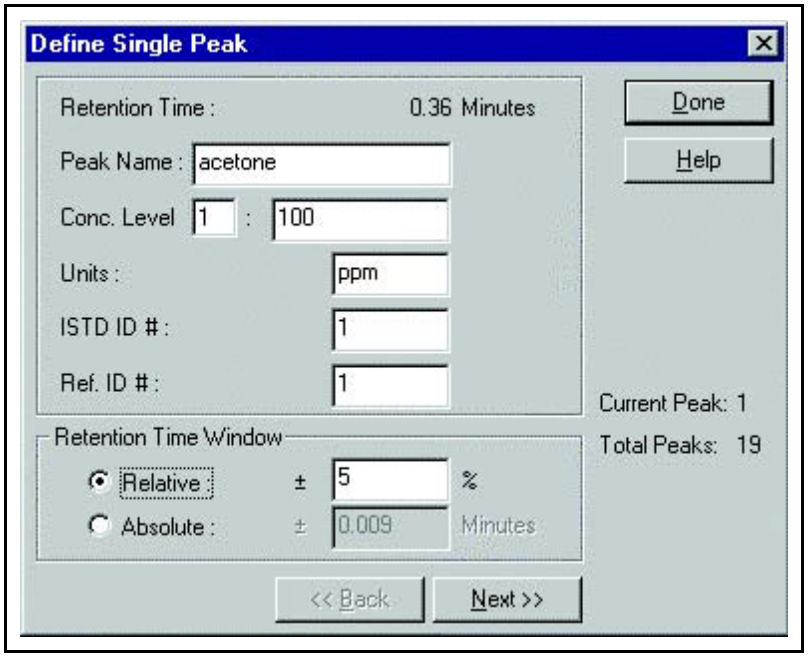

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Table 13-2 Define Single Peak Window Parameters

Retention Time	The retention time of the first detected peak will appear. 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 on the specific peak. The retention time shown in the window will change to reflect the selected peak.
Peak Name	Enter 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, for instance as a label attached to the gas cylinder. **NOTE:** For setting up more than one level for this compound, enter 2 for the **Concentration 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 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.

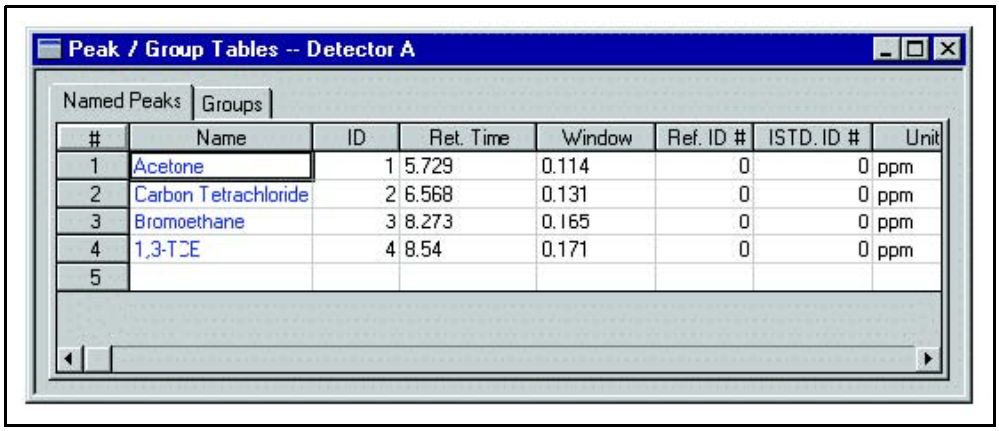
Table 13-2 Define Single Peak Window Parameters (continued)

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 for calculation of the window.
Absolute	Click **Absolute** to enter an absolute 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...** to display the **Peak/Group Tables** window. See Figure 13-11. Click 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 13-11 Calibration Peak Table



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.

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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**.)

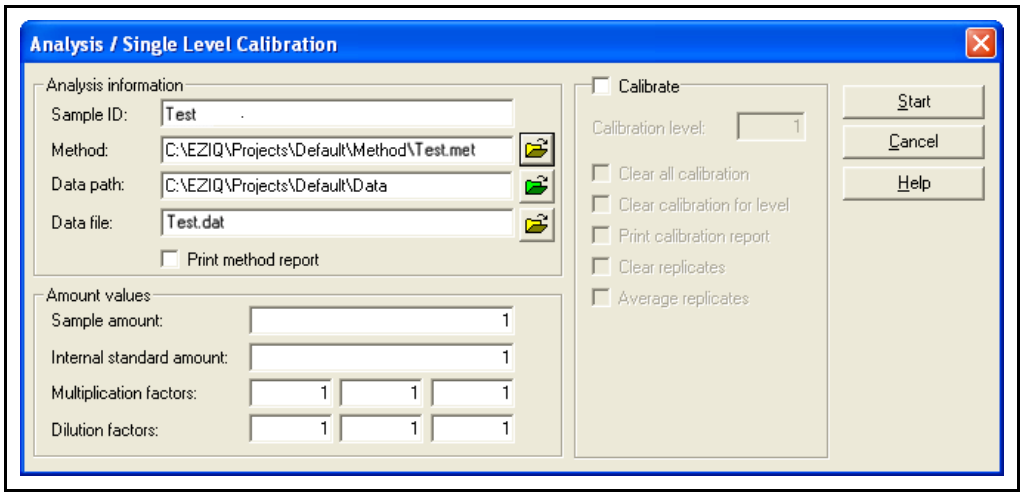
13.3.7 Calibrate Using a Stored Data File

In order for the software to calculate concentrations for unknown samples, the method must contain the areas generated for each component in the standard sample. To store these areas into the method, either run the standard sample again, designated as a calibration run, or calibrate the method using the stored data file created earlier in this tutorial, using **Analysis >> Single Level Calibration**. To use the stored data file to calibrate the method:

1 Click **Analysis >> Analysis Single Level Calibration**. A window will display where file information for the calibration must be set. See Figure 13-12.

2 In the **Sample ID** field, enter sample identification information. If following this tutorial, enter **Test**.

Figure 13-12 Analysis/Single Level Calibration Window



3 In the **Method** field, type the data path name for the method to calibrate. Click the **Open 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 **Open File** icon.

5 Type the name of the calibration data file in the **Data File** field. Click the **Open File** icon and select a saved filename—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** checkbox and enter **1** for **Calibration Level**. Since this method is currently uncalibrated, it is unnecessary to select any of the checkboxes dealing with calibrations or replicates. However, if unsure of the method contents, select **Clear all calibration** before starting.

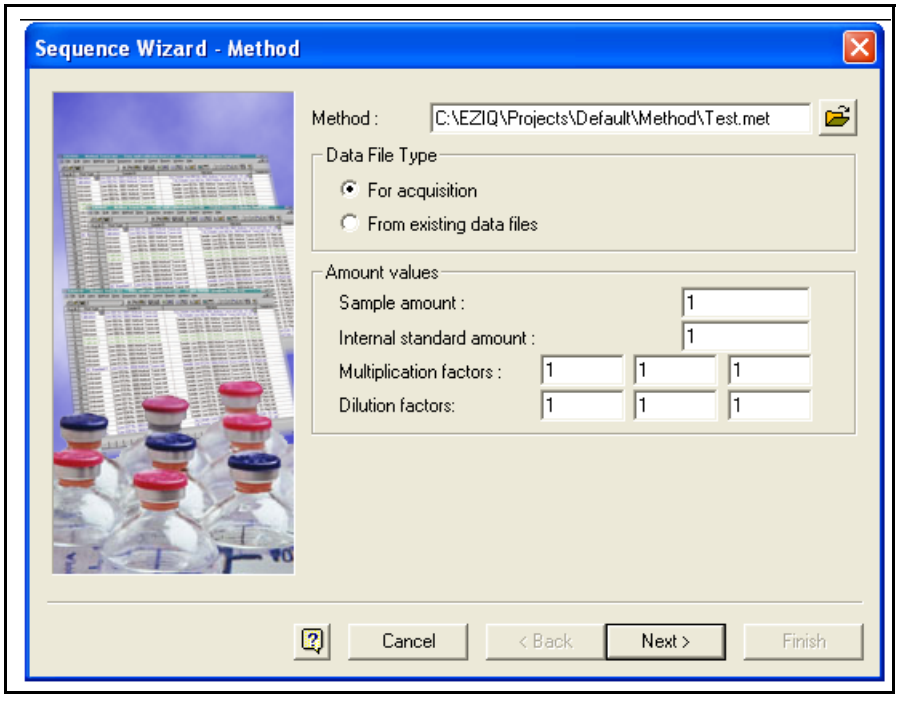
8 When the window is populated, click **Start**. When the analysis is complete, the chromatogram will be integrated, and the areas for the peaks identified as calibration compounds will be entered into the method. Enter the concentration of the calibration gas into corresponding Level field in the **Peak / 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.

1 To create a new sequence, click **File >> Sequence >> Sequence Wizard**. A **Sequence Wizard** window will display. See Figure 13-13.

Figure 13-13 Sequence Wizard - Methods Window



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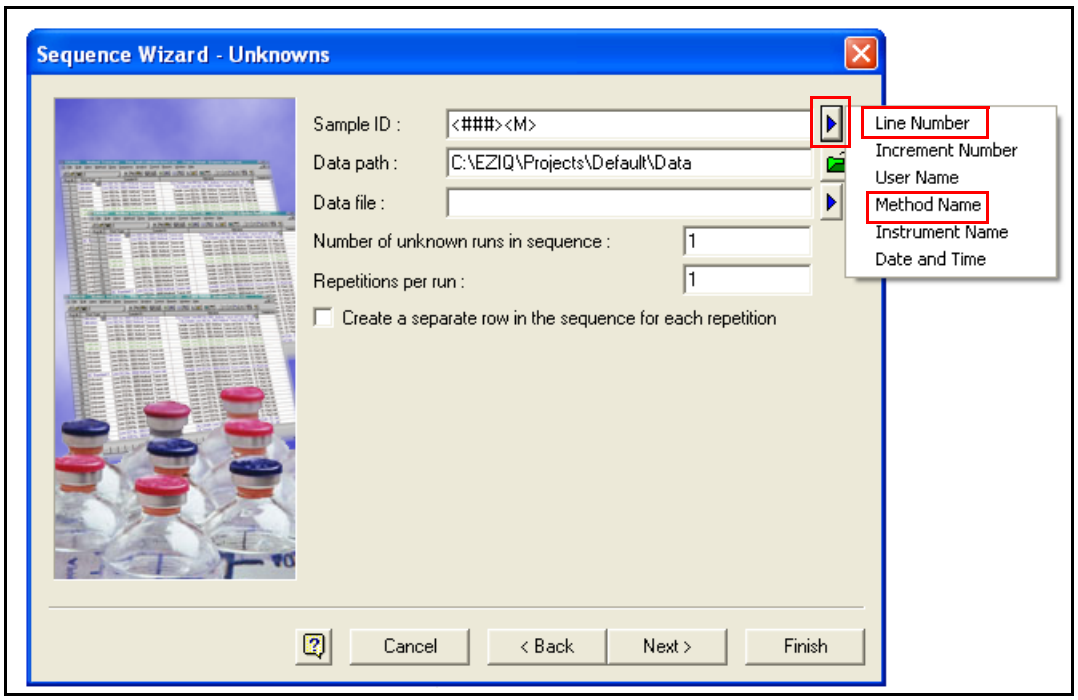
2 Enter the method to be used for the acquisition, or select it from a list of available methods by clicking the **File Open** icon.

3 For **Method**, enter the method name (including path) for the method created in this Tutorial. The user can select the entire path name by clicking the **File** icon next to the field, and selecting the method name from the list displayed. If the user is following this Tutorial, select **Test.met** as the method name. Leave the **Amount Values** at their default values.

4 Select **For acquisition**. The Sequence Wizard will prompt for information required for data acquisition.

5 Click **Next**. The **Sequence Wizard - Unknowns** window will display. See Figure 13-14.

Figure 13-14 Sequence Wizard - Unknowns Window

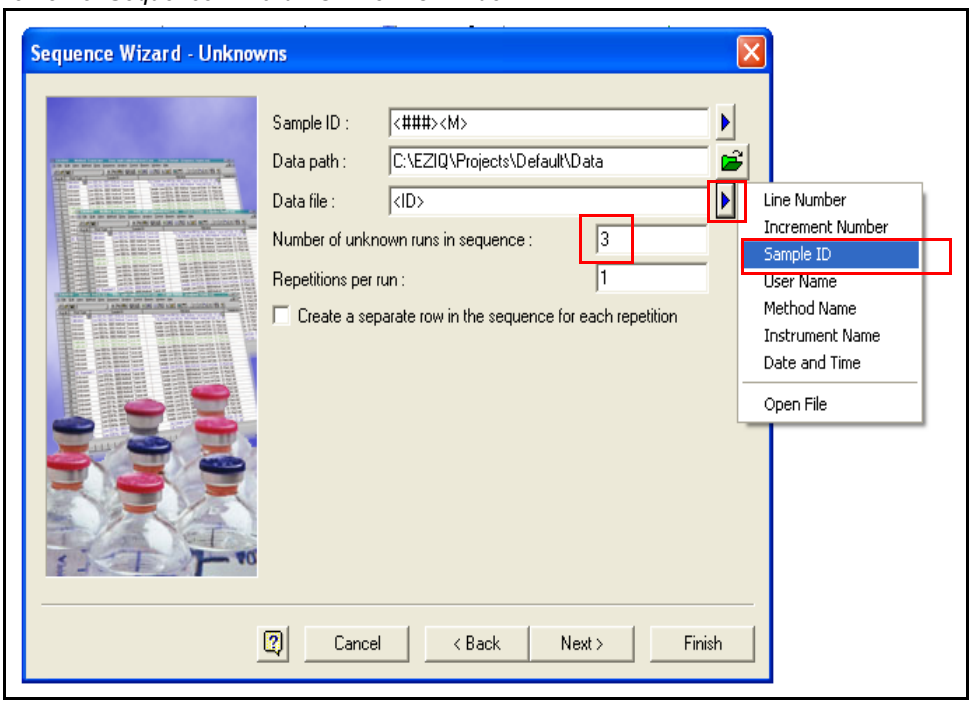


6 The **Sample ID** field is used to identify the samples. Click the blue arrow and select the **Line Number** and **Method Name**. Each **Sample ID** will contain the sequence line number and the current method name.

7 In the **Data path** field, enter the path to where the data will be stored, or select an existing path by clicking the **File Open** icon.

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 13-15.

Figure 13-15 Sequence Wizard - Unknowns Window



9 For **Number of unknown runs in sequence,** enter 3. Leave the other fields at their default values.

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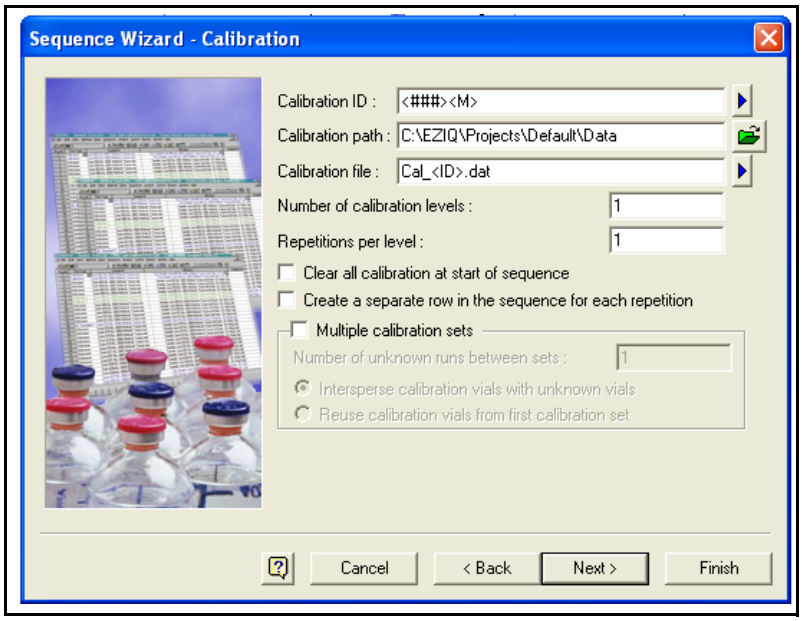
10 Click **Next** to continue.

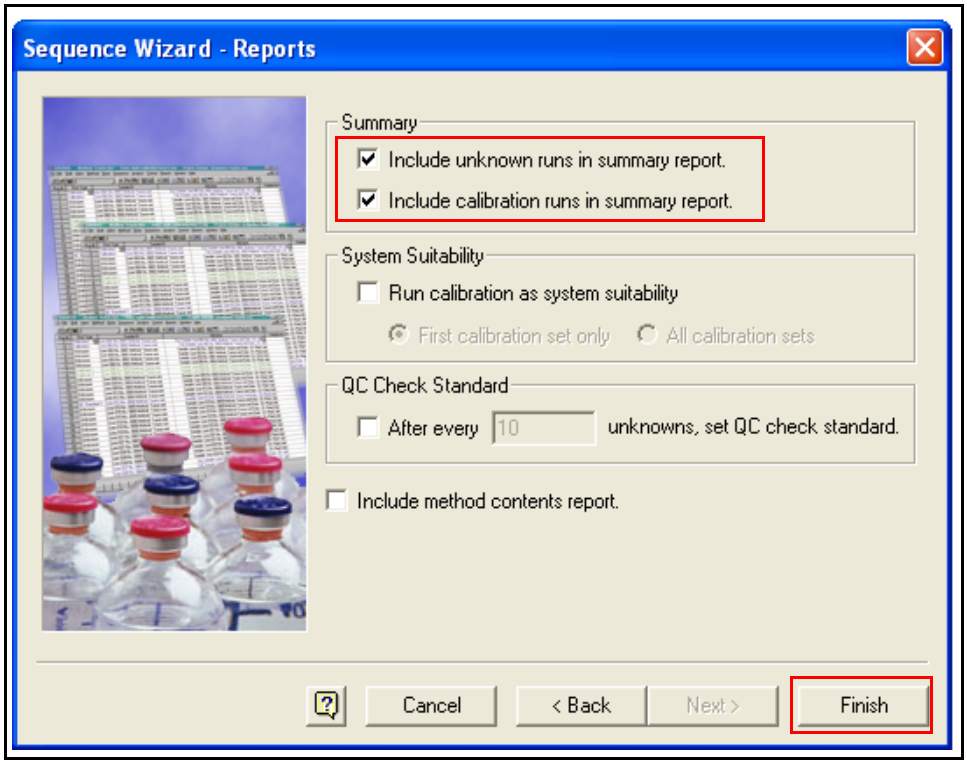
Figure 13-16 Sequence Wizard - Calibration Window



11 In Figure 13-16, 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. Click **Next**.

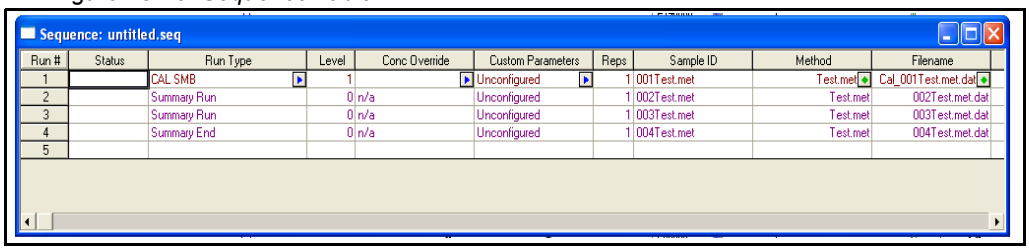
12 Select **Include unknown runs in summary report** and **Include calibration runs in summary report**. Do not check the other boxes. See Figure 13-17.

Figure 13-17 Sequence Wizard - Reports Window



13 Click **Finish**. A sequence table will appear, with the file and method names specified. See Figure 13-18.

Figure 13-18 Sequence Table



14 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 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 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.

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15 To save the sample sequence file, click **Save\Save Sequence** to go to the **Save Sequence** window, or click **File >> Sequence >> Save As**. Select the **C:\datasystem\Sequence** folder (where datasystem is the program installation folder), then type the name **Test** or **Test.seq** for the sequence file name.

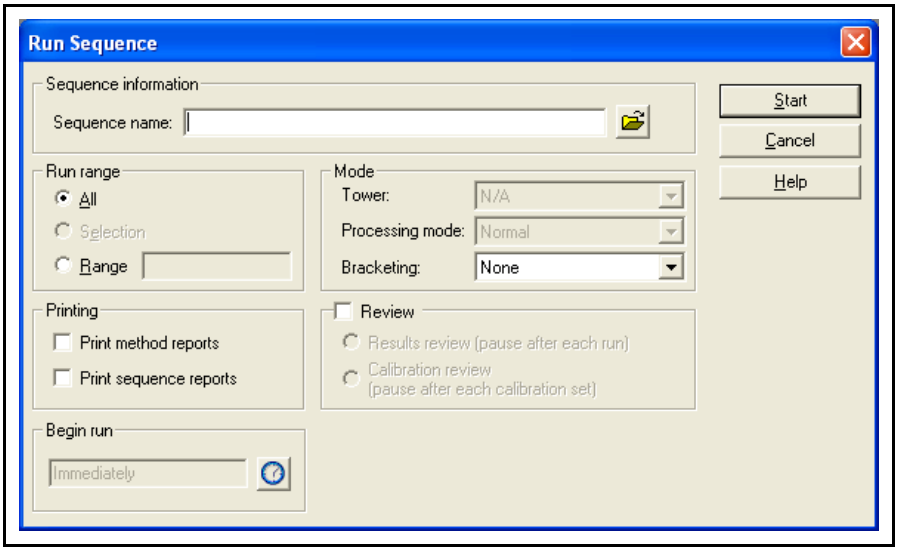
NOTE: By default, sequence files are saved with the .seq extension.

13.3.9 Run a Sequence

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 13-19.

Figure 13-19 Run Sequence Window



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.

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.

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

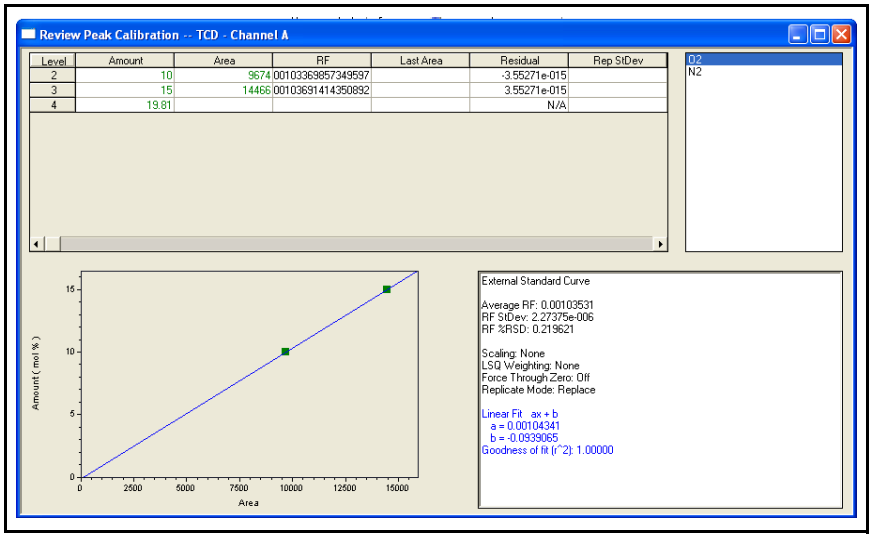
13.4 Review Multi-level Calibration Curves

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.

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. Once the **Multi Calibration.met** method has been opened, click **Method >> Review Calibration**. The window shown in Figure 13-20 is displayed.

   Figure 13-20 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 calibration curve box and select **Fit Type >> Linear**. Notice the new linear calibration curve is overlaid 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.

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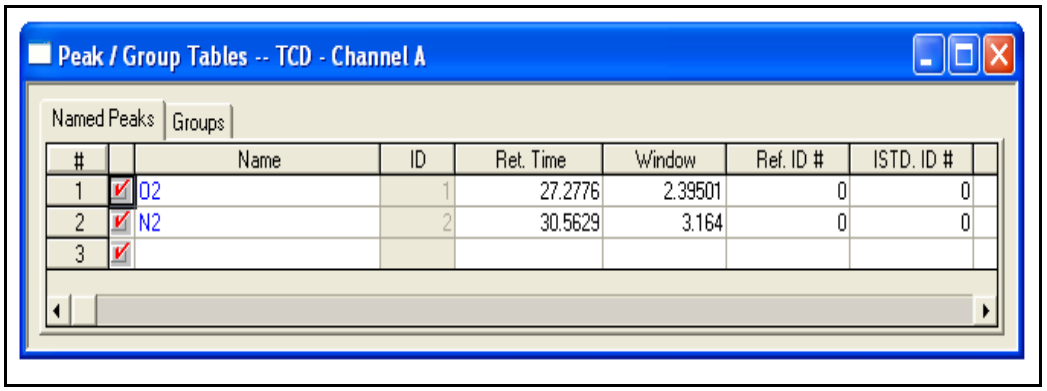
13.5 Explore a Peak Table

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 a Peak Table 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.

2 Open the **Multi Calibration.met** method. View the **Peak / Group Tables** by clicking **Method >> Peak/Groups**. The following table will display. See Figure 13-21.

Figure 13-21 Peak Table

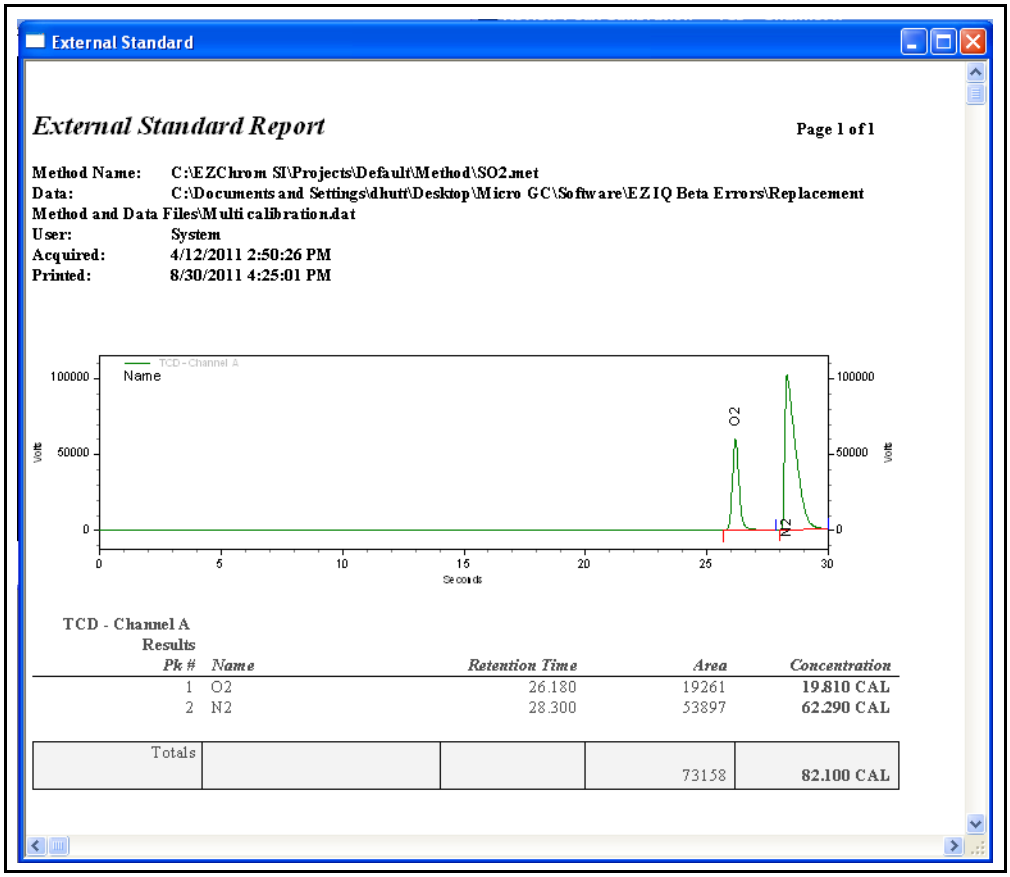


3 In the **Named Peaks** tab, a table containing all of the calibration information for the calibrated peaks in this method is displayed. By scrolling to the right, many different columns appear, each of which represent a parameter for the calibration, such as **Levels**, which contain the calibration 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.

13.6 Examine a Custom Report

A complete suite 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 be displayed. See Figure 13-22.

Figure 13-22 External Standard Report



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.

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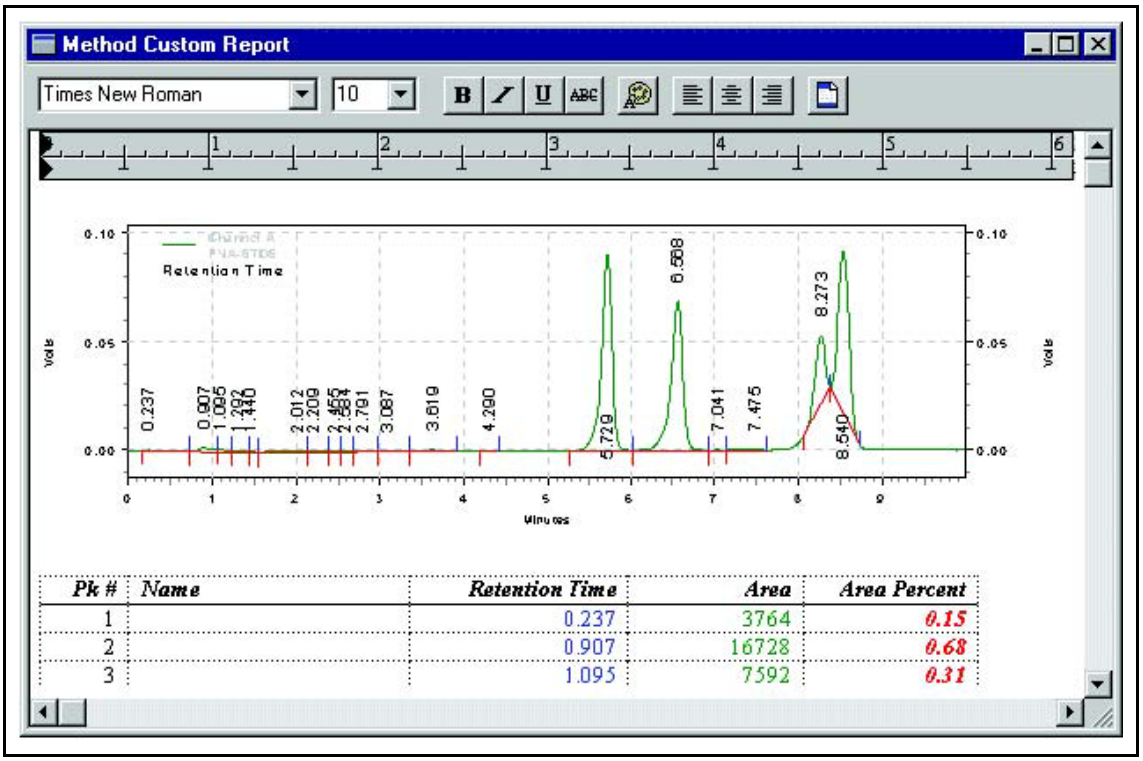
To view the custom report in the **Multi Calibration.met** file, open the file if it is not already open (click **File >> Method >> Open**, then select **Multi Calibration.met** from the file list). Click **Method >> Custom Report** to access the method custom report editor. The current method custom report will appear. See Figure 13-23.

Figure 13-23 Method Custom Report



Pk #	Name	Retention Time	Area	Area Percent
1		0.237	3764	0.15
2		0.907	16728	0.68
3		1.095	7592	0.31

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

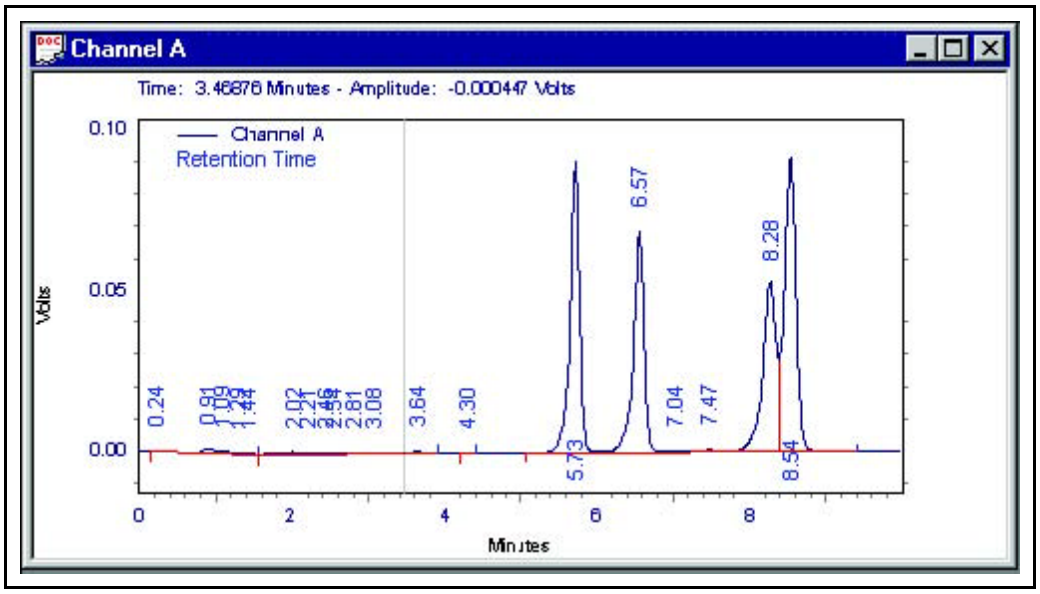
13.7 Changing Integration Parameters

Another important aspect of using a computerized data system is the ability to customize the integration using Integration Timed Events. In this part of the Tutorial, use the **Multi Calibration.dat** data file to become familiar with how to enter integration timed events into the method, and to view the effects of some of these events. Complete details on how each integration timed event functions are given in the **Calibration** chapter in the online help file.

1. Open the **Multi Calibration.dat** data file by clicking **File >> Data >> Open**, and then select the **Multi Calibration.dat** file from the **\Data** folder. Click **Open with Method** to open the **Multi Calibration.met** method file that was used to acquire the data file.

2. Click **Analysis >> Analyze** to analyze the chromatogram and display the baselines. See Figure 13-24.

Figure 13-24 Analyzing Channel A



NOTE: The vertical line pointer moves with the mouse. The retention time where the pointer is located is shown at the top of the chromatogram window.

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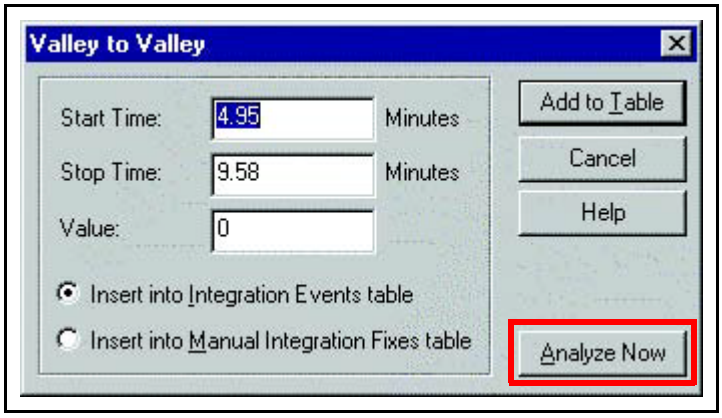
3 Add the Valley to Valley timed event to integrate the cluster of 4 large peaks with Valley to Valley baselines. To do this, right click on the chromatogram and then select **Graphical Programming >> Valley to Valley**.

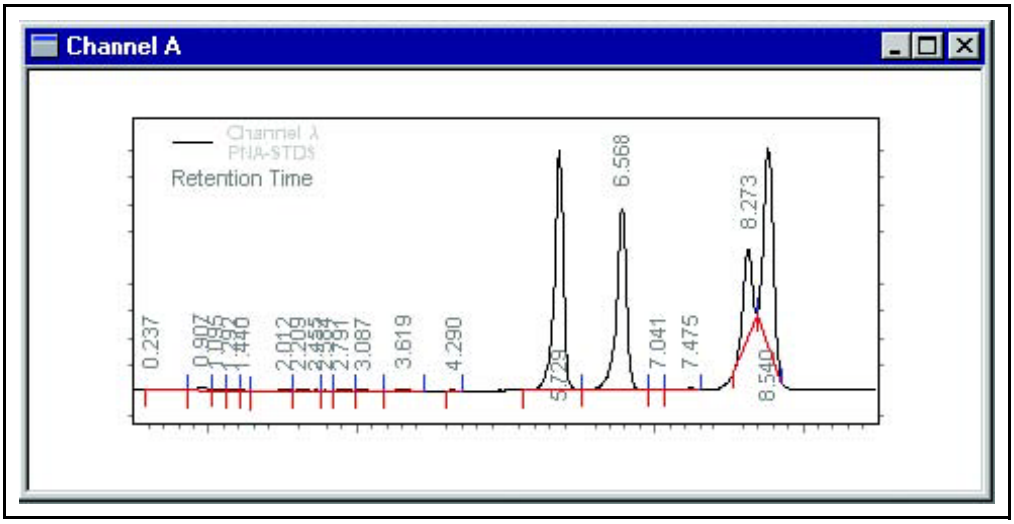
4 Then, click once before the first large peak, then click again just after the last peak. See Figure 13-25.

Figure 13-25 Valley To Valley Window



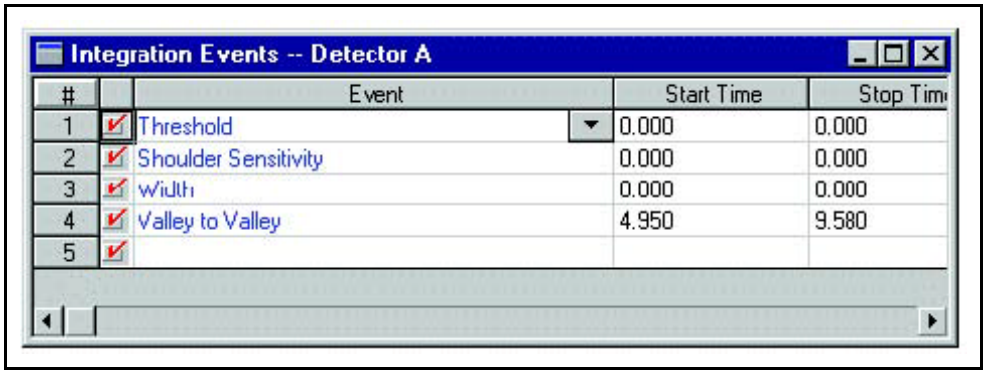
When the **Valley to Valley** window appears displaying the start and stop points for the event, click **Analyze Now** and view the chromatogram. Notice the peaks within the region of the event are now integrated using the valley-to-valley event, and the baselines are adjusted accordingly. See Figure 13-26.

Figure 13-26 Chromatogram



5 Click **Method >> Integration Events**. Note the addition of the **Valley to Valley** event in the table. See Figure 13-27.

Figure 13-27 Integration Events Table



6 Remove the **Valley to Valley** event by selecting the checkbox next to it, then press **Delete** on the keyboard. The integration can be tested without the event, and left in the timed event table, by clearing the check box next to the **Valley to Valley** event and then re-integrating the chromatogram.

7 Close the **Integration Events** table.

Practice adding and deleting integration timed events using the **Multi Calibration.dat** data.

This completes the Tutorial chapter. Refer to earlier chapters of this manual or online Help within the software for more detailed descriptions of each function.

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