Agilent OpenLab Chromatography Data System (CDS) EZChrom Edition

Users Guide

Agilent Technologies

Notices

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Safety Notices

CAUTION

A **CAUTION** notice de**note**s a hazard. It calls attention to an operating procedure, practice, or the like that, if not correctly performed or adhered to, could result in damage to the product or loss of important data. Do not proceed beyond a **CAUTION** notice until the indicated conditions are fully understood and met.

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A WARNING notice denotes a hazard. It calls attention to an operating procedure, practice, or the like that, if not correctly performed or adhered to, could result in personal injury or death. Do not proceed beyond a WARNING notice until the indicated conditions are fully understood and met.

Contents

Getting Started

Use the data system to control and acquire data from a variety of instruments. Once an instrument has been properly connected and configured in the Control Panel, data acquisition and control will require that you perform the following general steps:

As a data system user

- Create and save a data acquisition and control method. A method contains several sections, including acquisition and instrument control parameters, calibration information, integration timed events, and reporting options. A method may also contain special items such as export instructions and customized parameters or user programs that can be run after analysis.
- Create and save a sequence that contains details of calibration runs and unknown samples.
- Run the sequence to calibrate the method and generate results.

Note Privileges/Roles assigned in the Control Panel may prevent a user from performing all of these tasks.

See Also

Basics of Operation

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About Instruments

About Methods

About Integration

About Sequences

About Calibration

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Basics of Operation

This section covers the basics of operation.

See Also

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EZChrom eFamiliarization modules

EZChrom User Resources are included with your OpenLab software to help you get started and familiarize yourself with EZChrom.

To access the eFamiliarization modules, go to **Start > Agient Technologies > OpenLAB CDS Resources**.

Access the help files

There are two types of help file topics, optional and main.

The help topics for optional software are located in separate help files that are unique for each option. These help files are only accessed by the system when you are in a dialog or window that is specific to that option. When you access the help file for an optional program, the index and table of contents displayed will be for the help file for that optional program.

All other topics are located in the main help file. To access the main help file topics, you must first close the optional help file.

To access the help file:

From the Toolbar select **Help > Contents**, or select the Help  icon.

View version Information

Software version information for your system can be found in the About Agilent OpenLab CDS (EZChrom Edition) dialog box.

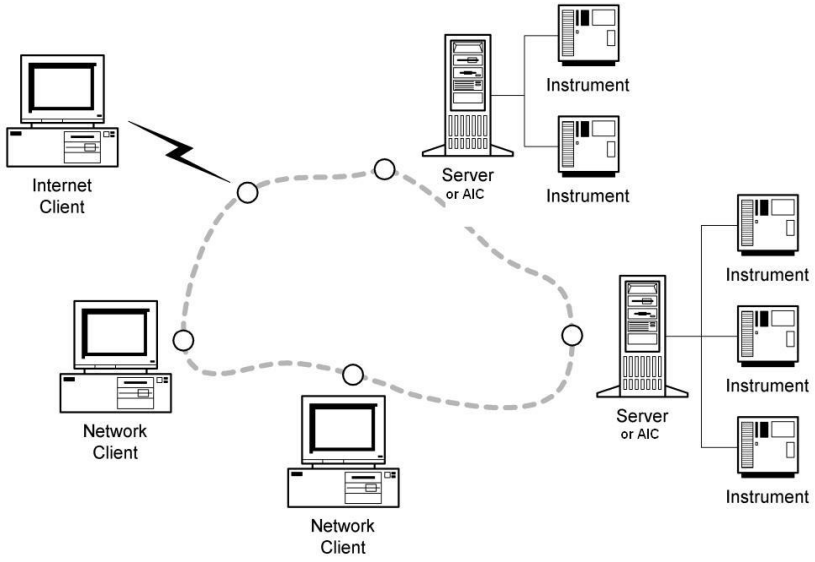
1 From the main menu select **Help > About**. The About Agilent OpenLab CDS (EZChrom Edition) dialog box is displayed listing the version of your Agilent OpenLab CDS (EZChrom

Edition) software.

2 To view version information for installed modules and drivers, select **Module Version**. The Module Version Info window displays the Product Name, Product Version, and Driver Version of your installed modules.

System architecture

An Enterprise is a combination of data system clients, servers, and instruments configured on a network. It can be as simple as two laboratories with Agilent Instrument Controllers connected together on a network, or as complex as a large pharmaceutical company with multiple locations, many buildings, and hundreds of laboratories, each with a wide range of instruments.



The data system can be installed as a single, stand-alone data system, as a series of stand-alone data systems networked together, or in a networked, client/server mode.

Agilent Instrument Controller's (AICs) are the machines where the actual data acquisition and control of instruments occur. All instruments are physically attached to the AICs.

Client workstations are where the users of the systems perform all operations of the system such as developing methods and sequences, and submitting data acquisition runs and sequences to the AICs. Clients can access the servers or AIC through direct network connection, or from remote locations using the Internet.

A client/server system is comprised of servers and clients configured together on a network, using a Windows computer as a domain controller.

In client/server mode when you start a run or a sequence from a client workstation, you are actually submitting that run or sequence to the Acquisition Controller where the instrument is attached. Once you have submitted a run or sequence, the server or

AIC assumes control over the acquisition and control functions. All methods and sequences are copied to the Acquisition Controller when a run queue item is submitted to the server. If the network goes down, the Acquisition Controller will continue to run with the files it has on its hard disk.

About new file templates

The system provides several pre-made file templates for:

- Methods
- Sequences
- Sample Preps
- Spectral Libraries
- Reports

See Also Open a Template

About the instrument window

In the Instrument Window many aspects of using the instrument are performed, including:

Methods

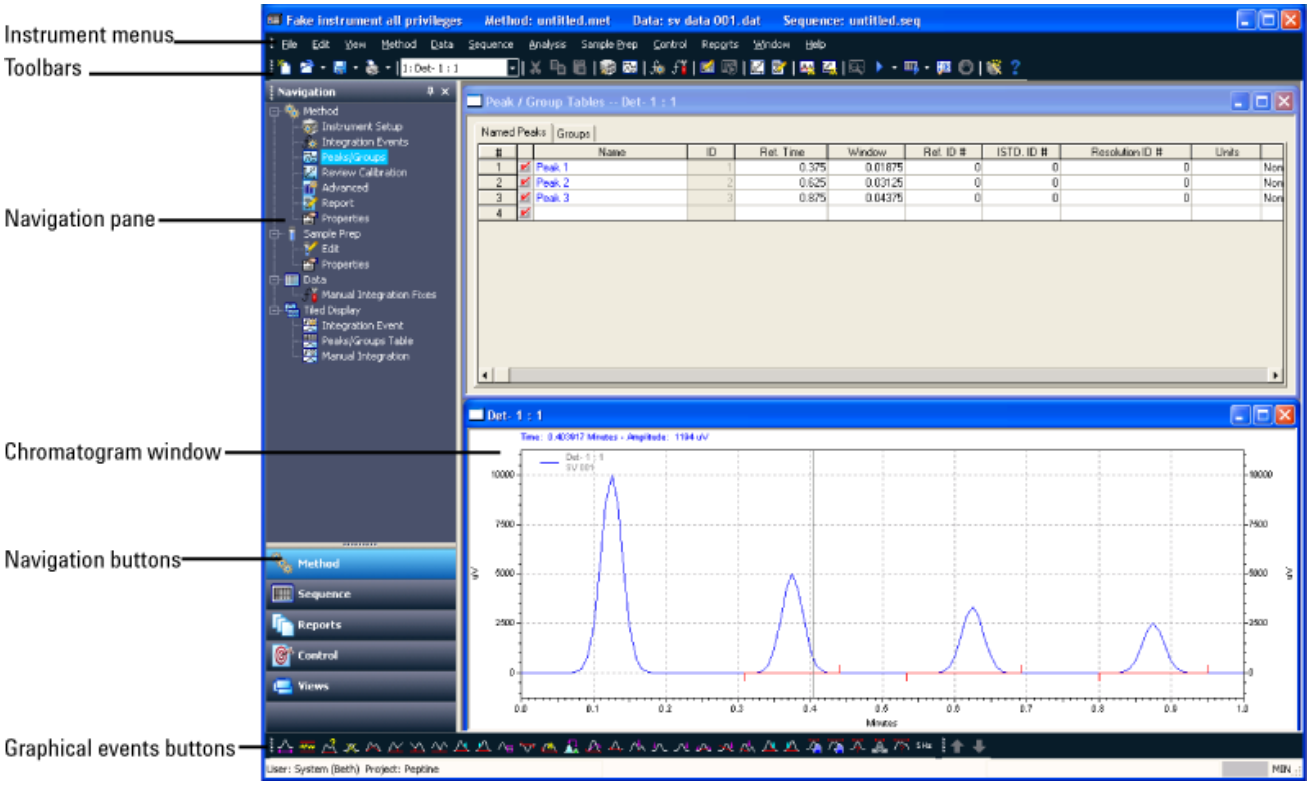
Sequences

Calibration

Reporting

Integration

You can customize the appearance of the application window by right clicking the toolbars or graphical events buttons and selecting which buttons to show. See also Change View Preferences.



See Also

Chromatogram Window

Navigation Buttons

Graphical Events Buttons

View Online Signals

Change View Preferences

Instrument Wizard

To Lock or Unlock the Instrument Window

About navigation pane buttons

The navigation pane buttons in the instrument window give you single-click access to method, sequence, report, control, and viewing options. The navigation buttons at the bottom of the navigation pane open command trees that give you access to commands that are also available from the menu bar of the instrument window.

Method	Method, Sample Prep, Data,and Tiled Display (to display current data tiled with selected Integration or Calibration/Peak Table information)
Sequence	Edit, Properties
Reports	Standard Report, Advanced Report, Intelligent Report, Area %, Config Contents Report, Current Baseline Check, External Standard, Internal Standard, Normalization, Properties
Control	Instrument Setup, Run Queue, Instrument Status
Views	Data Display (see View Online Signals), Data/Manual Integration Fixes, Tiled Display/Sample Entry View Use the sample entry view during data acquisition to set up the instrument window for display of the most commonly used functions. When you select this view, the instrument window will provide a tiled view containing Instrument Status, Current Data, and the Run Queue. This single view enables you to monitor the current run, check or modify instrument parameters, and submit runs or sequences.

To view the Navigation pane, select View > Navigation Pane.

To close the Navigation pane, select the x button at the top of the Navigation pane.

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

To unpark the Navigation pane, select the Navigation tab, and then select the **push-pin** button.

To customize the bars that are shown in the Navigation pane, select the small arrow at the bottom right corner of the Navigation pane, and select **Show More Buttons**, **Show Fewer Buttons**, or **Add or Remove Buttons.**

View online signals

The Online Signals View enables you to monitor the current online signals, and, if supported by the instrument, the instrument parameter curves. This data in this view is not acquired and stored, and is not associated with any runs.

Note: In order to view the Online Signals, the instrument must be Monitored using the Control>Monitor function. Not all instruments support View Online Signals.

To view online signals:

1. In the **Navigation Pane**, click **Views** and then under **Data Display** select **Online Signals.**
2. From the online signals view window, click **Change** to open the **Edit Signal Plot** dialog box where you can select signals and define the x- and y-axis ranges.

3 Once you have the desired signals selected for view, you can perform the following functions in this window:

- Click **Balance** to balance the detector. This button is only available for detectors that support this function.
- Click **Adjust** to adjust the signal window for data that exceed the absorbance range set.
- Click on the **horizontal arrows** to adjust the x-axis range.
- Click on the **vertical arrows** to adjust the y-axis range.

Note: The horizontal and vertical arrows are active only if the signal is not zoomed.

To display the individual y-axis for a signal select the signal in the display or the signal description in the header. The y-axis is the same color as the signal displayed.

Use the thick crosshair cursor to trace the signal and display the absorbance values at the foot of the window.

Zooming the Window

To zoom inside the online signal plot, hold down the left mouse button and draw a rectangle around the area of interest. Double-click to zoom out. The horizontal and vertical arrows are not active in a zoomed signal window. When changing x-axis or y-axis range or selecting **Adjust**, the window is automatically zoomed out.

Edit the Online Signal Plot

This dialog box is used to select and modify the ranges for signals to be displayed in the **Online Signal** view. To open this dialog box, click **Change** from the online signals view window. The signals available for viewing for this instrument will appear in the **Available Signals** list.

To select signals for display, highlight the signal in the list of **Available Signals** and select the **Add** button.

To remove signals from display highlight the signal in the list of **Selected Signals** and select the **Remove** button.

To change offsets and ranges for a given signal, select the signal to highlight it, then use the range parameters shown to enter values that will be used to display the signal in the Online Signal view:

- Select **Predictable Range** to enter absolute values for the y-axis range.
- Select **Floating Range** to provide an Offset that is used when the Adjust button in the Signal Plot window is selected. The current maximum value is then displayed at the proportion of the screen provided in offset. You can use this function also to display multiple signals with an offset. Just set a different offset for each signal and then select **Adjust**.

- The y-axis range defines the absolute length of the y-axis for your signal. For signals that support it, you can also select **Auto y-adjust** to automatically adjust the y-axis such that the latest data point is always visible.
- For setpoint (parameter) signals you can directly provide the starting point from and offset for your y-axis. No offset and y-adjust is possible.

Change view preferences

The **View** menu is used to set up view preferences in the instrument window. These preferences are set by each user for each instrument.

To change the appearance of the instrument window

1. In the toolbar select **View > Preferences**.
2. In the **Preferences** dialog box, select the **General** tab. The following options are displayed:

Toolbar options	For each area of the window listed, you can turn on or off the toolbar and tooltips if available. Click the toolbar area, then select the **Show toolbar** and **Tooltips** check boxes to enable your choices for that area.
Status bar options	Select the check box to turn on the status bar. The status bar provides brief information at the bottom of the instrument window, if enabled.
Time units	Select the time units for display of chromatographic information.
Tooltips options	Select the **Show graphical programming tooltips** or **Show trace operations tooltips** check box or both to enable your choices for that area.
Recent Files	Set the maximum number of recent files shown under **Files > Recent Files.**
Trace Stacking	Select the **Default to Normalized** check box to normalize one or more chromatograms to the first chromatogram by default. This adjusts the heights such that the apex height of a selected peak matches that of the peak selected on the first trace. If this option is not selected, the default will be Trace 1.

Instrument wizard

This wizard is designed to direct you to the basic functions of the instrument window.

To open the instrument wizard:

There are two ways to open the instrument wizard from the Instrument Window

- Select the **Instrument Wizard** icon. 
- Select **Help > Instrument Wizard**.

The following options are displayed in the **Instrument Wizard** dialog box:

Create a new method	This button starts the **Method Wizard** that will enable you to step through creating a method.
Modify the current method	This button starts the **Method Wizard** that will enable you to step through modifying a method.
Modify a method on disk	This button starts the **Method Wizard** that will enable you to step through modifying a method on disk.
Create a sequence	This button starts the **Sequence Wizard** that will enable you to step through creation of an acquisition or reprocessing sequence.
Intelligent Report with Wizard	This button starts the **Report Wizard** that will enable you to step through creating reports.
Run one sample	This button opens a dialog where you can use a stored method to run a single sample.
Run a sequence of samples	This button opens the Run Sequence dialog where you can start 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.

See Also Create a Method with the Method Wizard

To lock or unlock the instrument window:

This lock command is useful for multiple user labs, where you may want to lock your current work while you are temporarily away from the computer. When you choose this command, all menu items will be Locked except the **Window** and **Help** menu. Locked commands will not be accessible until you unlock them again.

To lock the instrument window, select **Window > Lock**.

To unlock the instrument window, select **Window > Lock.** In the **Login** dialog box, enter your **Username** and **Password** that were set in the Control Panel.

Open and save files

Opening and saving files is part of the basics of operation.

The appearance of the Open and Save dialog boxes will vary depending on your storage system.

See Also

Open a Method File

Open a Sequence File

Open a Result Set

Open a Data File

Open a Recently Opened File

Open a Template

Save a Method

Save a Master Method

Save a Sequence

Save a Result Set

Save a Data File

Save as a Template

Open a method file

When you open a method file you will be presented with a dialog box that allows you to open the file, and specify parameters for searching.

The dialog appearance and behavior will be slightly different for systems with advanced file security enabled. Users will be limited to storing files within the current project folder and the Enterprise Common folder.

To open a method file:

1. Select **File > Open > Method.**
2. The **Open Method File** dialog box opens to the method folder in your project files, and the **Files of type** is set to **.met**.
3. The dialog box appearance and behavior will vary depending on your storage type. Continue procedure for:

   File Based storage

   a. Use the **Look in** and **File name** fields to navigate to the file.

   b. To search for a file, complete the **Text in Desc.**, **Analyst** name, and date **Created** or last **Modified** fields and select **Find Now**.

c. **Note**: When using the Search feature, make sure the Windows **Hide Extensions for Known File Types** option is turned off. To turn this off select **My Computer > Tools > Folder Options > View**. Then deselect **Hide Extensions for Known File Types**.

Data Store

a. To search for files, select **Advanced**.

b. For more information, select the **Data Store Help**.

4 Select the method and select **Open**.

Open a sequence file

When you open a sequence file you will be presented with a dialog box that allows you to open the file, and specify parameters for searching.

The dialog appearance and behavior will be slightly different for systems with advanced file security enabled. Users will be limited to storing files within the current project folder and the Enterprise Common folder.

To open a sequence file:

1 Select **File > Open > Sequence.**

2 The **Open Sequence File** dialog box opens to the sequence folder in your project files, and the **Files of type** is set to **.seq**.

3 The dialog box appearance and behavior will vary depending on your storage type. Continue procedure for:

File Based storage

a. Use the **Look in** and **File name** fields to navigate to the file.

b. To search for a file, complete the **Text in Desc.**, **Analyst** name, and date **Created** or last **Modified** fields and select **Find Now**.

Note: When using the Search feature, make sure the Windows **Hide Extensions for Known File Types** option is turned off. To turn this off select **My Computer > Tools > Folder Options > View**. Then deselect **Hide Extensions for Known File Types**.

Data Store

a. To search for files, select **Advanced**.

b. For more information, select the **Data Store Help**.

4 Select the sequence and select **Open**.

See Also

Edit a Sequence

Save a Sequence

Open a result set

After you have run a sequence you can view your results in the **Result Sequence** dialog box.

To open a result set file:

1. Select **File > Open > Result Set.**
2. The **Open Result File** dialog box opens to the result folder in your project files, and the **Files of type** is set to **.rst**.
3. The dialog box appearance and behavior will vary depending on your storage type. Continue procedure for:

   File Based storage

   a. Use the **Look in** and **File name** fields to navigate to the file.

   b. To search for a file, complete the **Text in Desc.**, **Analyst** name, and date **Created** or last **Modified** fields and select **Find Now**.

   Note: When using the Search feature, make sure the Windows **Hide Extensions for Known File Types** option is turned off. To turn this off select **My Computer > Tools > Folder Options > View**. Then deselect **Hide Extensions for Known File Types**.

   Data Store

   a. To search for files, select **Advanced**.

   b. For more information, select the **Data Store Help**.
4. Select the method and select **Open**.
5. The data file chromatogram and the **Result Sequence** dialog box open. The yellow highlight in the **Result Sequence** dialog box lets you know you are in result review mode.
   - The columns in the **Result Sequence** dialog box are described under Sequence Spreadsheet Columns.
   - Right-click in the **Result Sequence** dialog box to open a context menu. These options are described under Sequence Spreadsheet Context Menu.

See Also

About the Sequence Spreadsheet

Sequence Spreadsheet Columns

Customize the Sequence Spreadsheet Columns

Sequence Spreadsheet Context Menu.

Open a data file

When you open a data file, you will be presented with a dialog box that allows you to not only open the file, but specify parameters for searching, as well as previewing file contents.

The dialog appearance and behavior will be slightly different for systems with advanced file security enabled. Users will be limited to storing files within the current project folder and the Enterprise Common folder.

To open a data file:

1. Select **File > Open > Data**.
2. The **Open Data File** dialog box opens to the result folder in your project files, and the **Files of type** is set to **.dat**.
3. The dialog box appearance and behavior will vary depending on your storage type. Continue the procedure for:

   File Based storage

   a. Use the **Look in** and **File name** fields to navigate to the file.

   b. To search for a file, complete the **Text in Desc.**, **Analyst** name, and date **Created** or last **Modified** fields and select **Find Now**.

      Note: When using the Search feature, make sure the Windows **Hide Extensions for Known File Types** option is turned off. To turn this off select **My Computer > Tools > Folder Options > View**. Then deselect **Hide Extensions for Known File Types**.

   c. Select the **Preview** button to view a preview of the chromatogram

   d. The **Options** box allows you to save time by loading additional information at the time the data file is opened. You can select **Method** or **Results**.

   If you select **Method**, select from the following options:

   - **Current:** The current method will not change when you open the data file. 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 your current active method.

If you select **Results**, 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 screen.

- If **Most Recent** is selected, the data file will be opened with the results from the last time the chromatogram was analyzed.
- If the **Save all analysis results** option is turned on in the Control Panel a list of all analysis results will be available for you to open with the file.
- If applicable, select **Open with Sample Prep**. When this box is selected, the sample prep file (if applicable) used at the time the data was acquired will be opened when the data file is opened. See Sample Prep.

Data Store

a. To search for files, select **Advanced**.

b. For more information, select the **Data Store Help**.

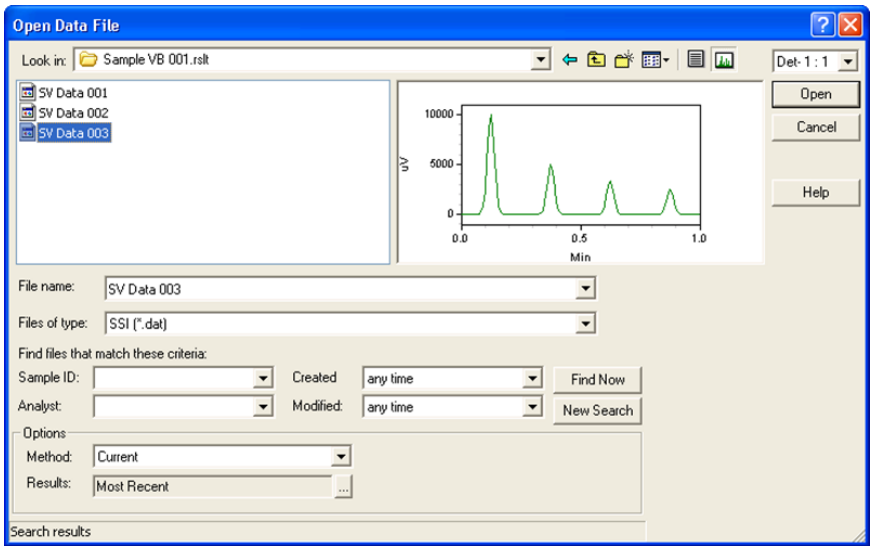
You can open an archived data file if **Allow user to navigate outside of project** is enabled in the Control Panel for this project. To enable this option, see the Control Panel Help, **Edit a Project.**

If this option is not enabled you must first:

a. De-archive the files in Data Store. See the Data Store Help, **Archive and de-archive folders and files**.

b. Restore the project in the Control Panel. See the Control Panel Help, **Restoring a project from the Data Store archive.**

4 Select the data file and select **Open**.



Open a recently opened file

To open a recently opened file, select **Files > Recent Files** and select the file from the list.

To change the number of recent files listed, see Change View Preferences.

Save a method

When you have completed the sections for creation of a data acquisition method, save the file on your hard disk before you use it for data acquisition.

The dialog appearance and behavior will be slightly different for systems with advanced file security enabled. Users will be limited to storing files within the current project folder and the Enterprise Common folder.

The **Save As > Method** command will only impact the selected method. It won't impact the method if the sequence is run again. To update the Master Method see Update the Master Method.

To save a method with the current file name:

Select **File > Save > Method**.

To save a method with a new file name:

1. Select **File > Save As > Method.**
2. The **Save Method File As** dialog box opens to the method folder in your project files, and the file type is set to **.met**.
3. In the **File name** field, type the filename.
4. Select **Save**.

Save a master method

To impact the method if the sequence is run again, update the Master method.

To save your changes to the Master method, from the toolbar, select **File > Update Master > Method**.

The **Save As > Method** command will only impact the selected method. It won't impact the method if the sequence is run again. To save as a regular method see Save a Method.

Save a sequence

Once you have created or edited a sequence, you must save it on disk before you can use it to acquire or process data.

The dialog box appearance and behavior will be slightly different for systems with advanced file security enabled. Users will be limited to storing files within the current project folder and the Enterprise Common folder.

To save a sequence with the current file name:

Select **File > Save > Sequence**.

To save a sequence with a new file name:

1. Select **File > Save As > Sequence.**
2. The **Save Sequence File As** dialog box opens to the sequence folder in your project files, and the file type is set to **.seq**.
3. In the **File name** field, type the filename.
4. Select **Save**.

See Also

Open a Sequence File

Edit a Sequence

Save a result set

To save a result set, select **File > Save > Result Set**.

See Also

About the Result Sequence

Save a data file

In your data system you can open many different 3rd party formats such as AIA, CDF, and PE. When you open one of these the Save As 32-Bit option is enabled. This allows the user to save the file in the native format and structure listed in About Data File Structure.

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 Ezchrom data format (such as 16-bit or converted files). In order to comply with good laboratory practices, you will not be allowed to save as 32-bit using the 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.

The dialog appearance and behavior will be slightly different for systems with advanced file security enabled. Users will be limited to storing files within the current project folder and the Enterprise Common folder.

To save a data file:

1. In the toolbar select **File > Save As > Data as 32-bit**.
2. The **Save Data File As** dialog box opens to the data folder in your project files, and the file type is set to **.dat**.
3. In the **File name** field, type the filename.
4. The dialog box appearance and behavior will vary depending on your storage type. Continue procedure for:

File Based storage

a. To save your data in a different folder, select it from the **Save in** drop down menu.

b. In the **Description** field, review or change the data description if necessary.

c. To save the file in a compressed format, select the **Compress Data** box. Once saved in compressed format, it will automatically be decompressed whenever the file is opened. However, once a file is saved in compressed format, you must do a save as command to save it in decompressed format again.

Data Store

a. To save your data in a different folder, select it in the navigation pane.

b. For more information, select the Data Store Help.

5 Select **Save**.

Open a template

To open and create a method, sequence, sample prep, or report with a template:

1 Select **File > New**.

2 In the **New File Templates** dialog box, select the template you wish to base your new method, sequence, sample prep, or report on.

3 Select **OK**.

See Also About New File Templates

Save as a template

To save a file as a Template, select **File > Save As > Method**, **Sequence**, or **Data as 32 bit** and navigate to the **Template** folder in your directory.

About the Chromatogram Window

When there is data to be viewed, it displays in a Chromatogram Window.

To access specialized commands for the Chromatogram Wiindow, right-click in the Chromatogram Window. These commands allow you to add graphs or chromatograms to the window, change the appearance, annotations, and axes, perform mathematical operations on chromatograms, and view or change the properties of existing traces in the window.

See Also

View Tiled or Overlay Data

Scroll the chromatogram

Add a Trace

Axis Setup

Annotations

Change the Chromatogram Appearance

Zooming

Clear Overlaid Traces

Operations

Copy to Clipboard

Print a Trace

Save a Trace

Remove a Trace

Graphical Programming

Set Limits for X-Axis and Y-Axis

About Integration

View tiled or overlay data

When viewing data from multiple channel methods, you can choose to view each channel in a separate window (**View > Tile Data)**, or you can overlay all channels in a single window (**View/Overlay Data**). When all channels are overlaid in a single window, you can still zoom, and change the individual channel appearances, as described below.

When in **Tiled** mode, you can arrange how the windows are tiled on your screen by using the **Window > Cascade, Window > Tile Horizontally,** or **Window > Tile Vertically** command.

Scroll the chromatogram

Once you have zoomed in on a chromatogram, you can scroll the chromatogram to the right or left without losing the zoom. This is done by pressing the **CTRL SHIFT** keys down and moving the mouse until the cursor changes to a hand and dragging it to the left or right.

You can also scroll the X- or Y- axis to view features which may be out of the range. To do this, press the **CRTL SHIFT** keys down while the mouse cursor is outside the graph area, yet near the axis of interest. The cursor will change to an up/down arrow near the y-axis, or a left/right arrow near the X-axis. 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, click the right mouse button and then click **Full Unzoom**.

Add a trace

You can view multiple traces in a single Chromatogram Window. This is convenient if, for example, you want to compare a past run with your current data or overlay an oven or pump profile.

To add a new trace to the Chromatogram Window:

1 Right-click in the Chromatogram Window and select **Add Trace**. Select from the following options:

- **From Current Data** - This selection allows you to select a trace from the current chromatography data.
- **From Other Data Files** - This allows you to select a stored data file from which you can select a trace for display. If you select this option, in the **Open Data File** dialog box, select the data file.
- **From Current Method** - This selection enables you to select a trace from your current method (if available). For example, you could load an oven temperature program from an HP5890 instrument method.

2 In the **Data Graph Properties** dialog box, select the **Trace Setup** tab. 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 dialog box where you can view or change them. Complete the following fields:

Show	Click this box to show the trace in the Chromatogram Window. De-select this box to remove the trace from the display (but leaving it open). This is a convenient way to temporarily remove a trace from the viewing window.
Legend	Click 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. Deselect this box to remove the legend for this trace from the Chromatogram Window. Setup for the appearance of the legend (color, etc.) is done in the **Appearance tab** for the Graph item. **Note**: If you have not turned on the Legend in the **Axis Setup** dialog, this box will have no effect.
Data Source	Enter the name of the file from which to get the trace. You can also click the **File** button adjacent to the field and select a data source from the options listed above.
Trace	Select the trace to be displayed. Click the button to display available traces.
Scale to	Select one of the scaling options: **Trace x** Scales to another trace in the window. **User Defined** Allows you to enter a value for Y max and min. **Normalized** Allows you to normalize one trace to fit on the graph.

Y min	If you have selected a User Defined scale, enter a minimum value for the Y-axis.
Y max	If you have selected a User Defined scale, 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.
x Scale	If desired, enter a multiplier that will be applied to the entire trace here.
Y Offset	Enter a value in units for offset of the Y-axis.
Y Scale	If desired, enter a multiplier that will be applied to the entire trace here.
Annotations	Click this button to display the trace annotations dialog.
Hide Details	Click this button to hide the current trace details and display only the spreadsheet.
Reset Scaling	Click this button to reset the scaling values to their original values.

3 Select **OK**.

To perform mathematical operations on the two chromatograms, see About Chromatogram Operations.

See Also Remove a Trace

Axis setup

The Axis Setup tab allows you to configure the appearance of the axis on your chromatogram. These settings apply to active traces.

To change the axis properties:

1 In the **Chromatogram Window**, right-click and then select **Axis Setup**, or select **Properties > Axis Setup.**

2 The following fields are available:

- **Graph Title** - Enter a title for the graph, if desired. This appears at the top of the graph.
- **Axis** - Using the drop-down list, select the axis of interest: Left Y-Axis, Right Y-Axis, or X-Axis. Then for your selection, you can choose the limits for the axis.

  For Y-Axis selections, you may choose **Use limits of trace** to get the limits from one of the traces in the window, or you can select the **Manually set trace's limits to** box and set the Y-Axis limits to your desired range. If you choose **None**, no Y-Axis values will be displayed.

For the X-Axis, you may either choose to **Autoscale**, where the X-Axis is set to the longest trace. Or, you may set an absolute range for the X-Axis by clicking the **Use This Range** button, then enter a minimum and maximum X-Axis value for the trace. Click the **Get Current Axis Limits** button to retrieve the X-Axis range from the screen view.

- **Margins** - Enter a value for the trace margins, in percent, for top and bottom of the graph.
- **General Options** - Select the check boxes to turn these 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.
- **Orientation** - Select portrait or landscape orientation for your graph by clicking the appropriate button.

Annotations

To change the annotations on the chromatogram:

1. From the Chromatogram Window, do a right mouse click and then select **Annotations**.
2. Select the **Trace**.
3. In the drop down box, select **Peaks**, **Groups, Fractions**, or **SEC**. If you have the SEC option installed, you can select SEC to annotate specific SEC features on your chromatogram.
4. Click on an **Available Annotation**. When an annotation is highlighted, you can add it to the annotations to be shown by clicking the **Green** arrow key (pointing to the right). This can also be done by double-clicking the selection.
5. For certain annotations, you can also designate the number of places to be displayed to the right of the decimal point. Enter this value in the **Decimals** box for the highlighted item.
6. Click the check box(s) to display **Baseline**, **USP Width**, or **Retention Time Windows, Show undetected named peaks, Group ranges,** and **FRC Actual** on the trace. With the SEC option installed, you will have access to additional SEC annotation features. You must have a Fraction Collector installed for FRC Actual to be available.

   Note: The Reference Peak window annotation displays the window set in the Peak Table. This window is not adjusted for relative retention time.
7. If you want to apply the annotation changes to all open channels, click the **Apply To All** button. If you want to apply the changes to the open chromatogram, select **OK**.
   Annotations are not saved as part of the method and are considered a function of the instrument application. If you close a method and re-open it, the current settings will apply.

Change the chromatogram appearance

You can change the appearance of the trace (line type, color, etc.) from the **Appearance** tab in the Properties box. Click on this tab to display the Appearance tab dialog.

To change the appearance of a chromatogram or trace:

1 In the **Chromatogram Window**, do a right mouse click and select **Properties**.

2 Click the **Appearance** tab. The following fields are available:

- **Scheme** - If you have previously saved an appearance scheme on disk, you can select it from this box. The **Save As** button allows you to save the existing appearance scheme on disk by giving it a name. The **Delete** button allows you to delete a scheme and start again.
- **Item** - This drop-down list lets you select which part of the Chromatogram Window for which you wish to change the appearance. The choices will include the graph itself (including background and legends), and the available traces.
- **Sub-item** - Select the sub-item you wish to modify. The choices for this will change based on the item you have selected. For example, if the Item selected is the Graph, you will have access to setting up appearances of sub-items including the background, axes and labels for the graph. If the item selected is a chromatogram data channel, you will have access to setting appearances of sub-items such as baselines, start and stop tic marks, and annotation. If the item selected is text, you will have access to the **Font** formatting commands as well.

  When a sub-item is selected, you will have access to fields appropriate to that item. For example, if you have chosen the **baseline** sub-item, you can choose the color and line type. If you have chosen the **annotation** sub-item, you can choose the font appearance and color.

  You can change the appearance of any trace without adding a new trace, by doing a right click in the **Chromatogram Window**, then selecting the **Appearance...** command. When you select this command, you will see an identical dialog to that shown above for the Appearance Tab.

Table 1 is an example of sub-items available in the Appearance tab.

Table 1 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 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 of the graph.
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 hand 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 display.
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 font for display of the trace Annotation(s). The items to be annotated for a trace are selected in the Annotations tab.
Data	Baseline	Select a color and/or line type for display of the baseline.
Data	Baseline Start Tick	Select a color and/or line type for display of baseline start ticks.
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.

Zooming

You may want to examine a chromatogram in more detail, or zoom in on a portion of the chromatogram. To do this, drag a box around the area of interest by holding down the left mouse button and dragging the box until it highlights the section of interest. Then release the mouse button. To move quickly to the previous level of zoom, double-

click on the chromatogram. To zoom to the full chromatogram again after multiple zooming operations, click the right-hand mouse button anywhere in the Chromatogram Window, then select **Full Unzoom** from the menu displayed. You can also execute a full unzoom of your chromatogram with CTRL+Z or SHIFT+double click in the Chromatogram Window. Once the chromatogram is in a zoomed view, you can scroll it. See Scrolling the chromatogram.

At the top of the Chromatogram Window is a display of **Time** and **Amplitude**. These values change as you move the cursor and reflect the time and amplitude of the trace where the cursor is located. If you have more than one trace, you can change the display to another trace by clicking on the chromatogram trace with the mouse. If the traces are displayed in different colors, the color of the Time and Amplitude display will reflect the color of the trace displayed.

Clear overlaid traces

You can clear all overlaid traces from the current Chromatogram Window by doing a right mouse click, then select the **Clear Overlays** command from the pop up menu.

Copy to clipboard

The Copy to Clipboard command copies the current Chromatogram Window to the clipboard as a metafile. From here, you can paste the view into a word processing document or other application that supports the clipboard. To paste into Microsoft Word, you need to use the **Edit/Paste Special/Picture** command.

To copy the contents of the window to the clipboard:

From the Chromatogram Window, do a right mouse click and select **Utilities** followed by **Copy to clipboard**.

Print a trace

This command sends the current Chromatogram Window view to the printer.

1. In the **Chromatogram Window**, right-click, and then select **Utilities**.
2. From the **Utilities** menu, select **Print Trace**.

Save a trace

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

1. In the **Chromatogram Window**, right-click, and then select **Utilities**.
2. From the **Utilities** menu, select **Save Trace**.
3. Click on the trace you wish to save.
4. In the **Save Data File As** dialog, browse to the location for saving the file and type the name for the file.

Remove a trace

If you have multiple traces in your Chromatogram Window, and you want to remove one or more of them from the Chromatogram Window, right-click anywhere within the window, and select the **Properties** command. A spreadsheet will appear where the currently displayed traces are listed.

To completely remove a trace from the **Chromatogram Window**, select the row by clicking on the **#** number, then press the **Delete** key on your keyboard.

To temporarily remove the trace from the window, clear the check box in the **Show** column. Click **OK** to return to the Chromatogram Window.

Set limits for X-axis and Y-axis

Occasionally, you may want to set an absolute range for either the X-Axis or Y-Axis, or both.

To set limits for the X- and Y- axis

1. Right-click in the **Chromatogram Window**, and then select **Properties**.
2. Click the **Trace Setup** tab to set Y-Axis minimum and maximum values for the trace. To set an absolute voltage range for all chromatograms, use the **User-Defined** option for the **Scale To** field. You must then enter a **Y-Min** (minimum Y-Axis value) and **Y-Max** (maximum Y-Axis value) for each chromatogram. If you want all chromatograms to be displayed using this same voltage scale, enter the same values for all chromatograms.
3. Click the **Axis Setup** tab to set absolute ranges for the trace. Select **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 you to use the zoom function to identify the desired region of the chromatogram and automatically enter the range values.
4. Once you have set an absolute range for one or both of these axes, the designated chromatogram(s) will always be displayed in the Chromatogram Window using these ranges until you change or reset them.
5. To reset the scaling of all chromatograms to default values, click the **Reset Scaling** button.

Chromatogram operations

There are a number of chromatogram comparison and mathematical operations that are available from the **Chromatogram Window**. These are accessed by doing a right mouse click in the Chromatogram Window and then selecting **Operations**.

Move Trace	Lets you 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.
Normalize	Normalizes one or more chromatograms to the first chromatogram, adjusting the heights such that the apex height of a selected peak matches that of the peak selected on the first trace.
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.

Move a trace

To grab a trace and move it with your mouse:

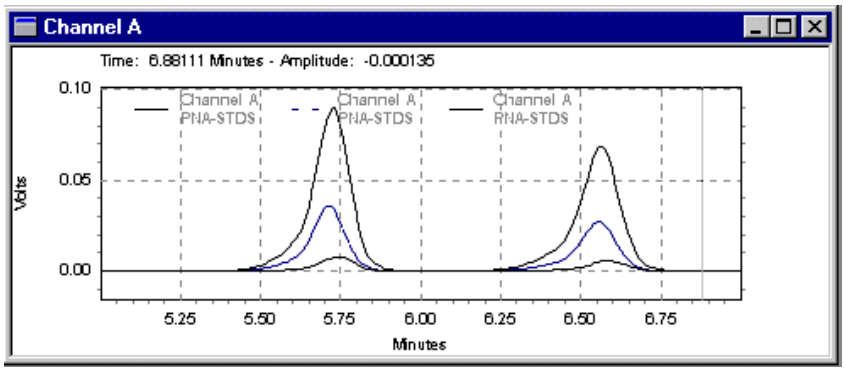
1. In the Chromatogram Window, do a right mouse click and select **Operations** followed by **Move Trace**.
2. Grab the trace by clicking the left mouse button and dragging the trace to a new location. When you release the mouse button, the trace will be placed where your cursor was located when you released the button.
3. You can continue to move traces. When finished, do a right mouse click and select **Operations** followed by the **Move Trace** command again to turn off the move trace operation.

Stack traces

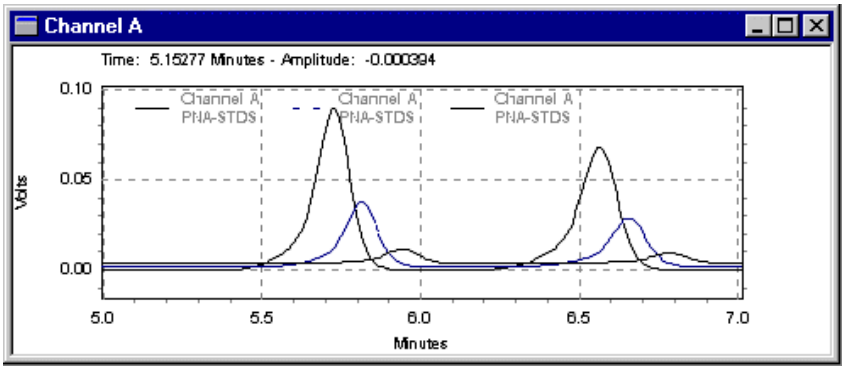
To quickly change the X-axis and Y-Axis offset for a trace:

1. In the Chromatogram Window, do a right mouse click and then select **Operations** followed by **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.



Chromatograms before stacking



Chromatograms after stacking

To remove these offsets:

1 In the **Chromatogram Window**, click the right mouse button and then select **Properties.**

2 Click the **Trace Setup** tab, then scroll to the right to the X-axis and Y-axis offset columns where you can delete or change these settings.

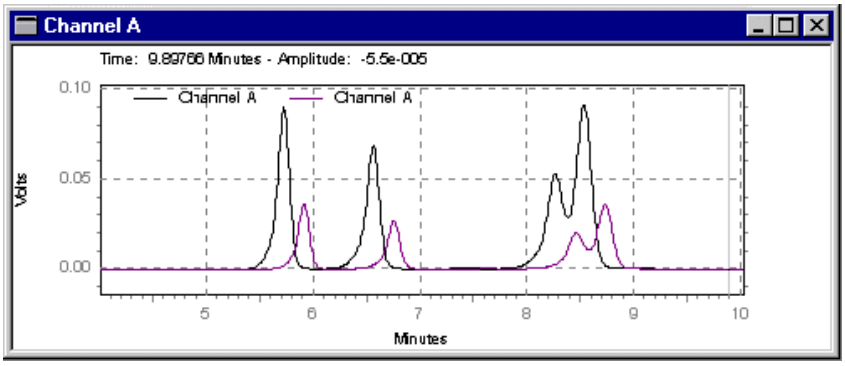
3 Click the **Reset Scaling** button to restore ALL settings to their original values. Or, you can use the **Stack** command again, entering 0 for both stack parameters.

Align two traces

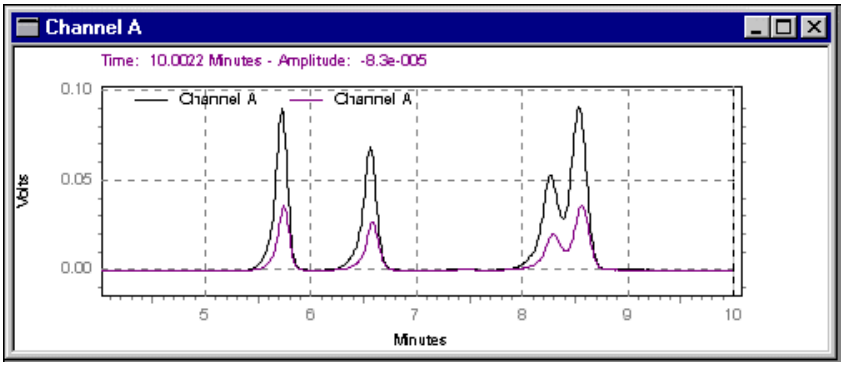
To align one chromatogram to another:

1 In the **Chromatogram Window**, do a right mouse click, and then select **Operations** followed by **Align**. Click first on the point of the first chromatogram to which you wish to align, then click on the peak (or point) of the second chromatogram which you wish to align to the first point. The second chromatogram will be adjusted such that the peak (or point) you clicked second will be aligned with the first point you clicked.

2 To remove the alignment, use the right mouse button/ **Properties** command to view the trace spreadsheet. Click the **Trace Setup** tab, then scroll to the right to the X-axis and Y-axis offset columns where you can delete or change these settings. Click the **Reset Scaling** button to restore ALL settings to their original values.



Chromatograms before alignment.



First peak of top chromatogram aligned to first peak on bottom chromatogram.

Stretch a chromatogram

The stretch function allows you to perform a two-point contraction or expansion of chromatograms relative to another.

To stretch a chromatogram:

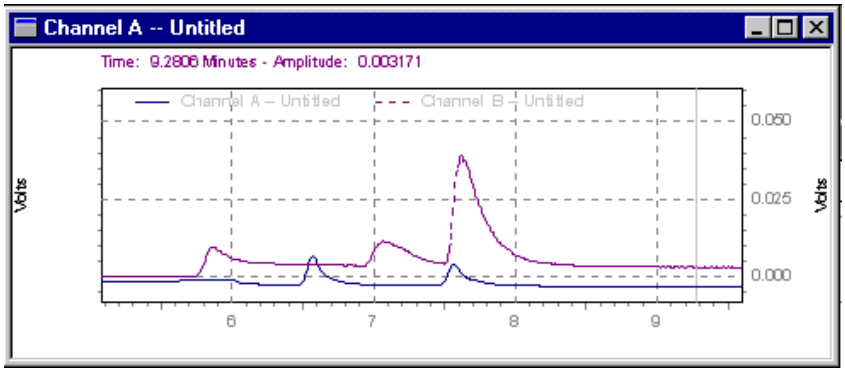
1 In the **Chromatogram Window**, do a right mouse click and then select **Operations** followed by **Stretch**.

2 Select points (or peaks) on the first chromatogram to which the second will be stretched (or contracted).

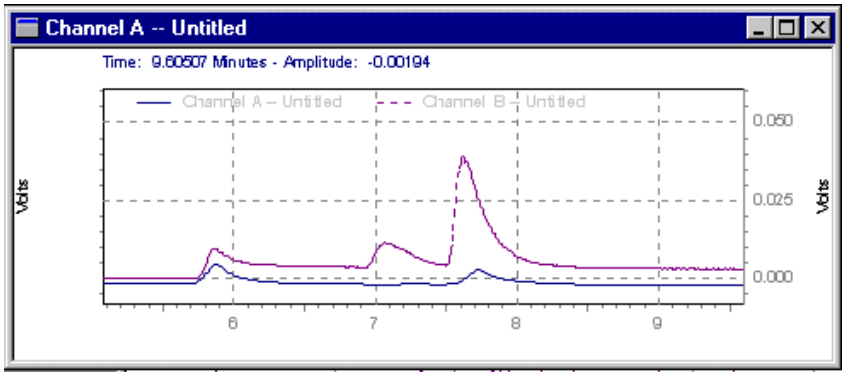
3 Select two points on the second chromatogram. The chromatogram between these two points will be stretched or contracted to fit the two points specified on the original chromatogram.

To undo the stretch:

1. In the **Chromatogram Window**, do a right mouse click and then select **Properties**. Click the **Trace Setup** tab, then scroll to the right to the X-axis and Y-axis offset columns where you can delete or change these settings.
2. Click the **Reset Scaling** button to restore ALL settings to their original values.



Chromatograms before stretching.

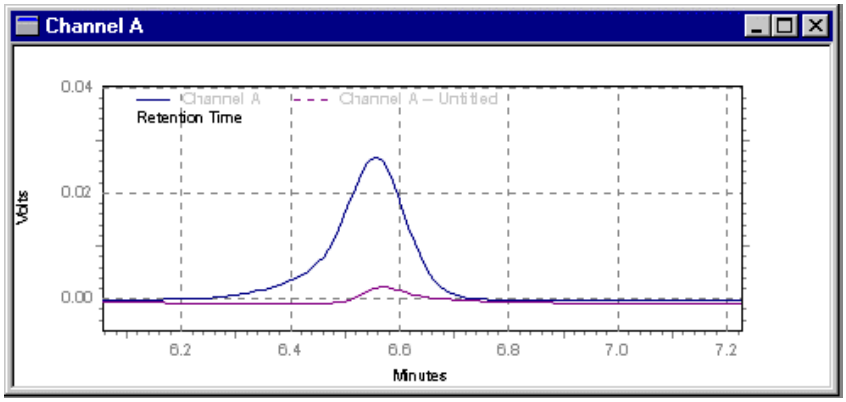


Bottom chromatogram stretched relative to top chromatogram.

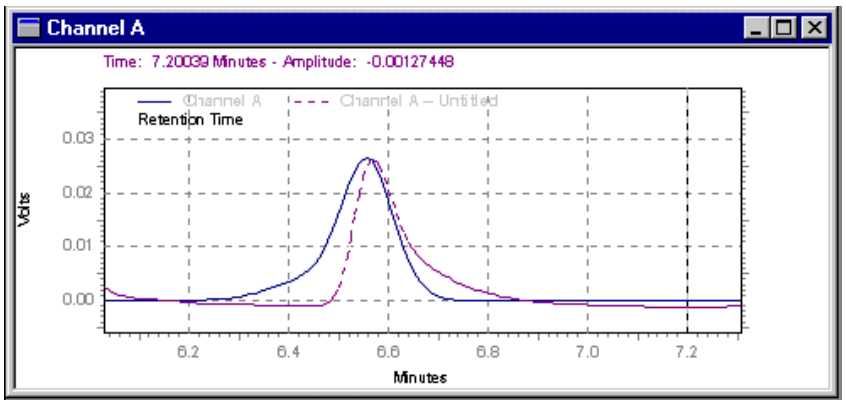
Normalize traces

This function allows you to 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 you have selected this command, you will be prompted to select the start and then the apex of a peak in the first trace. Then you will be prompted to click on the start and apex of a peak in the second trace for normalization.

To un-do the normalization, use the right mouse button/ **Properties** command to view the trace spreadsheet. Click the **Trace Setup** tab, then scroll to the right to the X-axis and Y-axis offset columns where you can delete or change these settings. Click the **Reset Scaling** button to restore ALL settings to their original values.



Chromatograms before normalization.



After Normalization.

You can set the default trace to Normalized for each instrument per user. See Change View Preferences for more information.

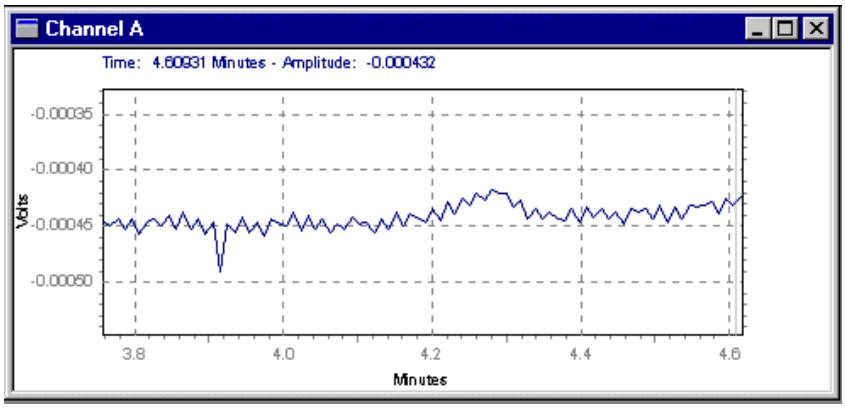
Smoothing

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

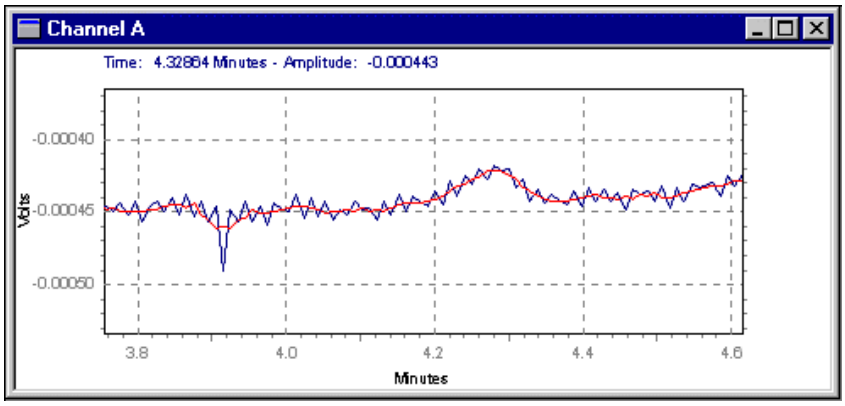
1 Right-click in the **Chromatogram Window**, point to **Operations**, and then click **Smooth**. A prompt will appear in the window instructing you to **Click on trace**.

2 Click the chromatogram to be smoothed. The result trace will appear in the window.

Chromatogram before smoothing.



Smoothed result trace is displayed with original trace.

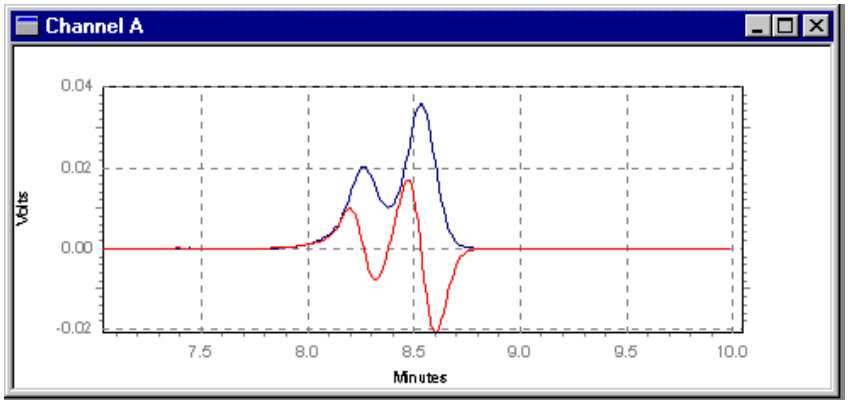


Calculate derivatives

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

1 Do a right mouse click on the chromatogram, and then select **Operations** followed by **1st Derivative** or **2nd Derivative**. A prompt will appear in the window **Click on trace**.

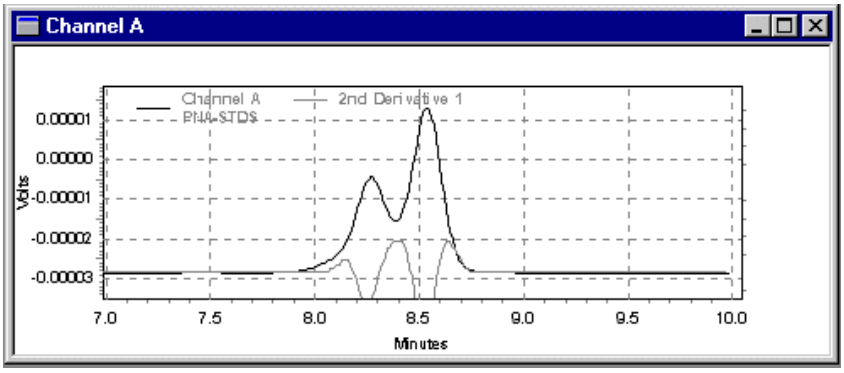
2 Click on the chromatogram for which you wish to perform the



operation. The result trace will appear in the window.

Trace before 1st derivative.

1st derivative trace displayed with original trace.



2nd Derivative displayed with original trace

Add two traces

To add two traces to a Chromatogram Window:

1. In the **Chromatogram Window**, do a right mouse click, and select **Operations** followed by **Add**.
2. Click on 1st trace to select the first file by clicking the mouse on the chromatogram.
3. Click on the 2nd trace to select the trace to be added to the first by clicking on the trace with the mouse. The result trace will appear in the window. Note that in order for this operation to be valid, both traces must have the same sampling frequency.

Subtract two chromatograms

To subtract two traces:

1. In the **Chromatogram Window**, do a right mouse click and then select **Operations** followed by **Subtract**.
2. At the prompt, click on the 1st trace. Select the first trace by clicking the mouse on the chromatogram.
3. Select the trace to be subtracted from the first by clicking on the trace with the mouse. The result trace will appear in the window.

Note: In order for this operation to be valid, both traces must have the same sampling frequency.

Multiply two traces

1. Right-click in the **Chromatogram Window**, point to **Operations**, and then click **Multiply.**
2. Select the first trace by clicking the mouse on the chromatogram or trace.

3 Select the trace to be multiplied by the first by clicking on the 2nd trace with the mouse. The result trace will appear in the window. For the multiply operation, the units of the resulting trace are <trace 1 units> x <trace 2 units>.

Divide chromatograms or traces

To divide two traces:

1 In the **Chromatogram Window**, do a right mouse click and then select **Operations** followed by **Divide**.

2 A prompt will appear in the window **Click on 1st trace**. Select the first trace by clicking the mouse on the chromatogram.

3 A second prompt **Click on 2**nd **trace** will appear. Select the trace to be divided into the first by clicking on the trace with the mouse. The result trace will appear in the window. The equation used to calculate the result trace is as follows.

$$p = \left(\frac{y_1}{\sqrt{y_1^2 + y_2^2}} \right) \div y_{mult}$$

Where

p = the calculated point for the result trace at time t

y1 = a point from the first trace at time t

y2 = a point from the second trace at time t

ymult = the y multiplier for the trace that converts it from microvolts to the trace's displayed units

Tutorial

Use the tutorial to learn how to set up a method, acquire a data file, optimize the method for integration, and set up calibration. Perform all steps in the order presented.

See Also

Create a Method

Run a Sample

Set Integration Parameters Graphically

Prepare a Method for Calibration

Calibrate a Method

Create a Sample Sequence

Run a Sequence

Review Multi-level Calibration Curves

Change Integration Parameters

Create a method

The first step of the tutorial is to create a method. A method contains the information needed to acquire data. Use the Method Wizard to create a method.

Create a method using the Method Wizard:

1. Select the **Instrument Wizard** icon  .
2. In the **Instrument Wizard** dialog box, select **Create a new method**.
3. In the **Instrument Setup** dialog box, each tab in the dialog box corresponds to one of the configured modules of your instrument. The tabs will vary depending on the type of instrument and its configured modules. Select each tab to set up the parameters for that module. Click the **F1** key when each tab is displayed to see specific help topics for each module. See Instrument Setup.
4. Once you have completed the acquisition setup information, select **File > Save > Method.**
5. The **Save Method File As** dialog box opens to the method folder in your project files, and **Save as type** is set to **.met**. In the **File name** field, type **Test.met**.
6. In the **Description** field, review or change the method description if necessary.
7. Select **Save**.
8. Exit the dialog box.
9. Next Run a Sample.

Run a sample

You will now use the method you just created to make your first data acquisition run.

1. To start the run, in the toolbar select **Control > Single Run.**
2. In the **Single Run** dialog box, locate the **Sample ID** field and enter **Test**.
3. In the **Method** field, enter the name of the method you want to run, including the full path name. Select the **Open File** button to select **Test.met** from a list.
4. In the **Data file** field, enter **Test.dat** as the name for storing your data. You must enter a unique file name in this field. Therefore, if you have performed this tutorial before, you must first delete this file from your disk, or move it to a different directory before proceeding.
5. In the **Result path** field, enter the location where your results will be saved, including the full path name. Select the **Browse for folder** button to select the result **.rslt** folder.
6. In the **Result name** field, enter **Test**. This is the name of your result file.
7. Select **Submit**. You will see the data as it is acquired in the Chromatogram Window on your screen.
8. Next, Set Integration Parameters Graphically.

Set integration parameters graphically

The data system 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 your 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 so only some peaks are effected.

To add a timed event to turn off integration to your method:

1. At this point, your recently acquired chromatogram should be displayed in your Chromatogram Window. If it is not, select **File > Open > Data**, and select your result **.rst** file.
2. In the top toolbar, select the **Analyze** button  . This will integrate the chromatogram and display the baselines.
3. In the bottom toolbar, select the **Integration Off** button  .
4. Follow the instructions in the **Integration Off** message window (see To view the integration message window). As instructed in the message window, click your mouse once prior to a part of the chromatogram where you want to turn integration off. (Select a section of chromatogram where one or more peaks elute.) Then click the mouse again at the point on the chromatogram where you want to turn integration on again.

5 In the **Integration Off** dialog box, complete the following fields:

- **Start Time** and **Stop Time** indicate the points where you clicked your mouse. The integration will be turned off between these points on your chromatogram.
- **Value** is set at zero, as no numeric value is required for this event.
- **Add event to Method (all data)** select this to add the event to the Method. It will be used on all chromatograms analyzed using this method.
- **Add event to this data file only** select this to add the event to this data file only. It will be applied only to this chromatogram.
- **Add to Table** will add the event to the integration timed events table without re-integration.

6 Select **Analyze Now** to add the event to the method and re-integrate the chromatogram. Your chromatogram will be redrawn using the new integration event. Notice that the area you selected has no baselines drawn because the integration has been turned off for these peaks.

7 In the top toolbar, select the **Integration Events** button  to open the **Integration Timed Events** table. The **Integration Off** timed event has been added to the table.

8 To remove the event from your method, select the **Integration Off** row number and select the **Delete** key on your keyboard. You can also delete the event using the **Edit > Cut** command, and re-insert the event using the **Edit > Paste** command.

9 To temporarily view the effect of removing an event without actually removing it from the table, click the check box adjacent to the event to deselect it. To reselect the event, click the check box once again.

10 When you are finished with the **Integration Events** table, close it and return to your chromatogram.

11 Next, Prepare a Method for Calibration.

Prepare a method for calibration

If you are interested in peak quantitation (calculation of results based on the running of standards), you must prepare your method for calibration. Further details on how to set up multiple level calibrations are given in the Methods section of this manual. For this tutorial, however, you will set up a single level of calibration.

Setting up any type of calibration involves the following steps:

1 Identify the Calibrated Peaks and enter standard amounts in the method.

2 Run the standard sample(s).

3 Review the calibration curve.

To enter calibration peak data run the standard sample first, then use the stored data file to graphically define your calibration peaks. Run a standard sample using the steps shown in Run a Preliminary Sample, or select one of the data files provided.

1 Select **File > Open > Data** and select a standard samples result file. The chromatogram opens.

2 On the top toolbar, select the **Analyze** button  to integrate the chromatogram and show the baselines.

3 On the bottom toolbar, select the **Define Single Peak** button  .

4 In the **Define Single Peak** dialog box, the retention time of the first detected peak will appear. To add this peak to the peak table, complete the fields listed below. If you do not wish to add this peak to the peak table, select the **Next** button. To move to a specific peak in the chromatogram, select the peak with your mouse.

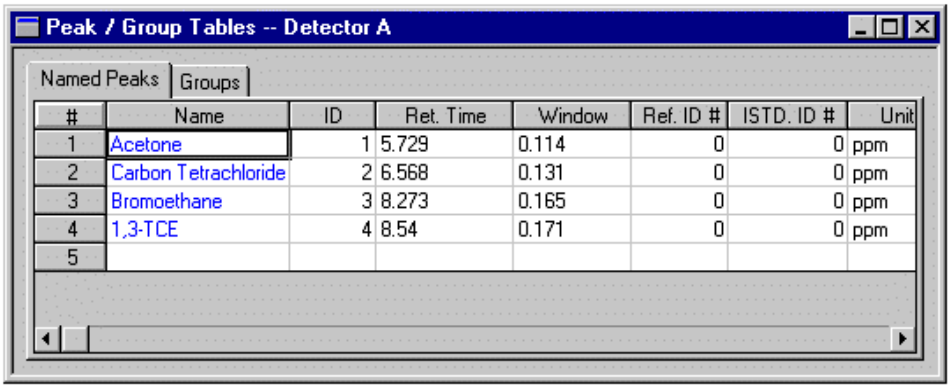
Peak Name	Enter the name of the compound in this field.
Conc Level	Concentration Level 1 is shown. Enter the amount of this compound for this concentration level. (**Note**: For setting up more than one level for this compound, you would enter Concentration Level 2 and the amount for that level. Continue to enter level concentrations until you have completed the number of calibration levels desired.)
Units	Enter the units to be used for display of results.
ISTD ID #	If you are doing 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 you don't know it, you can add it in the peak table later.
Ref ID #	Enter a retention time reference peak ID # to be used for this peak. This is the peak ID number from the peak table. If you don't know it, you can add it later in the peak table. Reference peaks are used to locate calibrated peaks when chromatographic conditions change such that retention times shift.
Retention Time Window	Select how you want 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	Select this if you want the system to calculate the retention time window based on a % of the expected retention time of the peak. Enter the % you want to use for calculation of the window.
Absolute	Select this if you want to enter an absolute window for the peak. Enter the value you want to use for the retention time window, in minutes.
Next	Select this to move to the next peak in the chromatogram.
Back	Select this to move to the previous detected peak in the chromatogram.

5 Select Done.

6 On the top toolbar, select the Peak/Group Tables button  .

7 In the Peak/Group Tables dialog box, select the Named Peaks tab. Each peak you defined is a row in the Peak Table spreadsheet, along with its retention time and other parameters you entered.

8 Information in the spreadsheet can be edited. Each column



represents a parameter for the calibration, including the Levels, which contain the calibration amounts for each compound at each level of calibration. It is possible to customize the Peak Table so 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 given in the Calibration chapter of this manual.

9 Select File > Save > Method. If you wish to save the method using a different name, select File > Save As > Method. See Save a Method.

10 Close the **Peak Table**.

11 Next, Calibrate a Method.

Calibrate a method

Once you have Prepared a Method for Calibration you are ready to calibrate the method.

1 From the menu bar, select **Analysis > Analysis/Single Level Calibration**. In the **Analysis/Single Level Calibration** dialog box, designate the file information for your calibration.

2 In the **Sample ID** field enter **Test**.

3 In the **Method** field, enter the name of the method you want to calibrate, including the full path name. Select the **Open File** button to select **Test.met** from a list.

4 In the **Data file** field, enter the name of the data file you are using to calibrate the method, including the full path name. Select the **Open File** button to select **Test.dat** from a list.

5 In the **Result path** field, enter the location where your results will be saved, including the full path name. Select the **Browse for folder** button to select the result **. rslt** folder.

6 In the **Result name** field, enter **Test**. This is the name of your result file.

7 Leave the **Amount Values** set to 1. For details on how these values are used, see About Methods.

8 Click on the **Calibration** checkbox, then enter a 1 for **Calibration Level**.
Since this method is currently uncalibrated, it is unnecessary to select any of the boxes dealing with calibrations or replicates. However, if you are unsure of the method contents, click the **Clear all calibration** box before starting.

9 Select **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. 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.

10 Next, Create a Sample Sequence.

Create a sample sequence

If you are using an autosampler to inject samples, you must define the samples to be injected and how they are to be acquired and analyzed. This is done 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 are located in the Sequence section. In this part of the tutorial you will create and use a simple sequence to acquire a calibration sample and two or three unknown samples.

To create a new sequence:

1 Select the **Instrument Wizard** button  .

2 In the **Instrument Wizard** dialog box, select **Create a sequence.**

3 In the **Method** field, enter the method to be used for acquisition, including the full path name. Select the **Open File** button to select **Test.met** from a list.

4 Select the **For Acquisition** button. This will cause the Sequence Wizard to prompt you for information required for data acquisition.

5 Leave the **Amount values** at their default values. Then select **Next.**

6 In the **Sample ID** field, select the blue right arrow and select the **Line number** and **Method name.** This will cause each sample to be identified with the sequence line number and current method name.

7 In the **Data File** field, select the blue right arrow and select **Sample ID.** This will cause the data files to be named by the sample ID you selected above. Using a numbered identification ensures the data file name for each run is a unique name, preventing errors that will occur if you try to acquire data using an existing data file name.

8 In the **Number of unknown runs in sequence** field, enter **3**. Leave the other fields at default values.

9 Click **Next**.

10 In this dialog, the **Calibration ID** and **Calibration file** names are automatically set to the identifications from the previous dialog.

11 Set the **Number of calibration levels** to **1**, and leave the **Repetitions per level** at **1**.

12 Leave all other boxes unchecked, then click **Next**.

13 Select the check boxes **Include unknown runs in summary report** and **Include calibration runs in summary report**. Do not select the other boxes.

14 Select **Finish**.

15 A sequence spreadsheet will appear, with the file and method names you specified shown.
At this point, the sequence is set up to run 1 calibration sample and 3 unknown runs. Notice the Sample ID's and Data File names are numbered automatically to prevent duplication. In order to run a calibration standard as the first run, you must designate that run to be a calibration run. This has been done 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, see Set Sample Run Types and About Sequences. Since the method we have been creating in this Tutorial is a single level calibration, only one calibration standard run is necessary.

16 To save the sample sequence file, select **File > Save > Sequence**. Navigate to the **Sequence** folder, under **File name** enter **Test.** By default, sequence files are saved with the **.seq** extension. Select **Save**.

17 Next, Run a Sequence.

Run a sequence

Once you have Created a Sample Sequence you are ready to run the sequence.

1 In the toolbar, select the **Sequence Run** button  , or right-click in the sequence spreadsheet, and select **Run Sequence**. In the **Sequence Run** dialog box designate the file information for your sequence.

2 In the **Sequence name** field, enter the name of the sequence file you want to run, including the full path name. Select the **Open File** button to select **Test.seq** from a list.

3 In the **Result path** field, enter the location where your results will be saved, including the full path name. Select the **Open File** button to select the result **. rslt** folder.

4 In the **Result name** field, enter **Test**. This is the name of your result file.

5 Prepare your autosampler to inject your standard sample, followed by 3 unknown samples.

6 Select **Submit**.
When the sequence is completed, you will have acquired and saved the data files for one standard and three unknown runs.

7 Next, Review multilevel calibration curves.

Review multilevel calibration curves

Once you have fully calibrated a method, the calibration curves and associated data can be viewed using the **Review Calibration** function. In order to see a fully calibrated multilevel calibration, use the **multilevel calibration.met** file provided with the data system. For additional details on using Review Calibration, see Review Calibration Curves.

1 Select **File > Open > Method**.

2 Select the **multilevel calibration.met** file from your disk. It will be located in the \datasystem\Methods folder. (Where datasystem = your installation program folder.)

3 Select the **Review Calibration** button  , or select the **Method > Review Calibration** command.

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 peak that is highlighted. You can view the other curves by highlighting their peak name. At the top of the screen is a spreadsheet that displays all the calibration information, including areas used to create the current calibration curve.

4 The calibration curve fit type by default is Point_to_Point. To overlay a different fit type, click the **right** mouse button anywhere in the calibration curve box. Select **Fit Type** and then select **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, R^2, which is not calculated for the Point_to_Point curve since it is by definition a perfect fit to the data.

5 To close the window, click the **X** box at the upper right corner of the **Review Calibration** window.

6 Change Integration Parameters.

Change 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, you will become familiar with how to enter integration timed events into your method, and to view the effects of some of these events. Complete details on how each integration timed event works are given in the Integration section.

1 Select **File > Open > Data** and select the **Test.rst** file.

2 Select the **Analyze** button  to analyze the chromatogram and display the baselines. The vertical line cursor moves with your mouse. The retention time where the cursor is located is shown at the top of the Chromatogram Window.

3 Add the **Valley-to-Valley** timed event to integrate the cluster of 4 large peaks with valley-to-valley baselines. On the integration toolbar, select the **Valley to Valley** button  . Then, select the mouse once before the first large peak, then again just after the last peak.

4 In the **Valley to Valley** dialog box, select the **Analyze Now** button and view the chromatogram. Notice the peaks within the region of the event are now integrated using the **Valley-to-Valley** event, and baselines are adjusted accordingly.

5 Select the **Integration Events**  button from the command ribbon. Note the addition of the **Valley to Valley** event in the table.

6 Remove the **Valley to Valley** event by clicking its number with the mouse, then select **Delete** on your keyboard. You can also test integration without the event, yet leave it in the timed event table, by deselecting the check box next to the **Valley to Valley** event and then reintegrating the chromatogram.

7 Close the **Integration Events** table by clicking the **x** box at the top right corner of the table.

You have now completed the tutorial. Detailed explanations on how to create multilevel calibrations, create custom reports, and create and use sample sequences are given in later sections. Use the online Help as you work with the software.

About Instruments

Use the Instruments pane in the Control Panel to setup and control the instruments connected to your system. See your Control Panel help for more information about the Instruments pane.

See Also

Configure instrument

Configure an analog detector

Configure an external event

Configuration options

Configure a fraction collector

Instrument Activity Log

View the instrument status

Set the instrument to Sleep or Wake mode

Configure instrument

Configuration is the process by which you tell the software about the installed detectors, injectors, or other components for an instrument. Each instrument must be configured before the program can be used to acquire data from it.

Before you can configure an instrument, it must be added to the instruments list in the Control Panel.

To have the program automatically detect and configure your installed devices:

1. From the **Control Panel** navigation pane, select **Instruments**.
2. Select the instrument.
3. In the **Actions** toolbar, select **Configure Instrument**.
4. In the dialog box, select **Auto Configuration**.
5. In the **Auto Configuration** dialog box, enter the **Number of Detectors**, and **Number of Pumps**.
6. Select **Autosampler** if necessary.
7. Select **OK**.

To manually choose which devices to configure:

1. From the **Control Panel** navigation pane, select **Instruments**.
2. Select the instrument.
3. In the **Actions** toolbar, select **Configure Instrument**.
4. In the dialog box, select a module from the **Available modules** and select the arrow to move it under **Configured modules**.
5. Double-click on a **Configured module** to open a dialog box pertaining to that module. If applicable see Configure an analog detector, Configure an external event, or Configure a fraction collector.
6. Select **Options**.
7. In the **Configuration Options** dialog box, select from the following General options: **System Suitability**, **SEC**, **PDA**, and **Baseline check**.
8. Select **OK**.

Configure an analog detector

1. From the **Control Panel** navigation pane, select **Instruments**.
2. Select the instrument.
3. In the **Actions** toolbar, select **Configure Instrument**.
4. In the dialog box, select an analog detector from the **Available modules** and select the arrow to move it under **Configured modules**.
5. Under **Configured module**, double-click an analog detector.

6 In the **Detector Configuration** dialog box complete the following fields:

Detector Name	Enter a descriptive name for the detector. For example FID or TCD.
Detector Model	Select the type of detector from the drop-down list.
Acquisition Source	Select the type of A/D board or device you are using from the drop-down list. Then click the adjacent button to configure it.
Y-Axis Units	Type in the units to be displayed on the Y-Axis of your chromatogram. For example, microvolts or AU, depending on the detector units of measurement. Your analog signal is acquired and stored in microvolts. If you want to display the signal in different units, you must use the correct multiplier. Consult the table below.
Y-Axis Multiplier	The chromatogram is usually displayed in volts. If you wish to display another unit, enter the conversion factor to be applied. Consult the table below.

Commonly used Y-axis labels and corresponding multipliers

Y-Axis Label	Y-Axis Multiplier
Volts	0.000001
Millivolts	0.001
Microvolts	1

Configure an external event

Events include instrument triggers, valves, and other user-defined external events.

To configure events for an instrument:

1 Insure that your event is properly connected to the data system.

2 From the **Control Panel** navigation pane, select **Instruments**.

3 Select the instrument.

4 In the **Actions** toolbar, select **Configure Instrument**.

5 In the dialog box, select **Events** from the **Available modules** and select the arrow to move it under **Configured modules**.

6 Under **Configured module**, double-click **Events**.

7 In the **Event Configuration** dialog box complete the following fields:

Name	To configure a **Trigger** or **Ready** line, select the drop-down button and select **Trigger** or **Ready**. To configure a value or other external event, enter the name of your event.
Source	Select the drop-down button and select the source of the event (the hardware from which the event comes).
Setup	Select the button in the **Setup** field to open a dialog box. Enter information for the operation of this event.

Note: It is possible to assign the same events to more than one instrument. Be careful to assign events such that conflicts between instruments will not happen.

8 The **External Events** tab is now available in **EZChrom** under Instrument Setup.

Enable optional analysis software

To select the optional software or features to enable for an instrument:

1 From the **Control Panel** navigation pane, select **Instruments**.

2 Select the instrument.

3 In the **Actions** toolbar, select **Configure Instrument**.

4 In the dialog box, select **Options**.

5 In the **Configuration Options** dialog box, select from the available analysis options such as: **System Suitability**, **SEC**, **PDA**, and **Baseline check**.

6 Select **OK**.

Configure a fraction collector

1 From the **Control Panel** navigation pane, select **Instruments**.

2 Select the instrument.

3 In the **Actions** toolbar, select **Configure Instrument**.

4 In the dialog box, select **Auto Configuration**.

5 Under **Configured modules**, select **FRC**.

6 In the **Fraction Collector (FRC) Configuration** dialog box, select **Help** or press **F1** in a section for more information.

See Also Fraction collector configuration

Instrument activity log

To view the instrument activity log, select **View > Instrument Activity Log.**

The following information is displayed:

- User
- Logged
- Source
- Activity

The following options are available:

- To refresh the Instrument Activity Log select, **Refresh**.
- To add a manual entry, select **Add Manual Entry**.
- To print a selection, select an item or items then select **Print Selection**.
- To print the entire Instrument Activity Log, select **Print All**.

View the instrument status

You can view the selected instrument status in the message bar at the bottom of the screen at all times.

The status is shown as:

Not connected (gray)

The selected instrument is configured with the system and available to use but the AIC/workstation is not currently running.

To use this instrument, select **Launch** from the **Control Panel** or **Run a sample** or **sequence** from the **Data System**. Your specific hardware and method will determine how long before the instrument reaches the **Idle** state and is ready to process samples.

Stand by (teal)

The selected instrument is running in a **Sleep** resource saving mode (for example, gases and lamps turned off).

To use this instrument, select **Control >*Instrument*> Wake** or add a run to the run queue and wait until the scheduled instrument **Wake Up** time. Your specific hardware and method will determine how long before the instrument reaches the **Idle** state and is ready to process samples.

Idle (green)

The selected instrument is running and ready to process samples.

To use this instrument, select **Launch** from the **Control Panel** or **Run a sample** or **sequence** from the **Data System**.

Running (blue)

The selected instrument is currently collecting data.

To use this instrument, submit a run to the run queue or wait until it is **Idle**.

See Also Set the instrument to Sleep or Wake mode

Set the instrument to Sleep or Wake mode

You can set the selected instrument in the **Not connected** or **Idle** state to the **Stand by** state by selecting **Control >*Instrument*> Sleep** or by scheduling specific sleep and wake times through the instrument driver.

You can set the selected instrument in the **Stand by** state to the **Idle** state by selecting **Control >*Instrument*> Wake** or by scheduling specific sleep and wake times through the instrument driver. Your specific hardware and method will determine how long before the instrument reaches the **Idle** state and is ready to process samples.

See Also View the instrument status

About Methods

A method contains the information for how a sample is processed. It contains instructions for data acquisition (run time, sampling rate, etc.), integration, calibration and peak information, and 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.

Use the Method Wizard and the Instrument Setup information to create and save a method. You can also select a new project, view method reports, and edit method and data properties.

Use Advanced Method Options to customize results, or link to external data systems or networks.

If Pretreatment, Lab Monitor, or System Suitability software is supported by your instrument refer to those topics.

To add integration to your method see About Integration.

See Also

Create a Method with the Method Wizard

Instrument Setup

Open a Method File

Save a Method

Save a Master Method

Select a New Project

View Method Reports

Method Properties

Data Properties

Advanced Method Options

Sample Prep

Launch Lab Monitor Software

About System Suitability

Create a method with the method wizard

In order to acquire data and save it on the hard drive of your computer, you need to create a method that contains data acquisition information such as run time and sampling rate. To create a new method or edit an existing method, use the **Method Wizard**.

You can create a new method whether or not the instrument is on line. However, you only have access to starting actual data acquisition when you have an on line instrument connected.

1. Select the **Instrument Wizard** icon  .
2. In the **Instrument Wizard** dialog box, select from the following:
   - Select **Create a new method** to start a new method with the system default method parameters.
   - Select **Modify the current method** to step through the current method and make changes.
   - Select **Modify a method on disk** to open a file saved on disk and step through it to make changes.
3. In the **Instrument Setup** dialog box, each tab in the dialog box corresponds to one of the configured modules of your instrument. The tabs will vary depending on the type of instrument and its configured modules. Select each tab to set up the parameters for that module. Click the **F1** key when each tab is displayed to see specific help topics for each module. See Instrument Setup.
4. Once you have completed the instrument setup information Save the Method.

Instrument setup

The instrument setup portion of your method is where you define instrument control parameters and define acquisition parameters. If you are using a Generic instrument, parameters appear that enable you to set up the acquisition. If you have installed one of the instrument control options and are using one of those configured instruments, the instrument setup will contain parameters that are specific for the control of the selected instrument.

In the **Instrument Setup** dialog box, each tab in the dialog box corresponds to one of the configured modules of your instrument. The tabs will vary depending on the type of instrument and its configured modules. Select each tab to set up the parameters for that module. Select the **F1** key when each tab is displayed to see specific help topics for each module. A few of the common modules are listed below.

See Also

Open Instrument Setup

Import Instrument Setup

Detector 1

Trigger

External Events

Baseline Check

Aux Traces

Fraction Collector

Open instrument setup

There are three ways to open the Instrument Setup dialog box:

- In the toolbar, select the **Method Wizard** button  , then select **Create a new method**.
- In the navigation pane, select **Method > Instrument Setup**.
- In the toolbar, select the **Instrument Setup** button  .

Import instrument setup

This command enables you to open the instrument setup parameters from a saved method.

To import instrument setup:

1. Select **Method > Import Instrument Setup**.
2. In the **Open Method File** dialog box, select the method from which you wish to import the instrument setup parameters.
3. Select **Open**.

Detector 1

To configure the detector to use for a method:

1 Open Instrument Setup

2 In the **Instrument Setup** dialog box, select the **Detector** tab. If no trigger is configured, this tab will not appear.

3 For each detector channel configured on the instrument, define the following acquisition information:

Acquisition Channel On	Select this box to turn the acquisition for this channel ON. If this box is not selected, no data will be acquired for this channel.
Sampling	This is the rate at which data will be sampled by the system. You can choose how you want to specify the sampling rate. When you select a sampling rate, a prompt will appear indicating the narrowest peak width for which this sampling rate will be adequate. **It is recommended that you use the Graphical Events Programming to determine the optimum sampling rate for your chromatography.**
Frequency	This selection is in Hz (samples per second). This is the selection for most chromatography applications. Click on the down-arrow to get a list of the frequencies available for the configuration of your system.
Period	When you select this type of sampling, you must select the number of seconds (or milliseconds) between data points. Enter the value, then select whether the period is in milliseconds (mSec) or seconds.
Run Time	Run Time determines the length of time data will be sampled.
Acquisition Delay	Acquisition Delay is the interval between the start of run (Trigger) and the time when sampling starts for this channel.

Trigger

The trigger determines how the data sampling is started.

To select the type of trigger to use for a method:

1 Open Instrument Setup

2 In the **Instrument Setup** dialog box, select the **Trigger** tab. If no trigger is configured, this tab will not appear.

3 Select the Trigger **Type** for the type of remote start (if any) you have installed for the instrument you will be using. The trigger for each instrument is set up during configuration.

None	Sampling starts immediately after clicking on Start. Sequence acquisitions do not pause between runs.
Manual	Operator has to press **ENTER** to start the run. Sequence acquisitions pause for confirmation between runs.
External	If the data sampling is started from an external trigger, select this option. The type of trigger is designated when the instrument is configured.

External events

Once you have configured external events for your instrument, you can program the events for your method. When you select this tab, a spreadsheet appears where you can select the events and designate when and how they activate during the run.

To configure external events:

1. Open Instrument Setup
2. In the **Instrument Setup** dialog box, select the **External Events**. This tab will not appear on your menu unless you have configured external events for your instrument.
3. To program an event, select it from the drop-down list of configured events by clicking the **Event** field.
4. Enter the time at which the event is to actuate, the length of time you wish the event to remain in the desired state (**Duration)**, and the **State** of the event during the event (**Close** or **Open**).
5. You may configure up to 25 events for the run.

To view and edit the current state of the event:

1. Select **Control > Instrument Status**. This option will not appear on your menu unless you have configured external events for your instrument.
2. In the **Instrument Status** dialog box, select the **External Events** tab.
3. Each configured event is displayed on a line, along with its current **Status**. To change the status, click on the field displayed in the **Change To** column.
4. Select **Apply**. If **Ignore** is selected in the **Change To** field for an event, pressing **Apply** will not change that event.

Baseline check

Use **Baseline Check** to set the parameters for a baseline check while acquiring data using this method.

When a method containing baseline check parameters is used for data acquisition, a baseline check will occur when either:

- The **Perform Baseline Check** checkbox is checked in the **Single Run** dialog, or
- The **Run Type** of the current **Sequence** line includes **Baseline Check**.

When a baseline check is to occur as part of data acquisition, the software will first download the initial conditions from the method to the instrument. These initial conditions are then used to acquire the baseline check data before the normal data acquisition. If the baseline check data fails to meet the threshold for any channel, then the data acquisition is aborted.

If the baseline check results indicate a failure of the test, then the current run is aborted and the baseline check data and results are stored in the data file without any other acquisition data. If the run is aborted (by the user or because of a hardware error) prior to the completion of the baseline check data acquisition, then no data is saved.

To set up the Baseline Check:

1 Open Instrument Setup

2 In the **Instrument Setup** dialog box, select the **Baseline Check** tab. For this tab to appear Baseline Check must be enabled in an instrument's configuration options.

3 The following fields are available:

To pass, the baseline must meet the test criteria for	This specifies the time during which the baseline must meet the criteria in order to pass the test.
Stop checking baseline if conditions are not met after	This specifies the maximum time that will be spent checking the baseline. If conditions are not satisfied in this time, then the baseline check fails.
Noise Test Method	This is used to specify the noise calculation method that should be applied to the acquired data.
Test Spreadsheet	This spreadsheet specifies the channels to be used for baseline calculations and the tests that should be performed on those channels. The number of rows of the spreadsheet equals the number of acquisition channels based on instrument configuration plus the number of PDA Multichromatogram channels defined in the **PDA Options** Window (if PDA is configured).
Channel	Each entry in this column contains the name of an acquisition channel specified by instrument configuration or the PDA multichromatogram definitions. The entries cannot be edited.
Enable Noise Test	Checking this box indicates that detector noise should be calculated on the corresponding channel. If this box is unchecked, the Threshold edit field to its right is disabled; otherwise it is enabled.
Threshold (Noise)	This is used to specify the maximum acceptable value for the calculated noise. If the calculated noise is greater than the Threshold, the baseline check is considered to have failed.
Enable Drift Test	Checking this box indicates that detector drift should be calculated on the corresponding channel. If this box is unchecked, the Threshold edit field to its right is disabled; otherwise it is enabled.
Threshold (Drift/hr)	This is used to specify the maximum acceptable value for the calculated drift. If the calculated drift is greater than the Threshold, the baseline check is considered to have failed.

To perform an on-demand baseline check:

Select **Control > Baseline Check**. A dialog will appear where you set the parameters for doing the baseline check.

To check the status of the Baseline Check function:

Select **View > Baseline Check Status**. A status box appears where you can view the status of the most recent Baseline Check test. This box contains status information only.

Aux traces

The **Aux Traces** tab is used to acquire traces of instrument status parameters during normal data acquisition. Many instruments have the ability to report continuous monitoring data on status parameters such as flow rate and oven temperature. When this option is enabled, this tab appears, allowing you to designate which status parameters you wish to monitor during the run. Changes to the aux. traces for the Agilent 1100 Column Comp, RI detector, Isocratic pump, Binary pump and Quaternary pump are logged in the audit trail.

To turn on acquisition and display of auxiliary traces for an instrument:

1. Open Instrument Setup
2. In the **Instrument Setup** dialog box, select the **Aux Traces** tab.
3. The actual entries in this list will vary depending on the instrument configuration.

To have status information logged for a parameter listed in this dialog, click on the check box for that row and select the appropriate units for that parameter. When data acquisition is performed, status information will also be acquired. The resultant data will be presented as an additional data channel whenever the data file is viewed.

Fraction collector

To configure the Fraction Collector to use for a method:

1. Open Instrument Setup
2. In the **Instrument Setup** dialog box, select the **Fraction Collector** tab. If no Fraction Collector is configured, this tab will not appear.
3. Select **F1** in any section of the **Fraction Collector** tab for more information.

Select a new project

You must select a project in the Control Panel before you can launch an instrument. If the instrument settings in the Control Panel include **Always use default project**, you will not be able to select a new project in the data system.

To change the project:

1 On the **File** menu, click **Select Project**.

2 From the list of projects to which you have rights, click the project you want to use for this instrument, and then click **Select Project**.

View method reports

To view the custom report, from the **Reports** menu, click **View** followed by **Method Report**. This command is available even when you are not editing the custom report. The current method custom report will appear in a window for viewing only. You cannot edit the report from this window. See About Reports and Standard Reports.

Method properties

Before you use a method to acquire data, be sure that the options such as automatic post-run analysis of the data (if desired) are turned on. To check these parameters, from the **Method** menu, click **Properties**.

See Also

Description

Options

Calibration

Audit Trail Log

Audit Trail

Method properties description

To enter a description for your method:

1 From the **Method** menu, click **Properties**.

2 In the **Method Properties** dialog box, select **Description**.

3 In the dialog box enter text information about your method. You can enter any information you wish. The description can be viewed from the **Open File** dialog, and therefore can be useful in sorting quickly through methods to find the right one.

Method properties options

To set the analysis options for your method:

1 From the **Method** menu, click **Properties.**

2 In the **Method Properties** dialog box, select **Options**.

3 Select from the following options:

- Analyze after acquisition - If this box is selected, the chromatogram will be analyzed automatically after every acquisition. This is the default condition. If this box is not selected, you must either manually analyze the

chromatogram by clicking the **Analyze** button, or analyze the sample as part of a sequence reprocessing after the run has been completed.

- **Enable compression for data file -** When this box is checked, the data files acquired using the data system will automatically be compressed before saving. (Compressed data files are smaller but take longer to load.) Once a file has been saved using compression, the only way to decompress it is to save it as another data file with compression turned off.

Method properties calibration

To set calibration defaults for your method:

1. From the **Method** menu, click **Properties.**
2. In the **Method Properties** dialog box, select **Calibration**.
3. Select from the following options:
   - **Automatically average consecutive replicates of the same level -** When this box is checked, calibration replicates (consecutive injections of a single calibration level) will always be averaged. If this box is not checked, calibration replicates will not be averaged unless you so specify at the time of calibration. See Automatically Average Replicates.
   - **Number of replicates in rolling average -** If you wish to use a rolling average, enter the number of replicates per average here.
   - **Response Factor Definition -** Select how the response factors are to be calculated and displayed - **Area/Amount** or **Amount/Area**.

Method properties audit trail log

Use this option to export, print, and search for audit trail information.

1. From the **Method** menu, select **Properties**.
2. In the **Method Properties** dialog box, select **Audit Trail Log**.
3. Enter the following:
   - **User**
   - **Location**
   - **Description**
   - **Reason**
   - **From date/time**
   - **To date/time**
4. Select from the following options:
   - **Export -** Select this to export the audit trail log
   - **Print -** Select this to print the audit trail log
   - **Search -** Select this to search the audit trail log

Method Properties Audit Trail Log

Use this option to export, print, and search for audit trail information.

1 From the Method menu, select Properties.

2 In the Method Properties dialog box, select Audit Trail Log.

3 Enter the following:

- **User**
- **Location**
- **Description**
- **Reason**
- **From date/time**
- **To date/time**

4 Select from the following options:

- **Export -** Select this to export the audit trail log
- **Print -** Select this to print the audit trail log
- **Search -** Select this to search the audit trail log

Method properties audit trail

Select the **Audit Trail** tab. The **Enable Audit Trail** checkbox is an important box because, if checked, subsequent changes to the method will be logged in the method.

To enable the method audit trail:

1 From the **Method** menu, click **Properties.**

2 In the **Method Properties** dialog box, select **Audit Trail**.

3 Select **Enable audit trail**. Once the Enable Audit Trail box is selected, it cannot be deselected. The method will continue to have audit trail enabled unless you save the file under a new filename.

4 In the **Warning** dialog box, select **Yes.** The Enable Audit Trail will be permanently checked for this method.

5 In the **Method Properties** dialog box, select from the following options:

- **Prompt for reason at every change -** This option requires the user to enter a reason for every subsequent change to the method at the time the change is made.
- **Prompt for reason when saving Method -** This option requires the user to enter a reason for each change when the method is saved. This records the changes to the data file.
- **Do not prompt for reason -** When this option is selected, changes are documented, but the user is not required to enter a reason for the changes.

When you have selected the **Audit Trail Option with reasons**, you

will be prompted for the reason for changes, either at the time of the change, or when the method/sequence/data/system is saved.

If you have selected the option to enter a reason at every change, the dialog will appear each time you make a change to the item being audit trailed. A description of the change appears in the **Source/Activity** box. Select the reason for the change in the **Reason** box or type in your own reason, then click **OK**.

If you selected the option to enter a reason upon saving the method/sequence/data, the dialog will appear when you save the method/sequence/data and you must enter a reason for all changes to the method/sequence/data. Use the **Back** and **Next** buttons to view the descriptions of the changes. A change item number is displayed on the lower right of the window, along with the total number of changes. If you want to enter one reason for all changes, type the reason, then click the **Apply to All** button. After you have entered changes for all reasons, click **OK**.

Data properties

Data is acquired each time you run a method. Select **Data > Properties** to edit and view the general information, description, electronic signatures, audit trail log, and audit trail of data files.

See Also

About Data File Structure

View Data File General Information

Data File Description

View Data File Electronic Signatures

Data File Audit Trail Log

Data File Audit Trail

About data file structure

A data file is created on the designated drive whenever you acquire a sample, or when you save a data file using the **Save As 32-bit** command. The Save As 32-bit is used to save files from other formats. You can open many different 3rd party formats such as AIA, CDF, and PE. When you open one of these the Save As 32-Bit will be enabled. This allows the user to save the file in the native format and structure listed below. The file contains the following information:

- **File Information Header.** This 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 you can acquire multiple channels of data simultaneously on a given chromatograph, 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 you analyze. The Sample ID for the results is also saved, as are manual integration fixes. If you did not select **Result Package Mode** when creating an EZChrom project in the Control Panel, the result name is used for the RST file, and ACAML file names. If you selected **Result Package Mode** when creating an EZChrom project in the Control Panel, the **Result Name** will also be used for the folder name. In ECM it will be the name of the SSIZip.
- **File Description.** If you entered a description 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 dialog.

- **Instrument Configuration.** The configuration of the instrument used to acquire the data file is saved.
- **Data File Audit Trail**. An audit trail log is always saved in the data file that tracks analysis of the data.
- Data files are saved using the file name and extension you specify when you initiate the data acquisition. The limit on file name length is 255 characters, including path..

View data file general information

1. From the **Data** menu, select **Properties**.
2. In the **Data File Properties** dialog box, select **General**.
3. The following information is displayed:
   - **Sample ID**
   - **Run Time**
   - **Analysis time**
   - **Analysis Computer Name**
   - **Vial**
   - **Injection Volume**

Data file description

To enter a description for your data file:

1. From the **Data** menu, select **Properties**.
2. In the **Data File Properties** dialog box, select **Description**.
3. In the dialog box enter text information about your data file. Because the description can be viewed from the Open File dialog, the description can be useful in sorting through the data files on your disk. If you want to change the description for the current data file, you can enter or edit from this box.

Data file descriptions can be entered in the sequence at time of data acquisition, or can be entered from the **Single Run** dialog when running a single sample.

View data file electronic signatures

To view the electronic signatures for a data file:

1. Open the data file.
2. From the **Data** menu, select **Properties.**
3. In the **Data File Properties** dialog box, select **Signatures**.

See Also Add Signatures to the Result Sequence

Data file audit trail log

1 From the **Data** menu, select **Properties**.

2 In the **Data File Properties** dialog box, select **Audit Trail Log**.

3 Enter the following:

- **User**
- **Location**
- **Description**
- **Reason**
- **From date/time**
- **To date/time**

4 Select from the following options:

- **Export** - Select this to export the audit trail log.
- **Print** - Select this to print the audit trail log.
- **Search** - Select this to search the audit trail log.

Data file audit trail

Data files always have an associated audit trail. Select **Audit Trail** to select whether or not you want the system to prompt you for reasons whenever a change is made

1 From the **Data** menu, select **Properties**.

2 In the **Data File Properties** dialog box, select **Audit Trail**.

3 Select from the following choices:

- **Prompt for reason** - This option requires the user to enter a reason for every subsequent change to the data file at the time the change is made.
- **Do not prompt for reason** - When this option is selected, changes are documented, but the user is not required to enter a reason for the changes.

Advanced method options

Advanced Method Options are available for users who have a need to go beyond the simple data acquisition and analysis provided by customizing results or linking to external data systems or networks.

To open the **Advanced Method Options** dialog box, select **Method > Advanced**. Select one of the following option tabs to set up advanced options for your method:

Data Export	Turn on data export and set export parameters. See also Data Export to Excel.
Graphics Export	Set up export for chromatograms and traces.
Custom Parameters	Define custom parameters.
Column/Performance	Set up automatic calculation of system performance values.
Files	Designate user programs and baseline file subtraction.

Advanced Reports	Turn on printing and export of advanced reports.

To export data as part of a method

You can export analyzed data automatically when the data is analyzed with a method. To export data, the export function must be enabled and defined in the method. In order to export advanced reports, a printer must be configured on the computer doing the exporting.

To export data as part of a method:

1. From the **Method** menu, select **Advanced**.
2. Select the **Data Export** tab.
3. Click the **Export Enabled** box to turn data export on for the method. While this option is enabled, data export will occur after each Analysis of the data. Since the export of data will occur whether the analysis occurs automatically at the end of a run, or when executed manually, you should turn this option off while you are developing methods.
4. Choose the type of information to export from the drop-down list from the following options:
   - **Peaks**
   - **Groups**
   - **Standard Reports**
   - **Chromatogram**
5. For each type of export chosen, you can select parameters for export. Select a parameter for export by double-clicking on it, or clicking on it to highlight it, then click the green (Top) arrow button to move it to the list of export items in the right box. To remove an item from the export box, highlight it, then click the red (bottom) arrow button.If you have defined any Custom Parameters, they appear in the appropriate list of items you can choose to export.
6. For each parameter you export, set the number of decimals reported by highlighting the parameter in the **Export these parameters** list and entering the number of decimals in the **Decimals** field.
7. If you select **Chromatograms to be exported**, you will be given the option to export in either/or **AIA (*.CDF), ASCII,** or **ASCII Double** file format. Selecting the **AIA** option causes EZchrom to create a ***.CDF** (Chromatograph Data File) in the standard format specified by the Analytical Instrument Association (AIA). AIA Level 2 file export is supported. This includes the raw chromatogram, and integration results. This is also called ANDI file format (Analytical Data Exchange). This allows the results to be read by other chromatography data systems.

8 The following character limitations exist for .CDF files:

- The detection_method_name must be less than 63 characters
- The peak_processing_method_name must be less than 63 characters
- The sample_name must be less than 29 characters
- The sample_ID must be less than 29 characters

9 If you selected **Standard Reports**, you may choose to use your local time or GMT time on your reports. Enable **Use Local Time** to display local time on your report. Disable **Use Local Time** to display GMT time on your report.

10 In the **Field Separator** drop down box, select **Tab, Space,** or **Comma**. If you want to import the file into a Microsoft Excel spreadsheet choose **Tab**.

11 In the **Path for export file** field, select a path name for the directory where you want to save your export files. If you do not know the name of the directory, you can select it from existing paths by clicking the **File** button adjacent to the field.

12 Select **Enable ODBC** if you want to use ODBC format for your data export. Open Database Connectivity (ODBC) is an industry-standard method of sharing data between databases and other programs.

- In the **Data source name** field, enter the name of the destination folder for export files or select the **Open** button and browse for the folder. To create a new data source, select the **New** button.
- Enter a **Table name** for your data export.

Exported data are saved in files using the following conventions:

Peak and Group Export Files

For each parameter selected, a file is created containing that value for each named peak, along with file and method name information. Each time the method is used to acquire or process data, a row is appended to the file containing the new calculated value for that file. Each file is saved with the method name, with an extension representing the type of value selected. For example, the following is an example of a file created for export of **area** for 5 runs.

Report	Channel	# Records							
Area	A	5							
Date	Time	Sample Id	File	Method	User	Peak1	Peak2	Peak3	
5/9/92	20:48:53	STDS	c:\system\	c:\system\	cathi	63088	52014	49749	
5/9/92	20:49:09	STDS	c:\system\	c:\system\	cathi	170789	142665	136661	
5/9/92	20:49:21	STDS	c:\system\	c:\system\	cathi	298854	251660	241049	
5/9/92	20:49:34	STDS	c:\system\	c:\system\	cathi	461695	394081	376339	
5/9/92	20:51:56	STDS	c:\system\	c:\system\	cathi	780025	668245	635081	

Note If you export data as part of a sequence, and you want to view the export file in another application while data is being acquired, you must make a copy of the file and save it with another name before you use it. Otherwise, a file sharing violation may occur when the software tries to update the file with data from a new run.

Standard Report Export Files

When you select a **Standard Report** option, a file is created each time an analysis is run. The file contains the information in the selected report.

Unlike peak and group export, Standard Report Export files are not appended with information from additional runs. Each time the method is used for acquisition or processing, a new file is created. The new file name is based on the data filename and it uses the export extension given below for the type of export data selected.

The following table shows an example of a file created for Standard Export of an External Standard report.

Report	Channel	# Peaks	Date	Time	Sample Id	File	Method	User	
ESTD	A	4	5/9/92	20:48:53	STDS	C:\system\	c:\system\	cathi	
Pkno	Name	Ret. Time	Conc	Area	Height				
1	Peak1	5.729	10.022	63088	7791				
2	Peak2	6.577	5	51884	5631				
3	Peak3	8.293	15.091	48187	4226				
4	Peak4	8.559	10.166	79647	7675				
Totals			40.279	242806	25323				

See Also About Advanced Method Options

Export graphics

The **Graphics Export** function of the method will cause designated graphics to be exported, in .WMF format, each time an analysis is performed using the method.

To enable graphics export for a method:

1. From the **Method** menu, select **Advanced > Graphics Export**.
2. In the spreadsheet, click **Export** and then type the filename to be used for the export.
3. The graphics window displays the current graphic for export. To change the graphic, do a right mouse click in the window. All the standard graphics parameters are available.
4. Select the **Path for export files**. The graphs exported will be saved with file name **<Data file name> + " _ " + <Export Name> + ".wmf"**

See Also About Advanced Method Options

Column/Performance parameters

The **Column/Performance** tab allows you to set up automatic calculation of system performance values such as Theoretical Plates, Capacity Factor, Resolution, or Peak Asymmetry.

To set up column performance calculations:

1 From the **Method** menu, select **Advanced > Column/ Performance**.

2 Click the **Calculate performance parameters for this channel** box. Then fill in the information for the following fields required for the calculations.

3 Once you have completed the **Column/Performance** tab, the system will calculate performance parameters after each analysis. These parameters can be exported, annotated on the chromatogram, and printed in a custom report.

Unretained peak time (min)	Enter the retention time of an unretained peak for this column.
Column length	Enter the length of the column, in meters or cm.
Particle diameter (microns)	Enter the particle diameter, in microns, for the column you are using (if applicable).
Column serial number	Enter the serial number for the column (if applicable). This information will be saved with the data and available for reporting.
Column installation date	Enter the date the column was installed in the instrument (if desired). This information will be saved with the data and available for reporting.
Column description	Enter column description if desired. This information will be saved with the data and available for reporting.
Calculate performance parameters for this channel	Select one or more calculation methods. The choices include USP, EMG (Exponential Modified Gaussian), DAB (German Pharmacopeia)/ BP (British Pharmacopeia)/EP (European Pharmacopeia)/ ASTM, AOH (Area/Height), and JP (Japanese Pharmacopeia), calculation methods.

See Also About Advanced Method Options

Select user programs and baseline files

To designate program files to associate with the method:

1 From the **Method** menu, select **Advanced > Files**.

2 Complete the following fields:

User Programs In this section you can designate user programs to be run:

- **Before** each run
- **Before Analysis** of the chromatogram
- **After Analysis** of the chromatogram
- **After export**.

	Enter the user program name, or select it from the drop down list. For details on writing User Programs, see the User Programs appendix at the end of this manual. (**Note**: Include the full UNC path name for the file.)
Baseline File	If you want the data system to automatically subtract a stored baseline file after each run, select the **Baseline File** box. Designate a baseline file name, and then check each channel from which the baseline file is to be subtracted. The chromatogram will be analyzed after the subtraction is performed. (**Note**: Include the full UNC path name for the file.)

Advanced method reports

To specify one or more reports to be printed and/or exported when the method is used to analyze data, select **Method > Advanced > Advanced Reports**. The following fields are available:

Print	Select this box if you want to print the designated report when data is analyzed with this method.
Export	Select this box if you want to export the designated report when data is analyzed with this method. This results in tab-delimited export only.
Report Template Name	Enter or select the name of the report template file to be used to generate this report.
Export Path	If the report is to be exported, enter or select the path for the export file to be saved.
Export File Name	Select the file naming from the types presented in the list. The export file name will be created using the identification selected.

See Also About Advanced Method Options

Sample prep

An autosampler sample prep (injector program) is comprised of a series of numbered lines, each of which defines an operation that the injector carries out sequentially.

If your autosampler supports a sample prep program, the **Sample Prep** menu will appear on the menu bar. From this menu, you can create/edit an autosampler sample prep program, and set up properties such as a description and audit trail for the sample prep program.

To open an existing sample prep file

1. From the **Instrument Window** menu bar, click **File > Open > Sample Prep.** A dialog will appear where you can select a sample prep file to open for the current instrument.
2. Select the file to open, or use the search boxes at the bottom to search for a file that matches criteria you select.

To turn on the audit trail for the sample prep file

1 From the **Sample Prep** menu, click **Properties > Audit Trail**.

2 To enable the audit trail function, select the **Enable** audit trail box. You will be prompted with a warning that if you proceed, you cannot disable the audit trail once it is turned on.

- **Prompt for reason at every change** - This option requires the user to enter a reason for every subsequent change to the sample prep file at the time the change is made.
- **Prompt for reason when saving Method** - This option requires the user to enter a reason for each change when the sample prep file is saved.
- **Do not prompt for reason** - When this option is selected, changes are documented, but the user is not required to enter a reason for the changes.

To enter a description for a sample prep file

1 From the **Sample Prep** menu, click **Properties > Description**.

2 Type a description for the sample prep file. The description is saved in the file and can be viewed when opening or used for searching.

To open a sample prep template

1 In the menu select **File > New**.

2 In the **New File Template** dialog box, select the **Sample Prep** tab.

3 Select the file you wish to open.

4 Select **OK**.

Launch lab monitor software

To run the Lab Monitor program for supported instruments, from the **Control** menu, click **Launch Lab Monitor Software**. This will only show when you are running the 7890 GC.

System suitability

System suitability testing, originally conceived by the pharmaceutical industry to determine if a chromatographic system is suitable for a particular analysis, is now used routinely in laboratories where quality of results is important. System suitability testing is often used in conjuction with method validation to provide a complete picture of laboratory quality and reproducibility of results.

System suitability involves running a mixture containing the analytes you will be running in your samples and examining various parameters that describe the ability of the chromatograph and column to separate those analytes.

System suitability is a license option that expands your Data System to include the ability to do automatic System Suitability calculations

for experimental variables such as efficiency, capacity, resolution, and reproducibility. The package includes five choices of calculation methods, including:

- USP (United States Pharmacopia)
- EMG (Exponential Modified Gaussian)
- DAB (German Pharmacopia) DAB calculation is also used for BP (British Pharmacopia), EP (European Pharmacopia), and ASTM.
- AOH (Area/Height)
- JP (Japanese Pharmacopia)

See Also

System Suitability Setup

Suitability Calculation Selection

Run a Suitability Test

Sequence Wizard - Reports

System suitability setup

Use the **System Suitability Setup** to enter the required acceptance ranges for the peaks of interest. This must be done before the data system can make System Suitability calculations.

To set up system suitability calculations:

1. To enable System Suitability, in the **Control Panel** select the Instrument and select **Configure Instrument > Options > System Suitability.** Launch the instrument.
2. In EZChrom, from the **Method** menu, select **System Suitability**.
3. Select the first peak to be used for calculations by highlighting it with the mouse in the **Compound** list.
4. In the adjacent spreadsheet, click on the first field in the **Parameter** column. A drop-down list of available parameters is displayed (See the table below). Select a parameter from the list. If you do not wish to perform a suitability test on any given peak, simply leave the **Parameter** fields blank. Similarly, if you do not wish to have one of the test criteria used (for example, %RSD), leave it blank. Some parameters have a choice of calculation methods. These parameters have the calculation method displayed after the parameter in parenthesis. (e.g. Plates/Meter (JP) indicates Plates/Meter calculated using the Japanese Pharmacopoeia calculation.) For details on these calculations, see Internal Calculations.
5. For each parameter selected, enter a minimum value **(Min)**, maximum value **(Max)**, and maximum allowed percent relative standard deviation **(%RSD)**.
6. To perform a test on the entire chromatogram, click on the lower spreadsheet in the column labeled **Test.** Select one of the noise calculations from the drop-down list. Enter a **Start** and **End** time for the test, and a threshold **Value** to determine acceptable limit.

The noise value for the portion of chromatogram between the start and stop times will be calculated and compared to the threshold value to determine whether the test passed or failed. Note that the times you enter for the noise test should be representative of a baseline area of your chromatogram where no peaks elute.

7 To perform a drift test, click on the lower spreadsheet in the column labeled **Test**. Select **Drift (drift/min)** from the drop-down list. If you select this box, you must enter a **Start** and **End** time for the test, and a threshold **Value** (in drift/Min) for the acceptable limit.

8 When you have completed the System Suitability Setup, close the box and set System Suitability Calculations.

Suitability Parameters

Suitability Resolution	This checks the ability of the column to separate one analyte from others in the mixture. Two peaks are considered resolved if the calculated R factor is greater than 1.5.
Suitability Repeatability	Injection of the same sample multiple times lets you determine if your chromatograph is providing reproducible results. Generally, 5 to 6 repeatability samples are necessary to provide adequate data for meaningful results. Repeatability can be determined through examination of the % relative standard deviation (%RSD) for such parameters as peak area, height, or concentration.
Suitability Peak Asymmetry (Tailing)	The quantitative values for peak asymmetry are important, especially when dealing with trace components. Also, since asymmetry can vary through the life of a column, it can be important to track this data on an ongoing basis.
Suitability Theoretical Plates	Calculation of plate count is an important indication of column efficiency. Many chromatographers like to monitor plate count as an indication of when to replace the column.
Suitability Noise and drift	Particularly important to trace analyses, the noise and drift values for your chromatograph indicate the limits of detection and quantification. Per-peak calculations include 6-sigma and ASTM signal to noise calculations. Noise and drift tests performed on a designated section of the chromatogram include rms Noise, drift, ASTM noise short (unscaled), ASTM noise short (scaled), ASTM noise long (scaled), and 6-sigma noise.

System suitability calculations

System Suitability calculations require information about your chromatography column. Do this after you have Setup System Suitability.

To select the calculation method:

1. From the **Method** menu, select **Advanced > Column/Performance**.
2. Enter values under **Column Information**. This is required for calculation of performance options.
3. Under **Calculation Method** select a method for calculation of the performance values from the following options:
   - **USP** (United States Pharmacopia)
   - **EMG** (Exponential Modified Gaussian)
   - **DAB** (German Pharmacopia) DAB calculation is also used for BP (British Pharmacopia), EP (European Pharmacopia), and ASTM.
   - **AOH** (Area/Height)
   - **JP** (Japanese Pharmacopia)
4. Select **Calculate performance parameters for this channel** to enable the suitability calculations for the method.
5. When you have completed the dialog box, exit to accept the parameters and Run a System Suitability Test.

See Also Column/Performance Parameters

Run a system suitability test and print a report

Run a System Suitability Test to create a sequence or modify an existing sequence to include one or more system suitability runs according to the needs and SOP's of your laboratory. Do this after completing the System Suitability Setup and System Suitability Calculations dialogs.

For example, following USP standards, five replicate standards are run at the beginning of the sequence. These are designated as system suitability standards in the sequence. At the end of the sequence, suitability calculations are made, and the software generates a system suitability report.

1. To open the Sequence Spreadsheet, select **Sequence > Edit.**
2. Set the **Run Type** of the first sample in your suitability set to **Begin System Suitability**. Additional suitability standards should be designated as **System Suitability Standard**s, and the final sample in your suitability set should be designated as **End System Suitability**. Multiple sample run types can be selected for a given sample.
3. A System Suitability Report will be generated at the end of the set of suitability standards when the sequence is run. To view the

Suitability Report on screen, click **Reports > View > Sequence Report**.

4 To print the Suitability Report, click on **Reports > Print > Sequence Report**, and select the **System Suitability Report** choice. In order to have your report printed automatically at the end of the sequence, you must have selected the **Print Sequence Reports** option in the **Sequence Properties** dialog. See Process a Sequence.

System Suitability Report Page 1 of 1 (1)

Sequence : \\nas\qa\Users\Elite Enterprises\Elite32\Projects\Amy\Sequence\TP005.002\syssuitp.seq
User : Amy T. Xu (qa3\axtech)
Printed : 9/6/2006 10:44:32 AM

Sample ID	Data Filename
PNA-STDS	\\nas\QA\Users\Elite Enterprises\Elite32\Projects\Amy\Data\TP005.002\multi calibration level 1.dat
PNA-STDS	\\nas\QA\Users\Elite Enterprises\Elite32\Projects\Amy\Data\TP005.002\multi calibration level 2.dat
PNA-STDS	\\nas\QA\Users\Elite Enterprises\Elite32\Projects\Amy\Data\TP005.002\multi calibration level 3.dat

System is Suitable

Channel A	Compound	Parameter	Min	Max	%RSD
	Peak 1	area	0	400000	70
	Peak 2	height	0	50000	70

Sample ID	Compound	Parameter	Average	Low	High	%RSD	Status
	Peak 1	area	178076	63056	299360	66.419	
PNA-STDS		63056					Passed
PNA-STDS		171813					Passed
PNA-STDS		299360					Passed
	Peak 2	height	15943	5631	26843	66.600	
PNA-STDS		5631					Passed
PNA-STDS		15356					Passed
PNA-STDS		26843					Passed

About Integration

Integration Timed Events are used to customize the integration of certain peaks or regions of the chromatogram.

There are two ways to add an integration timed event to a method: by manually adding the event to the Integration Timed Event Table, or graphically by clicking on the chromatogram.

Two Integration events are required for each run: Width, and Threshold. These events are used to detect peak start, stop, and apex, and to distinguish true peaks from noise. The system uses default values of Width = 0.2 minute and Threshold = 50.

Before attempting to add integration timed events, make sure your chromatogram has been analyzed using the current method. To make

sure, look for baselines and start/stop tic marks on your chromatogram. Or, click the **Analyze** button on the command ribbon.

See Also

About the Chromatogram Window

About Integration Tables

Integration Events Table

Manual Integration Fixes Table

Baseline Code Descriptions

Graphical Programming

About integration tables

There are two tables where integration timed events are saved.

- The method Integration Events Table is used for all data files integrated with the method.
- The Manual Integration Fixes Table is saved with the data file and used only for reintegration of the data file.

When you add an integration timed event graphically, a dialog box will appear, allowing you to choose what integration table is to be used for the event. The default table for each integration event is selected.

- To add the event to the Integration Events Table, select **Add event to Method (all data) > Add to Table**. If the method is saved, the event is applied to every data file integrated using this method.
- To add the event to the Manual Integration Fixes Table, select **Add event to this data file only > Add to Table**. The event is applied only to this data file.

Integration events table

The Integration Events table contains all current Integration Timed Events for the current method channel. All of the integration timed events can be added to your method using the Graphical Programming technique. Each row of the Integration Events table represents an integration event in the method.

When you add an integration event to the Integration Events table, the integration changes will be used on all subsequent samples analyzed using this method. (Assuming the method is saved.) This is the default selection for events that are normally used to modify integration of peaks that always occur in the sample.

To view the integration events table:

There are three ways to view the table.

- In the toolbar, select the **Integration Events**  button.
- In the **Method** menu, select **Integration Events.**
- In the navigation pane, select **Method > Method > Integration Events**

To add an event manually:

1. In a new line of the spreadsheet, click the **Event** field, and select the event you wish to add.
2. Type an appropriate **Start** and **Stop** time and a **Value** for the event (if required).
3. To remove an event's effect from an analysis, yet keep the event in the table, click on the checkmark next to the event. Only events with a red check-mark will be used in subsequent analyses.

To remove an event entirely from the table:

Click on the **row number** of the event, followed by the **DELETE** key on your keyboard.

To temporarily remove an event from the table:

Deselect the check mark adjacent to the event. When the check mark is not displayed, the event will not be applied to the integration.

To view the context menu:

A right mouse click anywhere in the table produces a menu of commands for manipulating cells and rows in the spreadsheet.

- The **Cut, Copy, and Paste** commands enable you to cut, copy, and paste the contents of a cell.
- The **Fill Down** command will copy the selected line into the following lines.
- The **Insert Paste** command will insert a line and at the same time do a paste to the location.
- The **Insert Line** command simply inserts a blank line where your cursor is located.
- The **Clear** command clears the contents of the current cell or selected row.
- The **Clear All** command clears the contents of the entire spreadsheet.

Manual integration fixes table

A Manual Integration Fix is an adjustment to integration required only for a particular chromatogram.

Manual integration corrections that are created using graphical integration are logged into the **Manual Integration Fixes** table. These manual changes can also be entered in the table by selecting the desired integration change from the **Event** drop-down list, then entering a **Start** and **Stop** time, and a **Value** if appropriate.

These integration changes are applied only to an individual chromatogram rather than becoming part of the method, and are saved in the data file only. The manual integration fixes are saved in the data file so that the integration of the chromatogram can be recreated at a later date.

The Manual Integration Fixes table contains all current Manual Integration Fixes for the current data file. When you add an integration event to the Manual Integration Fixes table, it will be applied only to this data file. Thus, Manual Integration Fixes are One-time integration events. This is the default selection for events that are normally used for one-time corrections to integration, such as Manual Baseline changes. The results using these events will also be stored in the data file. This allows you later to reproduce the results generated using a manual integration event that was only necessary for a single run.

To view the Manual Integration Fixes table:

There are three ways to view the table.

- In the toolbar, select the **MIF Table**  button.
- In the **Data** menu, select **Manual Integration Fixes.**
- In the navigation pane, select **Method > Data > Manual Integration Fixes.**

To add an event manually:

1. In a new line of the spreadsheet, click the **Event** field, and select the event you wish to add.
2. Type an appropriate **Start** and **Stop** time and a **Value** for the event (if required).
3. To remove an event's effect from an analysis, yet keep the event in the table, click on the check-mark next to the event. Only events with a red **check-mark** will be used in subsequent analyses.

To remove an event entirely from the table:

Click on the **row number** of the event, followed by the **DELETE** key on your keyboard.

To temporarily remove an event from the table:

Deselect the check mark adjacent to the event. When the check mark is not displayed, the event will not be applied to the integration.

To view the context menu:

A right click anywhere in the table produces a menu of commands for manipulating cells and rows in the spreadsheet.

- The **Cut, Copy, and Paste** commands enable you to cut, copy, and paste the contents of a cell.
- The **Fill Down** command will copy the selected line into the following lines.
- The **Insert Paste** command will insert a line and at the same time do a paste to the location.
- The **Insert Line** command simply inserts a blank line where your cursor is located.
- The **Clear** command clears the contents of the current cell or selected row.
- The **Clear All** command clears the contents of the entire spreadsheet.

Baseline code descriptions

Baseline codes can be included in custom reports, and also can be used to annotate chromatograms. A baseline code consists of two letters. The first letter denotes the peak beginning baseline type and the second letter indicates the peak ending baseline type.

Code	Baseline Type
B	Baseline
f	Force Peak Start or Stop (user defined)
I	Peak ended by Integration Off event
N	Begin negative peak
P	End negative peak
H	Forward horizontal
h	Backward horizontal
M	Manual baseline or Manual peak
m	Move baseline Start/Stop
S	Shoulder
T	Tangent skim
V	Valley
v	Forced valley point
x	Split peak

E	End of chromatogram encountered before the end of peak was found. End of chromatogram used as peak end.
R	Reset Baseline
L	Lowest Point Horiz

Graphical programming

The Graphical Programming menu enables you to add timed events and set up other method parameters graphically by clicking on the displayed chromatogram. These commands are also available from the Integration/Graphical Programming toolbar, which is displayed by default at the bottom of the Instrument Window. The examples in the following sections demonstrate how each integration timed event would affect the integration of the chromatogram displayed, in order to give you a feel for how an integration timed event might be used in your chromatography method.

The Integration/Graphical Programming toolbar is located at the bottom of the Instrument Window and contains graphical events buttons. For help with integration, set the integration message window to appear when you select a graphical event button.

To view the integration toolbar:

1. Select **View > Preferences**.
2. Under **Toolbar options** select **Integration**.
3. Select **Show toolbar** and **Tooltips**.

To view the integration message window:

1. Select **View > Preferences**.
2. Under **Toolbar options,** select **Integration**.
3. Under **Options**, select **Show the graphical programming tooltips**.

Parameters that can be set using graphical programming include:

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.
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.
Exponential Skimming	Integrate small peaks located on the tailing edge of a larger peak.
Front Exponent Skim	Force a exponential baseline for a daughter peak on the leading edge of a mother peak.
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.

Width

The Width event is used to calculate a value for bunching, or smoothing, the data points before the integration algorithm is applied. Integration works best when there are 20 points across a peak. If a peak is over sampled (i.e. the sampling frequency was too high), the **Width** parameter will be used to average the data such that the integration algorithm sees only 20 points across the peak. In setting a **Width** value graphically, the narrowest peak in the chromatogram should be used.

A **Width** event will be applied to a given peak as long as it occurs before or on the apex of the peak.

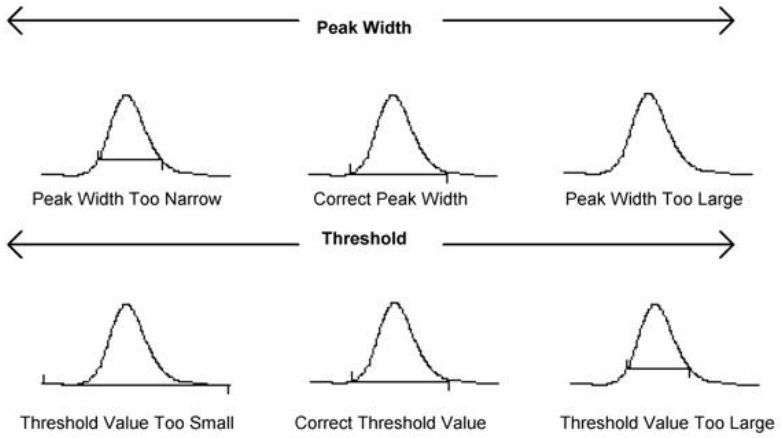
The **Width** parameter is only used to correct for over-sampling. It cannot correct for data that was under-sampled (i.e. sampling frequency too low causing fewer than 20 points acquired across the narrowest peak.)

Note: In most circumstances, an initial **Width** value based on the narrowest peak in the chromatogram will be adequate for proper integration of all peaks. However, a new **Width** timed event should be entered every time a peak width doubles.

Threshold

This parameter is the first derivative, used to allow the integration algorithm to distinguish the start and stop of peaks from baseline noise and drift. When setting the **Threshold** value graphically, you select a section of baseline. The recommended **Threshold** value is based on the highest first derivative value determined in that section of the chromatogram.

The diagram below shows examples of how incorrect values for peak Width and Threshold can effect the peak baseline.



Note that extreme values of both Width and Threshold (too large or too small) can result in peaks not detected.

Shoulder Sensitivity

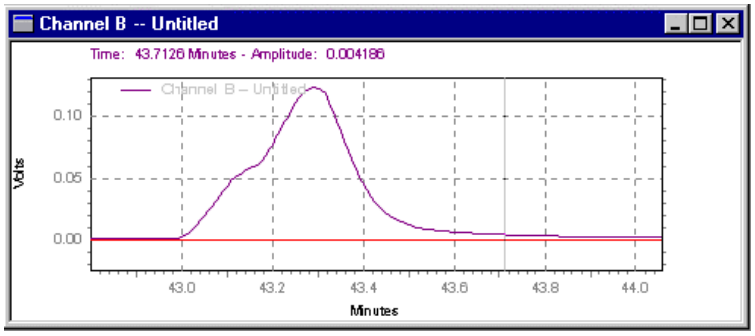
This parameter is used to enable the detection of shoulders on larger peaks. A larger value will decrease shoulder sensitivity, while smaller values increase sensitivity to shoulder peaks. When setting the **Shoulder Sensitivity** value graphically, you select a section of the baseline. The recommended **Shoulder Sensitivity** value is based on the highest second derivative value determined in that section of the chromatogram.

1. In the **Integration** toolbar located at the bottom of the Instrument window, select the **Shoulder Sensitivity** button.
2. In the chromatogram, select the **start** and **end points** of a baseline segment.
3. In the **Shoulder Sensitivity** dialog box, select **Add event to Method (all data)** or **Add event to this data file only.**
   - If you select **Add event to Method (all data)** the event will be added to the Integration Events table when you click the **Add**

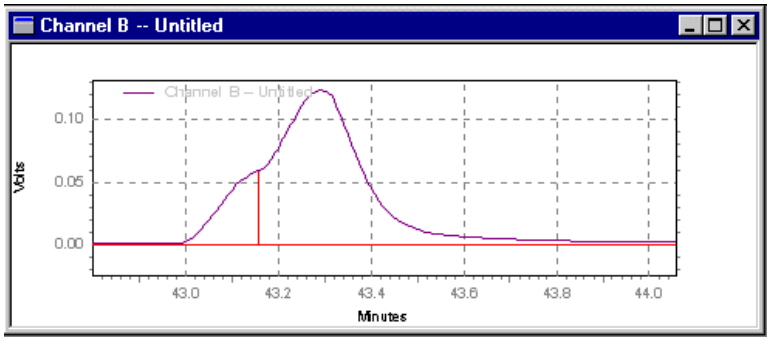
to Table button. If the method is then saved, the event will be applied to every data file integrated using this method.

- If you select **Add event to this data file only** the event will be added to the Manual Integration Fixes table when you click the **Add to Table** button, and will be applied only to this data file.

4 Click **Cancel** to ignore the timed event and cancel the operation, or click **Analyze Now** to add the event to the table and analyze the chromatogram using the event.



Shoulder Sensitivity value set too high



Shoulder Sensitivity value set correctly

Integration off

This event turns off the integration of your chromatogram during the range specified. This event is useful if you are not interested in certain areas of your chromatogram, and do not wish peaks to be reported for that section.

When using **Integration Off** to disable peaks, these regions will be included in the noise calculation. Leave all peaks integrated to get the correct noise values.

1 In the **Integration** toolbar located at the bottom of the Instrument window, select the **Integration Off** button.

2 In the chromatogram, select the **start** and **end points**.

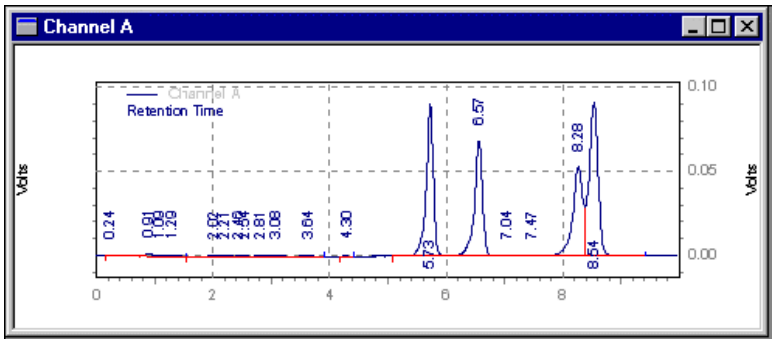
3 In the **Integration Off** dialog box, select **Add event to Method (all data)** or **Add event to this data file only**.

- If you select **Add event to Method (all data)** the event will be added to the Integration Events table when you click the **Add**

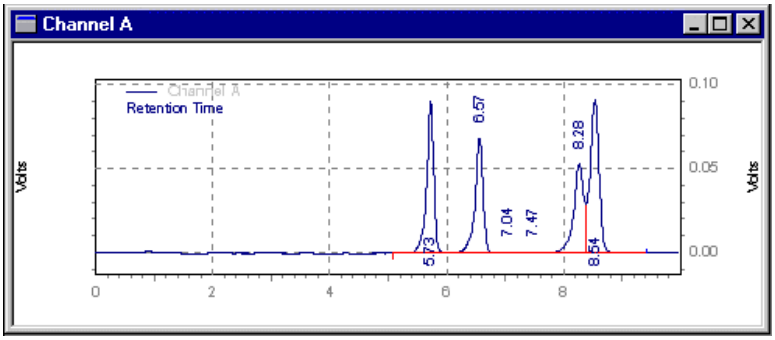
to Table button. If the method is then saved, the event will be applied to every data file integrated using this method.

- If you select **Add event to this data file only** the event will be added to the Manual Integration Fixes table when you click the **Add to Table** button, and will be applied only to this data file.

4 Click **Cancel** to ignore the timed event and cancel the operation, or click **Analyze Now** to add the event to the table and analyze the chromatogram using the event.



Default integration



Integration Off event from 0 to 5 minutes

Valley to valley

This event causes the baselines of peaks that are not totally resolved (i.e. do not return to baseline) to be drawn to the minimum point between the peaks. If this event is not used, a baseline is projected to the next point at which the chromatogram returns to baseline, and a perpendicular is dropped for peaks which do not reach baseline.

1 In the **Integration** toolbar located at the bottom of the Instrument window, select the **Valley to Valley** button.

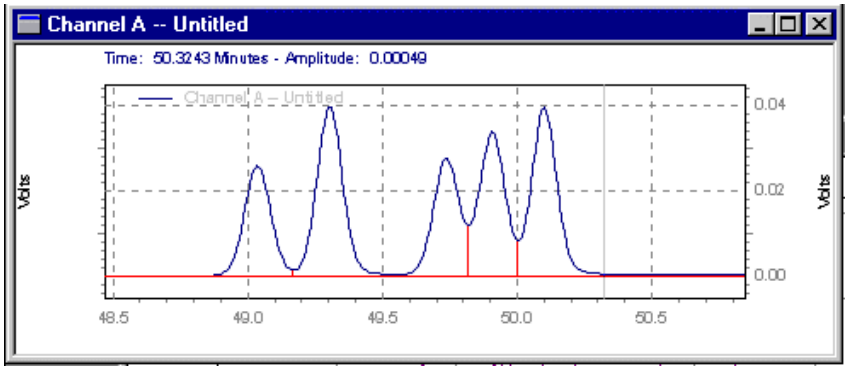
2 In the chromatogram, select the **start** and **end points**.

3 In the **Valley to Valley** dialog box, select **Add event to Method (all data)** or **Add event to this data file only.**

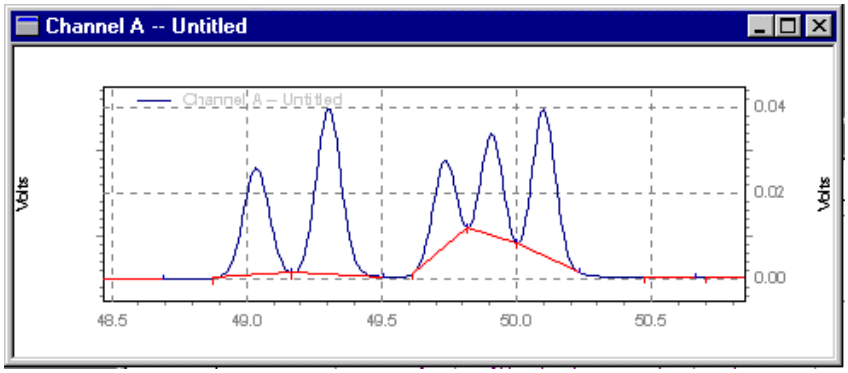
- If you select **Add event to Method (all data)** the event will be added to the Integration Events table when you click the **Add to Table** button. If the method is then saved, the event will be applied to every data file integrated using this method.

- If you select **Add event to this data file only** the event will be added to the Manual Integration Fixes table when you click the **Add to Table** button, and will be applied only to this data file.

4 Click **Cancel** to ignore the timed event and cancel the operation, or click **Analyze Now** to add the event to the table and analyze the chromatogram using the event.



Default Integration



Integration with **Valley to Valley** event

Horizontal baseline

This event allows you to project the baseline forward horizontally between the times specified for the event.

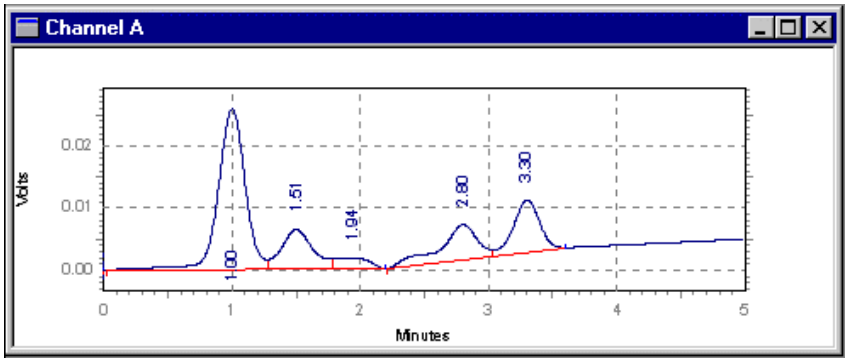
1 In the **Integration** toolbar located at the bottom of the Instrument window, select the **Horizontal Baseline** button.

2 In the chromatogram, select the **start** and **end points**.

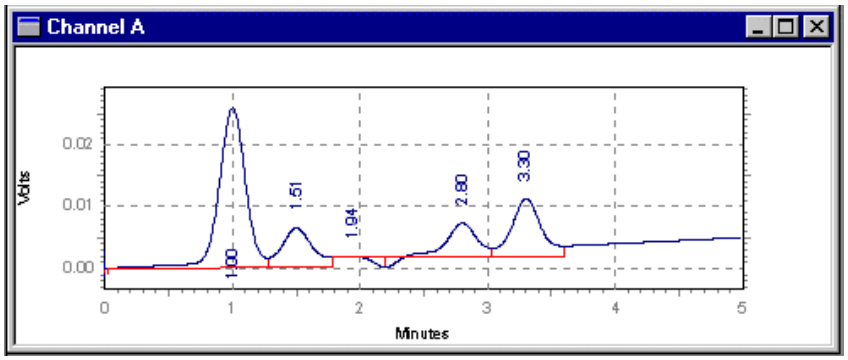
3 In the **Horizontal Baseline** dialog box, select **Add event to Method (all data)** or **Add event to this data file only.**

- If you select **Add event to Method (all data)** the event will be added to the Integration Events table when you click the **Add to Table** button. If the method is then saved, the event will be applied to every data file integrated using this method.
- If you select **Add event to this data file only** the event will be added to the Manual Integration Fixes table when you click the **Add to Table** button, and will be applied only to this data file.

4 Click **Cancel** to ignore the timed event and cancel the operation, or click **Analyze Now** to add the event to the table and analyze the chromatogram using the event.



Integration without Horizontal Baseline Event



Integration with Horizontal Baseline between 1.8 and 3.6 minutes

Backward horizontal baseline

This event is used to force a horizontal baseline in the direction of the beginning of the chromatogram. A backward horizontal baseline will be created between the times specified by the event.

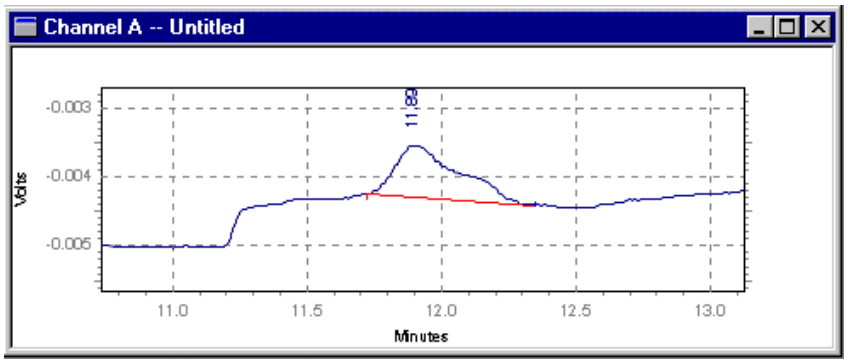
1 In the **Integration** toolbar located at the bottom of the Instrument window, select the **Backward Horizontal Baseline** button.

2 In the chromatogram, select the **start** and **end points**.

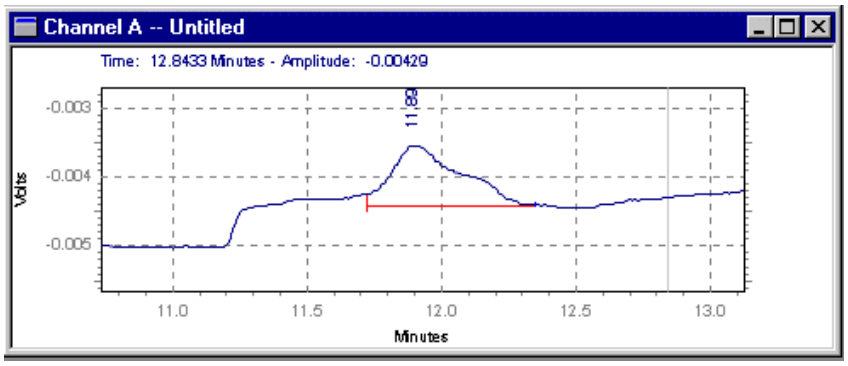
3 In the **Backward Horizontal Baseline** dialog box, select **Add event to Method (all data)** or **Add event to this data file only.**

- If you select **Add event to Method (all data)** the event will be added to the Integration Events table when you click the **Add to Table** button. If the method is then saved, the event will be applied to every data file integrated using this method.
- If you select **Add event to this data file only** the event will be added to the Manual Integration Fixes table when you click the **Add to Table** button, and will be applied only to this data file.

4 Click **Cancel** to ignore the timed event and cancel the operation, or click **Analyze Now** to add the event to the table and analyze the chromatogram using the event.



Default integration



Integration after backward horizontal baseline

Lowest point horizontal baseline

This event is similar to the Horizontal Baseline event, except that the lowest point in the chromatogram determines the baseline. The values you input for **Start Time** and **Stop Time** determine the region within the chromatogram where the lowest point horizontal baseline will be used.

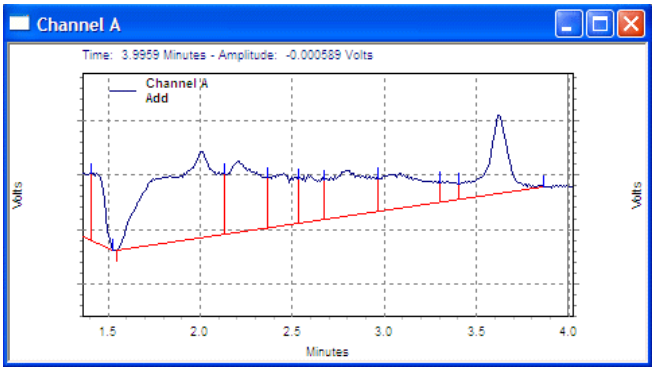
1 In the **Integration** toolbar located at the bottom of the Instrument window, select the **Lowest Point Horizontal Baseline** button.

2 In the chromatogram, select the **start** and **end points**.

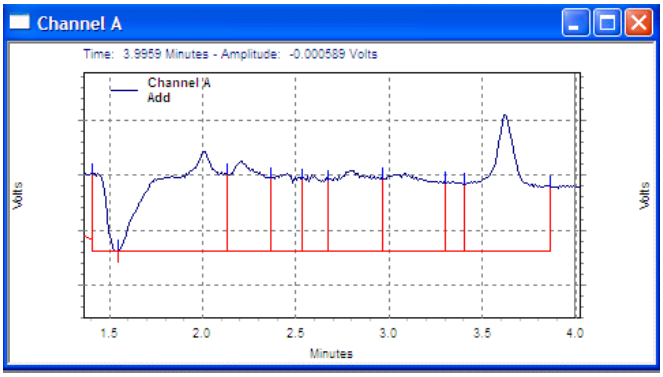
3 In the **Lowest Point Horizontal Baseline** dialog box, select **Add event to Method (all data)** or **Add event to this data file only.**

- If you select **Add event to Method (all data)** the event will be added to the Integration Events table when you click the **Add to Table** button. If the method is then saved, the event will be applied to every data file integrated using this method.
- If you select **Add event to this data file only** the event will be added to the Manual Integration Fixes table when you click the **Add to Table** button, and will be applied only to this data file.

4 Click **Cancel** to ignore the timed event and cancel the operation, or click **Analyze Now** to add the event to the table and analyze the chromatogram using the event.



Integration before using Lowest Point Horizontal event



Integration after using Lowest Point Horizontal event

Tangent skim

This event is used to integrate a small peak located on the tailing edge of a larger peak. The baseline of the small peak becomes a tangent drawn from the valley of the larger peak to the tangent point on the chromatogram.

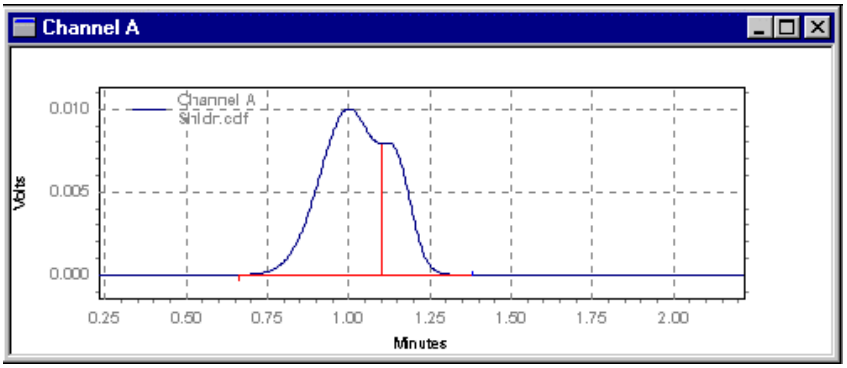
1 In the **Integration** toolbar located at the bottom of the Instrument window, select the **Tangent Skim** button.

2 In the chromatogram, select the **start** and **end points**.

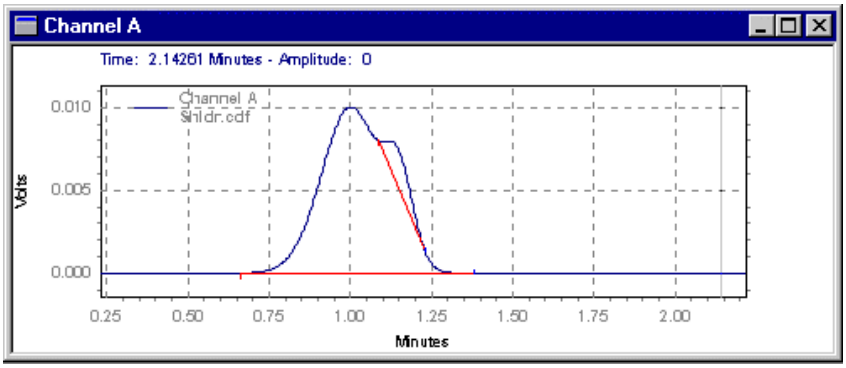
3 In the **Tangent Skim** dialog box, select **Add event to Method (all data)** or **Add event to this data file only.**

- If you select **Add event to Method (all data)** the event will be added to the Integration Events table when you click the **Add to Table** button. If the method is then saved, the event will be applied to every data file integrated using this method.
- If you select **Add event to this data file only** the event will be added to the Manual Integration Fixes table when you click the **Add to Table** button, and will be applied only to this data file.

4 Click **Cancel** to ignore the timed event and cancel the operation, or click **Analyze Now** to add the event to the table and analyze the chromatogram using the event.



Integration without Tangent Skim Event



Integration with Tangent Skim Event

Front tangent skim

The Front Tangent Skim event is used to force a tangential baseline for a daughter peak on the leading edge of a mother peak.

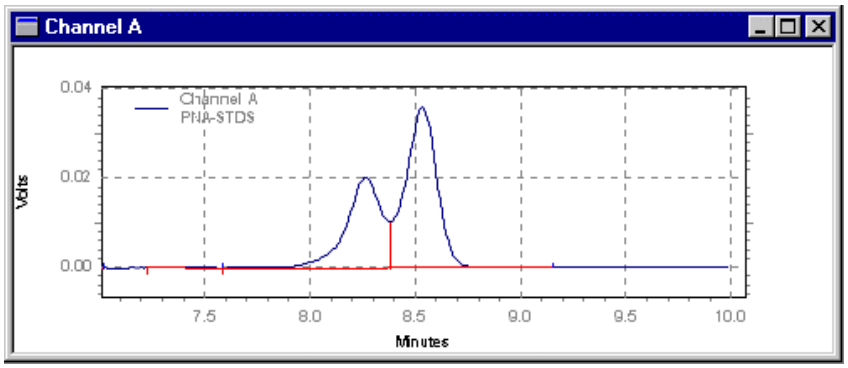
1 In the **Integration** toolbar located at the bottom of the Instrument window, select the **Front Tangent Skim** button.

2 In the chromatogram, select the **start** and **end points**.

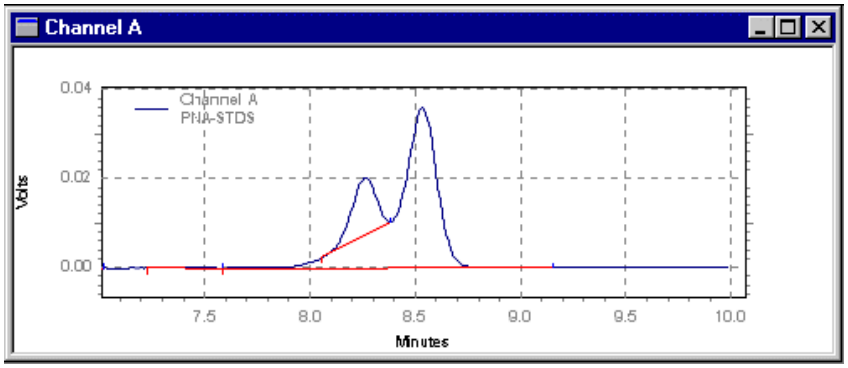
3 In the **Front Tangent Skim** dialog box, select **Add event to Method (all data)** or **Add event to this data file only.**

- If you select **Add event to Method (all data)** the event will be added to the Integration Events table when you click the **Add to Table** button. If the method is then saved, the event will be applied to every data file integrated using this method.
- If you select **Add event to this data file only** the event will be added to the Manual Integration Fixes table when you click the **Add to Table** button, and will be applied only to this data file.

4 Click **Cancel** to ignore the timed event and cancel the operation, or click **Analyze Now** to add the event to the table and analyze the chromatogram using the event.



Before Tangent Skim Event



After Front Tangent Skim Event

Minimum area

This event allows you to enter an area limit for peak detection. Peaks whose areas fall below this minimum area will not be integrated and reported as peaks. This event is useful for eliminating noise or contaminant peaks from your report.

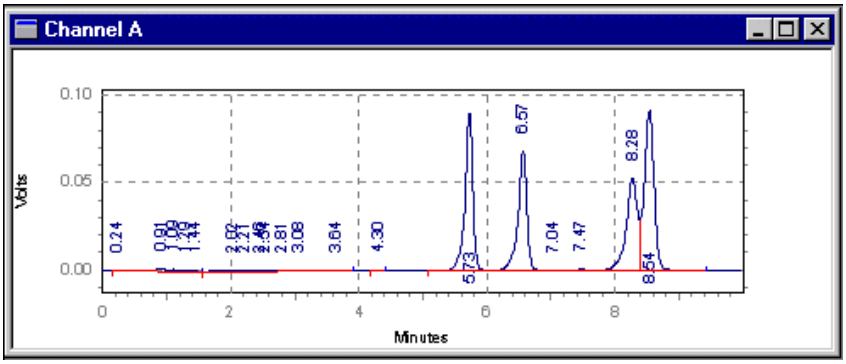
1 In the **Integration** toolbar located at the bottom of the Instrument window, select the **Minimum Area** button.

2 In the chromatogram, select the **start** and **end points**.

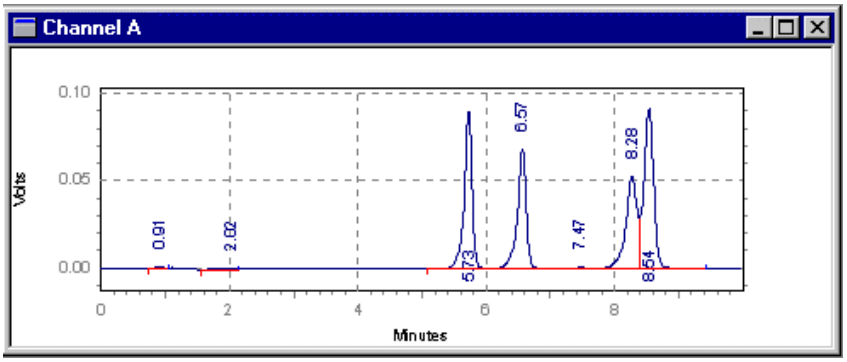
3 In the **Minimum Area** dialog box, select **Add event to Method (all data)** or **Add event to this data file only.**

- If you select **Add event to Method (all data)** the event will be added to the Integration Events table when you click the **Add to Table** button. If the method is then saved, the event will be applied to every data file integrated using this method.
- If you select **Add event to this data file only** the event will be added to the Manual Integration Fixes table when you click the **Add to Table** button, and will be applied only to this data file.

4 Click **Cancel** to ignore the timed event and cancel the operation, or click **Analyze Now** to add the event to the table and analyze the chromatogram using the event.



Integration without Minimum Area Event



Integration with Minimum Area Event

Negative peak

This event causes portions of the chromatogram that drop below the baseline to be integrated using the normal peak logic and reported as true peaks. This event is useful when using detectors such as Refractive Index types which give a negative response to certain compounds.

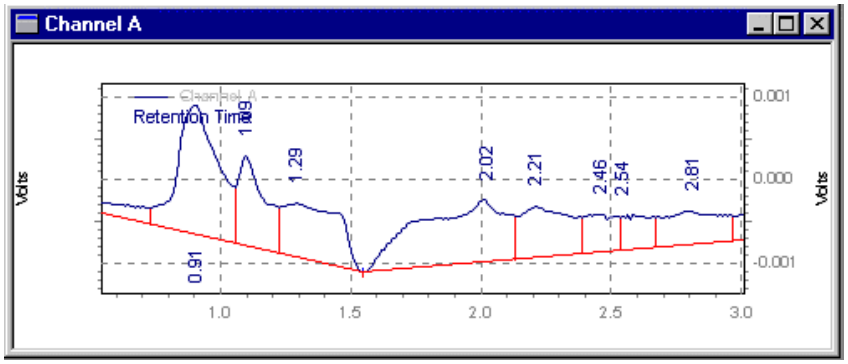
1 In the **Integration** toolbar located at the bottom of the Instrument window, select the **Negative Peak** button.

2 In the chromatogram, select the **start** and **end points**.

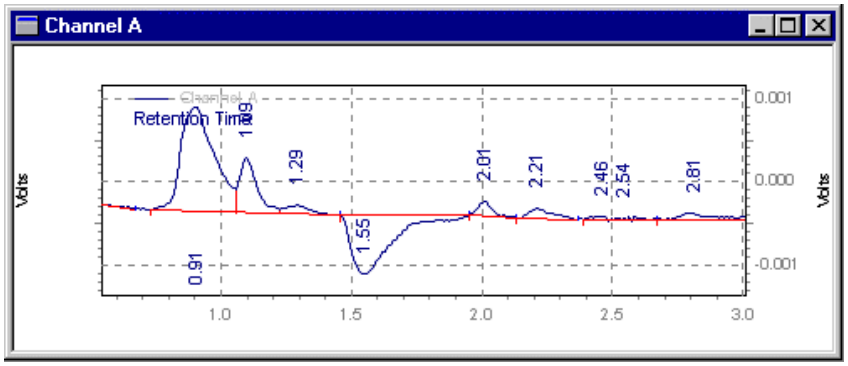
3 In the **Negative Peak** dialog box, select **Add event to Method (all data)** or **Add event to this data file only.**

- If you select **Add event to Method (all data)** the event will be added to the Integration Events table when you click the **Add to Table** button. If the method is then saved, the event will be applied to every data file integrated using this method.
- If you select **Add event to this data file only** the event will be added to the Manual Integration Fixes table when you click the **Add to Table** button, and will be applied only to this data file.

4 Click **Cancel** to ignore the timed event and cancel the operation, or click **Analyze Now** to add the event to the table and analyze the chromatogram using the event.



Default integration



Integration with Negative Peak event

Disable end of peak detection

This event is used to turn off end of peak detection between the specified times, forcing the software to treat peaks falling within the window of the event as a single peak. This event is a useful way to combine the areas of a series of contiguous peaks into one area. Because the peaks are considered to be part of a single peak, the retention time is assigned to the time of the first apex after the Disable End of Peak Detection event.

1 In the **Integration** toolbar located at the bottom of the Instrument window, select the **Disable End Peak Detection** button.

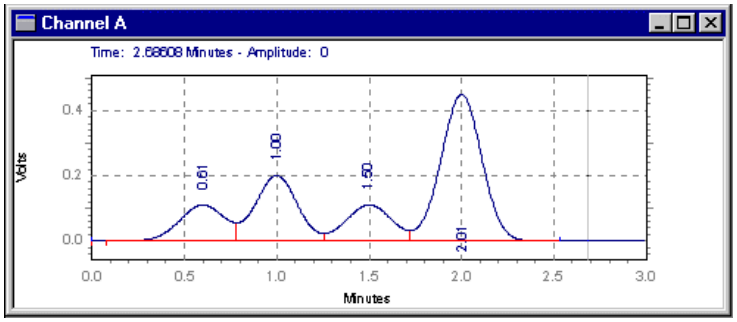
2 In the chromatogram, select the **start** and **end points**.

3 In the **Disable End Peak Detection** dialog box, select **Add event to Method (all data)** or **Add event to this data file only.**

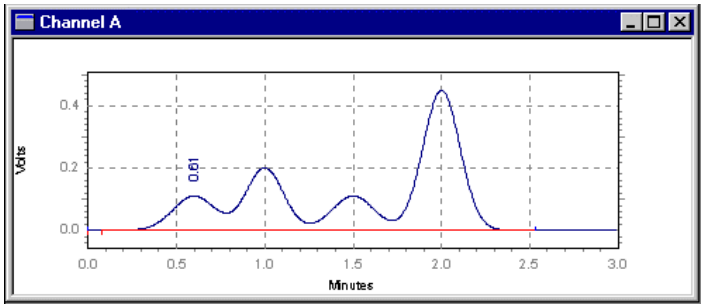
- If you select **Add event to Method (all data)** the event will be added to the Integration Events table when you click the **Add to Table** button. If the method is then saved, the event will be applied to every data file integrated using this method.
- If you select **Add event to this data file only** the event will be added to the Manual Integration Fixes table when you

click the **Add to Table** button, and will be applied only to this data file.

4 Click **Cancel** to ignore the timed event and cancel the operation, or click **Analyze Now** to add the event to the table and analyze the chromatogram using the event.



Default Integration



Disable End of Peak Detection between 0.4 and 2.2 minutes

Reassign peak

This event allows you to graphically designate a different peak as the calibrated peak in place of the peak which has been identified. This event does not change the values in the Peak Table.

1 In the **Integration** toolbar located at the bottom of the Instrument window, select the **Reassign Peak** button.

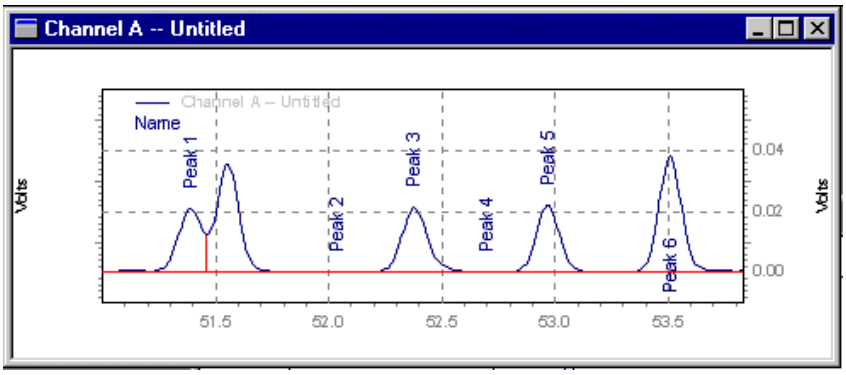
2 In the chromatogram, select the **start** and **end points**.

3 In the **Reassign Peak** dialog box, select **Add event to Method (all data)** or **Add event to this data file only.**

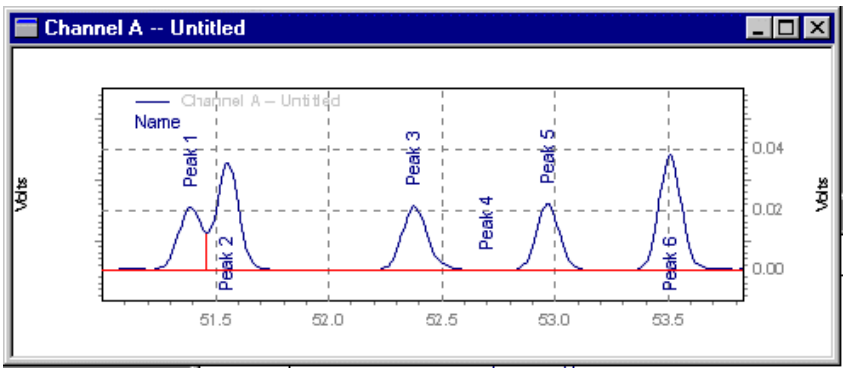
- If you select **Add event to Method (all data)** the event will be added to the Integration Events table when you click the **Add to Table** button. If the method is then saved, the event will be applied to every data file integrated using this method.
- If you select **Add event to this data file only** the event will be added to the Manual Integration Fixes table when you click the **Add to Table** button, and will be applied only to this data file.

4 Click **Cancel** to ignore the timed event and cancel the operation, or click **Analyze Now** to add the event to the table and analyze the chromatogram using the event.

In the following example, Peak 2 has been reassigned to a new peak.



Before Peak 2 reassignment



After reassignment of Peak 2

Manual baseline

This event allows you to change the way the baseline for a peak is drawn without changing the integration parameters. This is convenient when you want to change where a baseline is drawn for a peak without changing how the baseline is drawn for other peaks in the chromatogram.

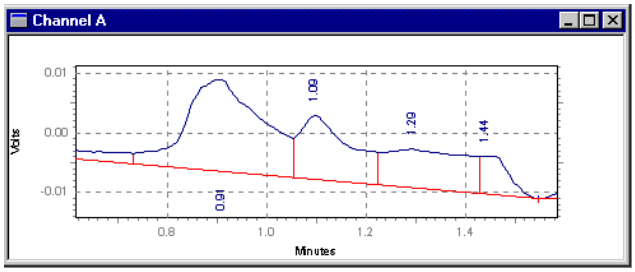
The **Manual Baseline** event was used to draw a new baseline for the second peak. To draw the new baseline, select the **Manual Baseline** command, then click your mouse at the start of the desired baseline, and again at the end of the desired baseline.

1. In the **Integration** toolbar located at the bottom of the Instrument window, select the **Manual Baseline** button.
2. In the chromatogram, select the **start** and **end points**.
3. In the **Manual Baseline** dialog box, select **Add event to Method (all data)** or **Add event to this data file only.**
   - If you select **Add event to Method (all data)** the event will be added to the Integration Events table when you click the **Add to Table** button. If the method is then saved, the event will be applied to every data file integrated using this method.
   - If you select **Add event to this data file only** the event will be added to the Manual Integration Fixes table when you

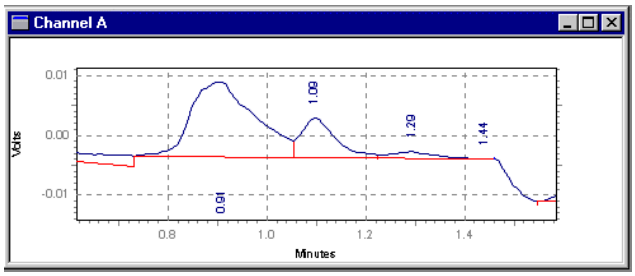
click the **Add to Table** button, and will be applied only to this data file.

4 Click **Cancel** to ignore the timed event and cancel the operation, or click **Analyze Now** to add the event to the table and analyze the chromatogram using the event.

Manual Baseline events are stored in the Manual Integration Fixes table by default.



Default Integration



Integration with Manual Baseline between 0.765 and 1.43 minutes

Manual peak

This command allows you to graphically define a peak that was not previously detected. This is convenient when you want to force integration of a peak, but do not want to change your overall integration parameters.

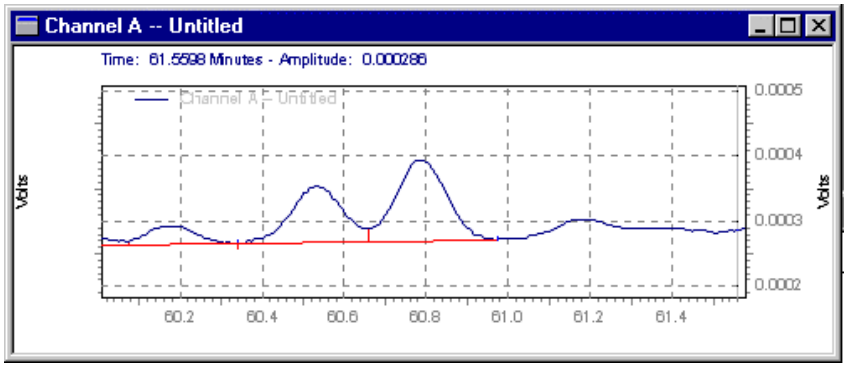
1 In the **Integration** toolbar located at the bottom of the Instrument window, select the **Manual Peak** button.

2 In the chromatogram, select the **start** and **end points**.

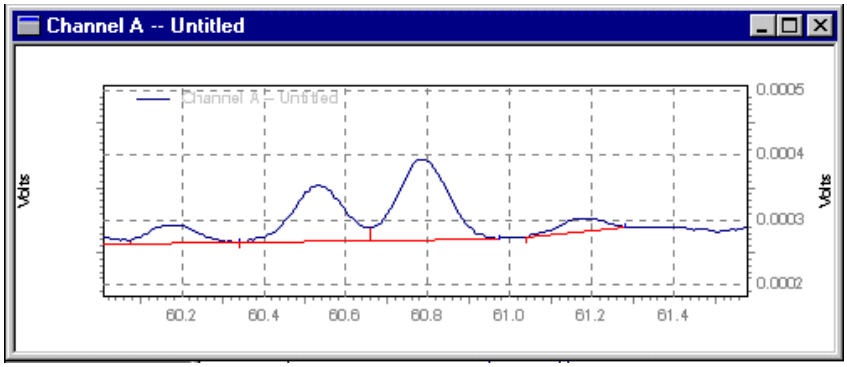
3 In the **Manual Peak** dialog box, select **Add event to Method (all data)** or **Add event to this data file only.**

- If you select **Add event to Method (all data)** the event will be added to the Integration Events table when you click the **Add to Table** button. If the method is then saved, the event will be applied to every data file integrated using this method.
- If you select **Add event to this data file only** the event will be added to the Manual Integration Fixes table when you click the **Add to Table** button, and will be applied only to this data file.

4 Click **Cancel** to ignore the timed event and cancel the operation, or click **Analyze Now** to add the event to the table and analyze the chromatogram using the event.



Default Integration



Small peak integration forced using Manual Peak event

Split peak

This event is used to force a perpendicular drop-line integration in a peak. The perpendicular will be dropped at the point where the event is inserted.

1 In the **Integration** toolbar located at the bottom of the Instrument window, select the **Split Peak** button.

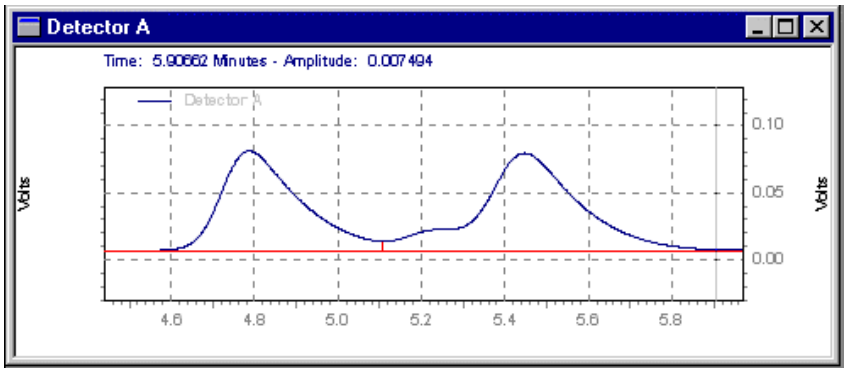
2 In the chromatogram, select the **start** and **end points**.

3 In the **Split Peak** dialog box, select **Add event to Method (all data)** or **Add event to this data file only.**

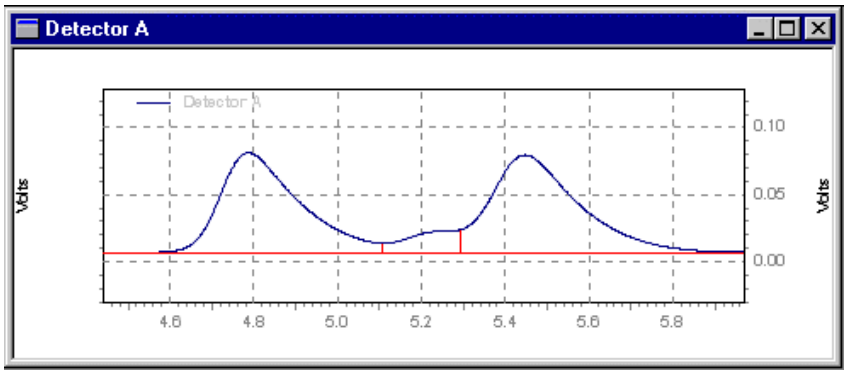
- If you select **Add event to Method (all data)** the event will be added to the Integration Events table when you click the **Add to Table** button. If the method is then saved, the event will be applied to every data file integrated using this method.
- If you select **Add event to this data file only** the event will be added to the Manual Integration Fixes table when you click the **Add to Table** button, and will be applied only to this data file.

4 Click **Cancel** to ignore the timed event and cancel the operation, or click **Analyze Now** to add the event to the table and analyze the chromatogram using the event.

This event is stored in the Manual Integration Fixes table by default.



Integration before split peak



Integration after split peak added at 5.3 minutes

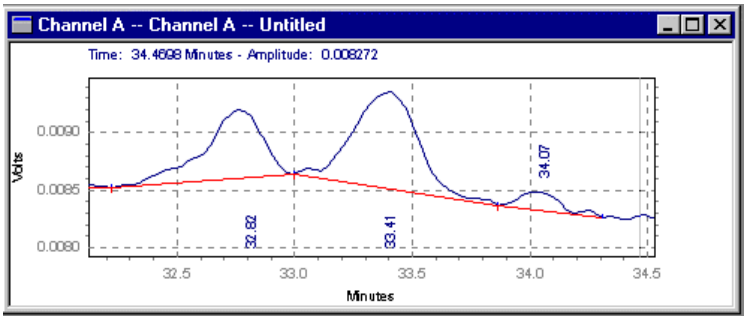
Force peak start /Force peak stop

These events are used to force the start or stop of the peak integration to a specific point.

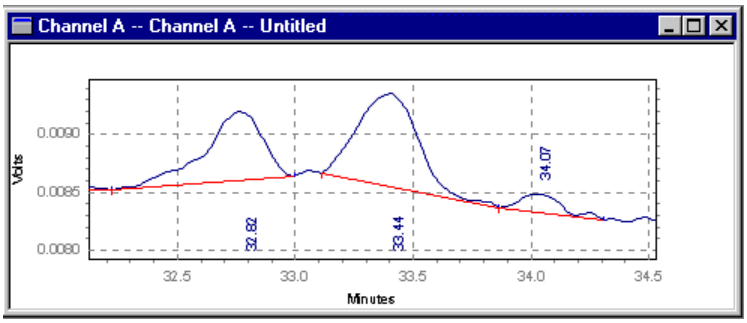
1. In the **Integration** toolbar located at the bottom of the Instrument window, select the **Force Peak Start** or **Force Peak Stop** button.
2. In the chromatogram, select the **start** or **stop points**.
3. In the **Force Peak Start** or **Force Peak Stop** dialog box, click **Add event to Method (all data)** or **Add event to this data file only.**
   - If you select **Add event to Method (all data)** the event will be added to the Integration Events table when you click the **Add to Table** button. If the method is then saved, the event will be applied to every data file integrated using this method.
   - If you select **Add event to this data file only** the event will be added to the Manual Integration Fixes table when you click the **Add to Table** button, and will be applied only to this data file.
4. Click **Cancel** to ignore the timed event and cancel the operation. Click **Analyze Now** to add the event to the table and analyze the chromatogram using the event.0

This event is stored in the Manual Integration Fixes table by default.

Default Integration



Integration after force middle peak start to 33.1 minutes



Move baseline

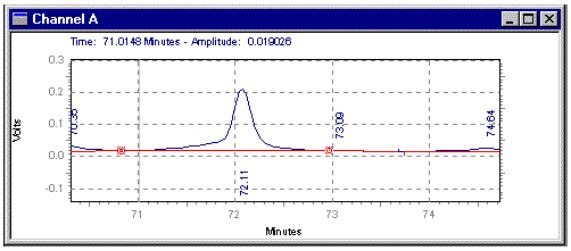
This event allows you to move the start or stop of a baseline by clicking and dragging it to a new location.

1. When you select **Move Baseline,** you will be prompted to click on the baseline segment you want to modify. The start and end points of the baseline will then appear highlighted with a box.
2. When you move the cursor to a location within range of the start or stop point, it will turn into an anchor. Click the left mouse button and drag the baseline start-point to the new location, then let go.
3. You can continue to click and drag the baseline in this manner until it is in the correct location. Then press the **Esc** key. A dialog will appear with the old and new baseline start and stop values.
4. Click **Select** to include the modified baseline. When this box is not selected, the baseline move event will not be used for integration.
5. Select **Add event to Method (all data)** to make this baseline change a part of the method to be used whenever the method is used to integrate data. Select **Add events to this data file only** to make this baseline change only for the current data file (manual integration fix).

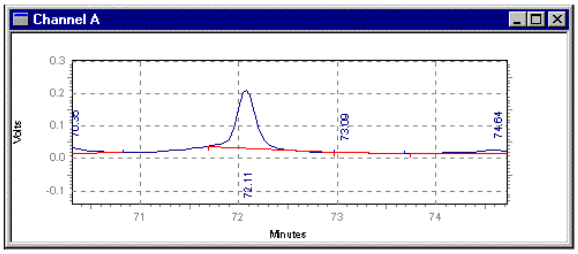
6 Click the **Add to Table** button, and the timed event will be inserted in either the **Integration Events Table**, or the **Manual Integration Fixes Table**, depending on which item in step 5 above is selected. Click **Cancel** to ignore the timed event and cancel the operation. Click **Analyze Now** to add the event to the table and analyze the chromatogram using the event.

7 Move Baseline Start and Move Baseline Stop events are stored in the Manual Integration Fixes table by default.

The following is an example of the **Move Baseline Start** event.



Before baseline is moved. Baseline start and stop points are indicated



Peak baseline start moved to approximately 71.7 minutes

Reset baseline

This event lets you set the baseline at a designated point on the chromatogram.

To enter the event graphically:

1 In the Chromatogram Window, click the **Reset Baseline** graphic event button.

2 Click the mouse on the point of the chromatogram to add the event.

3 Click **Add event to Method (all data)** or **Add event to this data file only.**

4 Click **Add to Table** to add the event to the integration events table.

5 In the **Reset Baseline** dialog box:

- Select **Add event to Method (all data)** to add the event to the Integration Events table when you click the **Add to Table** button. If the method is then saved, the event will be applied to every data file integrated using this method.

- Select **Add event to this data file only** to add the event to the Manual Integration Fixes table when you click the **Add to Table** button, and will be applied only to this data file.
- Click **Cancel** to ignore the timed event and cancel the operation. Click **Analyze Now** to add the event to the table and analyze the chromatogram using the event.

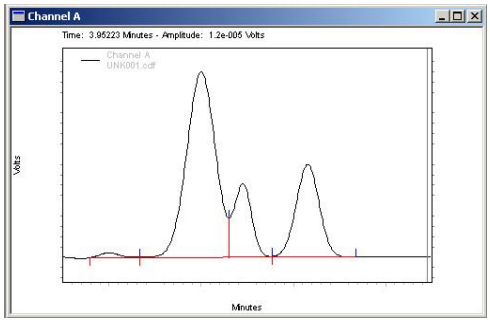
Reset baseline at valley

This event will cause the baseline to be reset at the next valley detected after the event.

Note: The event should be placed after the start of the peak first peak in the cluster; otherwise the start of the peak will be identified as the valley.

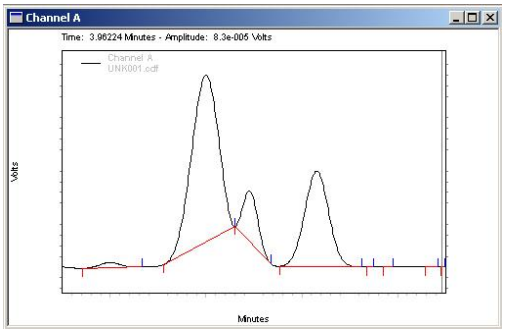
1. In the **Integration** toolbar located at the bottom of the Instrument window, select the **Reset Baseline at Valley** button.
2. In the chromatogram, select a location after the start of the peak first peak in the cluster; otherwise the start of the peak will be identified as the valley.
3. In the **Reset Baseline at Valley** dialog box, select **Add event to Method (all data)** or **Add event to this data file only.**
   - If you select **Add event to Method (all data)** the event will be added to the Integration Events table when you click the **Add to Table** button. If the method is then saved, the event will be applied to every data file integrated using this method.
   - If you select **Add event to this data file only** the event will be added to the Manual Integration Fixes table when you click the **Add to Table** button, and will be applied only to this data file.
4. Click **Cancel** to ignore the timed event and cancel the operation, or click **Analyze Now** to add the event to the table and analyze the chromatogram using the event.

An example of this event is shown below.



Baseline before Reset Baseline at Valley event

Baseline after Reset Baseline at Valley event



Exponential skimming

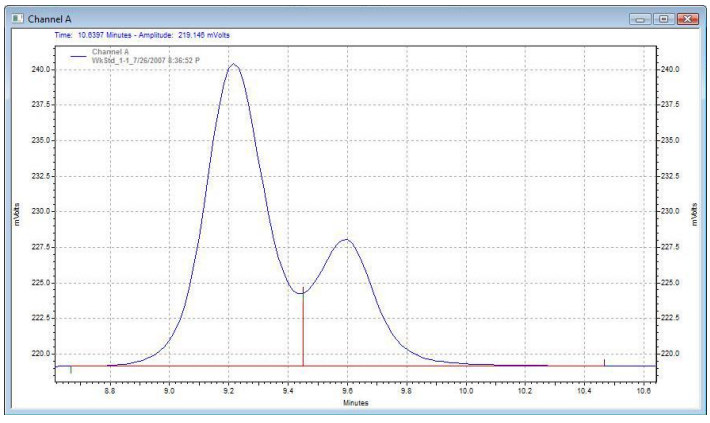
This event is used to integrate small peaks located on the tailing edge of a larger peak. The baseline of the small peak becomes an exponential drawn from the valley of the larger peak to the tangent point on the chromatogram.

1 In the **Integration** toolbar located at the bottom of the Instrument window, select the **Exponential Skimming** button.

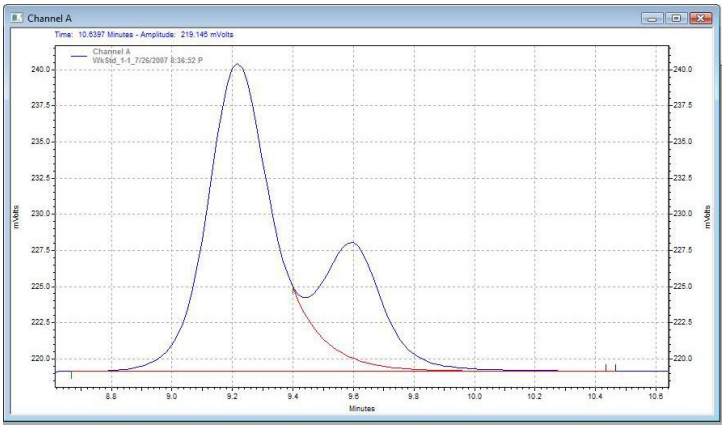
2 In the **Exponential Skim** dialog box, select **Add event to Method (all data)** or **Add event to this data file only.**

- If you select **Add event to Method (all data)** the event will be added to the Integration Events table when you click the **Add to Table** button. If the method is then saved, the event will be applied to every data file integrated using this method.
- If you select **Add event to this data file only** the event will be added to the Manual Integration Fixes table when you click the **Add to Table** button, and will be applied only to this data file.

3 Click **Cancel** to ignore the timed event and cancel the operation, or click **Analyze Now** to add the event to the table and analyze the chromatogram using the event.



Before Exponent Skim event



After Exponent Skim event

Front exponent skimming

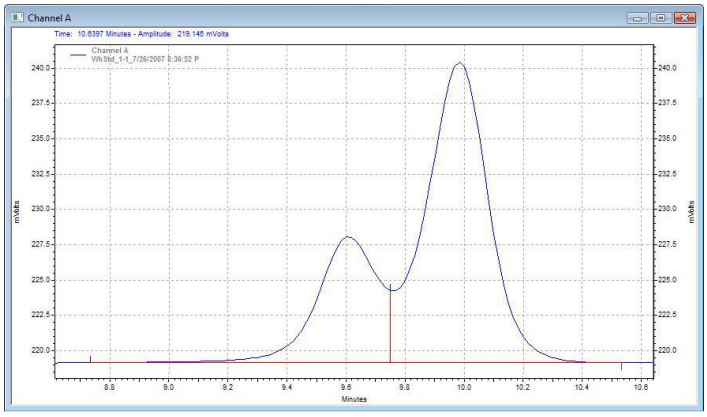
The Front Exponent Skim event is used to force a exponential baseline for a daughter peak on the leading edge of a mother peak.

1 In the **Integration** toolbar located at the bottom of the Instrument window, select the **Front Exponent Skimming** button.

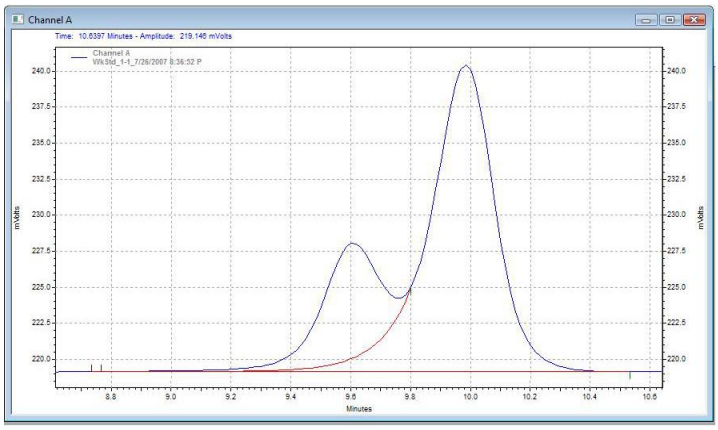
2 In the **Front Exponent Skim** dialog box, select **Add event to Method (all data)** or **Add event to this data file only.**

- If you select **Add event to Method (all data)** the event will be added to the Integration Events table when you click the **Add to Table** button. If the method is then saved, the event will be applied to every data file integrated using this method.
- If you select **Add event to this data file only** the event will be added to the Manual Integration Fixes table when you click the **Add to Table** button, and will be applied only to this data file.

3 Click **Cancel** to ignore the timed event and cancel the operation, or click **Analyze Now** to add the event to the table and analyze the chromatogram using the event.



Before Front Exponent Skim event



After Front Exponent Skim event

Adjust RT window

The expected retention time window is set when you add a peak to the calibration table. You can graphically change the retention time window for any calibrated peak using this graphical event.

Note: In order to graphically adjust the RT Window, you must have the RT Window annotation turned on. To turn on the RT Windows, in the Chromatogram Window do a right mouse click and then select Annotations. In **Trace Annotation Properties**, make sure **RT Window** is selected in the **Other** pane at the bottom.

To adjust the RT Window from the Chromatogram Window

1. Click the **Adj RT Window** button at the bottom of the Chromatogram Window and then click on the RT Window you wish to adjust. The cursor will turn into a two-ended arrow and two drag boxes will appear.
2. You can adjust the RT window by dragging either end or by dragging the RT bar itself.
3. If you grab the bar itself and move it, the Expected RT will be updated and the RT Window will remain the same.
4. If you grab either end of the bar and move it, the other end of the bar will stay in its current position and the Expected RT and the RT Window will be updated.
5. Repeat the procedure to adjust additional RT windows.
6. After you have adjusted the windows to your liking, press **ESC** to finish. A dialog will appear that displays a table with the RT Window changes you have made. Each row shows the peak **Name**, the **Old Ret. Time**, the **New Ret Time**, the **Old RT Window**, and the **New RT Window**. You can manually adjust the **New Ret Time** and **New RT Windows** by clicking the field and then typing the desired value.
7. By default, all RT Window updates are **Selected**. Clear the **Select** box for each RT Window adjustment update you do not wish to include.

8 Click **Update RT**, and the Retention Times will be updated in the peak table. Click **Cancel** to ignore the event and cancel the operation. Click **Analyze Now** to update the peak table and analyze the chromatogram using the updated Retention Time and RT Windows.

Sampling rate

The sampling rate used to acquire your data determines how much information the integration algorithm has for drawing and integrating the chromatogram. The sampling frequency is set in the Instrument Setup part of your method. To make sure you have the proper sampling rate, use the **Suggest Sampling Frequency** command in graphical programming. Slight over-sampling of data is corrected with the **Width** integration parameter and is not a problem. Try to avoid gross over-sampling of data, however, as it does not give better integration and it wastes space on the hard drive of your computer. More important, however, is not to under-sample, as there is no way to correct for data points that are not sufficient to define and integrate your peaks.

Before attempting to add integration timed events, make sure your chromatogram has been analyzed using the current method. To make sure, look for baselines and start/stop tic marks on your chromatogram. Or, click the **Analyze** button on the command ribbon.

Suggest Sampling Frequency

1 Right click the chromatogram and select **Graphical Programming > Suggest Sampling Frequency**.

2 Following the instructions on the status bar, click once at the beginning of your narrowest peak of interest, then once at the end of that peak. The software will suggest a sampling rate or period for acquisition of the sample. You can enter this value for your sampling rate using the **Instrument Setup** button.

About Sequences

The sequence is the cornerstone of automatic operation. With a sequence, you can automatically acquire, process, and store multiple runs. You can use a sequence to automate calibration, either at the time the runs are acquired, or post-acquisition by sequence reprocessing. You can set up run queues for automatic running of sequences, and you can trigger events based on results of a run in a sequence (see Set an Action for a Sequence Run.) Once a sequence is acquiring data, you can monitor the progress of the sequence(s) using the Run Queue function.

See Also

Create a Sequence using Sequence Wizard

Open a Sequence File

Edit a Sequence

Easy Sequence

Create a Sequence from a Container Sample List

Save a Sequence

Sequence Properties

About the Sequence Spreadsheet

About Data Acquisition and Control

About the Result Sequence

About Sequence Reports

Create a sequence with the sequence wizard

The Sequence Wizard is used to create a new sequence.

To start the Sequence Wizard:

1. From the **Instrument** window, click the **Instrument Wizard** button and then click **Create a Sequence**.
2. Complete the wizard to define your sequence. The wizard will step you through various parameter screens required to create an acquisition or reprocessing sequence depending on your choices and the instrument configured. The first screen of the Wizard is Sequence Wizard - Method.
3. When you have completed the wizard, click **Finish**.
4. To save the sequence, from the menu, click **File > Save As... > Sequence.** Browse to the location where you want to save your sequence, enter the name of the sequence, and then click **Save**. See Save a Sequence.

See Also

Tutorial - Create a Sample Sequence

Sequence Wizard - Method

Sequence Wizard - Unknowns

Sequence Wizard - Autosampler

Sequence Wizard - Calibration

Sequence Wizard - Reports

Create a Reprocessing Sequence

Sequence Wizard - Method

1 Specify a **Method** to be used for the sequence, or select it from a list of existing methods by clicking the **File Open** button.

2 Select a **Data File Type** from the following options:

- **For acquisition** enables you to designate new file names to be used for acquisition.
- **From existing data files** enables you to select the data file names from a list of existing data files from your data directory. This is normally used to create a sequence to be used for reprocessing. See Creating a Reprocessing Sequence for details.

3 In the **Amount Values** section, you can enter values that affect how the concentrations of unknown samples are calculated.

- **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 weighing 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 taken from the method Peak Table. For unknown runs, enter the amount of the Internal Standard in your unknown sample.
- **Multiplication factors -** Enter up to 3 multiplication factors to be used for these runs. All quantitated peaks will be multiplied by these factors.
- **Dilution factors -** Enter up to 3 dilution factors to be used for these runs. All quantitated peaks will be divided by these factors.

4 When you have completed this dialog, click **Next** to continue. See Sequence Wizard - Unknowns.

Sequence Wizard - Unknowns

In the dialog box shown below, you enter information for data storage and sequence runs.

Sample ID

Type a sample identification label. This can be numerical and/or text format, and will be saved with each data file.

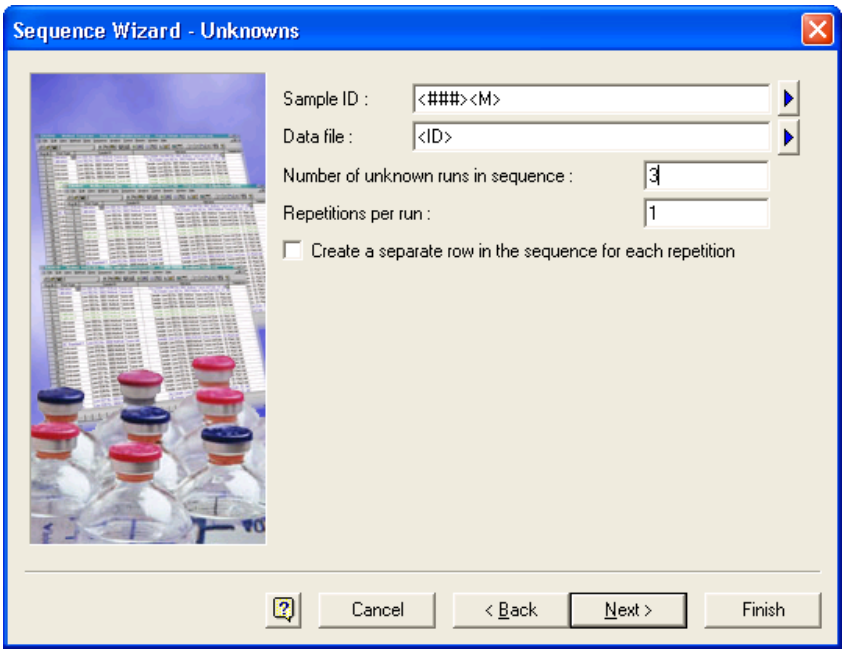
If you want the system to generate a Sample ID for you automatically, click on the blue arrow and select a parameter to be used for the basis of your Sample ID. You can select more than one parameter, which will be added sequentially to the Sample ID. You cannot use the date/time parameter (<D>) by itself as the Sample ID.

For example, if you select Line Number and Instrument name, the sample ID's generated will be the row number of the sequence followed by the instrument name: **3HPLC.**

To use the Increment Number option, enter a number to start the increment in angle brackets. For example, <33> would start

	numbering from 33. By default, the Increment Number option allows for 3 digits. To reduce or increase this number, adjust the digits in your brackets accordingly. For example <0033>.
Data File	Enter a name for the data files. In order for unique data file names to be created automatically, you can have the system generate file names for you automatically, based on a system parameter. Click the blue arrow and select a parameter to be used for the basis of your data file names. You can select more than one parameter. The software automatically appends the **.DAT** extension to the data file names. For example, you can use the Sample ID as the data file name. **Note**: In order to generate unique filenames automatically for each data file, you should make sure that the Line Number or Increment number is included somewhere in the file name.
Number of unknown runs in sequence	Enter the number of unknown samples to be acquired or reprocessed with the sequence.
Repetitions per run	Enter the number of times each unknown will be repeated or re-injected.
Create a separate row in the sequence for each repetition	Click this box if you wish to create a separate row in the sequence for each repetition. If you do not select this box, unknown repetitions will not be displayed in the sequence spreadsheet, although individual data files will be created and stored for each repetition acquired.

When you have completed this dialog, click **Next** to continue. See Sequence Wizard - Autosampler.



Sequence Wizard – Unknowns dialog box

Sequence Wizard - Autosampler

If you have an autosampler control option, this screen of the sequence wizard will appear. It is used to set up the vial numbers for the first unknown and calibration of the sequence, along with increment number. A default injection volume can also be entered. This can be changed on a per-run basis in the sequence spreadsheet.

When you have completed the dialog box, click **Next** to continue. See Sequence Wizard - Calibration.

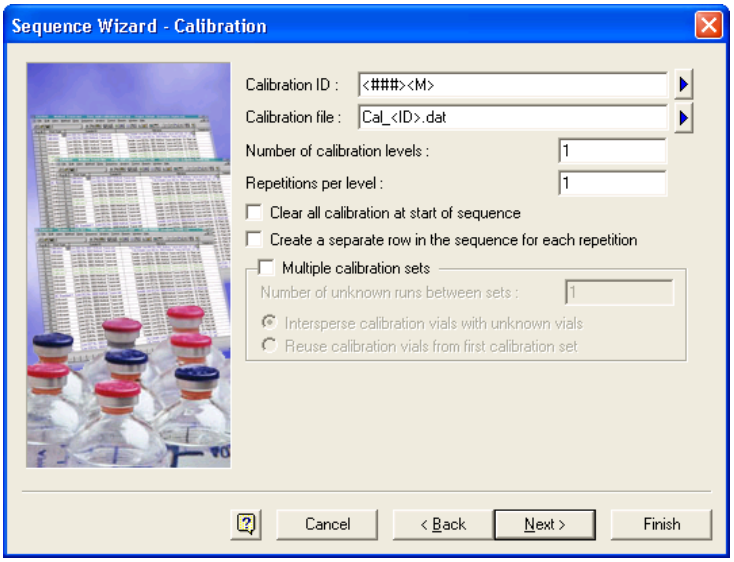
Sequence Wizard - Calibration

In the dialog box show below, allows you to set up calibration standards in your sequence.

Calibration ID	Enter a calibration sample identification. This is a text value that is stored in the calibration data file. The identifiers from Sample ID are automatically entered in order to associate calibration IDs with your data file IDs. If you wish, you can have the system generate a different Calibration ID for you automatically based on a system parameter. Click the blue arrow and select a parameter to be used for the basis of the Calibration ID.
Calibration file	Enter a name for the calibration data files. The system automatically will apply the **Cal_** prefix to each calibration file in the sequence. You can change this if you wish. The identifiers from Data File are automatically entered in order to associate calibration file names with your data file names. You can change these if you wish by clicking the blue button and selecting the parameter to be used for the basis of the calibration file name. You can select more than one parameter. **Note**: In order to generate unique filenames automatically for each data file, you should make sure that the Line Number or Increment Number is included somewhere in the file name.
Number of calibration levels	Enter the total number of calibration levels to be run in the sequence.
Repetitions per level	Enter the number of repetitions or re-injections for each calibration level. **Note**: If multiple repetitions are specified, a result file will be generated for each injection with the data file's name being created by appending Rep1, Rep2, etc. to the data file name.
Clear all calibration at start of sequence	Select this box if you want to clear all calibration information (response factors, replicates) before the first run of the sequence.
Create a separate row in the sequence for each repetition	Select this box if you want to create a separate row for each calibration repetition in your sequence. If you do not select this box, a separate data file will be created for each calibration repetition, however the repetitions will not appear in the sequence spreadsheet.
Multiple calibration sets	Select this box if you plan to run each calibration level (plus its replicates) more than once.

Number of unknown runs between sets	If you have selected **Multiple calibration sets** box, this option will appear. Enter the number of unknown samples to be run between each calibration set. If you have an autosampler with control installed, the vials options will become available.
Vials	Select **Intersperse calibration vials with unknown vials** if you wish to run unknown samples between calibration sets. Select **Reuse calibration vials from first calibration set** if you wish to reuse the same set of calibration vials for the entire sequence.

When you have completed this dialog, click **Next** to continue. See Sequence Wizard - Reports.



Sequence Wizard - Reports

Use this dialog (shown below) to set up summary reports for your sequence.

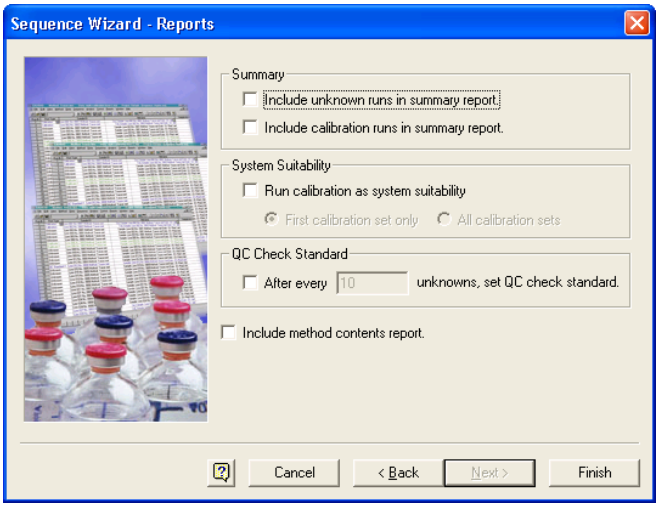
Summary	These options allow you to designate summary runs.
Include unknown runs in summary report	Select this box if you want your summary report to include unknown runs. These runs will have their Run Type set for a summary run.
Include calibration runs in summary report	Select this box if you want your summary report to include the calibration runs. These runs will have the Run Type set to be included as a summary run.
System Suitability	These options allow you to designate system suitability runs.
Run calibration as system suitability	Select this box if you have the system suitability software option, and you wish to designate calibration runs as system suitability types. This also will cause display of system suitability parameters in the sequence spreadsheet.

	Select either **First calibration set only** or **All calibration sets.** See About System Suitability.
QC Check Standard	**After every ___ unknowns, set QC check standard**
Include method contents report	When this box is selected, a method contents report will be automatically generated whenever the method changes in a sequence. When this option is enabled, the sequence will automatically add a **print additional reports** run type to each run where the method has changed from the previous run in the sequence. This can be changed or deleted for any given run in the Edit Sequence spreadsheet.

When you have finished this dialog, click the **Finish** button. A sequence will be created using the information specified in the dialogs and displayed as a spreadsheet.

The new sequence will be displayed as untitled. To save your new sequence, use the **File > Save As > Sequence** command and type the name of the new sequence.

To close the sequence spreadsheet, click the **X** box in the upper right corner of the spreadsheet. To open the current sequence spreadsheet, use the **Sequence>Edit** command, or click the **Edit Sequence** button on the command ribbon.



Create a reprocessing sequence

You can use the Sequence Wizard to create a sequence containing existing data files, for the purpose of reprocessing only.

To create a reprocessing sequence:

1 From the **Instrument** Window, click the **Instrument Wizard** button and then click **Create a Sequence**.

2 Complete the Sequence Wizard to select methods and data files to be used for the reprocessing.

3 In Sequence Wizard - Method, select **From existing data files** as the **Data File Type**. This will bypass the wizard screens necessary for creating an acquisition sequence and allow you to select data files to be reprocessed. In addition, amount values from the data files selected will be entered into the sequence.

4 When you have completed the wizard, click **Finish**.

5 To save the sequence, from the menu, click **File > Save As > Sequence.** Browse to the location where you want to save your sequence, enter the name of the sequence, and then click **Save**.

Edit a sequence

Once a sequence has been created, you can view or change the sequence from the Instrument Window.

To edit the current sequence:

1 From the **Sequence** menu, click **Edit.**

2 Modify the sequence using the displayed spreadsheet.

See Also

Open a Sequence File

Save a Sequence

Easy sequence

Easy Sequence is an easy to use interface for using and setting up sequences with predefined templates. Sequence setups can be created, modified, and then reused for different users and analysis types. This minimizes errors that occur each time a sequence is created.

Easy Sequence

The Easy Sequence... option allows a user to run a sequence using a predefined template.

To access Easy Sequence...:

1 From the main menu, select **Sequence**.

2 Select **Easy Sequence....** The Easy Sequence dialog box opens. See the **Easy Sequence Help** for more information.

Easy Sequence Setup

The Easy Sequence Setup... option allows a user to create and modify templates.

To access Easy Sequence Setup...:

1 From the main menu, select **Sequence**.

2 Select **Easy Sequence Setup....** The Easy Sequence Setup dialog box opens. See the **Easy Sequence Template Help** for more information.

Create a sequence from a container sample list

The Sample Entry option provides an easy to use graphical interface for setting up sequences from the container, such as 96-well plate or vial array. Sample list templates can be created, modified, and then reused for different users and analysis types.

This option is only active when supported devices are used in your system and the drivers are initialized when you start the instrument. You can view the status of the driver initialization in the Instrument Activity Log.

To use a container sample list template:

1. If you are launching an instrument for the first time, or are working with a sequence or method, select **Sequence > Sample Entry**. If you are working with a result set, select **Result Set > Sample Entry**. The Sample Entry dialog box opens.
2. Click **Help** in the Sample Entry window for detailed instructions on:
   - Using existing sample lists
   - Creating and modifying sample list templates
   - Opening and saving sample lists

A Sample List submitted from the Sample Entry interface is added to the Run Queue.

Once you submit your sequence, a sequence file is created in your project's Sequence folder. The file will be named after the Sample List name.

Sequence properties

Select **Sequence > Properties** to edit and view the description, export information, audit trail log, and audit trail of data files.

See Also

Sequence Properties Options

Sequence Properties Audit Trail Log

Sequence Properties Audit Trail

Sequence properties options

When you create a new sequence using the Sequence Wizard, you enter a description, specify a summary export path, and designate the default directories for data and methods.

To view or change these properties:

1. From the **Sequence** menu, select **Properties**.
2. In the **Sequence Properties** dialog box, select **Options**.
3. Enter the properties for the sequence.
   - **Description** - Enter a text description of the sequence, if desired. The description is saved in the sequence file and

may be viewed from the **Open Sequence** dialog box.

- **Export summary** - Click this box to export the summary report. Enter the path where you want the summary text file to be saved. The summary will be exported to a file entitled Sequence Summary - 000005000.txt Where the numbers represent nBatchTower, nReportRunTypeID, nReportNumber.
- **File Paths** - Select default paths to be used for methods, data, and autosampler, if appropriate. You can select a path from those available on the disk by clicking the file button adjacent to the field. These paths are used in the event that a file is specified in the sequence table without a path.

Sequence properties audit trail

To enable the audit trail for sequences:

1. From the **Sequence** menu, select **Properties**.
2. In the **Sequence Properties** dialog box, select **Audit Trail**.
3. Click **Enable Audit Trail**. Once the Enable Audit Trail box is selected, it cannot be deselected. The sequence will continue to have audit trail enabled unless you save the file under a new filename.
4. Once the **Enable Audit Trail** box is checked, the following options are available for documenting changes.
   - **Prompt for reason at every change** - This option requires the user to enter a reason for every subsequent change to the sequence at the time the change is made.
   - **Prompt for reason when saving Sequence** - This option requires the user to enter a reason for each change when the Sequence is saved.
   - **Do not prompt for reason** - When this option is selected, changes are documented, but the user is not required to enter a reason for the changes.

Sequence properties audit trail log

To view the audit trail log for the current sequence:

1. From the **Sequence** menu, select **Properties**.
2. In the **Sequence Properties** dialog box, select **Audit Trail Log**.
3. Enter the following:
   - **User**
   - **Location**
   - **Description**
   - **Reason**
   - **From date/time**
   - **To date/time**

4 Select from the following options:

- **Export** - Select this to export the audit trail log.
- **Print** - Select this to print the audit trail log.
- **Search** - Select this to search the audit trail log.

About the sequence spreadsheet

A sequence is displayed as a spreadsheet, with each row representing chromatography run or a file to be reprocessed. For each row, you designate a method, data file name, whether the sample is a calibration standard, along with various options for how you want the data to be processed. The following section describes the functions of the sequence spreadsheet.

See Also

Sequence Spreadsheet Context Menu

Fill Down

Insert a New Sequence into a Sequence Spreadsheet

Customize the Sequence Spreadsheet Columns

Sequence Spreadsheet Columns

Set Sample Run Types

Set up a QC Check Standard

Concentration Override

Set an Action for a Sequence Run

Sequence spreadsheet context menu

All sequences are displayed in a spreadsheet similar to the one shown below. Although the information in the fields will vary, the spreadsheets always support certain basic features. For a list of spreadsheet columns and their definitions, see Sequence Spreadsheet Columns.

Each row is assigned a **Run #**, followed by columns for information for each run in the sequence. Rows and field information can be cut, copied, pasted, and cleared. To access the menu for these commands, click the right mouse button anywhere within the spreadsheet.

Context Menu Commands

Cut	This command will cut the current selection and place it into the clipboard. You can subsequently paste the information to another application using the paste command, or move the selection to another location in the spreadsheet by selecting the location, then using the paste command. **Note**: Once you have cleared or deleted a row from your spreadsheet, the blank row will remain in the spreadsheet until you close the sequence spreadsheet and re-open it, or press the F5 key.
Copy	Use this command to make an exact copy of the selection in the clipboard. Once you select **Copy**, you can paste the selection to another application, or copy the selection to a location in your spreadsheet.
Paste	This command is used to paste the information currently in the clipboard into the spreadsheet at the location of the cursor.
Fill Down	This enables you to automatically copy spreadsheet information from one field or row down through the rest of the spreadsheet.
Insert Paste	This command works like a combination of insert line and paste commands. The item currently in the clipboard will be pasted into a new line above where the cursor is located.
Insert Line	This command inserts a blank line in the spreadsheet above where the cursor is located.
Clear	Use this command to clear the information in the selected location. (You can also use the Delete key from your keyboard for this function.) The F5 function key can be used to collapse rows that have been deleted from the spreadsheet.
Clear All	Use this command to clear the information from the entire spreadsheet.
Select All	Use this command to select the entire spreadsheet.
Open Method	This command will open the method associated with the currently selected run in the spreadsheet.
Open Data	This command will open the data file associated with the currently selected run in the spreadsheet. The data file will be opened with last results. If last results is not available, the data file will be recalled with the original results.
Process Sequence...	This command opens the Process Sequence dialog and enables you to reprocess all or part of the current sequence.
Run Sequence...	This command opens the Run Sequence dialog to enable you to start the sequence acquisition.
Insert New Sequence...	This command will start the sequence wizard to create a new sequence, which will be inserted into your current sequence below the currently selected row.
Set Run Types...	This command allows you to select a desired run type from the displayed list to be applied to the selected rows.
Properties...	This command opens the Sequence Properties dialog where you can add/edit the sequence description and select default paths for data and method files.

Note: When copying or pasting spreadsheets from the data system to other applications, hidden parameters that do not appear in the spreadsheet (such as action item parameters) will not be pasted.

Fill down

The **Fill Down** command enables you to automatically copy spreadsheet information from one field or row down through the rest of the spreadsheet.

To use the Fill Down command:

1. In the sequence spreadsheet, select a row or field by highlighting it with your mouse.
2. Do a right mouse click and select **Fill Down**. If you have selected a numeric field such as level or repetitions, the selected item will be automatically filled down the spreadsheet from where it is highlighted. If you select either a row, a Filename, or a Sample ID, a dialog will appear where you can designate a name and indicate whether you want to increment its associated numbering.
3. For Sample ID and Data File fields, you can opt to automatically increment the number or change the name by checking the **Increment** check box. You can select parameters for the increment in a manner similar to that used in the sequence wizard by clicking the blue arrow and selecting from the list. (Be sure to include the correct number of place holders. For example, if you start at number <10>, but the number of files is between 100 and 1000, you should enter <010>.) Click on **OK** to fill the information down the spreadsheet.

Insert a new sequence into a sequence spreadsheet

To create sequence rows and insert them into your spreadsheet:

1. In the sequence spreadsheet, do a right mouse click at the point where you want to insert new sequence rows and then click **Insert New Sequence**.
2. The Sequence Wizard will appear. Complete the wizard to define the new rows for the sequence.
3. Click **Finish**. The new sequence rows will be inserted **Above** the selected row.

Customize the sequence spreadsheet columns

You can customize the sequence spreadsheet to include only the columns you will be using. The selections are saved on a per-user/per instrument basis. That is, each user can set spreadsheet properties for each instrument.

1. In the sequence spreadsheet, do a right mouse click and then click **Properties**.
2. In the **Properties** dialog box, select the columns that will appear in the peak table. Columns with a check mark will be displayed in

the spreadsheet. Those without a check will not be displayed.

3 The blue anchor indicates what column will be used to anchor the right-left scrolling in your spreadsheet. Once this anchor is set, columns to the right of the anchor will scroll to the right and left. Columns to the left of the anchor will not scroll. To change the anchor, click on the name of the column you wish to use as anchor, and click the **Set Anchor** button. The blue anchor will move to the designated anchor column.

Note: When using the anchor, it is best to remove all unnecessary columns from the spreadsheet, and make the spreadsheet as wide as possible before you set the anchor. If you set the anchor to a column that does not currently show on the spreadsheet, you will not be able to scroll the spreadsheet.

Sequence spreadsheet columns

The following columns appear in the sequence spreadsheet and in the result sequence. Although the New Sequence Wizard allows you to automatically create a sequence, you should review the sequence to make sure the information for each run is correct before it is run.

To select a field, click on that field to highlight it. To select a row, click on the **Run #** to highlight the entire row. To select the entire spreadsheet, use the **right-click** menu, and click the **Select All** command.

To resize the columns, move the cursor to the title area above the column you wish to size. The cursor will turn into two vertical lines with arrows. Click and drag the cursor until the column is the desired size, then release the mouse key.

To view the spreadsheet, in the navigation pane, select **Sequence > Edit**.

Status	This field becomes active when a sequence acquisition or processing is in progress. It indicates the current status of the run.
Run Type	Select a Run Type from the available types by clicking the arrow button in the field. A dialog box will appear where you can select the run type(s). To see a list of the run types and their actions, see **Set Sample Run Types**. **Run Type Parameters** For each run type selected, you may be prompted to enter parameters necessary for the run type to be used. In most cases, this involves selecting a template to be used for a report. **Setting run types for multiple runs** You can quickly change the run type for multiple runs by highlighting the desired rows in the spreadsheet, then click the right mouse button and select **Set Run Types**. When you select the desired run type from the displayed list it will be applied to the rows you have selected.

Level	For a calibration run, you must enter the level number for the calibration standard. (For example, if you have 5 calibration concentration levels, each calibration run will have a **level** number representing the calibration concentration level being run. This number is NOT the concentration amount of the standards, however. Concentration amounts are entered in the peak table.)
Conc Override	This field lets you enter a concentration override for one or more peaks in the selected calibration run. This is not active unless the selected run is designated as a calibration run.
(Sequence) Custom Parameters	When you click this field, the **Custom Parameters** dialog box appears where you can define per-peak or system-wide sequence custom parameters. Custom parameters available are derived from the active method for the sequence line being configured. See About_Custom_Parameters and Set a Custom Parameter for a sequence.
Reps	Enter the number of repetitions per vial.
Vial	Enter the autosampler vial number to be used for the injection. For autosamplers that support it, in the drop down box, select **Use Method.** To enter a specific vial such as A2 first press **enter**, left or right arrow to exit the cell. Using the up or down arrow will always select **Use Method**.
Volume	Enter the volume to be injected. For autosamplers that support it, you can select **Use Method** to use the default injection volume specified in the method used. Use the Fill Down feature to populate one field or row down through the rest of the spreadsheet.
Frac. Start	Select the starting location (vial or well) for the fraction collector.
Sample ID	Enter a sample identification here. This can be text and numeric information. The Sample ID will have a unique number attached to it. Enter the new sequence dialog in the following format, <*SampleID*>. The Sample ID is saved in the data file. You cannot use the date/time parameter (<D>) by itself as the Sample ID.
Method	This is the name of the method to be used for data acquisition and processing. If you don't know the name of the method, click the button to select it from a list of available methods on your disk.
Filename	Enter a filename to be used for storing the raw data from the run. The filename will already have a unique number appended to it. Enter a data filename in the new sequence dialog in the following format, <*Filename*>. **Note**: If multiple repetitions are specified, a result file will be generated for each injection with the data file's name being created by appending Rep1, Rep2, etc. to the data file name.
Sample Amt	The Sample Amount value is used as a divisor during calculation of concentrations. It is intended to compensate for differences between samples due to weighing and when

	percentages of the total sample are being calculated rather than the amount detected in an injection.
ISTD Amt	For calibration runs, the Internal Standard Amount is taken from the method Peak Table. For unknown runs, enter the amount of the Internal Standard in your unknown sample.
Multiplier 1,2,3,4,5	Enter up to 3 multiplication factors to be used for this run. All quantitated peaks will be multiplied by these factors.
Dilutor 1,2,3,4 ,5	Enter up to 3 dilution factors to be used for this run. All quantitated peaks will be divided by these factors.
Action	Brings up the run action dialog, where you can specify test/result/action combinations for each run. For details on setting up an action, see **Set an Action for a Sequence Run**. **Note**: Action items that are user-interactive (e.g. pause and alarm) will not trigger user input on client machines when using client/server operation. This is because the server is controlling the instrument.
Description	Enter a description for this sample. This is text information that will be stored in the raw data file.

Set sample run types

Sample **Run Types** are used in a sequence to flag a run for designated processing, calibration, or reporting. Each sample can have multiple run types assigned. Some run types will be assigned automatically if you are using the Sequence Wizard to create a new sequence.

To change or add a run type after the sequence has been created:

1. In the sequence spreadsheet, click the arrow in the **Run Type** field for the sample of interest.
2. Select a run type from the available types listed below by clicking the check box for that run type.
3. Where required, parameter fields will appear where you must enter parameters or select templates to use for the processing of the designated run type.

Run Type	Action
Clear All Calibration	Clears all calibration response factors and coefficients for all calibration levels.
Clear Calibration at Level	Clears response factors and coefficients for current level only.
Print Calibration Report	Prints calibration report at end of calibration.
Average Replicates	Forces averaging of replicates. See **Calibration Averaging as Part of a Single Run or Sequence**.
Clear Replicates	Clears calibration replicates at this level before calibration.
Begin Loop	Flags the run as the start of an infinite loop. Runs between and including these flags will be continuously run until stopped.

End Loop	Flags the end of an infinite sequence loop.
Startup	Flags this sample as a startup sample. (Appears when supported by the instrument in use.)
Shutdown	Flags this sample as a shutdown sample.
Print Additional Reports	Enables you to select additional reports to print.
Begin System Suitability	First run of a System Suitability sample set.
System Suitability Standard	System Suitability Standard sample between Begin and End System suitability.
End System Suitability	Last run of a System Suitability sample set.
Begin Summary	First run to be included in a sequence summary, also indicates the summary report template to be used for the summary report. See About Sequence Reports.
Summary Run	Run to be included in a sequence summary. See About Sequence Reports.
End Summary	Last run to be included in a sequence summary. See About Sequence Reports.
Vial Summary	Create a vial summary report.
QC Check Std	Check standard sample. A check standard inserted in a sequence is used for generation of a Check Standard Report. It is a means for checking the chromatograph and conditions without calibrating.
Unspiked	Unspiked sample of a Spiked/Unspiked pair, used for Spike Report.
Spiked	Spiked sample used in single level spike analyses (unknown smp. & spiked smp.)
Spike 1 of 2	First spiked sample used for Spike Reports.
Spike 2 of 2	Duplicate sample used for Duplicate Reports.
Duplicate	Duplicate sample used for Duplicate Reports.
Begin Calibration	First calibration mixture to be used in Calibration Summary Report. When this run type is encountered, the data system stores the current retention times of all named peaks. These are displayed in the reports as the Old RT. After the End Calib sample is run, the updated retention times are stored and displayed as New RT in the Calibration Report. In addition, the average response factor for each peak is calculated, the % RSD is calculated, and compared to the expected % RSD from the peak table. Compounds falling above this % trigger the failure action.
End Calibration	Last calibration mixture to be used in Calibration Summary Report.
Baseline Check	Enable baseline check.
Baseline File	Designates this run as a baseline subtraction file. Select the channels to be subtracted from subsequent files in the sequence.

Set up a QC check standard

To designate a sample as a QC Check Standard:

1 In the sequence spreadsheet, click **Run Type** for the QC Check Standard sample.

2 In the **Run Type** dialog box, click **QC Check Standard.**

3 Enter the **Check Standard Number** and then select the **QC Check Standard.rep** template to be used for the report.

To automatically designate multiple runs in a sequence as QC Check Standard run types:

1 In the sequence spreadsheet, click and drag the mouse on the **Run #** of the rows to highlight.

2 Do a right mouse click in the highlighted rows, and then click **Set Run Types** followed by **QC Check Standard.**

3 Enter the number of runs between check standard runs. (For example, if you enter **2**, the first line will be set to QC Check Standard, followed by two runs that are not set to QC Check Standard, then the 4th run will be set to QC Check Standard, and so on to the end of the highlighted rows.) Click **OK**. The runs types will be set to QC Check Standard.

Concentration override

The **Concentration Override** allows you to modify a concentration for a calibration component that is different from the concentration in the method. This can be done from the **Sequence Spreadsheet**.

To enter a concentration override:

1 In the sequence spreadsheet, click **Concentration Override** for the run you wish to change a concentration.

2 Select the **Channel** you wish to edit.

3 Locate the peak for which you want to enter a new concentration, and click **NewConc**. Type the concentration you wish to use for this peak for the designated run. You can update the concentrations for as many of the component peaks as you wish.

4 Click **OK** to finish.

Note: The concentration override field is only available for runs designated as calibration runs.

Set an action for a sequence run

A sequence action enables you to program an action to occur based on a specified result of a sequence run. The action is designated in the sequence spreadsheet for the run of interest.

To designate an action for a sequence run:

1 In the **Instrument** window, click the **Edit Sequence** button 

to open the sequence spreadsheet.

2 Scroll the sequence to the right until the **Action** column is visible. (If the column is not visible, see Customizing the Sequence Spreadsheet Columns.)

3 Click **Action** for the desired run.

4 In the **Action** dialog box, select a **Test** whose result will trigger the post run action selected. Available conditions include:

- Any Condition
- Calibration
- QC
- System Suitability
- Hardware Status
- Conc. Limit
- Baseline Check

5 Click **Result** to select a result for the test that will trigger the action. Results can include:

- Pass
- Fail
- Recoverable
- Above limit
- Below limit

6 Click **Action** and select the action that will occur when the selected result occurs.

- Abort
- Pause
- Alarm
- Run Shutdown
- Continue
- Re-inject
- Run User Program
- Goto
- Restart System Suitability

7 If required, enter a **Parameter** for the action. (If no parameter is required, this field will not be available.)

8 In the **Rules and Alerts** table, you may set actions for the listed errors of each of your configured modules. Click **Action** and select the desired action for each module error.

9 When finished, click **OK**.

Note: Action items that are user-interactive (e.g. pause and alarm) will not trigger user input on client machines when using client/server operation. This is because the server is controlling the instrument.

The following Actions require no Action Parameters

Action	Effect
Abort	Abort the sequence.
Pause	Pause the sequence after the current run and wait for user to review and resume sequence.
Alarm	Trigger alarm.
Run Shutdown	On result, the sequence will search for and execute the next run with a shutdown run type. If no shutdown run type is found, it will search from the beginning of the sequence.
Continue	On result, continue sequence.

The following Actions require you to select Action Parameters

Action	Effect
Re-inject	Specify the number of times you wish to attempt re-injection of the sample if the injection fails.
Run User Program	Specify the UNC path for the program to be run. To ensure you have the correct path and file name, click the file button and browse to the location to select the file.
Goto	Specify a line in the sequence to **GO TO**, and enter a **Repeat count** for the number of retries before going to the new line.
Restart System Suitability	Specify the number of times you wish to attempt restarting system suitability.

About 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, where you acquire data for a single injection.

Sequence run, where you acquire data automatically for a series of runs using a preprogrammed 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.

See Also

Single Run Acquisition

Sequence Run Acquisition

- About Overlapped Sample Prep Mode
- Bracketed Calibrations
- Schedule Run

Reprocess a Sequence

Single run acquisition

There are two ways you can 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, you need to specify the method to be used for analysis, and a file name 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:

1. In the toolbar select the **Single Run** button  , or in the menu select **Control > Single Run**.
2. In the **Single Run** dialog box, complete the fields listed in the table below.
3. When you have completed the **Single Run** dialog box, click **Start** to begin the acquisition.
4. The current data will appear in the Chromatogram Window as it is acquired and stored on disk. At the end of the run, the chromatogram will be analyzed according to the method parameters, and a report generated if specified. If the sample is not analyzed at the end of the acquisition, click the **Analyze** button if you wish to view the results.

Run Information	This section allows you to specify 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. You can also click the arrow and select from a number of pre-defined ID's. You cannot use the date/time parameter (<D>) by itself as the Sample ID. • **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 your default method directory. You can select

the method from a list of methods available on your disk by clicking the **File** button adjacent to the field.

- **Data File** - Enter a file name to be used to save the data on disk. You can select from one of the pre-defined name types by clicking the arrow button adjacent to the field. It is not possible to use an existing file name, unless the file exists in located in a directory whose path contains the term public. For example, if you 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.
- **Result Path** - Enter a path name where the data acquired for this run will be stored. Click the File button to select a path from a list of those on your disk.
- **Result Name** - Enter a name for the result file. If you did not select **Result Package Mode** when creating an EZChrom project in the Control Panel, you will still need to enter a **Result Name**. The result name is used for the RST file, and ACAML file names. If you selected **Result Package Mode** when creating an EZChrom project in the Control Panel, the **Result Name** will also be used for the folder name. In ECM it will be the name of the SSIZip.

Number of runs

Enter the number of runs you wish to make. The runs will automatically proceed without review until completed, incrementing each file name as designated. If the sequence of single runs is aborted, and the user then repeats the single acquisition without changing any parameter, the run number will start with the next number as if the sequence not been aborted. For example, setting 4 runs with starting run number of 101, then abort during run 102. When restarting, the next run number will be 105. If the Sample ID is also incremented, it will increment in parallel.

Reports

- **Save as PDF** - When this box is checked, a report will be saved as a PDF at the end of the run.
- **Print Hardcopy** - When this box is checked, a report will be printed at the end of the run. If there is a loss of communication to the hard copy printer from the OpenLab EZChrom Print Server, files are copied from the monitor folder into the Quarantine folder. After communication to the hard copy printer has been established, files in the Quarantine folder can be copied back into the monitor folder for normal printing. Files in the Quarantine folder are automatically deleted in 24 hours by default. The time to delete folders from the Quarantine folder is set in the configuration file in the Print Server folder.
- **Select Printer** - If **Print Hardcopy** is checked, select a printer from the drop down menu.

Amount Values

In this section, you can enter values that affect how the concentrations are calculated. If you are making a single data acquisition prior to calibrating your method, simply leave these values at the default level.

- **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 weighing and when percentages of the total sample are being calculated rather than the amount detected in an injection.

- **ISTD** - For calibration runs, the Internal Standard Amount is taken from the method Peak Table. For unknown runs, enter the amount of the Internal Standard in your unknown sample.
- **Multipliers** - Enter one to five multiplication factors to be used for this run. All quantitated peaks will be multiplied by these factors.
- **Dilutors** - Enter one to five dilution factors to be used for this run. All quantitated peaks will be divided by these factors.

Calibrate

Select this box if the sample is to be a calibration sample. Once this box is clicked, the following fields and options will be available.

- **Calibration Level** - Enter the number of the calibration level represented by this calibration standard. If this is a single level calibration, enter 1.
- **Clear all calibration** - Click this box if you want to clear all existing calibration factors from your method before running the sample.
- **Clear calibration for level** - Click this box if you want to clear the existing response factors for this level only before running the sample.
- **Print calibration report** - Click this box if you want to print a calibration report after running the sample.
- **Clear replicates** - Click this box if you want to clear all existing replicates from the existing calibration level before running the sample.
- **Average replicates** - Click this box if you want to average the replicates for this calibration level. See **Calibration Averaging as Part of a Single Run or Sequence**.

Baseline Check

This box will appear if you have the **Baseline Check** option implemented in the instrument configuration. When this box is checked, it will trigger a baseline check prior to the start of the run.

Begin run

By default, the run will start immediately. To designate when you want the run to start, select the **Schedule Run**  button. In the **Schedule Run** dialog box, select from the following options:

- **Now** - immediately
- **After** - after a designated amount of time
- **On** - at a specific date and time

Description...

Click this button to enter a sample description for this run. This description is saved with the data file that will be collected. The user can view the description in the open dialog and in data properties when the run is complete.

Startup/Shutdown

For instruments that support it, boxes for Startup and Shutdown will appear in the dialog. These boxes enable you to designate the run as either a Startup or Shutdown sample. When one of these boxes is checked, it will trigger the Startup or Shutdown routine on your instrument. For details, see the control documentation for your instrument.

Autosampler

If the configured autosampler has the ability to use injection volume specified by the method, this section will appear.

- **Use program** - Click the checkbox if you want to use a sample prep program for your autosampler. After you click the checkbox,

click the folder button to browse to and select the sample prep file you wish to use.

- **Vial** - Enter the autosampler vial number to use for the injection.
- **Frac. Start** – Enter the fraction collector vial number to use for the injection.
- **Injection volume** - Enter the injection volume for this run. For autosamplers that support it, the Use method option will appear. When selected, this option will use the default injection volume specified in the Instrument Setup for the instrument.

Sequence run acquisition

Once you have created and saved a sequence, you can use it to acquire and process data.

To start a sequence acquisition:

1. From the **Instrument** window, click the **Sequence Run** button  , or from the **Control** menu, click **Sequence Run...**.
2. In the **Sequence Run** dialog box, complete the fields listed in the table below.
3. Click **Start** to initiate the sequence acquisition. You may see the data displayed in real time in the Chromatogram Window(s), if the current data is selected for viewing.

Sequence Information	This section allows you to specify files for the run. • **Sequence name** - Enter the sequence name to be used, or select the sequence file from a list of available sequence files by clicking the **File** button. The filename cannot be more than 70 characters long. • **Result path** - Enter a path name where the data acquired for this run will be stored. Click the **File** button to select a path from a list of those on your disk. • **Result Name** - Enter a name for the result file. If you did not select **Result Package Mode** when creating an EZChrom project in the Control Panel, you will still need to enter a **Result Name**. The result name is used for the RST file, and ACAML file names. If you selected **Result Package Mode** when creating an EZChrom project in the Control Panel, the **Result Name** will also be used for the folder name. In ECM it will be the name of the SSIZip.
Run Range	Select the range of the sequence to be run. • **All** - Click this to execute all runs in the sequence. • **Selection** - If you have currently selected a series of runs in your sequence spreadsheet by highlighting them, click this 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-** designates the 4th run through the end of the sequence.
Mode	Select the manner by which you want to handle autosampler dual towers (if any), processing mode, and bracketed calibration (if used.)

- **Tower** - If your instrument is configured for Dual Tower, you can 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 here will vary depending on the instrument configured. If the instrument does not support this feature, this option will be grayed out. For certain autosamplers, **Overlapped Sample Prep** mode will be available. See About Overlapped Sample Prep for information and restrictions for using this mode.
- **Bracketing** - Select the type of bracketing you wish to perform. (See Bracketed Calibrations for details.)
  - **None** Select this if you do not wish to bracket calibrations.
  - **Standard** Select this if you wish to perform the standard mode of bracketing calibrations.
  - **Sequence** Select this if you want to perform the sequence mode of bracketing calibrations.
  - **Seq. w/ Back Calc** Select this if you want to perform the sequence mode of bracketing calibrations and back-calculate calibration runs.

Reports

- **Save as PDF** - When this box is checked, a report will be saved as a PDF at the end of the run. Select either a **Method** or **Sequence** report.
- **Print Hardcopy** - When this box is checked, a report will be printed at the end of the run. Select either a **Method** or **Sequence** report. If there is a loss of communication to the hard copy printer from the OpenLab EZChrom Print Server, files are copied from the monitor folder into the Quarantine folder. After communication to the hard copy printer has been established, files in the Quarantine folder can be copied back into the monitor folder for normal printing. Files in the Quarantine folder are automatically deleted in 24 hours by default. The time to delete folders from the Quarantine folder is set in the configuration file in the Print Server folder.
- **Select Printer** - If **Print Hardcopy** is checked, select a printer from the drop down menu.

Review

- **Results Review** - Click this box if you want the sequence to pause between runs for you to review results.
- **Calibration Review** - Click this box if you want the sequence to pause after each calibration set, where a calibration set is defined as one or more calibration runs that occur in a sequence.

Begin run

By default, the run will start immediately. To designate when you want the run to start, select the **Schedule Run**  button. In the **Schedule Run** dialog box, select from the following options:

- **Now** - immediately
- **After** - after a designated amount of time
- **On** - at a specific date and time
- **Perform Run Every** – repeat the run at specific minute intervals

Email Recipient(s)	Use this field to enable email notification to be sent to a designated address (entered in the **To**: field). Select the **On start** box to send email notification when the sequence starts. Select the **On stop or error** box to send email notification when the sequence stops or if an error occurs.

About overlapped sample prep mode

When the **Overlapped Sample Prep** option is selected in the Sequence Run dialog box, when running a sequence the software will send the entire sequence to the hardware at once, instead of line-by-line. This option allows the autosampler to optimize throughput by performing overlapping pretreatment of samples.

When using Overlapped Sample Prep mode:

- Do not use Run Types Begin Loop or End Loop
- Do not specify Failure Action other than Alarm, Continue or Send E-Mail
- Do not edit the sequence after it has started.

For certain autosamplers that support it, as each line of the sequence is submitted to the instrument, the vial number and pretreatment program for the next sequence line will also be passed on for implementation of the sample overlap. Sample overlap will:

- Pre-fetch the next sample vial while a line of the sequence is being analyzed
- Pre-wash the syringe and load the sample

For these autosamplers, no sequence table options are prohibited. In the event that a change in processing order results from a priority run, sequence abort or Smart Sequence action, the pre-fetched sample will not be analyzed, but will instead be wasted.

Note: Overlapped Sample Prep mode is only available for autosamplers that support it. See the documentation provided with your autosampler to determine how sample overlap is handled.

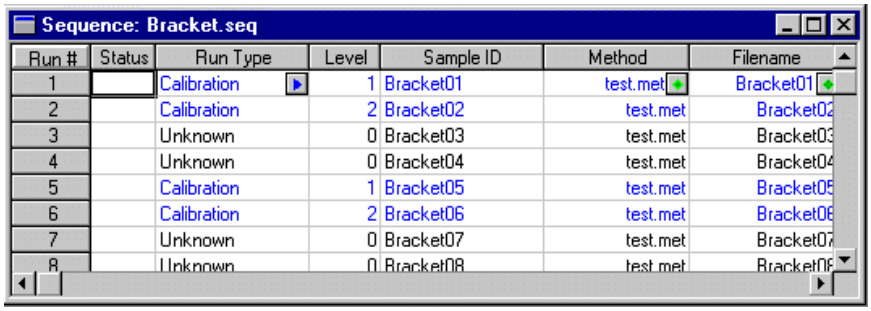
Bracketed calibrations

In the Sequence Run dialog box, the **Bracketing** option allows you to process data using calibration replicates that are run in brackets around your samples in the sequence. This enables you to process all your data files using consistent response factors. When you choose a bracketing option, calculation of results will be handled such that the calibration standards will be processed before calculation of the unknown results, regardless of the fact that the calibration standards are bracketed around the unknown samples. Bracketing can also be performed as part of sequence reprocessing.

- **Standard Bracketing** - If you choose this method of bracketing calibration, each group of unknowns will be calculated based on the response factors determined by the calibration standards directly before and after the unknown group in the sequence.
- **Sequence Bracketing** - If you choose this option for bracketing, the results for unknown samples will be calculated based on the response factors generated by the entire sequence of calibration standards, regardless of their position in the sequence. Calibration takes place after all samples and standards have been run.
- **Sequence Bracketing with Back-Calculation** - This method of bracketing uses the sequence bracketing method, then back-calculates and reports amounts for the calibration runs by using the final calibration curves.

Using the following sequence as an example, using the **Standard** method of bracketing, unknown samples number 3 and 4 will be calculated using response factors generated after calibration runs 1, 2, 5, and 6 are completed. Unknown sample runs 7 and 8 will be calculated using response factors generated after running calibration sample runs 5, 6, 9 and 10.

For the same example, using the **Sequence** method of bracketing, all unknown samples will be calculated using response factors generated after all calibration standards are completed (1,2,5,6,9, and 10).



Schedule run

This dialog box appears when you click the **Begin Run** button in the **Single Run Acquisition** or **Sequence Run** dialog box. It allows you to designate when you want the run to start: immediately (**Now**), after a designated amount of time (**After**), or at a specific date and time (**On**). You can also select to repeat the run at specific minute intervals (**Perform Run Every**).

Reprocess a sequence

After data has been acquired, you can use a sequence to automatically analyze or re-analyze all or some of the files in the sequence. Reprocessing a sequence is a convenient way to reanalyze data if you have changed integration or other method parameters and wish to generate new results for a series of data files. You can also use a sequence to calibrate or recalibrate a multilevel calibration method.

To reprocess a sequence:

1 Open the result set.

2 In the Instrument Window, select **Result Set > Process**  .

3 Complete the following fields:

Sequence Information	**Sequence Name, Result Path**, and **Result name** are automatically populated.
Run Range	Select the range of the sequence to be run. • **All** - Click this to execute all runs in the sequence. • **Selection*** - If you have currently selected a series of runs in your sequence spreadsheet by highlighting them, click this 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-** designates the 4th run through the end of the sequence.

*If using Data Store, selecting this option may cause data files in the result set to be associated with different method versions. To view the method associated with a specific data file, see Open the Method from a Data File.

Mode

Select the manner by which you want to handle autosampler dual towers (if any), processing mode, and bracketed calibration (if used.)

- **Tower** - If your instrument is configured for Dual Tower, you can 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. **Reintegrate** analyzes the raw data using the method designated for each row. **Use Last Results** prints out reports or sequence summaries using the last results saved in the data file. **Use Original Results** prints reports or sequence summaries using the original results stored in the data file. Select **Review Only** to simply review the files.
- **Bracketing** - Select the type of bracketing you wish to perform. (See Bracketed Calibrations for details.)
  - **None** Select this if you do not wish to bracket calibrations.
  - **Standard** Select this if you wish to perform the standard mode of bracketing calibrations.
  - **Sequence** Select this if you want to perform the sequence mode of bracketing calibrations.
  - **Seq. w/ Back Calc** Select this if you want to perform the sequence mode of bracketing calibrations and back-calculate calibration runs.

Report

- **Save as PDF** - Select **Method** or **Sequence**. When this box is checked, a report will be saved as a PDF at the end of the run.
- **Print Hardcopy** - Select **Method** or **Sequence**. When this box is checked, a report will be printed at the end of the run. If there is a **loss** of communication to the hard copy printer from the OpenLab EZChrom Print Server, files are copied from the monitor folder into the Quarantine folder. After communication to the hard copy printer has been established, files in the Quarantine folder can be copied back into the monitor folder for normal printing. Files in the Quarantine folder are automatically deleted in 24 hours by default. The time to delete folders from the Quarantine folder is set in the configuration file in the Print Server folder.
- **Select Printer** - Select a printer from the drop down menu.

Review

Results Review - Click this box if you want the sequence to pause between runs for you to review results.

Calibration Review - Click this box if you want the sequence to pause after each calibration set, where a calibration set is defined as one or more calibration runs that occur in a sequence.

See Also Turn off Processing for Data Acquisition

Open the Method from a Data File

If using Data Store, reprocessing selected runs may cause data files in the result set to be associated with different method versions. When you open a result set, only the latest version of the method is opened and associated with all of the data files in your result set. To associate the correct version of the method with your data file, you must open a method from a data file. Use the following steps to associate the correct version of your method with your data file from a result set that was partially reprocessed.

To open the method from a data file:

1. Click **File > Open > Data**.
2. Select and open the data file.
3. Click **Data > Open Method From Data...**
4. Select **From Results**.
5. Browse for and select the result from which you want to view the method.
6. Click **OK**.

About the run queue

The run queue is used to manage and schedule single runs and sequence runs. Once a sequence or single run is initiated, it is entered into the run queue automatically.

To view the current run queue, select the **View Run Queue** button . Each row in the run queue represents a sample or sequence that is in process or waiting. Both acquisition and reprocessing samples and sequences for this instrument will be displayed.

From the run queue, you can view details about each run or sequence in the queue, including the following:

- **Type** - single run or sequence
- **Name** - name of resulting data file
- **State** - Pending, Running, Completed
- **Status** - Completed Success, Aborted, Failed, Every X minutes.
- **User**
- **Vial**
- **Volume**
- **Description.**

If you are running a sequence, the **Status** shown in the sequence spreadsheet displays the status of an individual run in the sequence.

When there are items in the run queue, buttons at the top of the window will become available:

- **Start** will start the run queue again after the **Pause** button has been pressed. This button is disabled when a sample is running or if the run queue is empty.
- **Pause** will pause the run queue as soon as one run is completed and wait for your action. You do not have to wait for the entire sequence to be completed.
- **Abort** will immediately terminate the item currently running in the queue and pause the sequence.
- You can perform additional functions for the run queue by doing a right mouse click in the run queue window.

Submit a Run to the Queue

The **Submit** button appears when data is currently being acquired using a sequence or single run and you open either the single runs or sequence runs dialog box.

Select the **Submit** button to submit a single acquisition to be run at the completion of the current run. The run is entered at the end of the Run Queue if you are currently running a sequence of runs.

Add a run to the queue

To add a run to the queue:

1. In the toolbar, select the **View Run Queue** button  .
2. In the **Run Queue** dialog box, in the **Method** drop down box select the method to be used for the run. Methods displayed are from the current project.
3. In the **Sample ID** box, type a unique sample ID to be used for the sample. You can enter any valid Sample ID parameters supported by Sample ID in the Single Run dialog. You cannot use the date/time parameter (<D>) by itself as the Sample ID. This field will be incremented each time the **Submit** button is pressed.
4. To specify additional information for the run, select **Advanced** to open the **Single Run** dialog.
5. Click **Submit** to submit a single run to the run queue.

Add a run to the result

You may add multiple or single runs to an existing container.

To add a multiple runs to an existing container:

1. From the menu select **Control > Add Runs to Result.**
2. In the **Add Runs to Result** dialog box, the fields are populated with the open method. Make sure all fields are completed.
3. Select **Start**.

To add a single run to result:

1 From the menu select **Control > Add Single Run to Result.**

2 In the **Add Single Run to Result** dialog box, the fields are populated with the open method. Ensure all fields are completed.

3 Select **Start**.

View the new runs in the Result Sequence dialog box in result review mode.

User access to runs in progress

The user who submits the run or sequence, will have access to the Stop Run, Extend Run, or Stop Sequence functions.

Other users who did not submit the run or sequence, can view the run (if they have instrument rights), but cannot stop a run or sequence that has been started by another user. Users with **System Administration** or **Instrument Administration** rights have full access to the run and sequence functions.

Once you have submitted a run or sequence to an Acquisition Controller from a client workstation, you can modify the method. You must save the file (File > Save Method**)** in order for the changes to be used for subsequent sequence runs that use this method. If more than one client changes and saves the method, the last client's changes are saved and all others are lost. If the method is not saved before the start of the next sequence run using this method, the changes on a client will be lost when the next sequence run starts.

The user who submitted a sequence to the acquisition controller may add or remove runs from the submitted sequence from a client workstation (if the user has appropriate privilege assignment). In order for sequence changes to take effect, the sequence must be saved (File > Save > Sequence**)**. When the sequence is saved, all other clients will be notified of the change, and the next run of the sequence will be executed from the modified sequence.

Stop a run in progress

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. If you want to produce a report or view results from a run that was stopped, you must analyze the data file.

If you are not the user that submitted the run or sequence or are using an instrument offline, you do not have access to the Stop command.

Note: When using the **STOP** button, make sure to hold the mouse button down until the **STOP** button icon changes to the depressed appearance before releasing.

To stop data acquisition during a run:

1 Select **Control > Stop Run**.

2 Select how you want to stop the run:

- **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** - This selection stops the run currently in progress, and terminates the sequence it is a part of. Other queued items will proceed.
- **Stop sequence after current run completes** - This selection will abort the sequence after the current run in progress is

completed.

- **Stop all run queue items you submitted** - This selection stops the run currently in progress, and terminates all the items in the queue that were submitted by you. Queue items submitted by other users will be unaffected.
- **Stop all run queue items** - This selection stops the run currently in progress, and terminates all items in the run queue.

Extend a run

While a run is in progress, you can extend the data acquisition beyond the designated run time. If you are not the user that submitted the run or sequence or are using an instrument offline, you do not have access to the Stop or Extend Run command.

1. From the menu, click **Control** followed by **Extend Run**.
2. A dialog will appear where you can enter the amount of time by which you wish to extend the run.
3. Enter the number of minutes you wish to extend the run, then click the **OK** button.

Add and delete items in the run queue

The sample run queue is used to keep track of and acquisition and processing. Once a single run or sequence is initiated, it is entered into the run queue automatically.

To add or delete items from the run queue:

1. In the Instrument Window, click the  **Display Run Queue** button, or from the **Control** menu, click **Run Queue...** .
2. In the **Run Queue**, do a right mouse click on the run queue item where you want to make a change.
3. Select the change to be made.
4. When finished, close the **Run Queue**.

Delete	This command will delete the selected item from the run queue.
Delete My Runs	This command will delete only the runs you have submitted.
Delete All	This command deletes all items from the run queue.
Change Begin Time...	To designate when you want the run to start, select the **Schedule Run**  button. In the **Schedule Run** dialog box, select from the following options: • **Now** - Immediately • **After** - After a designated amount of time • **On** - At a specific date and time

Reports	• **Method as PDF** - When this box is checked, a method report will be saved as a PDF at the end of the run. • **Sequence as PDF** - When this box is checked, a sequence report will be saved as a PDF at the end of the run.* • **Method as Hardcopy** - When this box is checked, a method report will be printed at the end of the run. * • **Sequence as Hardcopy** - When this box is checked, a sequence report will be printed at the end of the run. • **Select Printer** - If **Method as Hardcopy** or **Sequence as Hardcopy** is checked, select a printer from the drop down menu. *If there is a loss of communication to the hard copy printer from the OpenLab EZChrom Print Server, files are copied from the monitor folder into the Quarantine folder. After communication to the hard copy printer has been established, files in the Quarantine folder can be copied back into the monitor folder for normal printing. Files in the Quarantine folder are automatically deleted in 24 hours by default. The time to delete folders from the Quarantine folder is set in the configuration file in the Print Server folder.

Note: If you are currently reprocessing a sequence, you must have the results review (pause after each run) option selected in order to submit an additional sequence to the queue. If you are reprocessing a sequence without this option selected, you must stop the sequence, select the Results review (pause after each run) option, then start it again. At this point you can submit one or more sequences to the queue.

Turn off processing for data acquisition

If you wish to acquire and store data on the hard disk, but postpone processing completely until you have reviewed the data, turn off the option to analyze after acquisition before you acquire the data.

To turn off post-acquisition processing:

1. From the menu bar, click **Method** followed by **Properties.**
2. Click **Options**.
3. Click the check box to clear the check mark for **Analyze after acquisition**. If the check box for **Analyze after acquisition** is selected, data files generated with this method will be integrated and results generated automatically after each acquisition. If you **deselect** this option in your method, no analysis will occur as you acquire runs with this method. The data will be saved on the disk, but no results will be generated.

Note: The option to turn off analysis after acquisition is part of the method. If you want to postpone processing of a sequence until after data acquisition is completed, make sure all methods specified in your sequence have this option turned off.

See Also Reprocess a Sequence

Submit a priority run

The **Submit Priority...** button appears when data is currently being acquired using a sequence or single run and you open either the Single Run or Sequence Run dialog. The **Submit Priority...** button allows you to submit a single acquisition to be run at the completion of the current run. The run is entered at the end of the Run Queue if you are currently running a sequence of runs.

Note: If the chromatogram is not integrated at the end of the run, or if you were expecting a report and none was printed, check the Method Properties section of your method to make sure data analysis and reporting are turned on for this method.

Fraction collector configuration

1. Select **Control > Configuration > Fraction Collector**.
2. In the **Fraction Collector Configuration** dialog box, select **Help** or press **F1** in a section for more information.

See Also Configure a fraction collector

About the result sequence

The result sequence is a sequence of runs you have acquired and the data that comes with it.

See Also View Result Review Mode

Open the Result Sequence

Add Signatures to the Result Sequence

Revoke Signatures

Result Set Properties

Save a Result Set

View result review mode

Result Review Mode notifies you that you are in data review.

1. In the toolbar select **View > Preferences**.
2. In the **Preferences dialog** box, under **Toolbar options** select **Result**.
3. Select **Show Toolbar**.
4. Select **OK**.

The yellow **Result Review Mode** appears in the instrument window.

Add signatures to the result sequence

Signatures are applied to a result sequence.

1 Open the Result Sequence.

2 In the toolbar select **Data > Apply Signature**.

3 In the **Apply Electronic Signature** dialog box, select from the following options:

- **Sign current file** - This will add a signature to the current file.
- **Range** - Select the range of the sequence to be run. It can be a set of rows or ranges of rows, for example **1, 3, 5, 7** or **1-3, 7-10**.
- **Sign all files** - This adds signatures to all files in the open result file.

4 Enter a **Username** and **Password**.

5 Select a **Reason** from the drop down list.

6 Add a **Comment** if necessary.

7 Select **Signoff**. The data is locked to further analysis.

Revoke signatures

Users with appropriate rights can revoke an electronic signature. Once you have revoked the electronic signature the data can be analyzed. When the signature is revoked an entry is made in the audit trail.

1 Open the Result Sequence.

2 In the toolbar select **Data > Revoke Signature**.

3 In the warning dialog box, select **Yes**.

4 In the **Revoke Electronic Signature** dialog box, select from the following options:

- **Revoke current file** - This revokes the signature in the current file.
- **Range** - Select the range of the sequence to be run. It can be a set of rows or ranges of rows, for example **1, 3, 5, 7** or **1-3, 7-10**.
- **Revoke all files** - This revokes signatures to all files in the open result file.

5 Enter a **Username** and **Password**.

6 Type a **Reason**.

7 Select **Signoff**. The data can now be analyzed.

Result set properties

From the menu select **Result Set > Properties** to view result set options, audit trail log, and enable the audit trail.

Result Set Options

1 Open a result (**.rst**) file.

2 From the **Result Set** menu, select **Properties**.

3 In the **Result Set Properties** dialog box, select the **Options** tab:

- **Description** - In the dialog box enter text information about your result file. Because the description can be viewed from the **Open File** dialog, the description can be useful in sorting through the files on your disk.
- **Export Summary** - Select this box to export the summary. Then select the location where the files will be saved:
- **Path** - Enter a summary export path
- **Method** - Enter a method path

View the result set audit trail log

1 Open a result (**.rst**) file.

2 From the **Result Set** menu, select **Properties**.

3 In the **Result Set Properties** dialog box, select **Audit Trail Log**.

4 Enter the following:

- **User**
- **Location**
- **Description**
- **Reason**
- **From date/time**
- **To date/time**

5 Select from the following options:

- **Export** - Select this to export the audit trail log
- **Print** - Select this to print the audit trail log
- **Search** - Select this to search the audit trail log

Enable the result set audit trail

1 Open a result (**.rst**) file.

2 From the **Result Set** menu, select **Properties**.

3 In the **Result Set Properties** dialog box, select **Audit Trail.**

4 Select **Enable audit trail**. Once the Enable Audit Trail box is selected, it cannot be de-selected.

5 In the warning dialog box, select **Yes.** The Enable Audit Trail will be permanently checked.

6 Select from the following options:

- **Prompt for reason at every change** - This option requires the user to enter a reason for every subsequent change to the method at the time the change is made.
- **Prompt for reason when saving Sequence** - This option requires the user to enter a reason for each change when the Sequence is saved.
- **Do not prompt for reason** - When this option is selected, changes are documented, but the user is not required to enter a reason for the changes.

About sequence reports

Reports can be generated that contain results from runs in a sequence. The sequence file does not contain the report, but points to an external template (or templates) that are used to generate the reports as the sequence is run or reprocessed.

Reporting for any given sample in the sequence spreadsheet is designated as part of its Run Type. If the **Summary Run** run type is selected, the sample will be included in the sequence summary report. If the **Print Additional Reports** box is selected, the designated reports will be printed for that sample.

To create a custom report template that contains sequence run information (such as a Sequence Summary report), in the menu select Advanced Report. The Advanced Reports application enables you to create a Sequence Summary template (.tpl file) that can be used to generate a report for a sequence. Because the template is not saved as part of a sequence, it can be used independently for summarizing data from any sequence.

For details on how to create a Sequence Summary template, see About Advanced Reporting.

See Also

Generate a Sequence Summary Report

View Sequence Reports

Print Sequence Reports

Edit a Sequence Report Template

Edit and Print a Sequence Contents Report

Generate a sequence report

To generate a sequence report either during acquisition or reprocessing, the runs to be included in the summary report must be designated as summary runs in the sequence. If you are using the **Sequence Wizard**, these files will be selected during the sequence creation at the **Reports** step in the wizard.

To designate runs to be included in a sequence report:

1. Open the sequence file if it is not already open.
2. To open the sequence spreadsheet, on the menu bar, click **Sequence** followed by **Edit**.
3. In the first row of the sequence to be included in the summary report, click **Run Type**.
4. In the **Sample Run Types** dialog box, click the **Begin Summary** box to select it.
5. Click the **open file** button  to browse for and select the report template to be used to generate the report (the summary.tpl report is provided as a default template).

6 For each row to be included in the summary report, click **Run Type** and select **Summary Run**.

7 For the last row to be included in the summary report, click **Run Type** and select **End Summary**.

8 Save the sequence. All designated Summary runs between and including the Begin Summary run and the End Summary run will be summarized by this report.

9 In the Single Run, Sequence Run, or Sequence Process dialog box, select the **Print hardcopy** box.

10 Run the sequence.

After the sequence has been acquired or reprocessed, the report will be printed on the default printer. You can also view the report from the Instrument Window.

If there is a loss of communication to the hard copy printer from the OpenLab EZChrom Print Server, files are copied from the monitor folder into the Quarantine folder. After communication to the hard copy printer has been established, files in the Quarantine folder can be copied back into the monitor folder for normal printing. Files in the Quarantine folder are automatically deleted in 24 hours by default. The time to delete folders from the Quarantine folder is set in the configuration file in the Print Server folder.

View sequence reports

To view the sequence report:

1 Generate a Sequence Summary Report.

2 From the **Reports** menu, click **View** followed by **Sequence Report**.

3 A list box appears with the sequence reports for the current sequence listed. For each sequence report, the Report Type is listed, along with the sequence rows included in the report, and the report template used to produce the report. To view a report on-screen, click on it with the mouse to highlight it, then click the **View** button.

Sequence reports will only appear in this window if the sequence has been run or analyzed.

In order to display a Sequence Summary report, you must have defined a sequence summary advance report template, and set the Run Type to include Summary in the Sequence Table for the sequence runs to be included in the report, designating the correct sequence summary template file to be used for generating the report.

Print sequence reports

To automatically print a sequence report:

1 Generate a Sequence Summary Report.

2 In the Single Run, Sequence Run, or Sequence Process dialog box, select the **Print hardcopy** box.

3 Run the sequence.

To manually print a sequence report:

1. Generate a Sequence Summary Report.
2. From the menu bar, select **Reports > Print > Sequence Report**.
3. In the **Print Sequence Reports** dialog box, select a sequence report. The report type, the sequence rows, and the report template are shown.
4. Select **Print**.

Sequence reports will only appear in this window if the sequence has been run or analyzed.

In order to display a Sequence report, you must have defined a sequence summary advance report template, and set the Run Type to include Summary in the Sequence Table for the sequence runs to be included in the report, designating the correct sequence summary template file to be used for generating the report.

If there is a loss of communication to the hard copy printer from the OpenLab EZChrom Print Server, files are copied from the monitor folder into the Quarantine folder. After communication to the hard copy printer has been established, files in the Quarantine folder can be copied back into the monitor folder for normal printing. Files in the Quarantine folder are automatically deleted in 24 hours by default. The time to delete folders from the Quarantine folder is set in the configuration file in the Print Server folder.

Edit a sequence report template

You can modify an existing Sequence Summary Report template using the Advanced Reports feature.

To open an existing template file for editing:

1. Select **File > Open > Advanced Report**.
2. Browse to and highlight the **Summary.tpl** template file (or the summary template you wish to modify), then click **Open**.
3. Modify the report template using the Advanced Reports editor and then save the template file by clicking **File > Save > Advanced Report.**

Edit and print a sequence contents report

The Sequence Contents Report uses the **SequenceContentsReport.rep** template file, which is located in the *Template* folder of the current project.

To edit the template for the current sequence:

1. From the **Instrument** window, select **File > Open > Standard Report** and then navigate to the Template folder of the current Project.
2. Select the **SequenceContentsReport.rep** and click **Open**.
3. In the **Standard Report** window, right click on the Sequence Print report table to customize the contents of the table. See

Using the Report Editor.

4 Select **File > Save As > Standard Report.** Navigate to the template folder and save the template as SequenceContentsReport.rep (overwriting the existing template).

To print the current sequence:

1. From the Instrument Window, select **File > Print > Sequence**.
2. In the **Print Setup** dialog box, select a printer from the **Name** drop down menu.
3. Select **OK**.

A Sequence Contents Report will be generated on the designated printer.

About Calibration

Before you can get accurate amounts calculated from the areas of unknown peaks, you must have a method that contains a calibration curve from which to calculate the answers. This involves setting up your acquisition method to receive the areas from calibrated standard peaks, then actually running the standards so that the standard areas are entered into your method. **Accurate results cannot be obtained until the method is completely calibrated**. In other words, standards for each level of calibration must be run to complete the calibrated method.

Once the method is set up for calibration, the calibration is not completed until the areas for peaks in the standard samples are entered into the method. Updating the method with these areas is called Calibration or Calibrating the Method. Calibration can be performed by updating the calibration in the method automatically as each standard sample is run, or it can be performed by sequence reprocessing using standard data files which were previously acquired and stored on disk.

For information on how to create a sequence for either running calibration samples, or for reprocessing stored data files, see About Sequences**.**

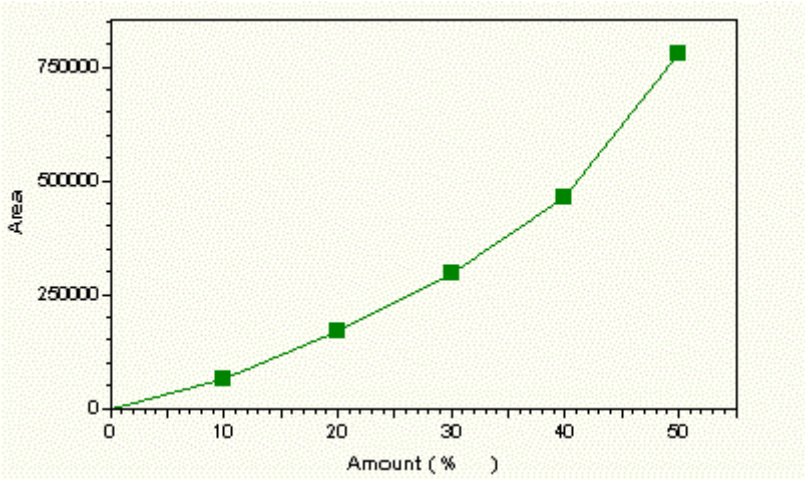
You can also run calibration standards one at a time using the Single Run procedure. To calibrate a single level method using a single calibration standard that has been saved on the disk, follow the procedure outlined in Single Level Calibration Using a Stored Data File.

See Also

Calibration Theory
Steps for Creating a Calibration
Run a Calibration Standard
Define Single Peak
Define Peaks
About the Peak Table
Change the Peak Table Properties
Single Level Calibration Using a Stored Data File
Renumbering Peak ID's
Review Calibration Curves
Concentration Calculator
Calibration Averaging
About Groups and Group Calibration
Insert a Calibration Report
Insert Calibration Information
Adding a Calibration Curve

Calibration theory

Calibration of chromatography instruments is usually necessary to obtain accurate results. The purpose of calibrating an instrument is to verify the response of a detector to a given component. The same detector may give different responses to equal amounts of different components under identical chromatographic conditions. Another reason for calibration involves the linearity of the detector. The rate of detector response to many compounds will decrease with increasing component concentration, therefore requiring calibration of the detector at varying concentration levels of the same component (a multilevel calibration).



Multi-Level Calibration Curve

When all calibration standards have been run, each calibrated component will have its own calibration curve, representing the response of that compound to the detector over the concentration range. When an unknown sample is run, each component concentration is determined from the calibration curve by finding the amount corresponding to the component area (or height). There are two general techniques for calibrating samples: Internal Standard and External Standard.

Internal Standards

With the Internal Standard technique, each sample (both standards and unknowns) is spiked with a known amount of a known compound. When samples are subsequently run, the areas are adjusted using the internal standard. This technique is used to compensate for variations in sample work-up and injection technique.

External Standards

The External Standard technique does not use a spiked standard component. All unknown samples are compared to the standards without correction, and therefore it is important that the injection size is accurate and reproducible.

Single Level and Multiple Level Calibrations

A calibration curve can have as few as one level, or can have multiple levels. A single level calibration curve is created from running just one standard sample. The calibration curve for each peak then becomes a line through the origin and a point representing the area/amount relationship of the peak in the standard.

Running several (two or more) standard samples with different concentration amounts creates a multiple level calibration curve (also called Multi-level). The calibration curve for a given component then becomes a line between the points that represent the area/amount relationships of the compound at each concentration. In some cases, the calibration curve is forced through zero, which causes the line to use the origin as one of the points. This eliminates the possibility of negative concentrations being calculated for low area peaks. Several types of calculations are available for calculation of the actual curve (called fit types). The best-fit type would be the one where the calibration points most closely fit on the line.

For details on calibrations and the equations used to calculate results, see Internal Calculations.

Steps for creating a calibration

Setting up a multilevel calibration for a method involves the following steps:

1. Using your data acquisition method, run one calibration standard, saving it on disk. Make sure your chromatography conditions and integration are correct.
2. Use your stored standard data file to graphically create your calibration peak table using the Define Single Peak or Define Peaks command.
3. All the calibration parameters for each calibrated compound are entered in the Calibration Peak Table. The peak information is filled out graphically, then specific information for each peak is entered manually. If you are doing multiple channel calibration, be sure to set your calibration parameters for **each** channel. Complete your peak table by typing the peak names and concentration amounts, reference peak, internal standard numbers, and other necessary parameters for your samples.
4. Save your method.
5. Calibrate your method. The method can be calibrated using previously acquired standard data files or automatically as you run your standard(s). A calibration can be performed in the following ways:

   Single Level Calibration

   - Calibrate using areas from a stored standard file.
   - Calibrate by running the standard sample.
   - Calibrate by running the standard sample as part of a sequence of runs.

   Multiple Level Calibration

   - Calibrate using stored standard files (one level at a time, or sequence reprocess).
   - Calibrate bracketed calibration using stored standard files (sequence reprocess using bracketed calibration).
   - Calibrate by running calibration standards as part of an acquisition sequence.

Note: Concentration results for an unknown run cannot be calculated until you have a complete calibration curve saved in your method.

Run a calibration standard

Before you can run a calibration standard, the method must contain the names of all the peaks you want to quantitate, their expected retention times for identification, and the amounts you will be injecting in the standard sample(s). These values are entered in a spreadsheet-like table called a Peak Table.

How to define named peaks graphically:

The most efficient and accurate way to enter this data into your method is to inject your first standard sample and save the data file on disk, then use the stored chromatogram to graphically enter most of the data you need.

Note: The following steps assume the acquisition sampling rate and integration portion of the method have been optimized for the samples to be acquired.

To acquire your first standard sample, follow the acquisition step below. If you have already acquired a calibration standard and it is saved on your disk, proceed to **Step 3**.

1 Select the **Control > Single Run** command from the menu, or click the **Single Run** button from the command ribbon. A dialog box will appear. Fill in the information listed below. At this point, leave the Amount Values at the default values.

Sample ID	Enter a Sample ID for the run. This can contain text and numbers, and is saved with the data file. You cannot use the date/time parameter (<D>) by itself as the Sample ID.
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 your default method directory. You can select the method from a list of methods available on your disk by clicking the File Folder button adjacent to the field.
Data file	Enter a file name to be used to save the data on disk. It is not possible to over-write an existing data file. To use an existing data file name, you should use the Windows utilities to rename the existing file, or move it to another location first.
Result path	Enter a path location where the data/result file will be stored. If you wish, you can select a path by clicking the File button.
Result name	Enter a name for the result file. If you did not select **Result Package Mode** when creating an EZChrom project in the Control Panel, you will still need to enter a **Result Name**. The result name is used for the RST file, and ACAML file names. If you selected **Result Package Mode** when creating an EZChrom project in the Control Panel, the **Result Name** will also be used for the folder name. In ECM it will be the name of the SSIZip.
Calibrate	Do not select this box at this point, as you have not prepared your method for calibration yet!

2 When ready, click **Start** to begin the acquisition of your sample.

3 When the run is completed, the chromatogram with baselines drawn should be shown on the screen. (If you are starting with an already-acquired data file, make sure the file is open and has been Analyzed.)

4 If the baselines are not displayed, click the **Analyze** button to make sure the chromatogram has been analyzed. If the baseline still does not appear, click the right mouse button within the Chromatogram Window, and select **Appearance...** Make sure the

baseline is displayed in a color that is visible on the screen. See Change the Chromatogram Appearance. You are now ready to define your calibrated peaks.

5 There are two ways to define calibration peaks. Using Define Peaks you add all of the peaks of interest to the peak table, then enter names and complete level information in the peak table. Using Define Single Peaks, you name and define each peak as you add it to the peak table.

Define single peak

The **Define Single Peak** button allows you to create a row in the calibration peak table for a single peak. You can then edit the peak in the Peak Table.

To add a single peak to the peak table:

1 Open the data file to display the chromatogram.

2 Right-click in the chromatogram and select **Graphical Programming > Define Single Peak**, or in the integration toolbar select the **Define Single Peak** button  .

3 Select the peaks you want to define.

4 In the **Define Single Peak** dialog box, the retention time of the first detected peak will appear. If you do not wish to add this peak to the peak table, click the **Next** button. If you want to move to a specific peak in the chromatogram, click on that peak with your mouse. The retention time shown in the dialog will change to reflect the selected peak. Complete the following fields:

Peak Name	Enter the name of the compound in this field.
Conc Level	Concentration Level 1 is shown. Enter the amount of this compound for this concentration level. If you are running more than one level for this compound, enter Concentration Level 2 and the amount for that level. Continue to enter level concentrations until you have completed the number of calibration levels desired. You can also enter or edit concentration level amounts from the method Peak Table.
Units	Enter the units to be used for display of results.
ISTD ID #	If you are doing 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 you don't know it, you can add it in the peak table later.
Ref ID #	Enter a retention time reference peak ID # to be used for this peak. This is the peak ID number from the peak table. If you don't know it, you can add it in the peak table later. Reference peaks are used to calculate Relative Retention Times.
Retention Time Window	The Retention Time Window values sets a window around the expected retention time of calibrated peaks. A retention time window is important because it allows a peak to drift slightly (within the window) and still be identified as a calibrated peak. If no retention time window is set, a calibrated peak must

ALWAYS occur at exactly the expected retention time in order to be identified as the calibrated component. You can select a **Relative** Retention Time Window or an **Absolute** Retention Time Window.

Relative — Relative retention time window is based on a % of the expected retention time of the component. By default, the Relative Retention Time Window is set to 2.5%, which means that the Retention Time Window for calibrated peaks will be set to 2.5% of their expected retention time. Setting a Relative Retention Time Window means that peaks eluting later in the chromatogram will have larger retention time windows than peaks eluting earlier in the chromatogram. Use a relative retention time window if your peaks tend to drift later in the run.

Absolute — Absolute retention time window sets up a retention time window that is the same for all calibrated peaks. You enter a value for the retention time window to be used for the peaks. An absolute retention time window does not vary with the retention time of the calibrated peak.

5 Click **Next** to move to the next detected peak. Click **Back** to move to the previous detected peak in the chromatogram. To move directly to a specific peak, click on that peak in the chromatogram. The current peak and total peaks in the chromatogram is displayed on the right of the dialog box.

6 When you are finished adding peaks to your peak table, click **Done.**

7 Complete the peak table for each calibrated compound, as described in About the Peak Table.

Define peaks

The **Define Peaks** button allows you to create a row in the calibration peak table for each detected peak in a selected range. You can then edit each peak in the Peak Table.

To add peaks to the peak table:

1 Open the data file to display the chromatogram.

2 Right-click in the chromatogram and select **Graphical Programming > Define Peaks**, or in the integration toolbar select the **Define Peaks** button  .

3 Select the peaks you want to define.

4 In the **Define Peaks** dialog box, enter the peaks for your calibration by clicking the mouse once to the left of the first calibration peak in the chromatogram, then once to the right of the last calibration peak in the chromatogram. A dialog box will appear where you set up some of the parameters for the peaks that will be added to the peak table. Complete the following fields:

Define peaks in range — All peaks detected within the range between the **Start Time** and **Stop Time** shown will be added to your peak table. This

	range was defined by your mouse clicks on the chromatogram. You may change these times manually in the boxes shown if you desire.
Retention time window	The Retention Time Window values sets a window around the expected retention time of calibrated peaks. A retention time window is important because it allows a peak to drift slightly (within the window) and still be identified as a calibrated peak. If no retention time window is set, a calibrated peak must ALWAYS occur at exactly the expected retention time in order to be identified as the calibrated component. You can select a **Relative** Retention Time Window or an **Absolute** Retention Time Window. **Relative** retention time window is based on a % of the expected retention time of the component. By default, the Relative Retention Time Window is set to 2.5%, which means that the Retention Time Window for calibrated peaks will be set to 2.5% of their expected retention time. Setting a Relative Retention Time Window means that peaks eluting later in the chromatogram will have larger retention time windows than peaks eluting earlier in the chromatogram. Use a relative retention time window if your peaks tend to drift later in the run. **Absolute** retention time window sets up a retention time window that is the same for all calibrated peaks. You enter a value for the retention time window to be used for the peaks. An absolute retention time window does not vary with the retention time of the calibrated peak.
Units	Enter the units to be used for labeling the concentration results using the calibrated peaks.
Quantitate Peaks On	Select **Area** or **Height** for the basis of calculation of response factors. **Note**: if you are doing both Peak and Group quantitation using internal standards, both Peaks and Groups must use the same quantitation measurement type (area or height).
Minimum Peak Area	If you enter a minimum peak area, any peaks found within the defined peak range whose areas fall below this limit will not be considered calibration peaks, and will not be entered in the calibration Peak Table.
Add all peaks to table	Select this button to add the peaks in the current defined peak range to existing peaks in your calibration table.
Replace existing peaks in table	Select this button if you want to replace all existing peaks in the current calibration peak table with the peaks from the defined peak range.

5 Click **OK** to accept your selections.

6 A spreadsheet view of the **Peak Table** will appear with the retention time of each peak in the selected peak range displayed. Complete the peak table for each calibrated compound, as described in About the Peak Table.

About the peak table

All of the information required to calculate concentrations for unknown peaks using a calibration is contained in the Peak Table. Each row of the peak table represents one of the calibrated components. Once you have graphically entered the peaks into the peak table (see Create Calibrations Graphically), you must complete the peak table with information required to correctly identify and calculate unknown concentrations for each peak. You may not need to use all the columns of the spreadsheet. Enter information only for columns that will be required for calculation of amounts for each peak of interest.

Note: Once you have become familiar with the parameter columns in the Peak Table, you can customize the appearance of the table to only display the columns of interest to you by doing a right mouse click in the table and selecting **Properties**. See Change the Peak Table Properties.

To open the Peak/Group tables:

1 There are three ways to open the Peak/Group tables:
   - In the navigation pane select **Method > Peaks/Groups.**
   - In the menu select **Method > Peaks/Groups.**
   - In the toolbar select the **Peaks/Groups** button  .

2 In the **Peak/Group Tables** dialog box, select the **Named Peak** tab.

3 The following columns in the Peak Table are used for calculating results for calibrated peaks.

#	Row number
Name	Type the name of the component that matches the retention time displayed.
ID	Peak identification number. The data system will automatically assign a peak ID# for each peak, starting with 1. This ID# is used to designate reference peak and internal standard peak number. If you are adding peaks to an existing peak table, you can renumber the new peak table automatically by doing a right mouse click in the peak table, followed by **Renumber Peak ID#**. **Note**: If you renumber the Peak ID#, make sure any custom parameter programs or other user programs that may use Peak ID# are updated to reflect the new Peak ID#'s.
Ret. Time	The calibrated peak's expected retention time. If you have used graphical events to enter the peaks into the peak table, Retention Times are automatically filled in using the retention times of the detected peaks in the standard file used to create the table.

Window	Retention time window for calibrated components, used for identification of calibrated peaks. The width of the window is indicated and is centered on the retention time value. If a peak's retention time (adjusted for reference peak shift) falls outside this window, it is not considered to be the calibrated peak. If more than one peak falls within the window, the peak closest to the center of the window is identified as the calibrated component. You can change the size of the window by entering a new value.
Resolution ID #	Enter a peak ID# to be used for calculation of resolution, if desired. If this is left blank, resolution will be calculated for the peak of interest based on the detected peak preceding it. If the peak entered here is not detected, or if a peak refers to itself for the Resolution ID #, the resolution will not be calculated.
Ref. ID#	ID# of the peak to be used as a reference peak for this component. A reference peak is used to adjust the expected retention time of a calibrated component to compensate for changes in the chromatograph such as flow rate. If more than one peak falls within the reference peak window, the largest peak in the window is used as the reference peak. Each peak can have its own reference peak. An ideal reference peak is one that is always present in the sample, and is well resolved from other peaks in the chromatogram. (Internal standards make excellent reference peaks.) If a named peak is assigned a reference peak, then its expected retention time is calculated as follows: Expected RT = (Actual Ref. Peak RT/Expected Ref. Peak RT) * Peak RT.
ISTD.ID#	ID# of the peak to be used as internal standard for this component, if you are using an internal standard method. **Note**: If you are doing an Internal Standard calibration, you must enter an ISTD ID# for each calibrated component. If the peak is an internal standard, enter its own ID# in the ISTD ID# column. If you are doing External Standard calibration, you should enter 0 in the ISTD ID# column for all components. You may designate more than one internal standard.
Units	Enter the concentration units to be used in reporting results, such as mg/ml or vol%.
RT Update	Select how you want to update the expected retention times in your Peak Table. The selection includes None, after every analysis (Run), after calibration runs only (Calib), or after every run and calibration (Run & Calib).
LOD	This parameter is used to calculate and report the ASTM LOD (Limit of Detection) value that is used to determine if the peak is within the Limits of Detection as previously determined for the method. The value entered here is the S/N ratio (signal to noise ratio) to be used for the calculation

for this peak. This calculation is valid only for ESTD or ISTD methods.

LOQ

This parameter is used to calculate and report the ASTM LOQ (Limit of Quantitation) value that is used to determine if the peak is within the Limit of Quantitation as previously determined for the method. The value entered here is the S/N ratio (signal to noise ratio) to be used for the calculation for this peak. This calculation is valid only for ESTD or ISTD methods.

Quantitate

Choose whether the calibration and quantitation are to be based on peak height or peak area. **Note**: if you are doing both Peak and Group quantitation using internal standards, both Peaks and Groups must use the same quantitation measurement type (area or height).

Fit Type

This option determines how the calibration curve will be fit to the data.

Note: You have five choices for how the calibration curves will be drawn: point-to-point, linear, and quadratic, cubic, and Average RF fits. You must have at least two calibration levels for a linear fit (not including zero), three levels for a quadratic and four levels for a cubic fit.

Force Zero

When this box is selected, the calibration curve will be forced through zero.

Calib Flag

The **Replace/WtAverage** selection allows you to determine how the calibration areas/heights for each peak in your method will be affected by running a standard: they will either be replaced, or averaged with the current replicate areas in the calibration method. If Calib Weight is set to a value other than 100, a weighted average of the areas/heights will be calculated. For details on calibration averaging, see About Replicates and Averaging Calibrations.

Each time a calibration average is performed, the value is saved in the method as Last Area, which is subsequently used for calculation of weighted averages.

Calib Weight

You can designate a weight for the average of the replicates. The weighting factor is applied to replicate injections as shown in the following example.

Current run value (area/height) 101

Replicate 1 104

Replicate 2 100

Replicate 3 102

Current Last Area Value = 102

Using a weighting factor of 60, the new method average is:

[((104 + 100 + 102) / 3) * .6] + [101 * .4] = 101.6

Note: For Internal Standard calibrations, each Replicate represents a ratio of the component area/height to internal standard area/height.

% Calib Margin

This selection creates an acceptance margin based on the % difference between the peak area or height found during calibration and the current peak area or height in the method. If the % difference between these values exceeds this limit, the calibration for this peak will not be updated.

Scale

This parameter allows you to apply a scaling factor to the calibration curve. This factor is applied to the entered amounts or response values prior to computing the calibration curve. The purpose of using a scaling factor is to create a relationship between areas (or heights) and amounts or response that can be approximated by a polynomial fit. A scaling factor can be applied to any fit type. The available scaling operations are:

None
1/Amount
$1/Amount^2$
ln[Amount]
1/ln[Amount]
sqrt[Amount]
$Amount^2$
1/Response
$1/Response^2$
ln[Response]
1/ln[Response]
sqrt[Response]
$Response^2$
Log (Amount)
1/ log (Amount)
log (Response)
1/ log (Response)
ln (Amt)&ln(Resp)
log(Amt)&log(Resp)
Weighting Method

Select a LSQ Weighting Method to be used for calculation of least squares regression fits, either 1/Response, $1/Response^2$, 1/Amount, $1/Amount^2$ or none. Weighting gives increased importance to smaller concentrations and areas in the regression calculation.

Level

Type in the exact amount of each compound (corrected for purity) in your first calibration standard in the column labeled Level1. If you are doing a single-level calibration, you do not need to fill in any other Level columns. If you are doing a multiple-level calibration (e.g. you have more than one calibration standard mixture) you should repeat this process for each standard concentration level you plan to inject.

For example, assume you have a multi-level calibration where component A is present in standard mixture 1 at 10 ppm, in standard mixture 2 at 20 ppm, and standard mixture 3 at 30 ppm. You would enter 10 in the **Level 1** column, 20 in the **Level 2** column, and 30 in the **Level 3** column.

Note: Occasionally, a situation may arise where one or more named components may not be present in the calibration level mixture. To avoid introducing error in your calibration curve, you can cause the component area to be ignored at that level by leaving the Level of interest blank for that component. (Click on the cell and press the delete key.)

STD ID#

If you wish to calculate the concentration of a peak for which you have no standard sample, you can designate that the calibration curve of a different peak be used. Using STD Mult (see below), you can multiply the result to arrive at a proportional number.

STD Mult

If you have designated another peak to be used to calculate concentration, enter a multiplier here to be used. The equation used to calculate the concentration of the peak of interest then becomes:

$$Conc_i = f(Area_i) x \frac{Mult_S}{Mult_i}$$

Where:

f = the calibration curve equation for the standard peak according to the fit type selected (linear, quadratic, point to point, etc.)

$Conc_I$ = concentration of peak of interest

$Area_i$ = area of the peak of interest

$Mult_S$ = STD Mult of designated STD peak

$Mult_I$ = STD Mult of peak of interest

Manual RF

If you wish to assign a response factor to be used for a peak instead of the response factor calculated from the standard data, enter that value here. If a manual response factor is present in this field, it will be used to calculate amounts for this peak instead of using the calibration curve.

Low Conc

You can enter a concentration lower limit in this column. After each analysis, the data system can compare the calculated concentration of the peak to this value. If the value falls below the lower limit value, in order for a message to be posted in the Instrument Activity log, a post-run sequence action must be selected. **Note**: If you enter a value of zero, this function will be disabled.

High Conc

You can enter a concentration upper limit in this column. After each analysis, the data system can compare the calculated concentration of the peak to this value. If the concentration value falls above the upper limit value, in order for a message to be posted in the Instrument Activity log, a post-run sequence action must be selected

QC Reports Parameters

The following parameters in the Peak Table are used for calculation of QC Reports.

Check Std 1...5 Conc	Enter the amount of component present in the designated Check Standard. (Up to 5 check standards can be defined.) If you enter a value of zero, this check will be disabled. **Note**: If you enter a value of 0, the check will be disabled.
Check Std 1...5 %RD	If you are generating a Check Standard Report, enter the value to be used for the percent relative difference limit here. When the run is made, the calculated concentration of the peak will be compared with the check standard concentration specified in the peak table (Check Std Conc). If the difference is less than the Check Std % RD, the component passes. If the difference is more than the Check Std % RD, the component fails, and the failure action for that line of the sequence will be taken. Up to 5 check standards can be defined. **Note**: If you enter a value of **0**, the check will be disabled.
Spike 1 Amt	For **Spike Recovery Report**, enter the amount(s) of the first component(s) used to spike the first spiked sample.
Spike 2 Amt	For **Spike Recovery Report**, enter the amount(s) of the second component(s) used to spike the second spiked sample (if you are spiking the sample twice).
Low Spike Limit	Enter the lower limit (in %) for spike recovery. The calculated spike recovery will be compared to this value. If it falls below the low spike limit, it fails. **Note**: If you enter a value of **0**, the check will be disabled.
High Spike Limit	Enter the high limit (in %) for spike recovery. The calculated spike recovery will be compared to this value. If it falls above the high spike limit, it fails.
Dup % RD Limit	Enter the value to be used for % relative difference for duplicate reports. If the % relative difference falls above this value, the sample fails. **Note**: If you enter a value of 0, the check will be disabled.
RF % RSD Limit	Enter the % relative standard deviation for calibration response factors. When a **Calib Start** and **Calib End** are designated in the sequence table, this value will be used to determine whether the calibration passes or fails. **Note**: If you enter a value of 0, the check will be disabled.
PDA Parameters	The following columns appear if you have a PDA detector configured.

Detection	Select the basis for the identification of the peak. If you choose **Ret Time**, only the retention time will be used for identification of the peak. If you choose **Ret Time with Spectral Confirm**, the Similarity of the peak's spectrum to that of a designated reference spectrum will be used in addition to the retention time as the basis of peak identification.
Spectrum	If you want Similarity to be used as a basis for peak identification, then click on the arrow to the right of this field to specify the stored reference spectrum to be used for comparison. During identification, this reference spectrum is compared to the peak apex spectrum and a similarity index is computed. A peak is considered identified if this calculated similarity index is at least the value specified in the Similarity column of the peak table. If Similarity is not specified as a basis for peak identification, then this field is ignored.
Similarity	If **Similarity** is specified as a basis for peak identification, then this field specifies required minimum similarity index for a peak to be considered identified. During identification, the reference spectrum (see previous section) is compared to the peak apex spectrum and a similarity index is computed. A peak is considered identified if the calculated similarity index is at least the value in this field. If Similarity is not specified as a basis for peak identification, then this field is ignored.
Analysis Channel	Specify which Diode Array wavelength channel is to be used for analysis of the peak. The choices will be those specified in **Instrument Setup/DAD**.

Change the peak table properties

If you are not using one or more of the parameters presented in the Peak Table, you can remove it from view. The selections entered are saved on a per-instrument/per-user basis. This allows each user to set his/her own peak table parameters for each instrument.

To change the columns displayed in the peak table:

1. In the peak table, do a right mouse click and then click **Properties**.
2. In the **Properties** dialog box, select the columns that will appear in the peak table. Columns with a check mark will be displayed in the Peak Table spreadsheet. Those without a check will not be displayed.
3. The blue **anchor**  indicates what column will be used to anchor the right-left scrolling in your spreadsheet. Once this anchor is set, columns to the right of the anchor will scroll to the right and left. Columns to the left of the anchor will not scroll. To change the anchor, click on the name of the column you wish to use as anchor, and click the **Set Anchor** button. The blue anchor will move to the designated anchor column.

Note: When using the anchor, it is best to remove all unnecessary columns from the spreadsheet, and make the spreadsheet as wide as possible before you set the anchor. If you set the anchor to a column that does not currently show on the spreadsheet, you will not be able to scroll the spreadsheet.

Single level calibration using a stored data file

If you already have your calibration standard saved on your disk, you can calibrate your method using the areas from this file. This does not initiate data acquisition. It updates the method specified using areas from the stored data file specified.

1. From the **Analysis** menu, click **Analysis/Single Level Calibration**.
2. Complete the fields listed below.
3. When you have completed the dialog box, click **Start**. The stored data file will be opened and the areas for calibrated peaks will be used to update the method specified.

Sample ID	The sample ID for the data file selected is displayed here.
Method	Enter the name of the method to be calibrated. Include the entire path name if the method is not in your default method directory. You can select the method from a list of methods available on your disk by clicking the File button adjacent to the field.
Data File	Enter the name of the file to be used to calibrate the method. You can select a data file by clicking the File button adjacent to the field.
Result Path	Enter the path name where the result file is located. You can select the path name from a list by clicking the File button.
Result Name	Enter a name for the result file. If you did not select **Result Package Mode** when creating an EZChrom project in the Control Panel, you will still need to enter a **Result Name**. The result name is used for the RST file, and ACAML file names. If you selected **Result Package Mode** when creating an EZChrom project in the Control Panel, the **Result Name** will also be used for the folder name. In ECM it will be the name of the SSIZip.
Save as PDF	When this box is checked, the method report(s) will be saved as a PDF.
Print Hardcopy	When this box is checked, the method report(s) will be printed. If there is a loss of communication to the hard copy printer from the OpenLab EZChrom Print Server, files are copied from the monitor folder into the Quarantine folder. After communication to the hard copy printer has been established, files in the Quarantine folder can be copied back into the monitor folder for normal printing. Files in the Quarantine folder are automatically deleted in 24 hours by default. The time to delete folders from the Quarantine folder is set in the configuration file in the Print Server folder.

Amount Values	In this section, you can enter values that affect how the concentrations are calculated. If you are making a single data acquisition prior to calibrating your method, simply leave these values at the default level.
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 weighing 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 taken from the method Peak Table. For unknown runs, enter the amount of the Internal Standard in your unknown sample.
Multiplication factors	Enter up to 3 multiplication factors to be used for this analysis/calibration. All quantitated peaks will be multiplied by these factors.
Dilution factors	Enter up to 3 dilution factors to be used for this analysis/calibration. All quantitated peaks will be divided by these factors.
Calibrate	Select this box to trigger calibration. Once this box is clicked, the following fields and options will be available.
Calibration Level	Enter the number of the calibration level represented by the stored calibration standard. If this is a single level calibration, enter **1**.
Clear all calibration	Click this box if you want to clear all existing calibration factors from your method before running the calibration.
Clear calibration for level	Click this box if you want to clear the existing response factors for this level only before running the calibration.
Print calibration report	Click this box if you want to print a calibration report after running the calibration.
Clear replicates	Click this box if you want to clear existing replicates from this level before running the calibration.
Average replicates	Click this box if you want to average replicates for this calibration level.

Renumbering peak ID's

Peak ID numbers are assigned to calibrated peaks in the order in which they are added. If you add peaks to your peak table renumber the Peak ID's so the ID numbers are in order of the peak retention times.

To renumber peak ID's, in the peak table, right click and select **Renumber Peak ID's**. The Peak ID numbers in the peak table will be renumbered (including Ref and ISTD Peak ID numbers to reflect the changes).

Note: Renumbering Peak ID#'s may require items identified by Peak ID# in custom parameters or custom reports to be re-defined using the new Peak ID#'s.

Review calibration curves

After you have completed running all of the calibration standards for your method, you can review the calibration curve and associated data by clicking the **Review Calibration** button. A window will appear with the calibration information from your current method.

From Review Calibration, you can

- Look at the calibration curve for each calibrated peak.
- Change and overlay calibration curve fit types.
- Review the equations for curve fit types, and examine the R-squared (goodness of fit) value for each.
- Temporarily remove points from the calibration curve.
- View response factors, replicate areas, and standard deviation values.
- Use the concentration calculator to calculate amounts from manually entered areas.

Viewing the Calibration Curve

Calibrated peaks are listed in the **Peak List**. To view the calibration information for a given calibrated peak, click on the peak name from the **Peak List**. It will be highlighted, and the spreadsheet and calibration curve will be updated to include the current calibration information for that peak.

The calibration curve for the peak selected appears in the lower left corner of the window.

The box at the lower right of the window displays parameters and calculation data for the calibration curve displayed. This includes Average Response Factor, the Response Factor Standard Deviation, the Response Factor % RSD, Scaling factor, LSQ Weighting factor, Force through zero On or Off, Replicate mode, and calculations for each fit type displayed, along with R^2 for the fit.

Temporarily removing points from the calibration curve

If you want to see the effect of removing one of the points from your calibration curve, you can temporarily remove it from the calculation by clicking the point once with your mouse. The point will turn red, which indicates it is not currently used for the calculation of the calibration curve. The spreadsheet cells represented by the point will also turn red. To return the point to the calculation of the curve, click on the point again. Points can also be disabled from the spreadsheet by clicking the cell in the spreadsheet, then pressing the **Delete** key. To restore the point, click the **Delete** key again.

Using the right mouse button

Clicking the right mouse button give you access to quick menus. When you right-click in the calibration curve region of the window, a menu will appear where you can change the characteristics of the displayed calibration curve.

View Fit Type	Select a new fit type to be displayed in the review peak calibration graph. The fit is overlaid with the current calibration curve. You can also select **View all fits** or **Clear all fits** from this menu.
Change Fit Type	Select a new fit type to be applied to the calibration curve. When you change the fit type, the change will also be entered into your peak table for this peak.
Scaling	Select a new scaling factor for the calibration curves. This scaling will be applied to all calibration fits displayed, and will be applied to the peak table for this peak.
LSQ Weighting	Select a least squares weighting factor to apply to the calibration curves. (Applies only to linear, cubic, and quadratic fits.) The LSQ Weighting selected will be entered in your peak table for this peak.
Force Through Zero	Select this to force the calibration curve(s) through the origin. Changing this will automatically change the peak table for this peak.
View Mode	Select **Peaks** or **Groups** for viewing.
Replicate View Mode	This selects how you want to view the replicate data in the calibration data spreadsheet. Select **Area/Height** to view the replicate area or heights. Select **Response Factor** to view the replicate response factors.
Response Factor Definition	Select how the response factors are to be calculated and displayed, **Area/Amount** or **Amount/Area**. The selection of **Area/Amount** or **Amount/Area** for your method is located in the **Method>Properties>Calibration** dialog.
Print Current Peak/Group	Select this to print the currently selected peak or group information.
Print All Peaks/Groups	Select this to print all the peaks or group information.
Full Unzoom	Restores calibration curve display to 100%.
Concentration Calculator	The Concentration Calculator lets you calculate amounts based on areas or heights you input. See Concentration Calculator.

Viewing Calibration Data

When you select a peak from the peak list, the calibration data for that peak will be displayed in the spreadsheet at the top of the window. Each row in the spreadsheet represents a calibration level for that compound.

Level	A calibration level corresponds to a point (or points, if replicates are used) on the calibration curve, and represents the relationship of peak area(s) to calibrated amount. The number of calibration levels may be different for each component. EZChrom software can handle an unlimited number of

	concentration levels per component. For each Level, the following fields are displayed.
Amount/Amount Ratio	This is the component Amount (external standard) or Amount Ratio (internal standard) represented by this level.
Area (or Height)/Area Ratio (Height Ratio)	This is the peak area or height (if external standard) or Area Ratio or Height Ratio (for internal standard) for the designated level.
RF	This is the response factor for the peak at the designated level.
Last Area (ratio)/Height (ration)	If no replicate injections are made, this is the last area or height (or area ratio/height ratio) for the peak at the designated level. If replicate injections have been made, this is the old average of the replicates, which is used for weighting purposes.
Residual	A residual is the difference between the user entered concentration and the concentration read back from the computed calibration curve.
Rep StDev	This is the standard deviation for the replicates.
Rep %RSD	This is the % relative standard deviation for the replicates.
Rep 1...x Area (ratio)/ height (ratio)	Each level can have multiple **replicates** (duplicate injections of a single standard level). Rep 1 is the first calibration replicate run, Rep 2 is the second replicate, etc. When replicate standards are used, and the Calib Weight is set to 100, the response factor will be based on the true average of all replicates in the calibration level. In order for replicates to be used, you must select the **Wt Average** option in the Peak Table Calib Flag column. Otherwise, each injection at a given level will replace the current calibration areas/heights.
Rep 1...x User	This is the logged user at the time the calibration was last performed using this replicate.
Rep 1...x Data File	This is the data file where the replicate data is stored.
Rep 1...x Sample ID	This is the Sample ID for the replicate sample.
Rep 1...x Calib. Time	This is the date and time the last calibration was performed using this replicate.

Concentration calculator

The Concentration Calculator lets you calculate amounts based on areas or heights you input. In order to use the concentration calculator, you must have a calibrated method open.

To open the Concentration Calculator:

1 In the Instrument Window, click the  **Review Peak Calibration** button.

2 Do a right mouse click in the calibration curve window, and then click **Concentration Calculator**.

3 Complete the following fields:

- **Fit Type** - Select a fit type to be used to calculate the concentration or area.
- **Scaling** - If desired, select a scaling factor to be used for the

calculation.

- **LSQ Weighting** - Select a least squares weighting factor to be used, if desired.
- **Force Through Zero** - Select this if you want the curve forced through the origin for the calculation.
- **Area** - If you want to calculate an **Amount**, enter an area that represents the peak to calculate, then click the **Calculate** button.

Calibration averaging

The following selections designate how calibration averaging is to be treated for the method.

To turn on automatic calibration averaging, select **Method > Properties > Calibration.** Check **Automatically average consecutive replicates of the same level.** To turn it off uncheck this box.
See Automatically Average Replicates.

To designate a calibration run type, select **Control > Single Run**. Check **Average Replicates**. To turn it off uncheck this box.
See Calibration Averaging as Part of a Single Run or Sequence.

To average a calibrated peak's areas, in the Peak Table set the Calib Flag for that peak to **Wt Average**. If you do not want a peak's areas to be averaged, set the Calib Flag for that peak to **Replace.**
See About Replicates and Averaging Calibrations.

Automatically average replicates

Automatic calibration averaging is a quick way to average calibration replicates that are grouped together, and is the most common use of averaging.

To set up your method such that all calibrations are averaged:

1. From the **Method** menu, click **Properties** and then click the **Calibration** tab. Here, you can select the option to automatically average after every calibration.
2. To turn averaging on, make sure there is a check mark next to the **Automatically average replicates** prompt. This is the default (recommended) selection. The default averaging is explained below. See Method Properties Calibration.

When the automatic averaging of replicates is selected, averaging of all replicates for a given level will be performed until the replicates are cleared. If a sequence calibration (or sequence reprocessing calibration) is performed, automatic averaging of all replicates for a given level will occur automatically at the end of a series of calibration replicates for that level. The area/height average at that point will be saved in the method as Last Area. When a new level is encountered, the replicates for the previous level will be cleared automatically from the method.

Note: Averaging only occurs for peaks where the Calib Flag is

designated as Wt Average.

If you turn the Automatic Averaging Off, be aware that for peaks whose Calib Flag is set to Wt Average, no results will be calculated until you force averaging by setting the Run Type to Average Replicates in either a single run or sequence run.

Rolling Average Calibration

If you have entered a number for replicates in rolling average in the **Method > Properties > Calibration** dialog, a rolling average will be calculated for replicates as described below. See Method Properties Calibration.

The rolling replicate average is done as in the following example:

For an acquisition sequence, where S = Standard and U = Unknown, and the number of replicates in rolling average = 4,

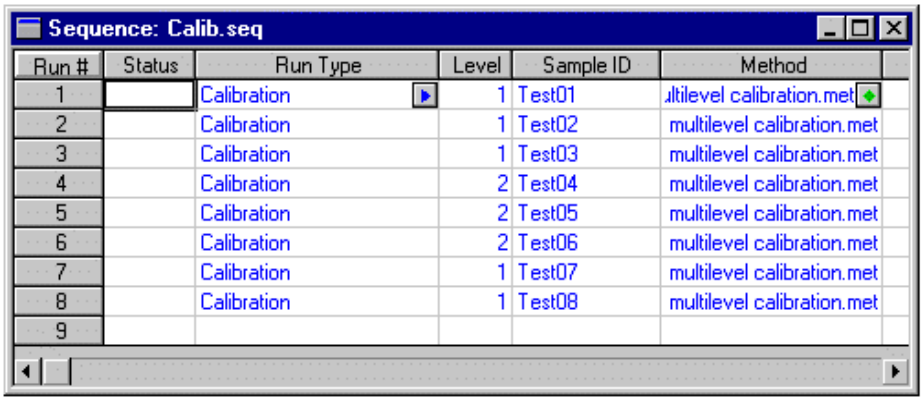
S1, U1, S2, U2, S3, U3, S4, U4, S5, U5, S6, U6, S7, U7

In the above acquisition sequence, U1 would be quantitated using S1, U2 would be quantitated using the average of S1 and S2, U3 would be quantitated using the average of S1, S2, and S3, U4 would be quantitated using the average of S1, S2, S3, and S4, and U5 would be quantitated with the average of S2, S3, S4, and S5. In this example, every 4 calibration replicates will roll the average forward.

The following example demonstrates how replicates are treated during a calibration sequence using Automatic Averaging:

1. As each run is analyzed, the area for each named peak is saved in the method as the current area. At the end of Run 3, a true average will be calculated from replicates for Runs 1 - 3 for Level 1. This value is the calibration area/height for this level.
2. At Run 4, the calibration for Level 2 begins. Replicates for Level 2 will be saved for runs 4, 5, and 6.
3. At the end of Run 6, the replicates for Level 2 will be averaged and used to calculate the calibration point for Level 2. This area/height is saved as Last Area for Level 2.
4. At the beginning of Run 7, the existing replicates for Level 1 will be cleared and new Level 1 replicates will be saved for Run 7 and Run 8.

5 At the end of Run 8, the existing calibration area/height becomes the Last Area, the true average of Runs 7 and 8 is calculated and a weighted average is calculated using this value and the Last Area (see calculation in Calib Weight section). **Note** that if the Calib Weight is set to 100, the Last Area value is not taken into account.



Calibration averaging as part of a single run or sequence

Single run

Whether or not you are doing Automatic Calibration Averaging, you can designate averaging at the start of a single run, or as part of the **Run Type** of a sequence entry.

To designate a calibration run type, select **Control > Single Run**. Check **Average Replicates**. The replicates are averaged and the average is used in conjunction with the Calib Weight and Calib Flag to calculate a new calibration point.

Sequence

For a sequence, calibration averaging is designated as part of a run's **Run Type**.

In the sequence spreadsheet select the **Run Type** field. In the **Sample Run Type(s)** dialog box, select **Average Replicates**. The replicates are averaged and the average is used in conjunction with the Calib Weight and Calib Flag to calculate a new calibration point.

You can quickly determine if a calibration run has an **Average Replicates** run type associated with it by looking at the sequence table. Runs that are designated for **Average Replicates** have the code **Average Replicates** in the **Run Type** column.

If you click on the **Run Type** for one of these runs, you will see the **Average Replicates** box has been checked for the Run Type of that sample. Click again on this check mark to remove the Average Replicates from the Run Type for this sample, if desired.

Note: When Automatic Averaging is turned OFF, calibration replicates will continue to be saved in the method until you clear or average them at the beginning of a calibration run.

About replicates and averaging calibrations

Initially, a method contains no calibration. When you run the first calibration standard, the areas/heights for each calibrated peak are entered into the method calibration. If you run a subsequent standard at the same calibration level (a **replicate**), you have a choice of how you want the data system to treat the new areas/heights for the calibration.

To average a calibrated peak's areas, in the Peak Table set the **Calib Flag** for that peak to **Wt Average**. If you do not want a peak's areas to be averaged, set the **Calib Flag** for that peak to **Replace.**

If you choose to **Replace** the existing calibration, the areas/heights for each replicate replaces the area/height for the previous replicate in the calibration. Only the most recent replicate areas/heights are used to create the calibration curve. Previous replicates are ignored.

If you choose **Wt Average**, each calibration point on the curve will be determined by performing the average of the current calibration with previous replicate areas/heights in the method. The following example describes how this is done.

Assume a starting method for a single-level calibration with no existing calibration data. After a series of n calibration replicate samples are run, the calibration curve is determined as shown below.

Level 1 Replicate Area

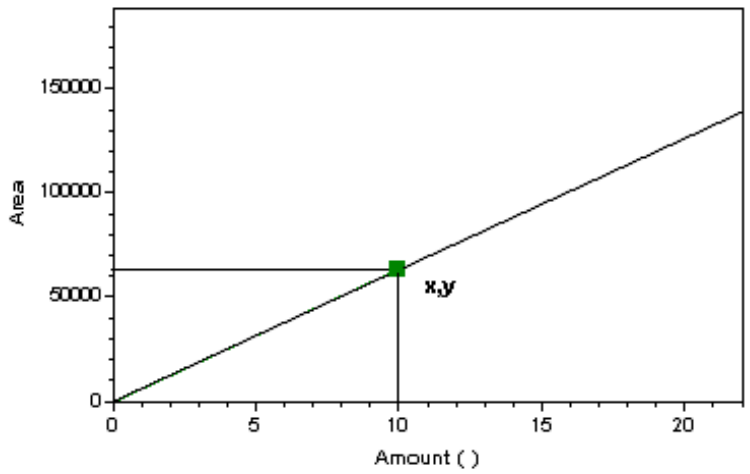
1. $Area_1$
2. $Area_2$
3. $Area_3$

. .

. .

. .

n $Area_n$



The resulting calibration curve is shown above, with the point **(x,y)** representing the calibration point for Level 1. The area, **y**, of this point is calculated by taking the average of the replicates at this level.

This average, y, is saved as the **last area** in the method. This value is

$$y = \frac{area_1 + area_2 + \ldots area_n}{n}$$

used to calculate the weighted average when a new series of replicates for this level is run, as shown below.

Level 1 Replicate Area

1 $Area_1$

2 $Area_2$

3 $Area_3$

. .

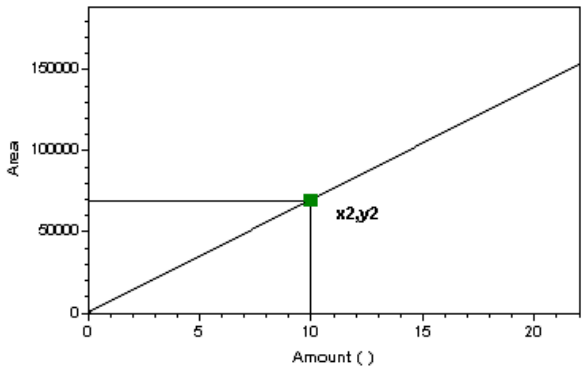
. .

. .

m $Area_m$

Because this is the second time a series of replicates was run for this level, a weighted average is now calculated, using the Calib Weight (weighting factor) set in the peak table.

A new calibration curve is calculated.



The new calibration point (**x2,y2**) is used to draw the calibration curve, with the area, **y2**, calculated as follows.

y2 =

$$\left[\left(\frac{area_1 + area_2 + \ldots area_m}{m}\right) * W\right] + \left[y * (1 - W)\right]$$

Where

y2 = area of calibration point x2,y2

W = Calib Weight, expressed as a percentage

y = Last area

About groups and group calibration

A group is a collection of peaks, which are somehow related. The data system allows you to define as many groups as you want. Peaks in a group do not have to be contiguous peaks in the chromatogram, and may be treated in one of three ways:

- Uncalibrated Range. In this type of grouping, you define a time range. A manual response factor will be applied to determine concentration of uncalibrated peaks eluting within that time range.
- Calibrated Range (Group Calibration). Using this technique, you calibrate peaks together as a group, creating a common response factor for the group. Peaks in the Calibrated Range will be reported as a single peak using the common response factor for the group as a basis for calculation of concentration.
- Designate Named Peaks to be included in a group (Calibrated Peak Grouping). Using this technique, a group report gives the concentration summation of all calibrated peaks designated as belonging to that group. All peaks in the group can also be reported individually because they also appear in the Peak Table.

See Also

Define a Group

Group Table Properties

Uncalibrated Group Range

Group Calibration (Calibrated Range)

Group Table

Group Range Definition

Calibrated Range Examples

Calibrated Peak Grouping (Named Peaks)

Peak Group Definition

Group Range Adjustment

Report Group Amounts

Define a group

Defining a group is similar to defining calibrated peaks. The group can either be defined manually, by typing information into the Groups table, or it can be defined graphically using an integrated chromatogram.

To define a group graphically:

1 Open the data file to display the chromatogram.

2 Right-click in the chromatogram and select **Graphical Programming > Define Groups**, or in the integration toolbar select the **Define Groups** button.

3 Select the group you want to define. Click once at the beginning and once at the end of a region of peaks you wish to add to the group. You may continue to add groups by clicking to define the group regions. When you are done defining the group regions, press the ESC key.

4 In the **Define Peaks** dialog box further define the group by completing the following fields:

Group name	Enter a name to be assigned to this group.
Group type	Select Uncalibrated Range, Calibrated Range, or Named Peaks for the type of group you want to define.
Quantitate group on	Select whether you want to use Area or Height for calculation of response factors. **Note**: If you are doing both Peak and Group quantitation using internal standards, both Peaks and Groups must use the same quantitation measurement type (area or height).
ISTD ID #	If you wish to use an internal standard method for the group calibration, you must add to your sample a known amount of an internal standard. The internal standard must be entered in your Peak Table, and must have a calibration amount assigned to it. Enter the Peak ID number of the internal standard from your Peak Table in this field.
Reference ID #	If you are using a reference peak, enter its Peak ID number from the Peak Table for the peak to be used as a reference peak. The retention time of the reference peak will be used to adjust the start and end times of the group windows. **Note** that the reference peak must be identified in the Peak Table and given an expected retention time. The reference peak does not need to have calibration levels assigned to it.
Units	Enter the units to be used for reporting group concentration results.
Include named peaks	Click this box if you want to include any individually calibrated peaks (named peaks) in this calibrated group. The areas of the named peaks will be used in calculation of the group response factor.
Calculate concentration for unnamed peaks in group	Selecting the **Calculate concentration for unnamed peaks in group** box will cause the concentrations of the unnamed (uncalibrated) peaks in the group to be calculated using the group response factor and listed in the peak report. The peak report will include the unnamed peak concentrations, but will not report the group concentration as a peak. The group concentration will be reported in a separate group report section. **Note**: When this box is checked, the total group area and height are not reported as part of the peak table, so the Area% and Height% columns in the peak report will add up to 100%. If Groups

are reported in the run report, a separate report section will be generated that only includes groups. This will be the only place where the total group concentration using this option can be viewed. If this box is not selected, the group will be reported as part of the peak table, and the Area%, Height%, concentrations may add up to more than 100%.

For examples of reports using various Calibrated Range options, see Calibrated Range Examples.

About the Group Table

To view the Group Table:

1 There are three ways to open the Peak/Group tables:
   - In the navigation pane select **Method > Peaks/Groups.**
   - In the menu select **Method > Peaks/Groups.**
   - In the toolbar select the **Peaks/Groups** button  .

2 In the **Peak/Group Tables** dialog box, select the **Groups** tab.

3 In order to calibrate the group(s), you need to enter calibration amount(s) for each group. In the columns of the group table labeled **Level 1,** etc., enter the calibration amount to be used in calculation of the calibration curve for that group. Also, enter the concentration units for reporting group results in the column labeled **Units**.

4 In order to properly do group calibration, you need to designate the following parameters:

#	Row number
Name	Type the name of the component.
Ref. ID#	ID# of the group to be used as a reference group for this component.
ISTD.ID#	ID# of the group to be used as internal standard for this component, if you are using an internal standard method. **NOTE**: If you are doing an Internal Standard calibration, you must enter an ISTD ID# for each calibrated component. If the peak is an internal standard, enter its own ID# in the ISTD ID# column. If you are doing External Standard calibration, you should enter 0 in the ISTD ID# column for all components. You may designate more than one internal standard.
Group Type	The **Group Type** should indicate **Calibrated Range**.
Group Def	If you click the **Group Def** field, you will see the retention time range for the region(s) you selected using the mouse to define the group.
Units	Enter the concentration units to be used in reporting results, such as mg/ml or vol%.
Quantitate	Choose whether the calibration and quantitation are to be based on peak height or peak area. **Note**: if you are doing both Peak and Group quantitation using internal standards, both Peaks and

Groups must use the same quantitation measurement type (area or height).

Fit Type

This option determines how the calibration curve will be fit to the data.

Note: You have five choices for how the calibration curves will be drawn: point-to-point, linear, and quadratic, cubic, and Average RF fits. You must have at least two calibration levels for a linear fit (not including zero), three levels for a quadratic and four levels for a cubic fit.

Zero

When this box is selected, the calibration curve will be forced through zero.

Calib Flag

The **Replace/WtAverage** selection allows you to determine how the calibration areas/heights for each group will be affected by running a standard: they will either be replaced, or averaged with the current replicate areas in the calibration method. If Calib Weight is set to a value other than 100, a weighted average of the areas/heights will be calculated. For details on calibration averaging, see the **Replicates and Calibration Averaging** section.

Each time a calibration average is performed, the value is saved in the method as Last Area, which is subsequently used for calculation of weighted averages.

Calib Weight

You can designate a weight for the average of the replicates. The weighting factor is applied to replicate injections as shown in the following example.

Current run value (area/height) 101

Replicate 1 104

Replicate 2 100

Replicate 3 102

Current Last Area Value = 102

Using a weighting factor of 60, the new method average is:

[(104 + 100 + 102) / 3) * .6] + [101 * .4] = 101.6

Note: For Internal Standard calibrations, each Replicate represents a ratio of the component area/height to internal standard area/height.

% Calib Margin

This selection creates an acceptance margin based on the % difference between the group area or height found during calibration and the current group area or height in the method. If the % difference between these values exceeds this limit, calibration for this group will not be updated.

Scale

This parameter allows you to apply a scaling factor to the calibration curve. This factor is applied to the entered amounts or response values prior to computing the calibration curve. The purpose of using a scaling factor is to create a relationship between areas (or heights) and amounts or response that can be approximated by a polynomial fit. A scaling factor can be applied to any fit type. The available scaling operations are:

None

1/Amount

$1/Amount^2$

ln[Amount]
1/ln[Amount]
sqrt[Amount]
Amount^2
1/Response
1/Response^2
ln[Response]
1/ln[Response]
sqrt[Response]
Response^2
Log (Amount)
1/ log (Amount)
log (Response)
1/ log (Response)
ln (Amt)&ln(Resp)
log(Amt)&log(Resp)

Weighting Method Select a Weighting Method to be used for calculation of least squares regression fits, either 1/Response, $1/Response^2$, 1/Amount, $1/Amount^2$ or none. Weighting gives increased importance to smaller concentrations and areas. A scaling factor can be applied to linear, quadratic, and cubic fits.

Level 1... x You must designate one or more calibration levels to be used in calculation of a group response factor. For each Level, enter the amount of the group in that calibration sample.

Occasionally, you may want to calibrate one group with fewer levels than the other groups in your group table. (For example, when you have more than one calibration mixture for the same concentration level.) To avoid introducing error in your calibration curve, you can cause the group area to be ignored at that level by leaving the Level of interest for that group blank. To insert a blank, double-click on the cell and press the Delete key.

If you are performing QC checks, you should fill out the appropriate columns for your groups. See the Calibration section for details on these columns.

Note: As with the Peak Table, the Group Table can be customized to include only those parameter columns that you need for your group calibration. To select the group parameters, click on the upper left corner of the group spreadsheet, and select Properties from the drop-down menu. From the dialog box, click on those parameters you wish to include in the spreadsheet.

Be sure to save your method. To complete the group calibration, you must run a calibration standard at each level for which you have entered an amount. This can be done manually using stored data files, or as a part of a sequence. For details on how to calibrate, see Calibration.

Change the Group Table properties

If you are not using one or more of the parameters presented in the Group Table, you can remove it from view. The selections entered are saved on a per-instrument/per-user basis. This allows each user to set his/her own peak table parameters for each instrument.

To change the columns displayed in the group table:

1. In the Group Table, do a right mouse click and then click **Properties**.
2. In the **Properties** dialog box, select the columns that will appear in the group table. Columns with a check mark will be displayed in the Group Table spreadsheet. Those without a check will not be displayed.
3. The blue **anchor**  indicates what column will be used to anchor the right-left scrolling in your spreadsheet. Once this anchor is set, columns to the right of the anchor will scroll to the right and left. Columns to the left of the anchor will not scroll. To change the anchor, click on the name of the column you wish to use as anchor, and click the **Set Anchor** button. The blue anchor will move to the designated anchor column.

Note: When using the **anchor**, it is best to remove all unnecessary columns from the spreadsheet, and make the spreadsheet as wide as possible before you set the **anchor**. If you set the anchor to a column that does not currently show on the spreadsheet, you will not be able to scroll the spreadsheet.

Uncalibrated group range

The Uncalibrated Range group type is used to enter a response factor for uncalibrated peaks eluting within a specified retention time range. When the chromatogram is analyzed, the concentration of unnamed peaks eluting within the uncalibrated range will be calculated using the response factor entered for the uncalibrated range.

Defining an Uncalibrated Range group is done using a stored chromatogram. Since you are simply defining a range for uncalibrated peaks, it is not necessary for the chromatogram to be analyzed in order to create the group.

To define an uncalibrated group range:

1. Select **File > Open > Data**. Navigate to the data file that contains the range(s) you wish to include in your group.
2. Click on **Analyze**. Make sure all the peaks you wish to include in the group are detected. (optional)
3. Click on the **Define Group** button, or select the Define Group command from the right mouse click> graphical programming menu. With this function, you define one or more group windows using the mouse. The regions defined by the mouse become the uncalibrated range(s) for the group. You can define any regions in the chromatogram, whether or not peaks are present.

4 Click the mouse once at a point on the chromatogram where you wish to define the beginning of the group region.

5 Click the mouse again to define the end of the group region.

6 If you want to add additional peak regions to the same group, repeat the above procedure as many times as necessary. When you are finished adding regions to the group, press the **[ESC]** key.

7 A dialog box will appear for the group. Select **Uncalibrated Range** for Group type, and enter a name for Group name. Because the concentration of the uncalibrated range is calculated from the manual response factor, it is not necessary to enter values for any other field, except **Units** for reporting.

8 When you have completed the dialog box, click on **OK**. A row will be added to your Group Table containing the information you entered.

9 To view the Group Table, click the **Peak/Group Tables** button on the command ribbon. Click the **Groups** tab to view the group information table.

10 Enter a response factor to be used for the uncalibrated range group in the **Manual RF** column for the group.

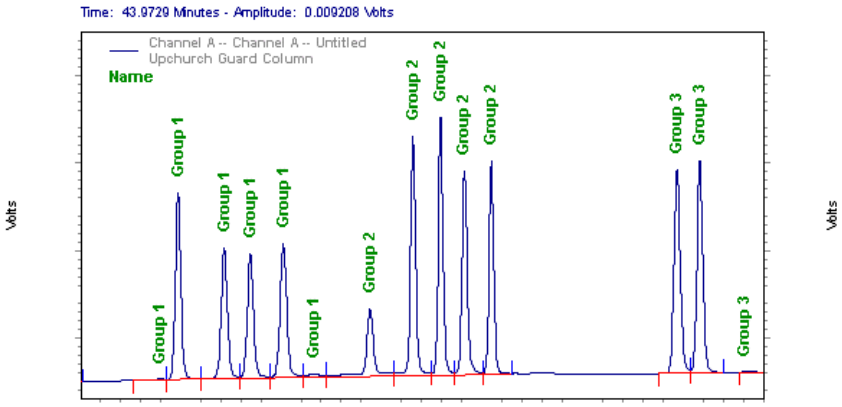
11 If you are using a reference peak, enter its **Peak ID** number from the Peak Table for the peak to be used as a reference peak. The retention time of the reference peak will be used to adjust the start and end times of the group windows. **Note** that the reference peak must be identified in the Peak Table and given an expected retention time. The reference peak does not need to have calibration levels assigned to it.

12 No other parameters are necessary. Click the **X** to exit the Peak/Group Tables box. Be sure to save your method.

Group calibration (Calibrated Range)

Calibrated Range grouping calibrates and analyzes peaks defined in the group as a single peak. A common response factor is calculated for the group, based on one or more calibration runs where concentration level(s) are defined for the group. In addition, you can choose to include calibrated (named) peaks in the group.

In the following example, we do not want to calibrate peaks individually. Instead, we want to combine peaks in certain regions of the chromatogram together and calibrate them in groups, creating a unique response factor for each group. Follow the steps to set up the groups.



To define a group of peaks graphically using the stored chromatogram:

1. Select **File > Open > Data**. Navigate to the data file that contains the peaks you wish to include in your group.
2. Click on **Analyze**. Make sure all the peaks you wish to include in the group are detected.
3. Click on the **Define Group** button, or select the Define Group command from the right mouse click> graphical programming menu. With this function, you define one or more group windows using the mouse. All detected peaks within the group window(s) will become part of the group being defined. This allows you to create a group that contains non-contiguous peaks in the chromatogram.
4. Click the mouse once to the left of the first peak to be included in the group. This defines the beginning of a group window.
5. Click the mouse again to the right of the last peak to be included in the group window. This defines the end of the group window.
6. If you want to add additional peak regions to the same group, repeat the above procedure as many times as necessary. When you are finished adding peaks to the group, press the **[ESC]** key.
7. A dialog box will appear where you can give the group a name, number, and designate a reference peak and internal standard for the group. Complete the following fields:

Group Name	Enter a name to be assigned to this group.
Group Type	Select **Calibrated Range** for the type of group you want to define.
Quantitate Group On	Select whether you want to use Area or Height for calculation of response factors. **Note**: If you are doing both Peak and Group

	quantitation using internal standards, both Peaks and Groups must use the same quantitation measurement type (area or height).
ISTD ID #	If you wish to use an internal standard method for the group calibration, you must add to your sample a known amount of an internal standard. The internal standard must be entered in your Peak Table, and must have a calibration amount assigned to it. Enter the Peak ID number of the internal standard from your Peak Table in this field.
Reference ID #	If you are using a reference peak, enter its Peak ID number from the Peak Table for the peak to be used as a reference peak. The retention time of the reference peak will be used to adjust the start and end times of the group windows. **Note** that the reference peak must be identified in the Peak Table and given an expected retention time. The reference peak does not need to have calibration levels assigned to it.
Units	Enter the units to be used for reporting group concentration results.
Include Named Peaks	Click this box if you want to include any individually calibrated peaks (named peaks) in this calibrated group. The areas of the named peaks will be used in calculation of the group response factor.
Calculate concentration for unnamed peaks in group	Selecting the **Calculate concentration for unnamed peaks in group** box will cause the concentrations of the unnamed (uncalibrated) peaks in the group to be calculated using the group response factor and listed in the peak report. The peak report will include the unnamed peak concentrations, but will not report the group concentration as a peak. The group concentration will be reported in a separate group report section. **Note**: When this box is checked, the total group area and height are not reported as part of the peak table, so the Area% and Height% columns in the peak report will add up to 100%. If Groups are reported in the run report, a separate report section will be generated that only includes groups. This will be the only place where the total group concentration using this option can be viewed. If this box is not selected, the group will be reported as part of the peak table, and the Area%, Height%, concentrations may add up to more than 100%.

8 When you have completed the dialog box, click on **Ok**. A row will be added to your Group Table containing the information you entered.

9 After the group has been defined, you must enter calibration levels into the group table and then run the calibration sample(s) to determine the group response factors.

10 After you have completed your group setup and calibration, the peaks in the defined groups will appear on your chromatogram if you have the peaks annotation on.

Group range definition

To review or change the chromatogram time range(s) currently selected for the group:

1 Open the Group Table by clicking the **Peak/Group Tables** button and then click **Groups**.

2 Click on the **Group Def** field. The **Group Range Definition** dialog box appears with the currently defined range(s) for the group. You can manually change the range(s) if desired.

Note: If the group selected is a Named Peaks group, a different dialog box will appear. See Peak Group Definition.

3 Click the **Include Named Peaks** option if you want to include in the group any named (calibrated) peaks that fall within the range. When this option is checked, the areas of named peaks falling within the defined ranges will be used in calculation of the group response factor. If this is not selected, the named peaks eluting within this region will not be considered part of the group, and the areas will not be used in calculation of group response factor.

4 Selecting the **Calculate concentration for unnamed peaks in group** box will cause the concentrations of the unnamed (uncalibrated) peaks in the group to be calculated using the group response factor and listed in the peak report. The peak report will include the unnamed peak concentrations, but will not report the group concentration as a peak. The group concentration will be reported in a separate group report section.

Note: When this box is checked, the total group area and height are not reported as part of the peak table, so the Area% and Height% columns in the peak report will add up to 100%. If Groups are reported in the run report, a separate report section will be generated that only includes groups. This will be the only place where the total group concentration using this option can be viewed. If this box is not selected, the group will be reported as part of the peak table, and the Area%, Height%, concentrations may add up to more than 100%.

Calibrated peak grouping (Named Peaks)

This technique assumes you have individually calibrated peaks in your chromatogram. You define the groups by designating in the Group Table the named peaks to be included in each group, and giving each group a name.

Note: In order to define a peak group graphically, 1) make sure the current chromatogram is the chromatogram you wish to use, 2) you have already created a calibrated peak table in your method, and 3) you have analyzed the chromatogram.

1. Open the data file containing the calibrated peaks you wish to include in your group. Click on **Analyze** to integrate the chromatogram and make sure the peaks are detected.
2. Define the peaks belonging to the group by graphically defining the group using a stored chromatogram. To do this, click the **Define Group** button on the toolbar, or select the Define Group command from the right-mouse click /graphical programming menu. Click the mouse to the left of the first peak to be included in the group, then click the mouse again to the right of the last peak to be included in the group (if they are contiguous peaks). You may continue to add peaks to the group by clicking the mouse to define peak regions. When you are done adding peaks to the group, press the **Esc** key on your keyboard. A dialog box will appear.
3. Type a name to be used for the group in the **Group Name** field.
4. Select **Named Peaks** for the **Group Type.** Click **OK** to accept and exit the dialog.
5. Click the **Peak/Group Tables** button from the command ribbon. Click the **Groups** tab to view the group table.
6. The **Group Type** field should show **Named Peaks**. Click the **Group Def** arrow to review the calibrated peaks selected for this group. See Peak Group Definition for details on defining the named peaks for this group.

Peak group definition

To review or edit the peaks in a group:

1. On the command toolbar, click the **Peak/Group Tables** button and then select the **Groups** tab.
2. For the group you wish to review or edit, click the **Group Def** field. If this group is a **Named Peaks** group, the **Peak Group Definition** dialog box will appear.
3. **Note**: If the group selected is not a Named Peaks group, a different dialog box will appear. See Group Range Definition.
4. Review the list of peaks on the right. If there is a peak that you do not want in the group, click on it with the mouse, then click **Remove Selection.**
5. To add a peak to the group, select it from the **Named Peaks** list, then click on **Add Selection**. You can quickly add or remove all of the peaks using the **Add All** or **Remove All** buttons.
6. When you are finished, click **OK**. The peaks in the box labeled **Peaks in this Group** will become the defined peaks for this group, and the Group Table will appear once more.
7. If you are using a calibrated peak group, you should not enter any **Level** information in the table, as the group total will be calculated using the calibrated amounts for the individual peaks in the group. To leave the group table, click on the upper left corner of the Group Table spreadsheet.

Once your peak group has been defined, it can be reported by selecting the **Report groups** option in the report properties.

Group range adjustment

To graphically change the Group Range, you must have the option to display the Group Range annotation turned on.

1. To turn on the Group Range annotation, do a right mouse click on the chromatogram and select **Annotations**. In the Trace Annotation Properties dialog, select **Group Range**.
2. Click the **Adj Group Range** button  .
3. Select the Group Range you wish to adjust. The cursor will turn into a two-ended arrow and two drag boxes will appear. You can adjust the Group Range by dragging either end or by dragging the Group Range bar itself. If you grab the bar itself and move it, both the start and stop of the Group Range will be updated. If you grab either end of the bar and move it, the other end of the bar will stay in its current position and the Group Range will be updated accordingly.

   Note: The groups from results and the method are matched based on group #. Therefore, you must analyze first (if the method has changed) before doing group range graphical programming.
4. After you have adjusted the window to your liking, press **ESC** to finish.
5. In the **Adjust Group Range** dialog box, select **Update Group**. The Group Range will be updated in the group table. Select **Analyze Now** to analyze the chromatogram using the updated Group Range.

Report group amounts

To report the group amounts in a new standard report:

1. In the navigation pane select **Reports > Standard Report**.
2. Right click in the report editor and select **Insert Report > Run Report**.
3. In the **Run Report** dialog box select **Groups**.

4 To report peaks that are part of an Uncalibrated Range group, select **Unnamed peaks**.

5 Select **OK**.

To add the group amounts to an existing run report table:

1 In the existing run report table, right click and select **Report Properties.**

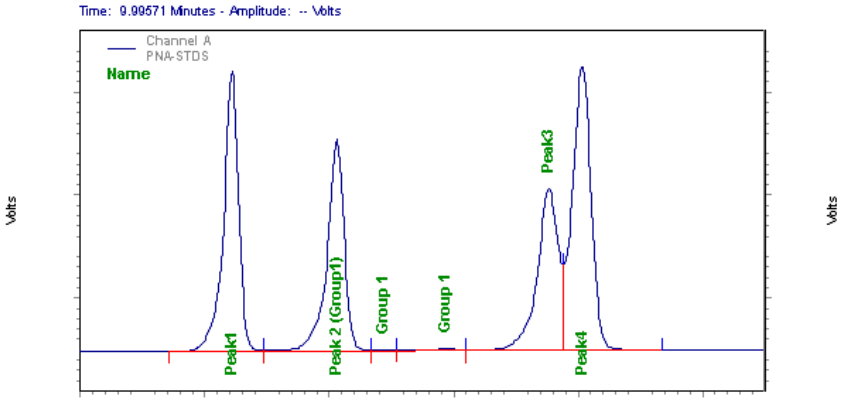
2 In the **Run Report** dialog box select **Groups**.

3 To report peaks that are part of an Uncalibrated Range group, select **Unnamed peaks**.

4 Select **OK**.

Calibrated range examples

The following example reports were generated using the peak options for calibrated range groups, using the simple chromatogram shown below. In this example, there are four named (calibrated) peaks **Peak 1...Peak 4**, and one calibrated range group defined, **Group 1**, where Peak 2 falls within the time range defined for the group. In this situation, there are various options on how to treat the named peak as part of the group.



The various reports are generated based on the options selected in the **Group Range Definition** dialog. This appears when you define the group graphically, or when you click the group def field in the Group Table.

Example 1

In this example, the concentration of Peak 2 is calculated using its own response factor and its area is used in the calculation of the group response factor. (**Include named peaks** option is **On**.) The concentrations of unnamed peaks in the group range are calculated using the group response factor. The group concentration is calculated by summing the concentrations of the peaks defined for the group. The total group is not included in the individual peak report, but is listed separately in the group report section. Because the group total is not included as a separate line in the peak table, the Area% and Norm concentrations add up to 100%. (**Calculate**

Name	Retention Time	Area	Area Percent	ESTD Conc	NORM Conc	Response Factor
Peak1	5.719	462656	25.363	40.000	30.891	10405.54
Peak 2 (Group1)	6.558	394564	21.630	8.000	6.178	38653.03
Group 1	6.932	1750	0.096	2.479	1.914	705.93
Group 1	7.435	6360	0.349	9.009	6.958	705.93
Peak3	8.264	375582	20.589	30.000	23.168	10020.50
Peak4	8.530	583249	31.974	40.000	30.891	13135.42
Totals		1824161	100.000	129.488	100.000	
Group 1		402674	22.074	19.488	15.050	705.93
Totals		402674	22.074	19.488	15.050	

concentration for unnamed peaks option is **On**.)

Example 2

In this example, the concentration of Peak 2 is calculated using its own response factor and its area is used in the calculation of the group response factor. (**Include named peaks** option is **On**.) The concentrations of unnamed peaks in the group range are not calculated and reported individually. The group concentration is calculated using the total area of all defined group peaks and the group response factor. The total group concentration is included in the individual peak report. Because the group total is included as a separate line in the peak table, the Area% and Norm concentrations do not add up to 100%. (**Calculate concentration for unnamed peaks** option is **Off**.)

Name	Retention Time	Area	Area Percent	ESTD Conc	NORM Conc	Response Factor
Peak1	5.719	462656	25.363	40.000	5.810	10405.54
Peak 2 (Group1)	6.558	394564	21.630	8.000	1.162	38653.03
Group 1	6.932	1750	0.096	0.000	0.000	705.93
Group 1	7.435	6360	0.349	0.000	0.000	705.93
Peak3	8.264	375582	20.589	30.000	4.358	10020.50
Peak4	8.530	583249	31.974	40.000	5.810	13135.42
Group 1		402674	22.074	570.414	82.859	705.93
Totals		2226835	122.074	688.414	100.000	

Example 3

In this example, the concentration of Peak 2 is calculated and reported using its own response factor. Its area is NOT used in the calculation of the group response factor. (**Include named peaks** option is **Off**.) The concentrations of unnamed peaks in the group range are calculated using the group response factor. The group concentration is calculated by summing the concentrations of the peaks defined for the group. The total group is not included in the individual peak report, but is listed separately in the group report section. Because the group total is not included as a separate line in the peak table, the Area% and Norm concentrations add up to 100%. (**Calculate concentration for unnamed peaks** option is **On**.)

Name	Retention Time	Area	Area Percent	ESTD Conc	NORM Conc	Response Factor
Peak1	5.719	462656	25.363	40.000	2.649	10405.54
Peak 2 (Group1)	6.558	394564	21.630	8.000	0.530	38653.03
Group 1	6.932	1750	0.096	300.343	19.892	5.83
Group 1	7.435	6360	0.349	1091.533	72.293	5.83
Peak3	8.264	375582	20.589	30.000	1.987	10020.50
Peak4	8.530	583249	31.974	40.000	2.649	13135.42
Totals		1824161	100.000	1509.876	100.000	
Group 1		8110	0.445	1391.876	92.185	5.83
Totals		8110	0.445	1391.876	92.185	

Example 4

In this example, the concentration of Peak 2 is calculated and reported using its own response factor. Its area is NOT used in the calculation of the group response factor. (**Include named peaks** option is **Off**.) The concentrations of unnamed peaks in the group range are not calculated and reported individually. The group concentration is calculated using the total area of all defined group peaks and the group response factor. The total group concentration is included in the individual peak report. Because the group total is included as a separate line in the peak table, the Area% and Norm concentrations do not add up to 100%. (**Calculate concentration for unnamed peaks** option is **Off**.)

Name	Retention Time	Area	Area Percent	ESTD Conc	NORM Conc	Response Factor
Peak1	5.719	462656	25.363	40.000	2.649	10405.54
Peak 2 (Group1)	6.558	394564	21.630	8.000	0.530	38653.03
Group 1	6.932	1750	0.096	0.000	0.000	5.83
Group 1	7.435	6360	0.349	0.000	0.000	5.83
Peak3	8.264	375582	20.589	30.000	1.987	10020.50
Peak4	8.530	583249	31.974	40.000	2.649	13135.42
Group 1		8110	0.445	1391.876	92.185	5.83
Totals		1832271	100.445	1509.876	100.000	

About Reports

Standard Reports and Method Reports use the Report Editor, which is similar to a word processing program. You can change fonts, colors, margins, insert chromatograms, graphics, system information, even multimedia sound and video clips.

Advanced Reports use a spreadsheet approach. Formulas can be entered for creating a customized display of simple statistics or complex mathematical computations for the data.

Intelligent Reports provide an easy way to create and modify

templates.

Standard report templates are provided to enable you to easily print reports.

See Also

About Report Templates

Standard Reports

Advanced Reports

Intelligent Reports

Standard Report Templates

About Sequence Reports

About report templates

Report templates are report designs that enable you to customize your reporting by creating a report design that can be reused or modified as desired.

A suite of standard report templates for all types of reports is provided. These can be used as-is or can be modified and saved as new templates.

Standard Report Templates

Standard templates for all reports are provided with the data system, however you may wish to create your own or edit the templates provided. Standard report templates (Area %, External Standard, Internal Standard, and Normalization) are provided and have the **.SRP** extension. You can create new standard report templates by saving your report template using the **.SRP** extension. Examples of the standard reports can be found in the Standard Report Templates section.

Sequence Reports

Sequence summary reports are created and saved using the Advanced Reports editor. Sequence report templates are not saved as part of the sequence file, and therefore must be saved as a template file if you want to use a sequence report template to generate a report. Standard sequence report templates provided (Calibration, Summary, Duplicate, QCCheckStd, Spike, and SysSuit), have the **.brp, .tpl,** or **.rdl** extension. See About Sequence Reports and About Sequence Summary Reports.

Sequence report templates are used for reporting data generated during batch sequence operations. For example, certain **Run Types** require a report template for reporting the data. When you designate a run as a **Begin Summary** run, for example, you will be required to designate a template name for the summary report. Other run types requiring templates include Suitability, QC Check Standards, and Duplicates.

Standard reports

Create and edit Standard reports and Method reports in the report editor.

See Also

Open a Standard Report

Open a Method Report

Save a Standard Report

Save a Method Report

Using the Report Editor

Open a standard report

To open a blank standard report, in the navigation pane select the **Report > Standard Report**.

Open a method report

To open a method report, select **Method > Report**. The report editor will open with either a blank page where you will create your report, or the current method custom report.

Click the **Edit the Custom Report** button  to open the method report for editing.

The Method Report is part of the method and is not saved as a template.

Save a standard report

To save a standard report with the current file name:

Select **File > Save > Standard Report**.

To save a standard report with a new file name:

1. Select **File > Save As > Standard Report.**
2. The **Save Standard Report Template File As** dialog box opens to the template folder in your project files, and **Save as type** is set to **.rep**.
3. In the **File name** field, type the filename, or select it from the drop down list.
4. Select **Save**.

Save a method report

The Method Report is part of the method and is not saved as a template.

If you have opened a method report that is linked to a method, it is saved automatically when you close the report.

Using the report editor

The Report Editor allows you to create and edit reports.

The Report Editor is similar to a word processing program. You can change fonts, colors, margins, insert chromatograms, graphics, system information, even multimedia sound and video clips.

In addition to free-form text, you can select a wide variety of information and objects to be placed in your report. These items are presented in four categories:

- Field items are individual fields of information related to the current data. File name, method name, and injection volume are examples of chromatography field items.
- Graph items generally contain groups of graphically related information that belong together. Chromatograms are examples of graph items. These items can be placed, moved, and edited independently of other items on the report.
- Reports are tables of information where the user defines the columns. A report table can include, for example, compound name, retention time, and concentration, and/or a variety of other sample-related items. Report tables can be formatted with fonts, centering, and decimal places. Reports are inserted as tables, because the number of rows is dynamic and can change from run to run.
- Object items are non-chromatography objects that enhance or aid in the usefulness of your report. These objects can include bitmap graphics, Excel spreadsheets or graphs, audio or video clips.

See Also

Basic Report Editor Functions

Using Print Preview

Short-Cuts

Create Headers and Footers

Add Lines and Boxes

Add Fields

Add a Chromatogram

Import a Report

Place a Graph Next to a Report

Add Objects

Adding a Calibration Curve

Print Reports

Insert a Report Table

Basic report editor functions

To set default font:

1. In the report editor, click the right mouse button and select **Edit > Text > Font**.
2. In the font dialog box, select font, font style, size, color, and effects.
3. Select **OK.**

These commands are also available on the toolbar. You can use the drop-down font selection to change the current font, or to quickly change a section of highlighted text without changing the default font. Use the color button, along with the Bold, Italic, Underline, and strike-through buttons to quickly format these aspects of the text.

To set justification:

In the report editor, click the right mouse button and select **Edit > Text > Left Justify, Center Justify,** or **Right Justify**. These commands are also available on the toolbar.

To add/remove bullets:

In the report editor, click the right mouse button and select **Edit > Text > Bullets**. `

This command is also available on the toolbar  .

To turn off the bullets, click the **Bullets** button again.

To add borders and shading:

1 In the report editor, click the right mouse button and select **Edit > Text > Borders and Shading**.

This command is also available on the toolbar  .

2 Select the check boxes where the border or shading is to appear.

3 Type the percent of shading to apply, if desired.

4 Click **OK** to apply the borders and shading.

To set the zoom Levels:

Select the level of magnification for viewing your report by clicking the **Zoom** button on the command ribbon, then selecting the zoom level. You can zoom in to get a close-up view of your document (increase %zoom), or zoom out to see more of the page at a reduced size (decrease %zoom).

To set default margins:

To set margins for the report, click the right mouse button, followed by **Margin Setup...** A dialog will appear for you to enter the units (inches or centimeters) and margins for the page (right, left, top, and bottom).

Other features:

- Ruler which shows position relative to the page. Black arrows that can be dragged to suit your needs indicate margins and indents.
- Command ribbon that contains frequently used commands for formatting. These buttons include bold, italic, underline, strike-through, color, left justify, center, right justify, view header/footer, add buttons, borders/shading, and zoom. When clicked, the formatting represented by these buttons will be applied to any text or item currently selected. Once a formatting button is clicked, it remains in effect for new text until the button is clicked again.
- Right mouse click access to menus for inserting chromatograms, report objects, chromatography, method information, and electronic results signoff fields.
- Items inserted into the report must first be activated by clicking on them in order to edit or move them.
- Report tables can be removed quickly with a right mouse click inside the table, followed by selecting the **Delete Table** command.

Using print preview

You can preview the current custom report by clicking the **Print Preview** button on the command ribbon, or by doing a right mouse click followed by **Print Preview...** . The Print Preview screen allows you to examine one or two pages of the current report at a time.

When you are in the print preview screen, the cursor temporarily

turns into a magnifying glass image. You can click on a location of the report to zoom in for details.

Print

Click this button to print the report.

Next Page

Click this button to view the next page of the report.

Prev Page

Click this button to view the previous page of the report.

Two Pages

Click this button to view two pages of the report at a time.

Zoom In

Click this button to zoom in on the chromatogram. This has the same effect as clicking on the report when the cursor has a magnifying glass shape.

Zoom Out

Click this button to zoom out one level.

Close

Click this button to return to the custom report editor.

Short-Cuts

There are a number of short-cut ways to customize the appearance of the information in the report editor.

Quick-Undo

If you want to reverse, or undoan action you just performed, press **Ctrl-Z**. The action (such as insert a field) most recently performed will be reversed. This is the same as doing a right mouse click followed by the **Edit > Undo** command.

Select all

Press **Ctrl-A** to select the entire custom report.

Quick copy/cut/paste

Press **Ctrl-C** to copy the selected item.

Press **Ctrl-V** to paste the item.

Press **Ctrl-X** to cut a selected item.

Forcing a Page Break

When you want to cause a certain element of your report to be printed always at the top of a new page, you should insert a page break before that item.

To insert a page break on your custom report, position your cursor at the point where you want the new page to begin, then press **Ctrl Enter** on your keyboard. This will force whatever follows in the report to be printed on a new page of paper when the report is printed. A page break is indicated on the custom report template by a dotted line that extends completely across the page. To remove a page break, move the cursor to just below

the page break line, and press the **Backspace** key until the page break is removed.

Tab Stops

Tab stops are used to align items on a page. By default, tab stops are set every ½ inch. However, you can move the tab stops so that there is room between items to accommodate changes (such as field items that change in length). To set a new tab stop, use your mouse to insertthe tab onto the ruler bar at the top of the page, as described below. Once you have inserted a new tab stop, you can move it by clicking and draggingit to a new location on the horizontal ruler. To remove a tab stop, click on it and dragit completely to the left of the horizontal ruler.

Left Tab Stop  Click the left mouse button on the ruler at the location for the new tab. A left tab stop left-justifies tabbed text to that location.

Right Tab Stop  Click the right mouse button on the ruler at the location for the new tab. A right tab stop right-justifies tabbed text to that location.

Center Tab Stop  Hold the shift key down and click the left mouse button on the ruler at the location for the new tab. A center tab stop center-justifies tabbed text to that location.

Numeric Tab Stop  Hold the shift key down and click the right mouse button on the ruler at the location for the new tab. A numeric tab stop aligns the tabbed text to the decimal point.

Create headers and footers

If you want to enter information that will appear on every page of your report, click the **View Header/Footer** button or click the right mouse button anywhere in the report area, then select **Header/Footer**. This will allow you view and edit the header and footer area of your report. To edit the header or footer, click your mouse in the displayed header or footer area and enter the information you want to include. **Note** that this area can contain both free text as well as chromatography fields and objects. It may not include report tables or drawing objects.

When you have finished formatting the header and/or footer, you can turn off the display of the header and footer by again clicking the **View Header/Footer** toolbar button, or the right mouse button, followed by **Header/Footer**. **Note** the check mark next to **Header/Footer** is turned off.

Add lines and boxes

You can add emphasis to your report by drawing lines, rectangles, and text boxes.

Draw and move a line

To add a line to your report, click the right mouse button and select **Drawing > Line**.

A line will appear at the location of your cursor. Activate the line by clicking on it with the mouse. A box will appear at each end of the line and the cursor will change to a +. You can click and drag the line handles to change its size and orientation on the page (angle). You can also drag and drop the line by selecting it with your mouse, holding down the mouse button and dragging the line to a new location on the report.

Draw and move a rectangle

To add a box to your report, click the right mouse button and select **Drawing > Rectangle**.

A rectangle will appear on the report where your cursor was located. To size the box, click on it, then drag the edges to the size desired. To move the box, click the box to activate it, then move the cursor to just **outside** the box, where the cursor becomes a +. Then hold down the mouse button and drag and drop the box in its new position.

Draw and move a text box

To add a text box to your report, click the right mouse button and select **Drawing > Text Box**.

A rectangle will appear with a cursor where you can type text. This tool creates an independent text box in the location of your cursor. To move the text box, click the text box to activate it, then move the cursor to just **outside** the text box, where the cursor becomes a +. Then hold down the mouse button and drag and drop the box in its new position.

Positioning Graphs Next to Tables

You can use the Text Box function to move a chromatogram or other graph to a position next to a report table. To do this, first create a text box. Then click inside the text box and insert a graph. Once the graph is inserted in the text box, you can use the drag and drop feature of the text box to move the chromatogram or graph to a position adjacent to a report table on your custom report. **Note** that you cannot place a report in a text box. See Place a Graph Next to a Report.

Add fields

To add a selected field of information:

1. In the report editor, do a right mouse click where you want to insert the field, and then click **Insert Field.**
2. Select the field you wish to insert from the selections shown.

When you click on any of the Field items, it will be placed on your report at the current location of your cursor. These items can be placed individually, or they can be grouped together to create a custom area of chromatography information for your report. These items are updated to reflect current data information whenever a report is printed or viewed. They can also be updated by choosing the **Update Fields** command from the right mouse click menu, or by pressing the **F9** key to update the current field.

Note: The directory path shown for data files in reports is the originally specified directory path, even if the data has been subsequently moved.

Once a field is added to the report, you can move it, change the font, and the appearance. The formatting will remain constant, however the field information will change as each report is printed to reflect the current information.

Add a chromatogram

You can include as many chromatograms in your report as you wish. Each chromatogram can appear in its own region, or you can display multiple chromatograms, pump profiles, or graphs in the same region. You can include chromatograms that have been saved on disk, and you can include current data that will change as each run is acquired.

To add a chromatogram or trace:

1. In the report editor, do a right mouse click where you want to insert the trace and then click **Insert Graph** followed by **Data Graph**.
2. In the **Data Graph Properties** dialog box, select the data source and set the appearance and annotations desired for the graph. The spreadsheet allows you to add chromatograms or other traces to the current graph. Each row represents a trace which will appear in this graph. For each row, you must designate how you want the data to be displayed.
3. After the graph has been inserted, to modify any of these items or add traces, click the right mouse button anywhere in the trace box, and make the desired changes.

Note: If you insert Current Data into your report, it will be updated whenever your current data changes. Therefore you can see the effects of integration by clicking the Analysis button while you are in the custom report screen.

Import a report

You can import an existing report template into a report in the report editor. When you import a report template, it will replace the current report template.

To import an existing report:

1. In the report editor, do a right mouse click and then select **Import Report** You will be asked if you want to overwrite your current report.
2. If you click **Yes**, a dialog box opens where you can select the report you want to import. When you select the new report and click **Open**, the current report information will be replaced with the selected report.
3. If you click **No**, the existing report will remain and no report import will be performed.

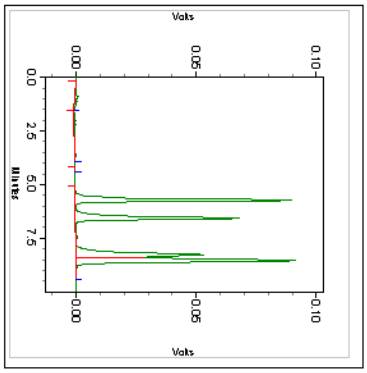
Place a graph next to a report

To insert a chromatogram (or other graph) adjacent to a report:

1. To draw a text box on your report, click the right mouse button and select **Drawing > Text Box.**
2. To insert a chromatogram (or other graph) into the text box, click the right mouse button and select **Insert Graph > Data Graph.**
3. To move the text box with the chromatogram/graph inside, click on the border of the text box until the black rectangular handles appear. Then move the cursor just outside the border until the cursor turns to crosshair +. Then hold down the left mouse button and drag the text box with the graph a new location (for example, next to a report) and then release the mouse button.
4. To edit the chromatogram/graph (annotations, etc.), double-click the mouse within the chromatogram/graph. Make sure you have selected the chromatogram and not the text box. To resize the chromatogram, select the text box (look for the text box handles), then click and drag the handles to the desired size.

   Note that you cannot place a report in a text box.

Name	Retention Time	Area
Peak1	5.729	779320
Peak2	6.568	667324
Peak3	8.283	633854
Peak4	8.540	994037
Totals		
		3074535



Add objects

Custom reports have full Object Linking and Embedding (OLE) support. This means you can add objects that are linked to other Windows applications, such as Excel. You can even add a video clip or voice recording to your report. These items are added as Objects to your report.

A variety of objects (graphs, charts, bitmaps, logos, word documents) can be added to a custom report.

To add an object to your report:

1. In the report editor, do a right mouse click at the location where you want to insert the object. Click **Insert Object...**.
2. In the Insert Object dialog box, select **Create New** to create a new object of the selected **Object Type**, or select **Create from file** to browse to and select the object from existing files. If creating from a file, click the **Link** box to create a link from the report to

the object in the report.

3 Click **Display as icon** to display the object as an icon in the editor. You can also select an icon to use for the object if this is selected.

There are a variety of object types to insert, based on the applications you have installed on your computer. For many selections, inserting an object will cause an application to runwithin your report editor, allowing you to modify and edit the object. To exit the application back into the custom report, simply click anywhere outside the object area on the report. You can create a new object to insert, or you can open an existing object file to insert.

For example, a Microsoft Excel chart can be inserted as an object into the custom report. When the Excel chart is inserted, the menus and ribbons from Microsoft Excel become available and are active for you to edit and modify the object.

If an OLE object, such as a Microsoft Excel chart, is inserted as a linked object it will be updated automatically in the custom report if the chart changes. This creates a very efficient way of combining data for reports.

Adding a calibration curve

1 In the report editor, click the right mouse button and select **Insert Graph/Calibration Curve.**

2 In the **Calibration Curve Properties** dialog box, complete the following fields:

- **Source** - Select the source of the calibration curve data from the **Source** drop-down list. Choose **Peaks, Groups, or Template** to select what calibration peak table to use. You should select **Template** only if you are editing a calibration report template. If you select this option within a method report template, the information will not be printed. If you select **Template**, calibration curves for all peaks in the calibration will automatically be printed as defined in the **.crp** calibration report template file.
- **Trace** - For the calibration curve trace, select the specific data to be displayed. When you select a data channel for the trace, you must then select a **Peak** from the list. This peak will always be displayed.
- **View Replicate Points** - Click this box if you want replicate data points to be displayed on the report calibration curve.

3 Click **OK** to enter the calibration curve into your custom report.

Print reports

You can print reports in one of four ways:

- From within the report editor. To print a report from the report editor, use either the Print button in **Print Preview**, or print the report directly by doing a right mouse click followed by **Print**.

- From an instrument window. To print the current method or sequence report, from the menu bar click **Reports** followed by **Print** and then select the report you want to print.
- As a part of data acquisition or reprocessing. A custom report can be printed at the end of each analysis, at the end of a data acquisition run, during or at the end of a sequence. When starting a single run, sequence run, or reprocessing a sequence, select the **Print Hardcopy** and select Method or Sequence. When this box is checked, a report will be printed at the end of the run.

  If there is a loss of communication to the hard copy printer from the OpenLab EZChrom Print Server, files are copied from the monitor folder into the Quarantine folder. After communication to the hard copy printer has been established, files in the Quarantine folder can be copied back into the monitor folder for normal printing. Files in the Quarantine folder are automatically deleted in 24 hours by default. The time to delete folders from the Quarantine folder is set in the configuration file in the Print Server folder.
- Sequence reports are not printed unless the **Print Sequence Reports** option is selected in the **Run Type** column of the sequence spreadsheet. See About Sequence Reports.

Note: When opening an instrument on-line, the configured printer is remembered for that instrument regardless of the user. When opening an instrument off-line, the configured printer is remembered for the user of that instrument.

Insert a report table

Report tables can be inserted into a standard report. The following topics describe the types, creation, and editing of report tables.

See Also

Add a Report Table

Change a Report Table Parameter

Edit the Appearance of a Report Table

Show Report Data at Design Time

Delete a Report Table

Types of Report Tables

Add a report table

There are a variety of report tables you can add to your standard report.

To add a report table:

1. In the report editor, do a right mouse click where you want to add the report table, then click **Insert Report...** A list of available report tables will be displayed.
2. Select the report type you want to insert from the following

options:

Baseline Check Report

Use this command to insert a table with Baseline Check information.

Calibration Info

Use this command to insert a table containing details of your calibration.

Calibration Table

Use this command to insert a table containing the peak calibration details into your report.

Data Audit Trail

Use this to insert the data file audit trail table into your report.

Electronic Signatures Table

Use this command to insert the electronic signatures table into the report.

Extra Sequence Columns

Use this command to insert a table containing name and data for extra sequence columns.

Fraction Report

Use this command to insert a table containing fraction report information.

Generic Report

Use this command to insert a report table file that was created by a user program. A dialog requests you to enter the filename for the generic report file. You can also select the file by clicking the **Open** button.

For details on the required format for generic reports, see About Generic Report Tables.

Instrument Activity Log

Use this command to create or update the template for viewing and printing Instrument Activity logs (LogViewInstActReport.lrp).

Instrument Configuration Report

Use this command to insert a configuration report for the instrument into your report.

Library Definition Report

Use this command to insert a table containing Library Definitions.

Library Search Report

Use this command to insert a library search report.

Method Audit Trail

Use this command to create or update the template for viewing and printing the Method Audit Trail (LogViewMethodAuditReport.lrp).

Method Report

Use this command to insert a report containing method details into your report.

Purity Report

Use this command to insert a purity report.

Run Report

Use this command to insert a table containing chromatography results into your report.

Sequence Audit Trail

Use this command to insert the sequence audit trail into your report.

Spectrum Report

Use this command to insert the spectrum report into your custom report.

Change a report table parameter

To change a report parameter without re-defining the entire report:

1. In the header of the report table, do a right mouse click and select **Change Parameter**.
2. The currently-selected parameter is highlighted. Select the new parameter from the list of available parameters.
3. Enter the number of decimal places to be displayed (for numerical parameters).
4. Type the parameter name as you want it to appear in **Column Header**.
5. Click **OK** to replace the selected parameter with the new one.

Note: This command can be used to replace existing parameters or to update them with new column header name or decimal places.

The current parameter is selected. To change it, simply click on another parameter in the list, then click **OK**.

Edit the appearance of a report table

The right mouse click gives you access to commands for modifying the report table.

Change Column Width

To change a column width, move the cursor over the border of the column until double vertical lines appear. Hold down the mouse button and drag the column border to the width you require.

Change Fonts

To change a font for text in the table, select the text by highlighting it with the mouse, or click once in the field. Then choose one of the formatting buttons to change the formatting to desired appearance. You can change formatting for both column headings and sample data areas.

Change Column Titles/Headers

Default titles for each parameter selected for the report will be displayed. You can change the column titles by editing them in the **Column Header** box in the **right mouse click/Report Properties** dialog. You cannot change the data fields other than formatting changes.

Delete a report table

Report tables can be removed quickly with a right mouse click inside the table, followed by selecting the **Delete Table** command.

Show report data at design time

By default, the software displays template fields when you create report tables in a standard report, without the actual data displayed.

To view the actual data while editing the template, in a table in the report editor, do a right mouse click and then click **Show Data at Design Time**. When this is enabled, the data for the report table will always be displayed in the template while you are editing.

Delete a report table

To delete a table:

1. In the report window, do a right mouse click inside the table, followed by selecting the **Delete Table** command.
2. Click **Yes** to confirm that you want to delete the table from the report.

Types of report tables

To place the following reports into a standard report, right click in the report editor and select **Insert Report**.

* A number of quality control reports can be generated automatically as you run a sequence. They are selected in the Run Type column of the Sequence. The values used to test the results of a sequence analysis are set in the Peak Table of the Method for each component in the analysis. See About Sequence Reports.

See Also

Insert Calibration Information

Insert a Calibration Report

Insert Electronic Signatures

Insert a Filtered Method Report

Insert a Generic Report

Insert an Instrument Activity Log

Insert an Instrument Configuration Report

Insert a Method Audit Trail Report

Insert a Method Report

Insert a Run Report

Modify Run Report Information

Insert a Sequence Spike Report *

Insert a Fraction Report

Insert calibration information

To add the calibration information:

1. In the report editor, do a right mouse click where you want to insert the calibration information, and then click **Insert Report** followed by **Calibration Info.**
2. In the **Calibration Info Setup** dialog box, complete the following fields:
   - **Source** - Select the source of the calibration information from the **Calibration Data Source/Source** drop-down list. Choose **Peaks, Groups,** or **Templates** to select what calibration peak table to use.
     Select **Template** only if you are creating or editing a calibration report template. If you select this for a method report, the information will not be printed. When you select **Template**, calibration information for all peaks in the calibration will automatically be printed, as defined in the **Calibration.brp** calibration report template file.
   - **Detector**
   - **Peak**

Insert a calibration report

To add a calibration table to a report:

1. In the report editor, do a right mouse click where you want to add the calibration table and then click **Insert Report** followed by **Calibration Report**.
2. Select the calibration report options in the dialog box and then click **OK**.
   - **Source** - Select the source of the calibration table from the **Calibration Data Source/Source** drop-down list. Choose **Peaks, Groups,** or **Templates** to select what calibration peak table to use. Do not select **Template** unless you are creating or editing a calibration report template. If you select **Template**, calibration tables for all peaks in the calibration will automatically be printed as defined in the .**crp** template.
   - **Detector**
   - **Peak**
   - **View Replicate RF** - Click this box if you want to display response factors for all replicates in the calibration table.

- **View Replicate Identification Information** - Click this box if you want to display the User, Sample ID, and Calib Time for each replicate.
- **Number of levels to print before break** - Enter the number of calibration levels to print on each line.

3 Click **OK** to accept and enter the calibration table on your custom report template. A calibration table can be removed quickly with a right mouse click inside the table, followed by selecting the **Delete Table** command

Insert electronic signatures

To add an electronic signature table, in the custom report window, do a right mouse click in the report, then select **Insert Report** followed by **Electronic signatures table**. This command will insert a table that contains the electronic signatures for this data file into your report.

To delete an electronic signatures table, do a right mouse click in the table, then select **Delete table** and click **OK**.

Insert a filtered method report

A filtered method report is a condensed method report that can be inserted into a custom report. The Filtered Method Report Layout must be created ahead of time in order to appear in the list of filtered method layouts.

To insert a Filtered Method Report:

1 In the report editor, do a right mouse click followed by **Insert Report** and then select **Filtered Method Report**.

2 Select the filtered method report layout to be inserted. A filtered method report layout must be available in order to use this feature. Once you have selected the report layout, it will be inserted into your report.

Insert a generic report

Use this command to insert a report table file that was created by a user program.

To insert a generic report:

1 In the navigation pane, select **Reports > Standard Report**.

2 In the report editor, right click and select **Insert Report > Generic Report**.

3 A dialog requests you to enter the filename for the generic report file. You can also select the file by clicking the **Open** button.

For details on the required format for generic reports, see the Generic Report Tables topic.

Insert an instrument activity log

To insert a copy of the instrument activity log:

1 In the report editor window, do a right mouse click at the location where you want to insert the report, then click **Insert Report** followed by **Instrument Activity Log**.

2 A table for the instrument activity log will be inserted in your report. This table is a template placeholder and will not display the actual instrument activity report until the custom report is printed.

User	Logged	Activity
Demo	01\02\99 12:34:56	What was changed and how

Insert an instrument configuration report

To add and view a listing of the current instrument configuration:

1 In the report editor window, do a right mouse click at the location where you want to insert the report, then click **Insert Report > Instrument Configuration Report**.

2 A table for the instrument configuration report will be inserted onto your report. The instrument configuration information can be viewed using **Print Preview.**

Instrument Configuration
==========

Instrument Name: Instrument 1
Instrument Type: Generic System

External Events:

Name	Source	Configuration
Trigger	SS420	Board: 0, In0, State : Closed

Detector Name : Detector A - Channel A
Detector Model: Analog
Acquisition Source: SS420
Board: 1, Analog Input: Chan A
Y-Axis Units: Volts
Y-Axis Multiplier: 0.00

Insert a method audit trail report

To insert a listing of the current method's Audit trail:

1 In the report editor window, do a right mouse click at the location where you want to insert the Audit Trail Report, then click **Insert Report** followed by **Method Audit Trail**.

2 A table template for the audit trail report will be inserted on your custom report template. This table is a template placeholder and will not display the actual audit trail report until the custom report is printed.

User	Logged	Source	Activity	Reason
Demo	01\02\99 12:34:56	Source of change	What was changed and how	Why it was changed

Insert a method report

To add details about the current method to your report, select the **Method Report** option from the right mouse click>**Insert Report** menu. A dialog box appears where you select the items from the method you wish to include in your report.

Use the drop-down menu to select the channel(s) from which to display method information. Then select the method items to display by clicking the check-boxes adjacent to the desired items. When finished, click OK.

A method report can be deleted from the custom report template by a right mouse click inside the table, followed by the **Delete Table** command.

Insert a run report

To add run details to a report:

1. In the report window, do a right mouse click where you want to insert the run information, and then click **Insert Report** followed by **Run Report**.
2. In the dialog box, designate items for your report.
3. Click **OK** to insert the run details table into your report.

Data Source	Select the Data Source (current data or stored data file) and the Channel from which you want to display information.
Report	Use the check boxes to select what peaks you want to report. **Named Peaks** Choose **All** if you want to report all calibrated peaks, whether detected or not. Choose **Detected Only** if you want to report only the calibrated peaks detected in the sample. **Unnamed Peaks** Click here if you want to include unnamed peaks in your report. A separate table is not generated. When an unnamed peak is part of an uncalibrated group, the group name is used for each peak in the peak name field in the report. **Groups** Click here if you want to include defined groups in your report. **Totals** Click here if you want to include totals for numeric columns in your report.
Available Parameters	A list of the possible parameters to report is displayed in this box. To add one of the parameters to your report, double-click on it, or click on it with the mouse to select it, then click the Green arrow to move it to the **Report the following parameters** box. You may select one or more of the parameters at a time by holding down either the **Shift** key (to select contiguous parameters), or the **Ctrl** key (to select non-contiguous parameters).

Decimals For each numeric parameter, you can enter the number of decimal places to be displayed. Click the parameter in the **Report the following parameters** box, then type the number of decimals to be shown for that parameter. Default decimals will appear for all numeric parameters.

Column Header Use this box to enter or edit the title that will appear at the top of the column.

Click **OK** to insert the report table into your custom report at the current location of your cursor. The report table will appear on your custom report page, with column headings and data placeholders shown.

Modify the run report information

Once you have inserted a Run Report in your report, you can edit that information.

To edit the run report information:

1. In the **report editor** window, do a right mouse click in the run report table, and select **Report Properties**.
2. In the dialog box, redefine or add items to your report.
3. When you are finished, click **OK**.

Insert a sequence spike report

To add a Sequence Spike report:

1. In the **report editor** window, do a right mouse click, and then click **Insert Report** followed by **Sequence Spike**.
2. Select the **Spike/Unspike** button if the report is to cover a spiked sample followed by an unspiked sample. Select the **Spike 2 of 2** button if you wish a QC Spike report where the unspiked sample is followed by the first spiked sample, followed by the second spiked sample.
3. Check the **Fully qualified filenames** box if you want to include full paths in the file names.
4. Click **OK**. A table template will be inserted into your report for the sequence Spike report. **Note** that this table contains placeholder information only - it does not contain data from your system.

Type	File	Sample ID	Acquired				
UnSpiked	D:\CHRO M\Data\Multical.001	Multi 1	1/30/97 9:28:38 Monday				
Spiked	D:\CHRO M\Data\Multical.001	Multi 1	1/30/97 9:28:38 Monday				
Channel A							
Compound	Unspiked Conc.	Spiked Amount	Spike Conc.	Spike Recovery	Low Limit	High Limit	Status
Peak 1	30.094	30.000	40.034	33.133	25.000	45.000	OK
Peak 1	30.094	30.000	40.034	33.133	45.000	55.000	Low
Peak 1	30.094	30.000	40.034	33.133	5.000	25.000	High

In order for your sequence report to contain valid spike information when it is printed, you must make sure your method and sequence are set up to create a sequence Spike report.

In the Peak Table of the Method, entries are made for the Spike 1 Amount and Spike 2 Amount (if two spiked samples are to be run), the Low Spike Limit and the High Spike Limit. The Low and High Spike limit values are entered as a percentage recovery used to determine whether the test passes or fails.

In the Sequence, one sample must have an **unspiked** Run Type. This is the sample that is not spiked. This sample must be followed by the **spiked** sample. This sample is identical to the **unspiked** sample, except that it has been spiked with the standard component(s).

After the unspiked and spiked samples are analyzed, a report is printed, showing the calculated concentration of the compound(s) in the unspiked sample, the amount(s) entered for the spiked amount(s), the calculated concentration(s) for the spiked sample(s) and the percentage(s) of the spiked amount(s) that is recovered. The recovery percent value is compared to the Low and High Limit values, and the status of the results (Low, High or OK) is printed.

The following is an example of a QC Spike report (template Spike1.brp), where the unspiked sample is followed by the spiked sample.

Type	File	Sample ID	Acquired
UnSpiked	C:\datasystem\data\multilevel003.dat	Multilevel Calibration Level 3	11/26/90 8:49:21 PM
Spiked	C:\datasystem\data\multilevel004.dat	Multilevel Calibration Level 4	11/26/90 8:49:34 PM

Channel A

Compound	Unspiked Conc.	Spiked Amount	Spike Conc.	Spike Recovery	Low Limit	High Limit	Status
Peak1	30.000	10.000	40.000	100.000	90.000	110.000	OK
Peak2	7.000	1.500	8.000	66.667	75.000	125.000	OK
Peak3	25.000	4.500	30.000	111.111	90.000	110.000	OK
Peak4	30.000	10.000	40.000	100.000	90.000	110.000	OK

Spike Report

The following equation is used in this QC Spike report:

$$\text{Spike Recovery} = \frac{100 \times \text{Spiked Conc.} - \text{Unspiked Conc}}{\text{Spiked Amt}}$$

Insert a fraction report

In the **report editor** window, do a right mouse click at the location where you want to insert the report, then select **Insert Report > Fraction Report**. A table for the fraction report will be inserted in your report. The following is an example of a Fraction Report.

Fraction Report

Sample ID:
Data File: C:\projects\Elite\Exe\Enterprise\Projects\Default\Data\4-7-2011 3-14-41 PM.dat
Method File: C:\Projects\Elite\Exe\Enterprise\Projects\Default\Method\VBSample.met
User Name: System
Acquisition Time: 4/7/2011 3:14:48 PM
Fraction Data Points: 4
Instrument Name: VB Sample

Fraction Number	Vial Number	Start Time (min.)	Stop Time (min.)
1	1	0.00	0.25
2	2	0.25	0.49
3	3	0.49	0.74
4	4	0.74	0.98

Advanced reporting

The Advanced Reporting feature uses a spreadsheet format to make it easy to create complex customized reports. A variety of advanced report templates are provided for you that can be easily modified to suit your application (sequence summary reports, for example, are created using an advanced report template). In addition, you can create completely customized report templates that extract virtually any data or file information and apply mathematical functions to it. For example, you can create reports that combine peak data from multiple channels into a single report. Or, you can take the results from a sequence of runs and calculate statistical analysis on them.

Each advanced report begins as an advanced report template. Once the report template is created and saved, it can be used to create and print reports from sequence runs or sequence reprocessing by designating the report template from the Run Type of the run in the sequence.

Note: In order to export advanced reports, a printer must be configured on the computer doing the exporting.

See Also

Create an Advanced Report Template

Format Cell Style for Advanced Reports

Define an Advanced Report Header/Footer

Add a Chart to an Advanced Report

Add Color to Cells in an Advanced Report

Change Advanced Report Grid Properties

Add a Table using the Table Wizard

Add a Function Using the Function Wizard

Advanced Report Audit Trail

View Advanced Reports Audit Trail Log

Save the Advanced Report as a Template

Create an advanced report template

To create a new advanced report template:

1. In the **Navigation** pane, select **Reports > Advanced Report**. A blank spreadsheet template will appear.
2. Define the new template by inserting data series, formulas and text into the cells of the spreadsheet. You can also define a header and footer, insert charts of data, and format the cells. See **Advanced Reporting** above for links to these topics.

3 Select **File > Save As > Advanced Report**. In the **Save Advanced Report File As** dialog box, navigate to the template folder. Enter a **File name** and select **Save**.

Format cell style for advanced reports

There are a wide variety of ways to automatically format the style of the selected cell (or cells).

1 Select a cell to format, and select the **Cell Style** button 

.

2 In the **Cell Style** dialog box, select a **Category**. Based on your selection, fields on the right may be come active to further define the cell style.

3 Under **Decimal places**, enter the number of decimal places to be displayed for numeric data.

4 Select from the following:

- **Floating** - If this is selected, text or numeric data that exceeds the width of the cell will automatically floatinto the next cell (if empty). If this selection is **Off**, the text or data that extends beyond the limits of the cell width will be either truncated, or displayed with an overflow indicator selected.
- **Word Wrap** - When this button is selected, information entered into a cell will be wrapped to the next line when the end of the cell is encountered.
- **Normal** - When this button is selected, information will be displayed in the default mode.

5 In the **Overflow indicator** drop down box, select the way cells that overflow are to be displayed: with no indicator, with ellipsis (e.g. **cell overflow is...**), or with pound sign (##########).

6 Select **OK.**

Define an advanced report header/footer

To define the header and/or footer for the report, click the right mouse button on the spreadsheet and select the **Header/Footer...** command. A dialog will appear where you define the contents of your header and footer.

Click in one of the fields of the **Left Aligned**, **Centered**, or **Right Aligned** columns. You can type text that will appear with the indicated alignment, or you can insert field codes for automatic insertion of items such as date, time, and page numbers. When you have a cell selected, you can change the font by clicking the **Font...** button and selecting the desired font and characteristics.

Note: Font colors are not supported in the header and footer sections.

Field codes that can be inserted in a header or footer:

$F Report Template Name

$P Page number

$N Number of pages

$SEQNUM Sequence page number

$D Date – you can specify the date formatting with an additional parameter, as for example $D{%h:%m}

Date format codes:

%a Abbreviated weekday name

%A Full weekday name

%b Abbreviated month name

%B Full month name

%c Date and time representation appropriate for locale

%d Day of month as decimal number (01 - 31)

%H Hour in 24-hour format (00 - 23)

%I Hour in 12-hour format (01 - 12)

%j Day of year as decimal number (001 - 366)

%m Month as decimal number (01 - 12)

%M Minute as decimal number (00 - 59)

%p A.M./P.M. indicator for 12-hour clock

%S Second as decimal number (00 - 59)

%U Week of year as decimal number, with Sunday as first day of week (00 - 51)

%w Weekday as decimal number (0 - 6; Sunday is 0)

%W Week of year as decimal number, with Monday as first day of week (00 - 51)

%x Default Date representation

%X Default Time representation

%y Year without century, as decimal number (00 - 99)

%Y Year with century, as decimal number

%z, %Z Time-zone name or abbreviation; no characters if time zone is unknown

Distance to frame

The values you enter here determine how far the header and footer are placed from the edge of the paper. This value is independent of the paper margin, and if set incorrectly can result in overlap with the body of the report.

To view headers and footers:

When you click the **OK** button, the header and footers defined will become part of your template, however they will not appear. To view the header and footer, click the **Print Preview** button and zoom in to see the details.

Add a chart to an advanced report

To add a chart to an advanced report:

1 Open the advanced report template.

2 In the advanced report template editor, do a right mouse click where you want to add the chart, and then click **Insert** followed by **Chart**.

3 Complete the parameters and then click **OK** to insert the chart.

Chart Title	Enter a title that will appear at the top of your chart.
Font	Click this button to change the font for your chart title.
Chart Style	Select the style for your chart from the drop-down list.
Initial Cell	Enter the cell where the initial data is located (the first cell of a series, for example). In many cases, the cell location you want to enter is the cell where the formula for the data series is defined.
Data Set	Select whether the data series extends vertically or horizontally on the spreadsheet.
Groups	Choose **Single** to display one series of data or **Multiple** to display more than one series of data. For example, in a sequence summary report where the summary table contains areas from 4 peaks in 5 runs, you would choose Single to chart areas from one peak, or Multiple to chart areas from all 4 peaks.
Group Titles	Enter a cell reference to be used for titles(legends) for the charted data series, or type in text to be used.
Show example chart	Check this box if you wish to view an example of the chart in your advanced report spreadsheet. (**Note**: This is not the actual data. To view the actual data in the chart, click the print preview button.)

Add a fill color to cells in an advanced report

Use the paint bucket tool to add color to cells in an advanced report.

To add a fill color to cells:

1 Open an advanced report.

2 Select the cells you wish to color.

3 Select a color using the arrow next to the paint bucket icon  .

Change advanced report grid properties

To format the general characteristics of your advanced report, click the right mouse button in the spreadsheet, and select **Grid Properties.** A dialog will appear where you can customize the grid size, margins, page order, and default cell style.

Grid Size	You can limit the size of the report spreadsheet to make it more manageable.
Row count	To limit the number of rows in your report, type in a number here.
Column count	Enter a number of columns for your report.

Autosize grid when generating reports	When this is selected, the spreadsheet grid will automatically be reduced to include only the number of rows and columns required for your report when printing. If this is not selected, empty rows and columns will be printed.
Page Order	Select the order for printing pages.
Margins	Enter the page margins in the fields indicated. This will establish the margins used for printing the body of the advanced report. **Note** that these margins are independent of the distance to frame setting in header and footer.
Default Cell Style	Select the default setting for your cell style. Any cell or range of cells can be changed from this independently.
Floating	If this is selected, text or numeric data that exceeds the width of the cell will automatically float into the next cell (if empty). If this selection is **Off**, the text or data that extends beyond the limits of the cell width will be either truncated, or displayed with an overflow indicator selected.
Overflow indicator	Select the way cells that overflow are to be displayed: with no indicator, with ellipsis (e.g. **cell overflow is...**), or with pound sign (##########).
Word Wrap	When this button is selected, information entered into a cell will be wrapped to the next line when the end of the cell is encountered.
Normal	When this button is selected, information will be displayed in the default mode.

Add a table using the table wizard

Use the **Table Wizard** to create tables in advanced reports.

1. In the navigation pane, select **Reports > Advanced Report**.
2. Select a cell where you would like your table to be located, and select the **Table Wizard** button.
3. In the **Table Type** dialog box, select the type of table from those available, and select **Next**.
4. In the **Parameters** dialog box, select **Peaks** or **Groups** from the drop down list.
5. Select a parameter from the list on the left by double-clicking it. You may select as many parameters as you wish. If the parameter is numeric, you can enter a value for **Precision**, or accept the value presented.
6. Select the **Trace index** of the channel you want to include (if using a multichannel file), where 1 = first trace, 2 = second trace, etc, and select **Next**.
7. In the **Types** dialog box, select the types of peaks or groups to be included in your summary by checking the box(es), and select **Next**.
8. In the **Run Parameters** dialog box, double click each parameter you want to include for each run in the summary table, and select

Next.

9 In the **Run Direction** dialog box, select which direction you want the runs to be displayed on the table, and select **Next.**

10 In the **Statistics** dialog box, select **Yes** if you want to include a statistics section in your table. Calculated statistics include Min, Max, Mean, Std. Deviation, and %RSD.

11 Select **Finish**. A sequence summary table will be inserted in your Advanced Report at the current cell location.

Add a function using the function wizard

Functions bring data into the report by extracting the desired information from the data system. The Function Wizard enables you to select the type of information to be displayed and how it will appear on the report. The result of your choices becomes a formula (a combination of functions) that is placed in the currently selected spreadsheet cell.

To use the Function Wizard:

1 In the **Navigation** pane, select **Reports > Advanced Report**.

2 Select a cell where you would like your table to be located, and select the **Function Wizard** button .

3 The Function Wizard will step you through the following dialogs that will help you define the information to be inserted in the selected cell.

See Also

Function Wizard Select Function

Function Wizard Dynamic Data

Function Wizard Data Direction

Function Wizard Types

Function Wizard Identification

Advanced Reporting Formulas and Functions

Functional Reference

Function wizard select function

The Function Wizard options will change depending on your selections in this dialog box.

1 In the **Select Function** dialog box, under **Data Source** select **Sequence file** or **Current data file**.

2 Select a category from the following options:

- **Data** - Data and parameters available in a data file
- **Group** - Information from the group table
- **Instrument** - Instrument parameters (ID, Name, User Name)
- **Peak** - Information from the peak table
- **Project** - Project name and associated paths

- **Sequence** - Sequence names, run numbers, and run types

3 Select a function from the list on the right. Detailed descriptions of all functions can be found under Advanced Reporting Formulas and Functions and Functional Reference.

4 Select **Repeating formula** if the formula is to be repeated for a series of peaks or files, then select **Next**.

Function wizard dynamic data

This screen only appears if you have selected the **Repeating formula** box. The questions here enable you to specify the source of data for repeated formulas.

When Advanced Report is used to display dynamic data, such as data from a sequence of runs, or peaks from every run where the number of peaks may change, the report uses Dynamic Data Functions. This type of function enables the report to expand or contract by repeating the function for all data that meet the specified requirements.

1 In the **Dynamic Data** dialog box, select from the following options:

- **Repeat formula for all runs in a sequence** - Select this box to extract the designated data from all runs of the sequence. For example, if the selected function is peak area from a sequence file, this option would enable you to select one peak from a trace of the sequence and then report its area for each run in the sequence.
- **Repeat formula for all peaks or groups** - This option will extract the designated information for all peaks or all groups of a sequence run you select. (Sequence run number prompt appears when this option is chosen.) For example if the selected function is peak area from a sequence file, this option would extract the area for all peaks or groups of the chosen sequence run.
- **Repeat formula for all runs in a sequence** and Repeat for all peaks or groups - If you select **both** options, the formula will be repeated for all runs and all peaks/groups of the sequence. For example, if the selected function is peak area from a sequence file, the combination of these options would produce a listing of areas for all peaks in every sequence run.

2 Select **Next.**

Function wizard data direction

In the **Data Direction** dialog box, select how you want the data series to be displayed:

- **Across** the row
- **Down** a column

Function wizard types

This dialog allows you to select the peak or group information.

Peaks

Using

Select the boxes for the type of peaks you will be using.

Trace Index

Select the trace number (if multichannel files), where the first trace = 1, second trace = 2, etc.

Groups

When you select groups to generate the data, the following choices appear.

Using

Select the type of group to be reported. Calibrated range and named peak groups are supported. For Calibrated range groups, if you have defined your group to calculate concentrations for unnamed peaks you can include these in your group reporting by selecting the appropriate button.

Trace Index

Select the trace number (if multichannel files), where the first trace = 1, second trace = 2, etc.

When you are done with this dialog, click **Finish**. The function defined by your answers to the Function Wizard will be inserted in the currently selected cell.

Function wizard identification

Peak

If a peak function is specified, this dialog allows you to designate which peak to report.

Trace Index

Select the trace number (if multichannel files), where the first trace = 1, second trace = 2, etc.

Peak Index

If you select this button, enter the peak index number for the peak of interest, where the first peak = 1, second peak = 2, etc.

Peak ID

If you select this button, enter the Peak ID number from the peak table for the peak of interest.

Using

Select the boxes for the type of peaks to include.

Group

If a group function is specified, this dialog allows you to designate which group to report.

Trace Index

Select the trace number (if multichannel files), where the first trace = 1, second trace = 2, etc.

Group Index

If you select this button, enter the group index number for the group of interest, where the first group = 1, second group = 2, etc.

Using

Select the type of group to be reported. Calibrated range and named peak groups are supported. For Calibrated range groups, if you have defined your group to calculate concentrations for unnamed peaks you can include these in your group reporting by selecting the appropriate button.

Advanced report audit trail

To turn on the Advanced Report Audit Trail:

1. From the **Reports** menu, click **Advanced Report Properties**.
2. Select the **Audit Trail** tab.
3. Select **Enable audit trail** to turn on the audit trail for Advanced Report Templates.
4. Select from the following options:
   - **Prompt for reason when saving file** - This option requires the user to enter a reason for each change when the template is saved.
   - **Do not prompt for reason** - When this option is selected, changes are documented, but the user is not required to enter a reason for the changes.

View advanced report audit trail log

To view the Advanced Reports Audit Trail Log:

1. In the toolbar, select **Reports > Advanced Report Properties**.
2. Select the **Audit Trail Log** tab.
3. Enter the following:
   - **User**
   - **Location**
   - **Description**
   - **Reason**
   - **From date/time**
   - **To date/time**
4. Select from the following options:
   - **Export** - Select this to export the audit trail log
   - **Print** - Select this to print the audit trail log
   - **Search** - Select this to search the audit trail log

Save the advanced report as a template

1 Select **File > Save As> Advanced Report**.

2 In the **Save Advanced Report File As** dialog box, select the templates folder.

3 Enter a **File name** and select **Save**.

Intelligent reports

You can easily create and modify templates using Intelligent reports. Report templates are saved in the standardized Report Definition Language (RDL) format that is also used by Microsoft Business Intelligence Studio.

See Also

Create an Intelligent Report

Open an Intelligent Report

Save an Intelligent Report

Create an intelligent report

To create a new Intelligent Report, in the navigation pane or the toolbar select **Report > Intelligent Report**. The Open Lab Intelligent Report (OLIR) editor opens.

To create a new Intelligent Report using the Report Wizard, in the toolbar select **Reports > Intelligent Report with Wizard**. The Report Wizard opens.

Open an Intelligent Report

To open an Intelligent Report from your project files:

1 In the toolbar select **File > Open > Intelligent Report**.

2 In the **Open Intelligent Report File** dialog box, navigate to the **Template** folder and select an **.rdl** file.

3 Select **Open**.

To open an Intelligent Report from the templates in your data system:

1 In the toolbar select **File > New**.

2 In the **New File Templates** dialog box, select the **Report** tab.

3 Select an **.rdl** file.

4 Select **OK**.

Save an intelligent report

To save an Intelligent Report:

In the toolbar select **File > Save > Intelligent Report**.

Or,

In the toolbar select the **drop down menu** next to the Save icon  and select **Save Intelligent Report**.

To save an Intelligent Report with a different name or location:

1. In the toolbar select **File > Save As > Intelligent Report**.
2. In the **Save Intelligent Report File As** dialog box, navigate to the folder where you wish to save the report.
3. Enter a **File name**, and **Type**, and select **Save**.

Standard report templates

Standard report templates are provided to enable you to easily print reports.

To open a standard report template:

Select **File > Open > Standard Report**. In the **Open Standard Report File** dialog box, navigate to the **Templates** folder.

Or,

In the **Navigation** pane, select **Reports** and select a standard report template. Some examples are listed below.

See Also

Area %

ConfigContents Report

Current Baseline Check

External Standard

Internal Standard

Normalization

Error Condition Flags

Area % report

This is an example of the Area % (**Area%.srp**) report template output.

Area % Report **Page 1 of 1**

Method Name: C:\datasystem\methods\multicalibration.met
Data: C:\datasystem\data\multicalibration001.dat
User: System
Acquired: 11/26/90 8:51:56 PM
Printed: 4/10/97 8:29:23 AM

Channel A Results

Pk #	*Retention Time*	*Area*	*Area %*	*Height*	*Height %*	*Codes*
1	5.729	779320	**25.26**	90135	29.67	BV
2	6.568	667324	**21.63**	68471	22.54	VV
3	7.041	2005	**0.06**	185	0.06	VV
4	7.475	8964	**0.29**	661	0.22	VV
5	8.273	633854	**20.54**	52979	17.44	VV
6	8.540	994037	**32.22**	91392	30.08	VV
Totals		3085504	**100.00**	303823	100.00	

ConfigContents report

This is an example of the ConfigContents Report (**ConfigContentsReport.srp**) report template output.

Page 1 of 1

User Name: System (Beth)
Print Time: 8/13/2010 11:33:21 AM (GMT -07:00)

```
Instrument Configuration
========================
   Instrument Name: Fake Instrument no privileges
   Instrument Type: Sample VB

General Options
===============
   System Suitability:       Disabled
   SEC:                      Disabled
   PDA:                      Disabled
   Baseline Check:           Disabled

   <No configured devices>
```

Current baseline check

This is an example of the Current Baseline Check (**Current Baseline Check.srp**) report template output.

```
Baseline Check Report
Noise Test                Test Not
                          Completed
Drift Test                Test Not
                          Completed
Required Stable Time      15.0 Minutes
Total Test Time           0.0 Minutes
Noise Test Type           rms
Test End Time             7/7/2010 1:02:08 PM (GMT
                          -07:00)

Channel                   Threshold       Status            Threshold     Status
                          (Noise Test)    (Noise Test)      (Drift/hr)    (Drift Test)
```

Internal standard report

This is an example of a report using the Internal Standard (**Internal Standard.srp**) template output.

Internal Standard Report

Page 1 of 1

Method Name: C:\datasystem\methods\istd.met
Data: C:\datasystem\data\multical005.dat
User: System
Acquired: 11/26/90 8:49:21 PM
Printed: 4/10/97 10:49:56 AM

Channel A Results

Pk #	*Name*	*Retention Time*	*Area*	*Conc*
6	Peak 1	5.710	298528	**1.000**
7	Peak 2	6.558	250174	**0.688**
9	Peak 3	8.264	239475	**0.985**
10	Peak 4	8.530	376822	**1.977**
Totals			1164999	**4.650**

External standard report

This is an example of a report using the External Standard (**External Standard.srp**) template.

External Standard Report **Page 1 of 1**

Method Name: C:\datasystem\methods\test.met
Data: C:\datasystem\data\multical005.dat
User: System
Acquired: 11/26/90 8:51:56 PM
Printed: 4/10/97 10:38:56 AM

Channel A Results

Pk #	*Name*	*Retention Time*	*Area*	*Conc*
2	Acetone	5.729	779320	**50.046**
3	Carbon Tetrachloride	6.568	667324	**9.017**
6	Bromoethane	8.273	633854	**35.026**
7	1,3-TCE	8.540	994037	**50.020**
Totals			3074535	**144.110**

Normalization report

This is an example of the Normalized Report (**Normalization.srp**) template output.

Normalization Report **Page 1 of 1**

Method Name: C:\datasystem\methods\test.met
Data: C:\datasystem\data\multilevel005.dat
User: System
Acquired: 11/26/90 8:51:56 PM
Printed: 4/10/97 10:43:48 AM

Channel A Results

Pk #	*Name*	*Retention Time*	*Area*	*Conc*
1	Peak1	5.729	779320	**34.728**
2	Peak2	6.568	667324	**6.257**
5	Peak3	8.273	633854	**24.305**
6	Peak4	8.540	994037	**34.710**
Totals			3074535	**100.000**

Error condition flags

When an error condition occurs for a calculated value, an error flag is printed that indicates the nature of the problem. These flags are used in reports, exported data, and for certain annotations.

0.00 BDL Below detection limit

0.00 ISTD Problem with ISTD peak

0.00 STD Problem with standard peak

0.00 FIT Problem with curve fit

<conc> CAL Currently calibrating, <conc> = peak table conc. for current level

0.00 NEG Negative concentration

<conc> LC Low conc, <conc> = calculated conc.

<conc> HC High conc, <conc> = calculated conc.

In cases where 0.00 is reported, the 0.00 is reported because the nature of the error prevents further calculation.

See Also

Open a Standard Report Template

About Custom Parameters

Custom Parameters are used to calculate specific values that are of interest to you, but are not normally calculated. This feature gives you access to the entire database of named and detected peaks. Custom parameters programs are called after all other analysis is finished.

Custom Parameter programs may be written in VB Script or be compiled DLLs written in C++. Compiled DLLs must implement a function called EvaluateCustomParam(). Please see the EZChrom CD for complete documentation and examples on developing custom parameter programs.

Custom parameters can be reported in a custom report, exported as a result, and annotated on chromatograms (per-peak parameters only).

Custom parameters are separate from Internal calculations. Internal calculations are available without configuring any custom parameter and are always calculated. See Internal Calculations.

See Also

Set a custom parameter for a method

Set a custom parameter for a sequence

Use the European Pharmacopeia(EP) System Suitability Signal To Noise custom parameter

Use the United States Pharmacopia(USP) Signal To Noise custom parameter

Use the Peak To Valley Ratio custom parameter

Use the Signal Conversion custom parameter

Use the Channel Wide Normalization custom parameter

Use the Relative Area Percent custom parameter

Use the Script Processor and Script Files to create a custom parameter

Add custom parameters to the method report

Set a custom parameter for a method

1. From the **Method** menu, select **Advanced > Custom Parameters**.
2. To define a Custom Parameter, enter the title you want to use to report the result in the **Parameter Name** field.
3. Next, move the cursor to the **Type** field and click your mouse. You will be given a choice of **System-wide** or **Per-peak**.
   - A **System-wide** parameter is one that is calculated once for the whole chromatogram. System-wide parameters can be displayed in a custom report, and will be printed at the bottom of the report. An example of a System-wide parameter would be a BTU calculation, where the program multiplies each peak by its BTU content, then sums the calculated BTU values providing a single value equal to the BTU content of the entire mixture.
   - A **Per-peak** parameter is one that is calculated once for each peak in the chromatogram. Per-peak parameters can be displayed in a custom report column similar to the way the peak number or concentration would be displayed. Per-peak parameters can also be annotated on the chromatogram. An example of a Per-peak parameter would be HETP (height equivalent to a theoretical plate). For HETP, the Custom Parameter program would take the length of the column (in centimeters) and divide it by n, the theoretical plates for the component which is already calculated by the system.

     Note: If the custom parameter is designated as a sequence table parameter, any change to the Type (per-peak or system-wide) will not be updated until you reopen the sequence custom parameter dialog from the sequence.
4. Select **Number** or **String** from the **Returns** drop-down list to select what type of value is returned by the parameter or calculation.
5. Click the **Source** field. From the **Parameter Source** dialog box, select from the following options:
   - **RelArea Perc**
   - **Script Processor** - Select this and double click on the Additional Parameters field to open the **Custom Parameter Scripter**.
   - **Sequence Table Parameter** - Select this if you want to define the custom parameter as part of the sequence.
6. Use the **Additional Parameters** field as necessary for your custom parameter application. The value entered here will be the default for the parameter, unless written over in the sequence table. See **Sequence Custom Parameters**.
7. Once you have a custom parameter defined in your method, the software will attempt to run the Custom Parameter Program(s) designated whenever you analyze your chromatogram.

Note: In order to enter a sequence custom parameter in a sequence spreadsheet, the method must have a custom parameter defined as sequence-based, and that method must be saved.

Set a custom parameter for a sequence

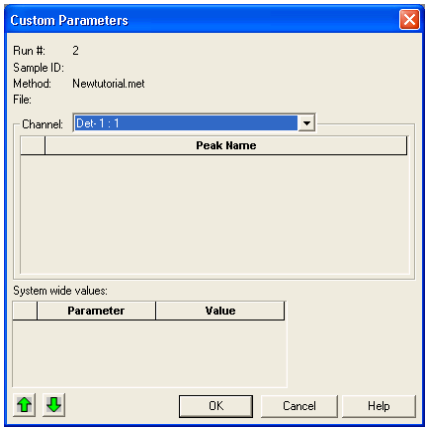
In order to enter a sequence custom parameter in a sequence spreadsheet, the method must have a custom parameter defined as sequence-based, and that method must be saved.

Define a sequence based custom parameter for a method

1. Open a method.
2. From the main instrument window, select **Method > Advanced**.
3. In the **Advanced Method Options** dialog box, select the **Custom Parameters** tab.
4. In the **Custom Parameters** table, in the **Source** list, select **Sequence Table Parameter**.
5. Save the **Method**.

Set a custom parameter for a sequence

1. From the **main instrument** window, select **Sequence > Edit**.
2. In the sequence spreadsheet, select the **Custom Parameters** field.
3. In the **Custom Parameters** dialog box, either the **Channel** or the **System wide values** area will be active. This is determined by how the custom parameter has been defined in the method designated for this line of the sequence.
   - If **Channel** is active, select the channel for which you want to define per-peak parameters from the drop down menu. The peaks defined for that channel will appear in the spreadsheet. Under **Peak Name**, enter a value for the custom parameter for each of the peaks displayed.
   - If **System wide values** is active, enter a **Value** to be used. This value applies to the entire chromatogram.
4. To set parameters for multiple runs, select the down and up arrows to move to the next or previous run in the sequence. You can also copy or fill-down parameters that do not change from run to run, if each run is using the same method.
5. Select **OK**.



Use the European Pharmacopeia (EP) System Suitability Signal To Noise custom parameter

The European Pharmacopeia System Suitability Signal to Noise custom parameter calculates a signal to noise ratio for peaks using the techniques documented for the European Pharmacopeia and influences the precision of quantification.

Do not use Integration Off when using the European Pharmacopeia System Suitability Signal to Noise custom parameter. Integration Off disables peaks, however these regions are still included in the noise calculation. Leave all peaks integrated to get the correct noise values.

Calculation

The European Pharmacopeia System Suitability Signal to Noise custom parameter is calculated using the following equation:

$$S/N = \frac{2H}{h}$$

H = The height of the peak corresponding to the component in the chromatogram obtained with the prescribed reference solution. It is measured from the maximum of the peak to the extrapolated baseline of the signal observed over a distance equal to 20 times the width at half-height.

h = The range of the background noise in a chromatogram obtained after injection or application of a blank. It is observed over a distance equal to 20 times the width at half-height of the peak in the chromatogram obtained with the prescribed reference solution. If possible, situated equally around the place where this peak would be found.

The time range for noise determination can either be entered manually or automatically determined. The time range for noise determination should be a minimum of five times the width at half-height of the peak. The automatic noise range determination uses 20 times the peak width at half-height, centered on the retention time of the peak of interest where possible. In cases where the automatically determined time range cannot be directly centered on the peak, (for example, when the peak is too close to the beginning or end of the chromatogram) the time range is shifted to remain within the limits of the chromatogram.

Use the parameter

In this example, noise is calculated using an ASTM unscaled short noise calculation over the noise range. For the ASTM unscaled short noise calculation, see ASTM Noise Calculations.

The parameter calculates values for named and unnamed peaks as appropriate and the results are stored with the peak information in the results file. This information may then be reported using the standard reporting tools in the system.

In order to use this custom parameter, you must include a blank run in your sequence. This blank run is used for the noise determination and, therefore, should be an appropriate representation of noise in the system. Only one blank run can be used within each sequence. The blank run should use the same acquisition method parameters as the sample runs and must contain the same signals as the sample runs.

1 From the **main instrument** window, select **Method > Advanced**.

2 In the **Advanced Method Options** dialog box, select the **Column/Performance** tab.

3 Enable the **Calculate performance parameters for this channel** option. This selection is necessary to trigger the determination of peak width at half-height for the noise range determination. It is not necessary to select any of the optional **Calculation method(s)** to generate the custom parameter values.

4 Select the **Custom Parameters** tab.

5 In the **Custom Parameters** table, complete the following fields:

Column	Value
Parameter Name	Enter **Signal to Noise EP** or any name desired. This name will show up for graph annotation purposes and reporting purposes. The name must not contain a /.
Type	Select **Per-peak** from the list.
Returns	Select **Number** from the list.
Source	Select **Signal Noise** from the list.
Additional Parameters	Enter additional arguments as described below.

In the **Additional Parameters** list, enter additional arguments as shown in the following examples:

- **BASELINE_FILE_NAME:** Name of the baseline file run in the current sequence
- **StartTime** and **StopTime** (optional): Indicates the time range (in minutes) for noise level determination
- Separate the arguments with a semicolon character (;). A trailing semicolon can be entered after the last argument, but is not necessary.
- If a start time is entered it must be accompanied by a stop time and *vice-versa*.
- Do not insert empty semicolon separators for start-stop times (baselinefile.dat;;) unless other parameters will follow (See Diagnostic codes section below) or the system will report an error and will not calculate a result.
- **BASELINE_FILE_NAME;StartTime;StopTime**
- To enter a baseline file with a manually designated start time of 1.5 minutes and a stop time of 3.5 minutes for noise

determination, in the Additional Parameters field enter **solvent002.dat;1.5;3.5**.

- You may also include reporting of intermediate values used in the calculations. These additional values can be reported by designating an optional fourth argument in the **Additional Parameters** field. The optional fourth argument is a two-character diagnostic code which controls the return value of the parameter DLL. When entering the diagnostic parameters, it is important that the method specifies the same baseline file and time range options as used for the calculation of the Signal to Noise parameter. Otherwise, the diagnostic parameter values will not reflect the intermediate values used for calculation of the Signal to Noise.

Diagnostic code	Value returned by system suitability signal/noise custom parameter DLL
NB	Begin time for noise determination (in minutes)
NE	End time for noise determination (in minutes)
NV	Noise Value (h) - Calculated as (Max signal value – Min signal value) within noise time range
SV	Signal Value (H) – Identical to Peak Height
VC	Flag to indicate whether a valid S/N value was calculated (1=Yes, 0=No) *See notes

- When determining noise using fixed time ranges, simply add the additional fourth parameter to the parameter list to return the diagnostic value of interest.
  BASELINE_FILE_NAME;StartTime;StopTime;DiagnosticCode
- When using automatic noise time ranges, place three semicolon characters between the baseline file name and the diagnostic code so the code is located in the fourth place in the parameter list.
  BASELINE_FILE_NAME;;;DiagnosticCode

The EP Signal to Noise calculation is not performed during acquisition. You need to reprocess in order to get this calculation.

Additional notes

Processing time

Please be aware that selecting multiple diagnostic values will significantly increase the time needed to process the results, as the custom parameter code is called once for each diagnostic value returned. Since the custom parameter must open two different signal files each time, processing times may be significant.

Signal matching

The custom parameter code attempts to calculate signal to noise for each signal trace in the data file. For the calculation to work, an exact

corresponding trace must exist in the baseline noise file. If no matching signal trace is found in the baseline noise file, the custom parameter code will post an error to the Instrument Activity log indicating that the matching signal could not be found. No S/N values will be calculated for any signal trace where no matching signal is present in the baseline noise file.

Values of zero

When no value can be calculated for signal to noise or the associated diagnostic parameters, the system will report a value of zero. This is necessary as the system must place a value in the return parameter. In these cases, the diagnostic parameter VC should also return a zero to indicate that the result is not valid.

Use the United States Pharmacopia(USP) Signal To Noise custom parameter

The USP Signal To Noise custom parameter performs a signal to noise calculation according to the guidelines presented by the US Pharmacopeia. Once the custom parameter is turned on in a method, the reporting variables become available for reports and annotations.

Do not use Integration Off when using Signal to Noise. Integration Off disables peaks, however these regions are still included in the noise calculation. Leave all peaks integrated to get the correct noise values.

In EZChrom Elite 3.3.2 & 3.3.2 SP1 the US Pharmacopeia custom parameter was not supported.

Calculation

The USP Signal To Noise custom parameter is calculated using the following equation:

$$S/N = \frac{2H}{h_n}$$

H = The height of the peak corresponding to the component concerned.

h_n = The difference between the largest and smallest noise values over a distance of 20 times the width at the half height of the peak.

The time range for the noise can be entered manually or automatically. If this value is to be calculated manually, the user must enter the first two parameters as the start time of the noise and the end time of the noise.

Use the parameter

To have this custom parameter automatically computed for peaks of a chromatogram, modify the method as follows:

1 From the main instrument window, select **Method > Advanced**.

2 In the **Advanced Method Options** dialog box, select the **Column/Performance** tab.

3 Select **Calculate performance parameters for this channel**.

4 Select the **Custom Parameters** tab.

5 In the **Custom parameters** table, complete the following fields:

Column	Value
Parameter Name	Enter **USP Signal to Noise** or any name desired. This name will show up for graph annotation purposes and reporting purposes. The name must not contain a /.
Type	Select **Per-peak** from the list.
Returns	Select **Number** from the list.
Source	Select **Signal Noise USP** from the list.
Additional Parameters	Additional parameters are optional. Parameter that will be used for actual calculation: **Start Time;StopTime** – To manually enter the start and stop time for the noise. These parameters will be used in the US Pharmacopeia signal to noise calculation. If these manual parameters are not entered, the system will automatically use start and stop values from the calculation above. Diagnostic parameters which give outputs: **;;NB** – Outputs Noise Beginning (Start Time) **;;NE** – Outputs Noise Ending (End Time) **;;VC** - Outputs if calculation is good or bad (1 is good and 0 is bad) **;;NV** – Outputs Noise Value – Calculated as (Max signal value – Min signal value) within noise time range **;;SV** – Outputs Signal Value – Identical to Peak Height

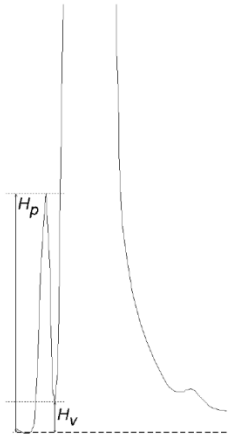
If this custom parameter was added after a run was acquired, you need to perform an analysis before the parameter will be calculated.

Use the Peak To Valley Ratio custom parameter

When a baseline separation between two peaks is not achieved, the Peak To Valley Ratio custom parameter may be used as a system suitability requirement in a test for related substances.

Calculation

The Peak To Valley Ratio custom parameter is calculated using the following equation:



Hp = The height above the extrapolated baseline of the minor peak.

Hv = The height above the extrapolated baseline at the lowest point of the curve separating the minor and major peaks.

Use the parameter

To have this custom parameter automatically computed for peaks of a chromatogram, modify the method as follows:

1. From the **main instrument** window, select **Method > Advanced**.
2. In the **Advanced Method Options** dialog box, select the **Custom Parameters** tab.
3. In the **Custom Parameters** table, complete the following fields:

Column	Value
Parameter Name	Enter **Peak To Valley Ratio** or any name desired. This name will show up for graph annotation purposes and reporting purposes. The name must not contain a /.
Type	Select **Per-peak** from the list.
Returns	Select **Number** from the list.
Source	Select **Peak To Valley Ratio** from the list.
Additional Parameters	Additional parameters are optional.

Use the Signal Conversion custom parameter

The Signal Conversion custom parameter allows you to calculate peak height and area using the actual signal numbers on the y-axis of the chromatogram without the use of multipliers. Once the custom parameter is turned on in a method, the reporting variables become available for reports and annotations.

In EZChrom Elite 3.3.2 & 3.3.2 SP1 the Signal Conversion custom parameter was not supported.

Calculation

The Signal Conversion custom parameter is calculated using the following equation:

Additional parameter 1: Peak Height/10^9

Additional parameter 2: Peak Area/10^9

Use the parameter

To have this custom parameter automatically computed for peaks of a chromatogram, modify the method as follows:

1 From the main instrument window, select **Method > Advanced**.

2 In the **Advanced Method Options** dialog box, select the **Custom Parameters** tab.

3 In the **Custom Parameters** table, complete the following fields:

Column	Value
Parameter Name	Enter **Signal Conversion** or any name desired. This name will show up for graph annotation purposes and reporting purposes. The name must not contain a /.
Type	Select **Per-peak** from the list.
Returns	Select **Number** from the list.
Source	Select **Signal Conversion** from the list.
Additional Parameters	Enter **1** for peak height and **2** for peak area.

If this custom parameter was added after a run was acquired, you need to perform an analysis before the parameter will be calculated.

Use the Channel Wide Normalization custom parameter

The Channel Wide Normalization custom parameter is used to calculate normalized concentration values across all available channels. This is a per-peak custom parameter.

Use the parameter

To have this custom parameter automatically computed for peaks of a chromatogram, modify the method as follows:

1 From the main instrument window, select **Method > Advanced**.

2 In the **Advanced Method Options** dialog box, select the **Custom Parameters** tab.

3 In the **Custom Parameters** table, complete the following fields:

Column	Value
Parameter Name	Enter **Channel Wide Normalization** or any name desired. This name will show up for graph annotation purposes and reporting purposes. The name must not contain a /.
Type	Select **Per-peak** from the list.
Returns	Select **Number** from the list.
Source	Select **Channel Wide Normalization** from the list.
Additional Parameters	Enter additional parameters as described below.

Additional Parameters are optional and may contain the following items. These items are not case sensitive:

- Normalization Type Flag
  - **/estd** Use to normalize the ESTD Concentrations across all channels.
  - **/istd** Use to normalize the ISTD Concentrations across all channels.
  - **/norm** Use to normalize the NORM Concentrations across all channels.
- Report Export Flag
  - **/report** Use to generate an export file of the normalized results.

If no additional parameters are specified, then the concentration used will either be ESTD or ISTD depending on what is available in the datafile. Also, no eport report will be generated.

Only one of the Normalization Type Flags may be specified at one time. It is not possible to combine these flags. For example, it is an error to specify **/estd /istd**.

If **/report** is specified, then the normalization type flag must also be specified. The exported report will end up in a subdirectory of the datafile directory. The subdirectory will be called **export**, and the name of the exported file will be the same as the datafile, with an extension of **.NOM**. For example, if the datafile was called **C:\EZChrom\Data\Test1.dat**, then the exported results would be called **C:\EZChrom\Data\Export\Test1.nom**. Any export file in this directory with this same name will be overwritten with the new file.

Use the Relative Area Percent custom parameter

This topic describes the installation and use of a custom parameter DLL to compute the Relative Area Percent for peaks of a chromatogram relative to a user specified reference peak.

The Relative Area Percent of a peak is the ratio of the area of the peak to the area of a user specified reference peak.

Calculation

The Relative Area Percent custom parameter is calculated using the following equation:

$$\text{Rel. Area Pct} = (\text{Area}_{\text{Peak}} / \text{Area}_{\text{Reference Peak}}) \times 100\%$$

Use the parameter

To have this custom parameter automatically computed for peaks of a chromatogram, modify the method as follows:

1. From the **main instrument** window, select **Method > Advanced**.
2. In the **Advanced Method Options** dialog box, select the **Custom Parameters** tab.
3. In the **Custom Parameters** table, complete the following fields:

Column	Value
Parameter Name	Enter **Relative Area Percent** or any name desired. This name will show up for graph annotation purposes and reporting purposes. The name must not contain a /.
Type	Select **Per-peak** from the list.
Returns	Select **Number** from the list.
Source	Select **Rel Area Perc** from the list.
Additional Parameters	Enter the peak number to be used as the reference peak in the calculation.

Once a chromatogram has been analyzed with this method, the relative area percent for each peak will available as a reportable result in custom and advanced reports, as well as for export and as a graph annotation.

Use the Script Processor and Script Files to create a custom parameter

The script processor allows advanced users to write simple VB script calculations. The script file allows you to reuse previously written script for your custom parameter.

For more information about scripting see the Scripting Custom Parameters Guide (CDS_EE-script-custom-param.pdf) found in the

documents folder of OpenLab CDS.

Use the script processor

1. From the **main instrument** window, select **Method > Advanced**.
2. In the Advanced Method Options dialog box, select the **Custom Parameters** tab.
3. In the **Custom Parameters** table, enter a **Parameter Name**. This can be any name desired.
4. Select a **Type** and **Returns**.
5. In the **Source** list, select **Script Processor**.
6. In the **Additional Parameters** field, click the arrow to edit script.
7. In the **Custom Parameter Script** dialog box, enter your script between **Sub EvaluatecustomParam()** and **End Sub**.
8. Select **OK**.

Use a script file

1. From the **main instrument** window, select **Method > Advanced**.
2. In the **Advanced Method Options** dialog box, select the **Custom Parameters** tab.
3. In the **Custom Parameters** table, enter a **Parameter Name.** This can be any name desired.
4. Select a **Type** and **Returns**.
5. In the **Source** list, select **Script File**.
6. In the **Select Custom Parameter File** dialog box, navigate to the script file.
7. Select **Open**.

Use the EZChrom Retention Index (Kovats Index) custom parameter

The EZChrom Retention Index is used to calculate the retention index of a solute based on the retention times of a series of normal alkanes at a given, isothermal temperature for a particular stationary phase. Retention indices can be used to compare the relative elution order of solutes for a given column and chromatographic conditions. The retention indices can also be used to compare the retention or selectivity of two columns.

Retention index rules

The normal alkanes are like reference peaks: regardless of their elution times, their retention indexes are determined by the number of carbon atoms in their molecules. The retention indexes of the other peaks in the mixture are determined by their times relative to the n-alkanes.

The retention index of an n-alkane is always 100 times its carbon

number and should be reported as such, for example, C-10 is 1000 and C-13 is 1300.

The retention time used in the calculation of the retention index is the peak's actual retention time in the chromatogram (corrected for the time of the unretained peak). The detected retention time of the first peak in the Peak Table is used as the time of the unretained peak.

I=100(y) + (100(z-y) ((log tRx - log tRy)/(log tRz - log tRy))

Where:

I = The retention index

x = Solute of interest

y = n-alkane with y carbon atoms, eluting before x

z = n-alkane with z carbon atoms, eluting after x

tR = Retention time minus time of unretained peak

To use the parameter:

1. Copy **RetentionIndex.DLL** and **RetIndex.CFG** into your EZChrom directory.
2. Create a standard mixture with the normal alkanes covering the boiling point range of the solutes you wish to measure.
3. Analyze this mixture using the chromatographic conditions (isothermal temperature and column-type) to be compared.
4. Create a Peak Table with the names and retention times of the n-alkanes and other solutes in the mixture. Note that the unretained peak (usually methane) must be in the Peak Table.
5. Using Microsoft NotePad or similar text editor, edit the **RETINDEX.CFG** file in your EZChrom directory to include for each of the n-alkane solutes in your calibration mixture. Use Tab to separate the values in a row. Do not use spaces between the values; doing so may cause the Custom Parameter to fail when it is executed.
   - The number of n-alkane peaks, as Peaks
   - The Channel (A,B,C,D),
   - Type (P for Peak),
   - The Peak ID# for each alkane from the Peak Table,
   - Number of carbon atoms in this peak's molecule (Carbon#),
   - Retention time (Ret.) of each peak
6. If you are using a Workstation/Networked Workstation, save the file in a local folder or a shared network location accessible by the workstation (for example, c:\RegIndexConfigFiles\MethodName.cfg).
   If you are using a Client-Server, save the file in a shared network location accessible by the client and the AIC (for example, \\RetIndexConfigShare\MethodName.cfg).
7. Set a custom parameter for a method.

8 Add custom parameters to the method report.

Add custom parameters to the method report

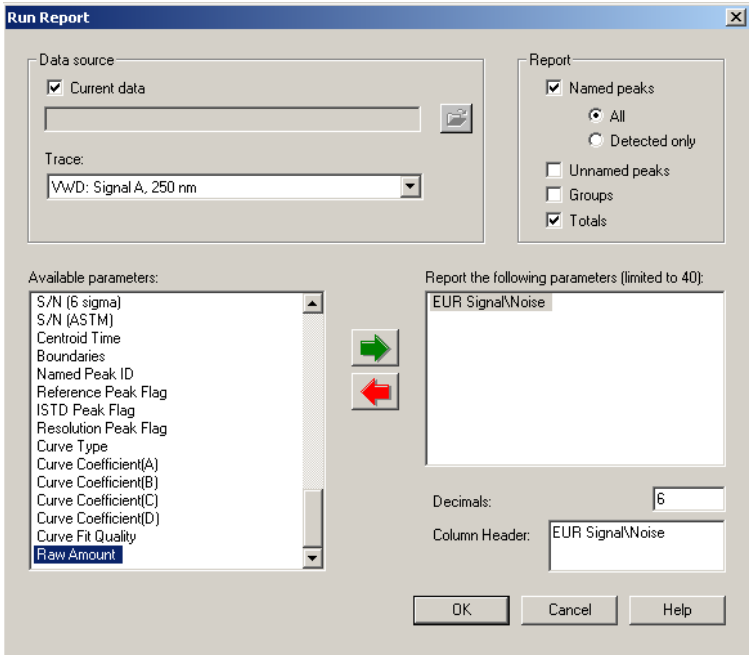
Once a custom parameter has been defined in the **Advanced Method Options** and the method has been saved, the parameter appears in the list of available parameters in the method report and can be included in the report definition.

1 From the **main instrument** window, select **Method > Report**.

2 In the **Method Report Editor**, right-click and select **Insert Report > Run Report**.

3 In the **Run Report** dialog box, add the additional custom parameter(s) from the **Available parameters** list.

4 Adjust the **Column Header** text and data reporting precision as needed.



The run report table preview will display the new parameter columns, but no preview data will be available until the data are processed.

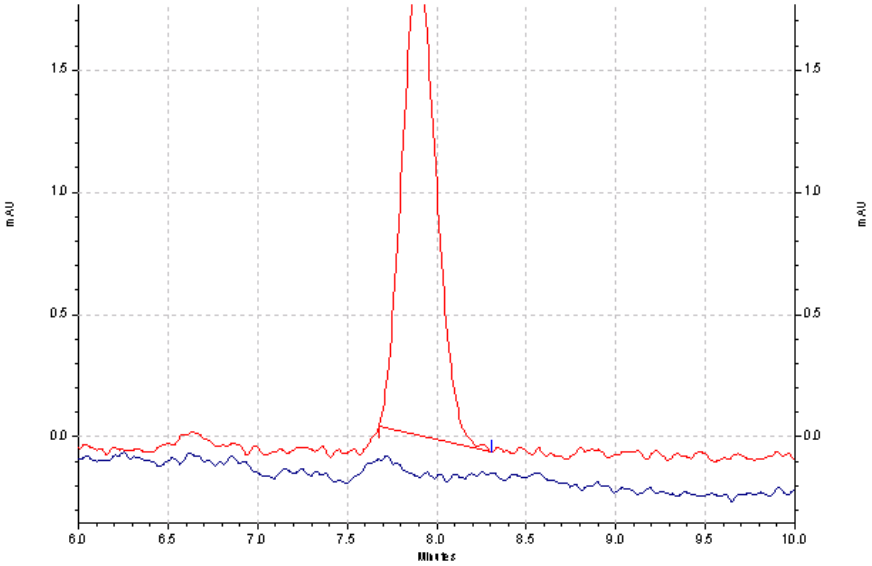
<Trace Data Header>						
Pk #	Name	Height	EP Signal/Noise	Noise Begin Time	Noise End Time	Noise Value
0	Sample Data	0	0.000	0.00	0.00	0.000

View and print the method report

Once the data has been reprocessed, the final report will display the custom parameter results and other run data that has been added to the report.

To view the final report, select **Reports > View > Method Report**.

To print the final report, from the instrument client select **Reports > Print > Method Report**.



DAD:
Signal
A, 214
nm/Bw:4
nm
Results

Pk #	Name	Height	EP Signal/Noise	Noise Begin Time	Noise End Time	Noise Value
4	Compound X	4016	19.033	5.78	10.01	422.000
Totals		4016				

Reference

See Also

Conversion of PENelson Data Files

Open a CDF File

Configure CIO/DIO Events

User Programs

Turn Off GPIB Instruments

Internal Calculations

About ASCII Sequence File Formats

Functional Reference

Advanced Reporting Formulas and Functions

Conversion of PENelson Data Files

The transparent conversion of TurboChrom Version 6.1 .RAW data files and AccessChrom .RAW files is supported. Some conversions may require the presence of PE software in order to work.

The following table summarizes the acceptable limitations in the conversion of data files:

Data File	PE Software Requirements
AccessChrom	None
TurboChrom 4.0 and earlier	None
TurboChrom 4.1 and later	TurboChrom must be installed on the client PC (The data system will automatically launch TurboChrom to perform the conversion)
TotalChrom	TotalChrom must be installed on the client PC and the user must log into the system. (The data system will automatically launch TotalChrom, but the user will need to login, in order for the data system to perform the conversion.)

In all cases, only the data points will be converted, not the results or other parts of the data file.

Open a CDF File

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

microvolts, uvolts, uv, uau or 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 based on the range of values.

If the CDF file being read is nonstandard, you need 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.

Configure CIO/DIO Events

If you are using one of the CIO/DIO boards, a dialog will appear when you click the **Setup** field in the event configuration spreadsheet.

- **Board** - Select the board for which you want to configure events.
- **Connector** - Select the connector to be used.
- **Signal** - Select the signal source for the event.
- **Idle State** - Select the idle state for the event: default, open, or closed.

When you have completed the dialog, click the **OK** button. Once the events are configured, you can program them from the **Instrument Setup** section of the methods for instruments using this board.

User programs

User Programs are external programs that are run before an acquisition or before or after an analysis. These programs are meant to synchronize actions between the data system and an instrument or another data processing program you may be running. A User Program may be an executable (.EXE) or a dynamic link library (.DLL) file.

If the User Program is an executable (.EXE) program, the data system will launch the program, and then wait until the program exits. The EXE is launched with a command line containing 3 string arguments:

addlParams - The contents of the 'Additional Parameters' field (from the dialog)

strMethod - The fully qualified path/filename of the current method (in quotes)

strData - The fully qualified path/filename of the current data file (in quotes)

Note that, although the user program receives the name of the current method and data file, the .EXE does not have access to the content of the files.

If the User Program is a .DLL, it has access to all data and parameters of the current method and data file. When the User Program is a .DLL, the data system will call the function RunUserProg() in the .DLL and wait for it to return before continuing. The .DLL should implement the following function:

void RunUserProg ((LPCTSTR)m_addlParams, (CClientInfo*) m_pInfo)

where 'm_addlParams' is the contents of the 'Additional Parameters' field (from the dialog.)

'm_pInfo' points to a CClientInfo object

Note: By default, all user program path/filenames are specified using drive letters. To instead use UNC naming conventions, create a DWORD values called 'UserProgramNetworkPaths' with a value of '1' in the following registry location (Replace 'c:/datasystem' with your install directory):

\HKEY_LOCAL_MACHINE\Software\ChromatographySystem\c:/datasystem\Inst\

Warning - always consult with your network administrator before editing the Windows registry.

Turn off GPIB instruments

If you are using two instruments attached to a GPIB board, it is important to close the instrument application (or close the instrument window and then close the server) prior to turning off the power to the instrument or instrument modules, otherwise the other instrument attached to the GPIB board may freeze.

Internal calculations

Internal calculations are available without configuring any custom parameter and are always calculated.

6-Sigma Noise Test	Calib Weight	Internal Standard Amounts	Plates/Meter
6-Sigma Signal-to-Noise	Calibration Averages	Internal Standard Report Calculation	Point-to-Point Fit
Area % Report Calculation	Calibration Curve Calculations	Internal Standard vs External Standard and Normalization	Quadratic Fit
Area/Amount Response Factor Definition	Calibration Curves	Internal Standards	Relative Retention

6-Sigma noise test

The 6-Sigma Noise is the standard deviation of the signal derived from n measurements multiplied by 6, defined over the time segment chosen. The equation uses a linear regression line, instead of the average measurement, to eliminate drift from the noise calculations.

$$6 \times \left[\frac{\sum_{i=1}^{n} \left(E_i - f(E_i)\right)^2}{n-1} \right]^{1/2}$$

Where *Ei* is a data point and $f(E_i)$ is the point on the linear regression line of all the data points.

The n measurements are made between the time limits entered.

6-Sigma Signal-to-Noise

To calculate the S/N, the 6-Sigma noise is calculated in 30 second intervals, back from the data point immediately preceding the peak's baseline (the integration Start time). It proceeds in 30 second intervals until it finds another peak's integration Stop time. Only 30 second intervals are used in the calculations. If an interval is less than 30 seconds, it is not considered.

The average of all the noise calculations is divided into the measured Height for the peak of interest to determine the Signal-to-Noise value.

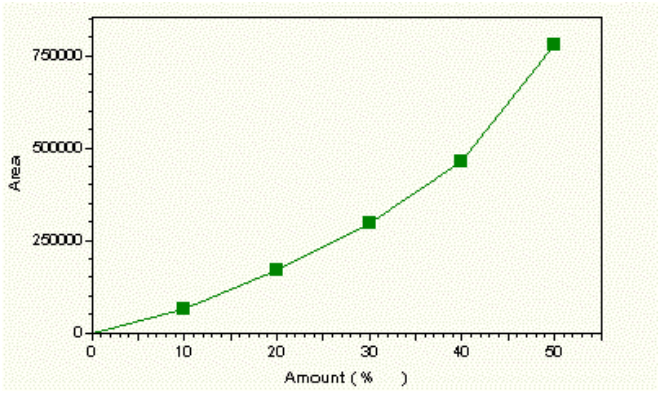
Do not use Integration Off when using Signal to Noise. Integration Off disables peaks, however these regions are still included in the noise calculation. Leave all peaks integrated to get the correct noise values.

Area % report calculation

$$\text{Area\%} = \frac{\text{Area of peak} * 100}{\text{Sum of all peak areas}}$$

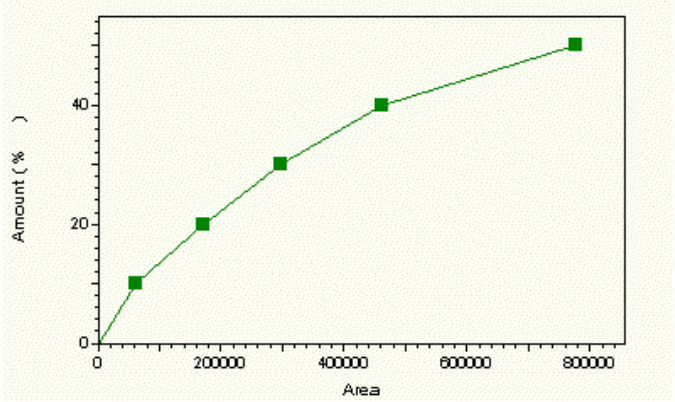
Area/Amount response factor definition

If you choose **Area/Amount** for your response factor definition, the calibration curve (which can be viewed in **Review Calibration**) is defined where **y = amount** and **x = area or height**. (For internal standard calibrations, y = amount ratio and x = area or height ratio.) An example calibration curve using **Area/Amount** response factor definition is given below.



Calibration Curve with Area/Amount Response Factor Definition

If you choose **Amount/Area** for your response factor definition, the calibration curve (which can be viewed in **Review Calibration**) is defined where **y = area or height** and **x = amount**. (For internal standard calibrations, y = area or height ratio and x = amount ratio.)



An example calibration curve using **Amount/Area** response factor definition is given below.

Calibration Curve with Amount/Area Response Factor Definition

Area/Height calculation method

Theoretical Plates

Where

$$N = 16 \times \left[\frac{t}{W}\right]^2$$

N = theoretical plates

t = The retention time of the component

W = The width of the base of the component peak.

$W = 4 \times \sigma$

Where

$$\sigma = \frac{1}{\sqrt{2\pi}} \times \left[\frac{A}{H}\right]$$

Where

$$= 0.399 \times \left[\frac{A}{H}\right]$$

A= Peak area

H= Peak height

Peak Asymmetry (Tailing Factor)

$$T = \frac{W_{0.05}}{2f}$$

Where

T = Peak asymmetry, or tailing factor

$W_{0.05}$ = The distance from the leading edge to the tailing edge of the peak, measured at a point 5% of the peak height from the baseline

f = The distance from the peak maximum to the leading edge of the peak at the position of 5% peak height

For peak asymmetry at 10%, the values for W and *f* are measured at 10% of peak height.

$$R = \frac{2(t_2 - t_1)}{W_2 + W_1}$$

Resolution

Where

R = Resolution between a peak of interest (peak 2) and the peak preceding it (peak 1).

t_2 = The retention time measured from point of injection of peak 2.

t_1 = The retention time measured from point of injection of peak 1.

W_2 = The width of the base of the component peak 2

W_1 = The width of the base of the component peak 1

ASTM LOD (Limit of Detection) calculation

This is a per peak result. The purpose of an LOD parameter is to determine whether the peak being evaluated is within the Limits of Detection as previously determined experimentally for that Method.

SNM = H/ ND t

LOD = C * SN / SNM

Where

SN: S/N ratio for LOD entered in Peak Table

SN_M: Calculated S/N ratio

H: Peak height

N_D: Measured noise level

C: Concentration result of peak being evaluated.

Note: The noise for a peak is calculated based on the first 30-second baseline segment prior to the peak start. The baseline after a peak is not used in the noise calculation for that peak.

ASTM LOQ (Limit of Quantitation)

This is a per peak result and should calculated and report as such. The purpose of a LOQ parameter is to determine if the peak being evaluated is within the Limits of Quantitation as previously determined experimentally for that Method.

SN = H/ ND

LOQ = C * SN / SNM

Where

SN: S/N ratio for LOQ entered in Peak Table

SN_M: Calculated S/N ratio

H: Peak height at concentration C

N_D: Measured noise level

C: Concentration result of peak being evaluated.

Note: The noise for a peak is calculated based on the first 30-second baseline segment prior to the peak start. The baseline after a peak is not used in the noise calculation for that peak.

ASTM noise calculations

As in the 6-Sigma noise calculations, the best fit Linear Least Squares is calculated for the time range chosen (30-second window for short or 60-second window for long). The noise value is calculated using the largest positive and negative differences between the actual points and the calculated points as shown below:

$$\mathbf{Noise = (Ei - f(Ei))max - (Ei - f(Ei))min}$$

Where:

E_i = individual data point

$f(E_i)$ = calculated data point using the LSQ formula

Note: For Scaled calculations, the results will be reported as scaled detector units rather than microvolts.

ASTM Signal to Noise

As with the 6-Sigma, the noise for this calculation is performed in 30 second intervals. The average of all the noise calculations is divided into the Height of the peak of interest to determine the Signal-to-Noise value.

Do not use Integration Off when using Signal to Noise. Integration Off disables peaks, however these regions are still included in the noise calculation. Leave all peaks integrated to get the correct noise values.

Automatic averaging

When you have the Automatic Averaging turned On for your method (in Method Properties), averaging will take place for all peaks designated with the WtAverage flag in the peak table. Replicates will continue to be saved in the method until a new level is calibrated for the method. When a new level is encountered, the replicates for the previous level will be cleared, and the average at that point will be saved in the method as Last Area.

If you want replicate areas to be continuously saved in the method, whether or not a new level is encountered, turn the Automatic Averaging OFF. You must then designate in your sequence where you want averaging to take place by designating Average Replicates in the Run Type of the sample.

Average RF

If the Average RF fit type is selected, the slope of the calibration line between each calibration point and zero is calculated independently. These values (the Response Factors, or RFs) are then averaged to give an Average RF value. The Average RF is then used to calculate the

uncorrected amount of the unknown component as follows:

ConcUnknown= (Average RF) * AreaUnknown

Where:

ConcUnknown = Area/RF if Response Factor is set to Area/Amount

ConcUnknown = Area * RF if Response Factor is set to Amount/Area

The slope of each calibration line is calculated as follows:

Cu = a Y

For an External Standard and Normalization:

C_u = Uncorrected Amount (With scaling factor applied, i.e. 1/x if applicable)

a = Slope of the calibration line segment

Y = Area or height value from Y-Axis

For an Internal Standard:

C_u = Uncorrected Amount Ratio

a = Slope of the calibration line segment

$$Y = \frac{\text{Component Area or Height}}{\text{Internal Standard Area or Height}}$$

Baseline check calculations

The following calculation is used for determining baseline drift in Baseline Check.

$$Drift = \left(\frac{N\sum xy - \sum x \sum y}{N\sum x^2 - \left(\sum x\right)^2} \right) * 60$$

N = Number of Points

x = X Values (in minutes)

y = Y values

For Noise calculations, see ASTM Noise Calculations and Noise Test topics, depending on your choice for this option. For Baseline check, the ASTM Noise Long selection is scaled to use Y-units scaled by the detector instead of microvolts.

Calib weight

You can designate a Calib Weight in the Peak Table for the average of

$$A_w = (x_c * W) + [x_0 * (1 - W)]$$

the replicates with the method Last Area. **Note** that a Calib Weight of 100 causes the Last Area value to be ignored.

A weighted average is calculated using the following equation:

Where

A_w is the weighted average result

Xc is the true average of replicates (if any) with current run area/height

W is the Calib Weight / 100

Xo is the Last area from the method

A weighted average is calculated for the following method example as shown:

Method Last Area	100
Current run area	101
Replicate 1	104
Replicate 2	100
Replicate 3	102

Using a Calib Weight of 60, the weighted average becomes:

[(101 +104 + 100 + 102)/4] * .6 + [100 * (1 - .6)]

Enter a weight factor of 50 to give equal weight to the Last Area average and the new calibration replicates.

Note: For Internal Standard calibrations, each replicate represents a ratio of the component area/height to internal standard area/height.

Calibration averages

The **Replace/Wt Average** Calib Flags in the Peak Table allow you to select whether or not calibration the calibration area will be averaged with previous replicates (Last Area). In general, when **Replace** is selected, the current calibration area will replace any existing calibration area or averaged area in the method. When **WtAverage** is selected, replicates are averaged, and then weighted with the Last Area value (if applicable).

For External Standard calibrations:

When **Wt Average** is selected, the current peak area/height replicates are averaged. When **Replace** is selected, each calibration run replaces the previous value in the method.

For Internal Standard calibrations:

When **Wt Average** is selected, the individual replicate ratios are calculated first, then the average of the ratios is taken. When **Replace** is selected, each calibration run replaces the previous value in the method.

For example, for a calibration component area, **U**, and its associated

internal standard component area, **I**, the average ratio, **Y**, for three replicates is calculated as follows:

Internal Standard Replicate Area (In)	Component Replicate Area (Un)
I1 = 100	U1 = 210
I2 = 99	U2 = 215
I3 = 104	U3 = 212

Ratio 1 = 210 / 100 = 2.1

Ratio 2 = 215 / 99 = 2.172

Ratio 3 = 212 / 104 = 2.039

Y = Average Ratio = 2.104

Note: In the Review Peak Calibration window, if you eliminate a replicate from the calibration curve of an internal standard peak by highlighting it with the mouse, then the associated replicates for peaks using that internal standard are ignored when calculating the average ratio.

If averaging, replicates for each peak level are saved in the method until they are cleared. Replicate 1 is the most recent replicate.

Calibration curve calculations

The calibration of a method results in the creation of a calibration curve for each calibrated component. The calibration curve equation is specified by the type of fit selected in the Peak Table, the definition of response factor for the method, whether it is an internal standard or external standard calibration, scaling factor selected, and weighting selected.

The Uncorrected Amount is the amount (or amount ratio) of a component represented by a given response (or response ratio). The term Uncorrected Amount is used because factors such as sample amount and multiplication factors have not been applied.

The Response Factor for a component is calculated from the calibration curve. It can be reported either as Amount/Area or Area/Amount. This is selected as part of the **Method/Properties** tab.

Note: When a calibration contains replicates, the average of the replicates is calculated prior to the fit calculation.

Calibration curves

A calibration curve relates the component amount to detector response, (or for an Internal Standard calibration, the amount ratio to the area or height ratio). The software fits a curve to the calibration points, according to the fit type, scaling, and weighting factors you select. The resulting calibration curve is used to calculate component concentrations in unknown samples, and is generally

defined by a least squares calculation

$$y = f(x)$$

where f = point to point

linear (with or without force through zero)

quadratic (with or without force through zero)

cubic (with or without force through zero)

average RF fit

Capacity factor (k')

$$k' = \frac{t_2}{t_a} - 1$$

Where

k' = Capacity Factor

t_2 = The retention time measured from point of injection

t_a = The retention time of an inert component not retained by the column, taken from Unretained Peak Time in the **Performance Options** section of the method.

Cubic fit

A cubic calibration fit uses a least squares calculation to determine the best curve fit for a series of calibration points. A minimum of four calibration points is required to determine a cubic fit. The equation for calculating the uncorrected amount is:

$$Y = aX^3 + bX^2 + cX + d$$

For External Standard:

Y = Uncorrected Amount (With scaling factor applied, i.e. 1/x if applicable)

a = Calibration Curve Coefficient

b = Calibration Curve Coefficient

c = Calibration Curve Coefficient

d = Y-Axis intercept

X = component area or height

For an Internal Standard:

Y = Uncorrected Amount Ratio

a = Calibration Curve Coefficient

b = Calibration Curve Coefficient

c = Calibration Curve Coefficient

d = Y-Axis intercept

$$X = \frac{\text{Component Area or Height}}{\text{Internal Standard Area or Height}}$$

DAB (German Pharmacopia) calculation method

NOTE: This calculation equation is also called the BP (British Pharmacopia), EP (European Pharmacopia), and ASTM.

Theoretical Plates

$$N = 5.54 \times \left[\frac{t}{W_{0.5}}\right]^2$$

Where

N = Theoretical plates

t = The retention time of the component

$W_{0.5}$ = Width of peak at the position of 50% peak height

Peak Asymmetry (Tailing Factor)

$$T = \frac{W_{0.05}}{2f}$$

Where

T = Peak asymmetry, or tailing factor

$W_{0.05}$ = The distance from the leading edge to the tailing edge of the peak, measured at a point 5% of the peak height from the baseline

f = The distance from the peak maximum to the leading edge of the peak at the position of 5% peak height

For peak asymmetry at 10%, the values for W and *f* are measured at 10% of peak height.

Resolution

$$R = 1.18 \times \frac{(t_2 - t_1)}{W_{0.5} + W_{p05}}$$

Where

R = Resolution between a peak of interest (peak 2) and the peak preceding it (peak 1).

t_2 = The retention time measured from point of injection of peak 2.

t_1 = The retention time measured from point of injection of peak

1.

$W_{0.5}$ = The width of the component peak at 50 % peak height.

$W_{p0.5}$ = The width of the previous component peak at 50 % peak height.

Determining concentrations for uncalibrated peaks

You can report concentrations for uncalibrated peaks by creating an Uncalibrated Range group and assigning a Manual Response Factor for this range in the Group Table. Once you have done this, any uncalibrated peak that falls within this range will have its concentration calculated using this response factor, and will be included in a run report that has unnamed peaks selected. **Note** that you can define as many uncalibrated ranges as you want for a given method.

Drift test for system suitability

The drift test measures the change in voltage over a given period of time.

$$\frac{y2 - y1}{x2 - x1}$$

Where

y_2 = voltage at time x_2 (drift test start time in minutes)

y_1 = voltage at time x_1 (drift test stop time in minutes)

Note: For SS420x, the voltage is in µv.

EMG (Exponential Modified Gaussian) calculation method

Theoretical Plates

$$41.7 \times \frac{\left[\frac{t}{W_{0.1}}\right]^2}{\frac{b_{0.1}}{a_{0.1}} + 1.25}$$

Where

N= The number of theoretical plates

t= The retention time of the component

$W_{0.1}$ = The width of the peak at the position of 10% peak height

$a_{0.1}$ = The width of the first half (start to top) of peak at the position of 10% peak height

$b_{0.1}$ = The width of the second half (top to end) of peak at the position of 10% of peak height

Peak Asymmetry (Tailing Factor)

$$T = \frac{W_{0.05}}{2f}$$

Where

T = Peak asymmetry, or tailing factor

$W_{0.05}$ = The distance from the leading edge to the tailing edge of the peak, measured at a point 5% of the peak height from the baseline

f = The distance from the peak maximum to the leading edge of the peak at the position of 5% peak height

For peak asymmetry at 10%, the values for W and *f* are measured at 10% of peak height.

Resolution

$$R = 2.15 \times \frac{(t_2 - t_1)}{W_{0.1} + W_{p0.1}}$$

Where

R = Resolution between a peak of interest (peak 2) and the peak preceding it (peak 1).

t_2 = The retention time measured from point of injection of peak 2.

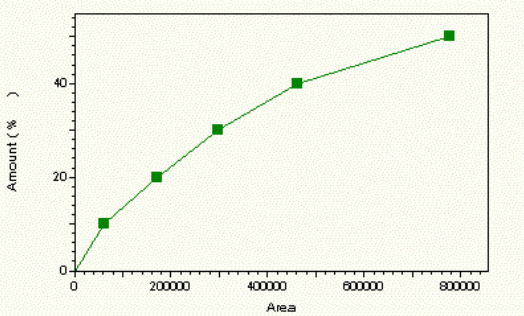
t_1 = The retention time measured from point of injection of peak 1.

$W_{0.1}$ = The width of peak at the position of 10% peak height

$W_{p0.1}$ = The width of previous peak at the position of 10% peak height

External standard calibration curves

In the following example for an External Standard and Normalization curve, the component Amount is plotted on the Y-Axis and the component Area is plotted on the X-Axis (Amount/Area Response Factor Definition).



The external calibration curve (for Response Factor definition **Area/Amount**) is calculated as:

Amtcal = f (Areacal)

Where:

f = the equation of the calibration points according to the fit type you have selected (linear, quadratic, point to point, etc.)

Amtcal = the amount of the calibration standard

Areacal = the area of the calibration standard

Therefore the unknown is determined by:

Amtunk(u) = f (Area unk)

Where:

Amtunk(u) = the uncorrected amount of the unknown component

f = the equation of the calibration points according to the fit type you have selected

Areaunk = the area of the unknown component

To calculate the concentration of the unknown sample:

$$\text{Conc} = \frac{\text{Amt}_{\text{unk(u)}}}{\text{SampleAmt}_{\text{u}}} \times \text{MF}$$

Where:

Conc = the concentration (in the same units used for calibration) of the unknown analyte of interest

Amtunk(u) = the uncorrected amount of the unknown component

Sample Amt_{u}= the amount of the unknown sample taken from the Sequence Table or Single Run dialog

MF = multiplication and dilution factors applied = $M_1{*}M_2{*}M_3/D_1{*}D_2{*}D_3$ for the unknown sample

External standard report calculation

$$Conc = \frac{Cu}{Samp.\ Amt.} * MF$$

Where:

Conc = Corrected Amount of component.

C_u = Amount value from calibration curve for a given unknown area

Samp.Amt = Sample amount

MF = multiplication and dilution factors applied = $M_1*M_2*M_3/D_1*D_2*D_3$

Internal standard amounts

The Internal Standard Amounts for any **calibration** run is always taken from the method Peak Table. Any value for Internal Standard Amount in the Sequence table or in the Single Run Acquisition dialog for a calibration run is ignored.

For an unknown run, the Internal Standard Amount is entered in the Single Run Acquisition dialog box, or in the Sequence Table. It is used as a multiplier in calculation of the unknown concentration.

Internal standard report calculation

$$Conc = \frac{Cu}{(Sample\ Amt.)} * ISTD_u * MF$$

Where:

Conc = Corrected Amount of component

ISTDu = Amount of Internal Standard

Samp.Amt = Sample amount

MF = multiplication and dilution factors applied = $M_1*M_2*M_3/D_1*D_2*D_3$

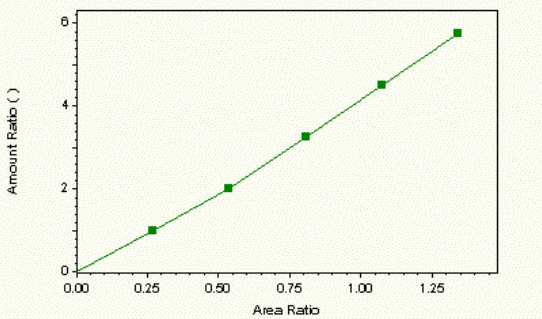
C_u = Amount ratio taken from the calibration curve for the given area/height ratio

Internal standard vs external standard and normalization

External Standard and Normalization calibration curve plots differ from Internal Standard calibration curves. This is because the amounts and responses in the Internal Standard calibration represent the ratios of the internal standard component to the amounts and responses of the calibrated components.

Internal standards

In this example of an Internal Standard calculation, the **ratio** of component amount to Internal Standard amount is plotted on the Y-Axis and the **ratio** of component area to Internal Standard area is plotted on the X-Axis (Amount/Area Response Factor definition):



The calibration is calculated as:

Amt RatioISCal = ƒ (Area RatioISCal)

Where:

Amt RatioISCal = amount ratio of the calibration standard

f = equation of the calibration points according to the fit type you have selected

Area RatioISCal = area ratio of the calibration standard

Therefore the unknown is determined by:

Amt Ratiounk(u) = ƒ (Area Ratiounk)

Where:

Amt Ratiounk(u) = the uncorrected amount ratio of the unknown component

f = the equation of the calibration points according to the fit type you have selected

Area Ratiounk = the area ratio of the unknown component

The concentration of the unknown sample is calculated by:

$$Conc_u = \frac{Amt_{IS}}{SampleAmt_u} \times MF \times AmtRatio_{unk}$$

$Conc_u$= Concentration (in the same units used for calibration) of the analyte of interest.

Amt_{IS} = Amount of the internal standard

$SampleAmt_u$ = Amount of the unknown sample from sequence or at start of single run

MF = multiplication and dilution factors applied = $M_1*M_2*M_3/D_1*D_2*D_3$ for the unknown sample

$AmtRatio_{Unk}$ = Amount ratio value taken from the calibration curve at the given area ratio for the unknown sample

Japanese Pharmacopoeia (JP) 15th Edition calculation

These equations are for the JP 15th Edition calculations.

Theoretical Plates

$$N = 5.54 \times \left[\frac{t}{W_{0.5}} \right]^2$$

Where

N = Theoretical plates

t = The retention time of the component

$W_{0.5}$ = Width of peak at the position of 50% peak height

Peak Asymmetry (Tailing Factor)

$$T = \frac{W_{0.05}}{2f}$$

Where

T = Peak asymmetry, or tailing factor

$W_{0.05}$ = The distance from the leading edge to the tailing edge of the peak, measured at a point 5% of the peak height from the baseline

f = The distance from the peak maximum to the leading edge of the peak at the position of 5% peak height

For peak asymmetry at 10%, the values for W and *f* are measured at 10% of peak height.

Resolution

$$R = 1.18 \times \frac{(t_2 - t_1)}{W_{0.5} + W_{p0.5}}$$

Where

R = Resolution between a peak of interest (peak 2) and the peak preceding it (peak 1).

t_2 = Retention time measured from point of injection of peak 2.

t_1 = Retention time measured from point of injection of peak 1.

$W_{0.5}$ = The width of the component peak at 50 % peak height.

$W_{p0.5}$ = The width of the previous component peak at 50 % peak height.

Linear fit

A linear calibration fit determines the best line (linear regression) for a series of calibration points. A minimum of two calibration points are required to determine a linear fit. The equation for calculating the uncorrected amount is:

$$Y = a X + b$$

For Response Factor definition Area/Amount,

External Standard:

Y = Component area or height

a = slope of the calibration line

X = Uncorrected Amount (With scaling factor applied, i.e. 1/x if applicable)

b = Y-Axis intercept of the calibration line

Internal Standard:

a = slope of the calibration line

X = Uncorrected Amount Ratio

b = Y-Axis intercept of the calibration line

For Response Factor definition Amount/Area,

External Standard:

Y = Uncorrected Amount (With scaling factor applied, i.e. 1/x if applicable)

a = slope of the calibration line

X = component area or height

b = Y-Axis intercept of the calibration line

Internal Standard:

Y = Uncorrected Amount Ratio

a = slope of the calibration line

b = Y-Axis intercept of the calibration line

Matrix operations

The following example illustrates the matrix operations used to determine curve coefficients for quadratic calibration curve fits.

The equation for the quadratic calibration curve is

For a series of amount/area pairs (x, y) representing calibration

$$Y = ax^z + bx + c$$

points (or averaged calibration points)

(x1, y1) (x2, y2) (x3, y3).....(xnyn)

These points produce n quadratic equations, which can be solved for the coefficients a, b, and c by writing the equations in matrix notation as follows.

$$\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix} = \begin{bmatrix} x_1^2 & x_1 & 1 \\ x_2^2 & x_2 & 1 \\ \vdots & \vdots & \vdots \\ x_n^2 & x_n & 1 \end{bmatrix} \bullet \begin{bmatrix} a \\ b \\ c \end{bmatrix}$$

or,

Y = M • Z

To ensure a square matrix, the equation is multiplied by M' to become

$$M^T Y = M^T MZ$$

where M^T is matrix **M** transposed

$$\begin{bmatrix} x_1^2 & x_2^2 & \cdots & x_n^2 \\ x_1 & x_2 & \cdots & x_n \\ 1 & 1 & \cdots & 1 \end{bmatrix}$$

then

$$Z = \left(M^T M\right)^{-1} M^T Y$$

If the curve is forced through zero, then c=0, and **M** becomes a 2-column matrix which is solved for coefficients a and b.

Modified least squares calculation

The following modified least squares formula is used to determine the calibration curve coefficients for linear fits:

$$\begin{vmatrix} a \\ b \end{vmatrix} = \begin{vmatrix} \sum WX & \sum W \\ \sum WX^2 & \sum WX \end{vmatrix}^{-1} \times \begin{vmatrix} \sum WY \\ \sum WXY \end{vmatrix}$$

Where:

a = the slope of the calibration line

b = the Y-Axis intercept of the calibration line

W is the weighting term = $1/X$ or $1/X^2$

where X = Response or Amount. This is selected as the Weighting Method in the peak table.

For Internal Standard calculations, X is the uncorrected amount ratio of the component of interest in the calibration sample Cu. Y is the corrected relative area = peak area/int std area

For External Standard calculations, X is the uncorrected amount of the component of interest in the calibration sample Cu. Y is the corrected relative area = peak area

The modified least squares calculation can be extended to higher order fits. As an example, the following formula is used to determine the calibration curve coefficients for weighted quadratic fits:

$$\begin{vmatrix} a \\ b \\ c \end{vmatrix} = \begin{vmatrix} \sum WX^2 & \sum WX & \sum W \\ \sum WX^3 & \sum WX^2 & \sum WX \\ \sum WX^4 & \sum WX^3 & \sum WX^2 \end{vmatrix}^{-1} X \begin{vmatrix} \sum WY \\ \sum WXY \\ \sum WX^2Y \end{vmatrix}$$

The following formula is used to determine the R-squared value for a series of values:

Where

$\hat{Y}$ is an ordinate of the least squares line.

$$R^2 \quad \overline{Y} = \frac{\sum Y_i - \hat{Y}_i)^2}{n} \quad \overline{\sum_{i=1}^{n} (Y_i - \overline{Y})^2}$$

Y_i is the observed value of Y.

Noise test (rms noise)

The rms noise is the standard deviation of the signal derived from n measurements, defined by the time segment chosen.

rms noise =

$$\left[\frac{\sum_{i=1}^{n} (E_i - \overline{E})^2}{n-1} \right]^{1/2}$$

Where E_I = individual voltage readings

and E bar = the average of n measurements.

Normalization report calculation

$$\text{Conc} = \frac{Cu * 100}{\text{Sum of } Cu \text{ for named peaks} + \text{Sum}CR}$$

Where:

Conc = Corrected Amount of component

Cu = Uncorrected Amount of component

Sum_{CR} = Sum of calibrated range groups

Peak centroid

The peak centroid is the position in the peak at which 50% of the area has been reached. This calculation is available for calculation, annotation, and export.

$$x_C = \frac{\int x\, dA}{A}$$

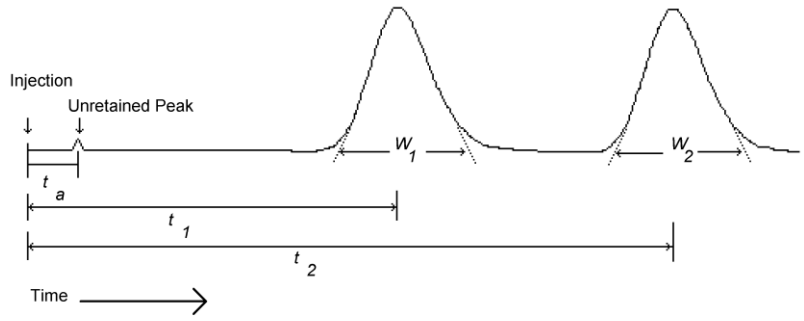
Performance calculations

The following values are calculated that can be used to assess overall system performance:

- Relative Retention
- Theoretical Plates
- Capacity Factor
- Resolution
- Peak Asymmetry
- Plates per Meter

These values can be included in a custom report.

The following diagram shows the parameters used to calculate these system performance values for the separation of two chromatographic components.



Separation of two chromatographic components

Note: To accurately calculate suitability values, the sampling frequency (set in Acquisition Setup) must be set to provide at least 20 data points for the narrowest peak of interest.

Plates/Meter

$$N = \frac{n}{L}$$

Where

N = Plates per meter

n = Theoretical plates in the column

L = Column length, in meters. This value is taken from the **Performance Options** section of the method.

Point-to-Point fit

A point-to-point calibration fit connects a series of calibration points with lines. The result for point-to-point calculations are the same regardless of Response Factor definition. The equation for calculating the uncorrected amount is:

$$\mathbf{Y = aX + b}$$

For an External Standard:

Y = Uncorrected Amount (With scaling factor applied, i.e. 1/x if applicable)

a = Slope of the calibration line segment

X = Area or height value from Y-Axis

b = Y-Axis intercept of the calibration line segment

For an Internal Standard:

Y = Uncorrected Amount Ratio

a = Slope of the calibration line segment

X = component area or height/internal standard area or height

b = Y-Axis intercept of the calibration line segment

NOTE: For points beyond the last calibration point, the line segment between the last two calibration points is extrapolated. If the value falls below the lowest calibration point, then the line segment is constructed between zero and the first calibration point.

Quadratic fit

A quadratic calibration fit determines the best quadratic curve fit for a series of calibration points. A minimum of three calibration points is required to determine a quadratic fit. The equation for calculating the uncorrected amount is:

$$Y = aX^2 + bX + c$$

For Response Factor definition Area/Amount,

External Standard:

Y = Uncorrected Amount (With scaling factor applied, i.e. 1/x if applicable)

a = Calibration Curve Coefficient

b = Calibration Curve Coefficient

c = Y-Axis intercept

X = component area or height

Internal Standard:

Y = Uncorrected Amount Ratio

a = Calibration Curve Coefficient

b = Calibration Curve Coefficient

c = Y-Axis intercept

$$X = \frac{\text{Component Area or Height}}{\text{Internal Standard Area or Height}}$$

For Response Factor definition Amount/Area,

External Standard:

Y = Component area or height

a = Calibration Curve Coefficient

b = Calibration Curve Coefficient

c = Y-Axis intercept

X = Uncorrected Amount (With scaling factor applied, i.e. 1/x if applicable)

Internal Standard:

a = Calibration Curve Coefficient

b = Calibration Curve Coefficient

c = Y-Axis intercept

X = Uncorrected Amount Ratio

$$Y = \frac{\text{Component Area or Height}}{\text{Internal Standard Area or Height}}$$

Relative retention

Relative retention is calculated for named peaks with reference peaks and detected unnamed peaks that are members of uncalibrated or calibrated range groups if a reference peak is specified. The reference peak specified in the group is used to calculate the Relative RT for the unnamed peaks using the same equation used for named peaks.

$$\alpha = \frac{t_2 - t_a}{t_1 - t_a}$$

Where

α = Relative retention.

t_2 = The retention time measured from point of injection

t_a = The retention time of an inert component not retained by the column, taken from Unretained Peak Time in the **Performance Options** section of the method.

t_1 = The retention time from point of injection for reference peak defined in the peak table. If no reference peak is found, this value becomes zero.

Relative retention (Selectivity)

$$\alpha = \frac{t_2 - t_a}{t_1 - t_a}$$

Where

α = Relative retention.

t_2 = The retention time measured from point of injection

t_a = The retention time of an inert component not retained by the column, taken from Unretained Peak Time in the **Performance Options** section of the method.

t_1 = The retention time from point of injection for reference peak defined in the peak table. If no reference peak is found, this value becomes zero.

Note: This parameter is labeled as Relative RT in reports.

Reporting Zero for internal standard concentrations

Internal standard components always have an RF value of 1.00. Normally a concentration is reported for internal standard components using the RF value.

To force the concentration of the internal standard component to be reported as zero (and therefore will not contribute to analyte concentration totals), enter a Manual RF value of zero for the internal standard components in the peak table.

Response factor definition

You can choose to have response factors defined as either Amount/Area or Area/Amount. This selection is made in the Method Properties>Options tab and will apply to the entire method. The calibration curve and assignment of x and y values will differ depending on the response factor selection you make.

Savitsky-Golay smoothing

A 9-point digital filter is applied as a sliding filter to the data points as shown in the following example for data points a1 through a3.

$$\frac{a1f1+a2f2+...a9f9}{norm} \quad \frac{a2f1+a3f2+...a10f9}{norm} \quad \frac{a3f1+a4f2+...a11f9}{norm}$$

Where a1....ax are the data points, f1...fx are the filtering factors, and norm is the normalization factor. The filtering factors and normalization factor are given below.

f0: -21

f1: 14

f2: 39

f3: 54

f4: 59

f5: 54

f6: 39

f7: 14

f8: -21

The normalization factor is 231.0.

Scaling

This parameter allows you to apply a scaling factor to the calibration curve. This factor is applied to the entered amounts prior to computing the calibration curve. The purpose of using a scaling factor is to create a relationship between areas (or heights) and amounts that can be approximated by a polynomial fit. A scaling factor can be applied to any fit type. The available scaling operations are:

None

1/Amount

ln[Amount]

1/ln[Amount]

sqrt[Amount]

Amount2

1/Response

1/Response2

ln[Response]

1/ln[Response]

sqrt[Response]

Response2

Log (Amount)

1/ log (Amount)

log (Response)

1/ log (Response)

ln (Amt)&ln(Resp)

log(Amt)&log(Resp)

USP (United States Pharmacopia) calculation method

Theoretical Plates

$$n = 16\left(\frac{t}{W}\right)^2$$

Where

n = theoretical plates

t = The retention time of the component

W = The width of the base of the component peak using tangent method.

Peak Asymmetry (Tailing Factor)

$$T = \frac{W_{0.05}}{2f}$$

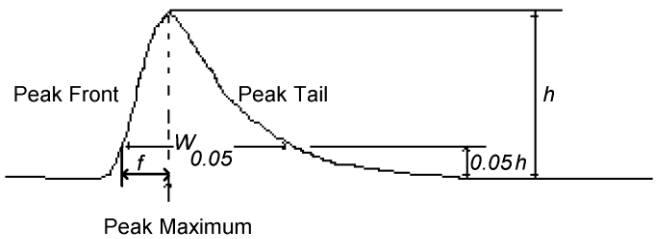
Where

T = Peak asymmetry, or tailing factor

$W_{0.05}$ = The distance from the leading edge to the tailing edge of the peak, measured at a point 5% of the peak height from the baseline

f = The distance from the peak maximum to the leading edge of the peak at the position of 5% peak height

Note: For peak asymmetry at 10%, the values for W and *f* are measured at 10% of peak height.



Asymmetric Peak

Resolution

Where

$$R = \frac{2(t_2 - t_1)}{W_2 + W_1}$$

R = Resolution between a peak of interest (peak 2) and the peak preceding it (peak 1).

t_2 = The retention time measured from point of injection of peak 2.

t_1 = The retention time measured from point of injection of peak 1.

W_2 = The width of the base of the component peak 2

W_1 = The width of the base of the component peak 1

Weighting and scaling

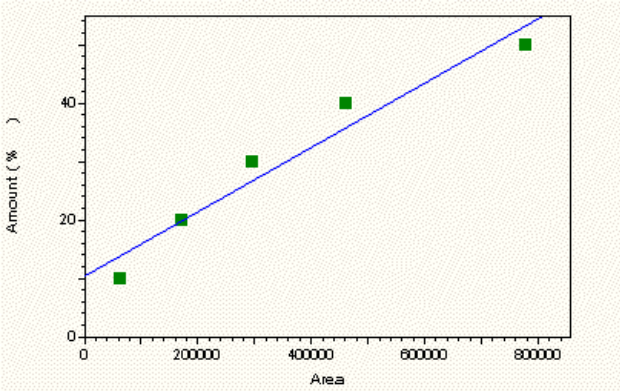
There are a number ways to do averaging and weighting. The following table summarizes the differences between these selections.

Table 2 Differences between averaging and weighing

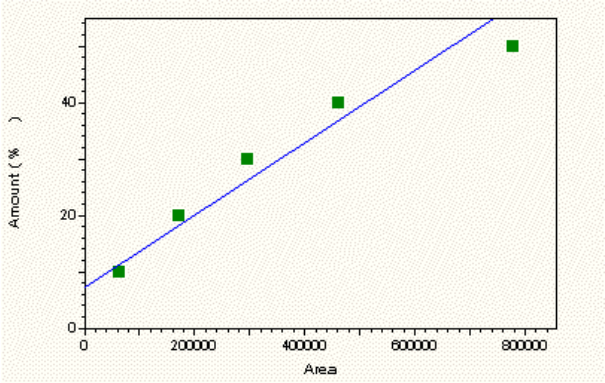
Selection	Located In	Effect or Use
Calib Flag Replace/WtAverage	Peak Table	If Replace, each new calibration area will replace previous calibration area in the method. If WtAverage, replicates will be averaged. Weighted average using Calib Weight will be calculated if method contains a Last Area. If Auto Averaging is also ON,calibration replicates will be cleared when the level is re-calibrated.
Calib Weight (Value)	Peak Table	A weighting factor used to calculate a weighted calibration average of current replicates with method Last Area.
Scaling	Peak Table	Applied to amounts prior to creating calibration curve for a peak, for purpose of creating a relationship between area and amounts that can be approximated by a polynomial fit.
Weighing Method	Peak Table	LSQ Weighting Method to be used for calculation of least squares regression fits. Generally gives more importance to points representing smaller areas and amounts.

Weighting method (LSQ Weight)

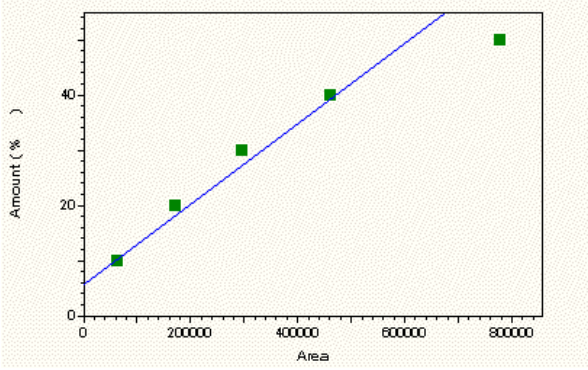
Selecting a LSQ Weighting Method to be used for calculation of least squares regression fits, either 1/x or $1/x^2$, gives increased importance to smaller concentrations and areas. LSQ Weight can be applied to linear, quadratic, and cubic fits only. Examples are shown below.



Linear fit with No LSQ Weighting



Linear Fit with 1/x LSQ Weighting



Linear Fit with $1/x^2$ LSQ Weighting

About ASCII sequence file formats

An ASCII sequence suitable for importing consists of lines of text (each line terminated with a newline character). The first line of the text file must be: ASCII Sequence n where n is the version number of the ASCII sequence. Currently, this number must be set to 1 (one), so the first line of the file should be ASCII Sequence 1. The ASCII double export is one version higher than the ASCII version number. An ASCII sequence file contains the following elements:

See Also

ASCII Sequence Header

ASCII Sequence Records

ASCII Action Record

Example of ASCII Sequence File

Example of ASCII Dual Tower Sequence File

ASCII sequence header

The next part of the text file contains sequence header information of the form

<keyword>=<value>

For example:

DATAPATH=C:\DATASYSTEM\DATA

The following keywords are recognized as elements of the sequence header (Keywords are case sensitive and should be typed as shown below):

CREATIONDATE=

LASTCHANGEDATE=

METHODPATH= (128 characters maximum)

PRINTREPORTS=(YES or NO)

DATAPATH= (128 characters maximum)

PRETREATPATH= (128 characters maximum)

SUMMARYPATH= (128 characters maximum)

DESCRIPTION=

None of these keywords are mandatory; if a keyword does not exist in the text file, a default value will be used.

Note: When creating description fields with multiple lines, a hex 0x07 character may be used to embed a <CR> (new line) within the text. Typically this should be done by a software program that can directly write hexadecimal characters. Some text editors support keyboard entry of hexadecimal characters by holding the alt key while typing 07 on the numeric keypad.

ASCII sequence records

After all sequence header elements have been specified, the rest of the text file consists of lines specifying the records of the sequence table. The record contains comma-delimited elements detailing the operation of that line of the sequence.

Note: Some autosamplers use a non-numeric designation for vial poisitons (e.g. 'A7' for a micro plate). If the instrument configuration includes such an autosampler, please refer to that driver's installation guide for detail on how to encode it in a manner that is compatible with ASCII sequence import.

These lines are of the form:

RECORD=a,b,c,d,e,f,g,h,i,j,k,l,m,n,o,p,q,r,s,t,u

Where:

a = Sample ID (63 characters maximum)

b = Method name (63 characters maximum)

c = File name (63 characters maximum)

d = Calibration level (0 - x, 0 = no calibration)

e = Sample amount (real number > 0)

f = Internal standard amount (real number > 0)

g = Multiplication factor 1 (real number > 0)

h = Injection vial

i = Injection volume

j = Pretreatment file name

k = Fraction collector file name

l = Reserved; do not specify anything between the commas

m = Run type (see list below)

n = Action (Leave blank. This is no longer used.)

o = Run description

p = Repetitions per vial (1 - 9)

q = Multiplication factor 2 (real number > 0)

r = Multiplication factor 3 (real number > 0)

s = Dilution factor 1 (real number > 0)

t = Dilution factor 2 (real number > 0)

u = Dilution factor 3 (real number > 0)

Run Types

Decimal Hex Name

4 0x0000004 UnSpiked

8 0x0000008 Spiked

16 0x0000010 Spike 1 of 2

32 0x0000020 Spike 2 of 2

64 0x0000040 Duplicate 1

128 0x0000080 Duplicate 2

256 0x0000100 System Suit Start

512 0x0000200 System Suit End

1024 0x0000400 System Suit Std.

2048 0x0000800 Shutdown

4096 0x0001000 Begin Calibration

8192 0x0002000 End Calibration

16384 0x0004000 QC Standard

32768 0x0008000 Summary Start

65536 0x0010000 Summary End

131072 0x0020000 Summary Run

262144 0x0040000 Clear All Response Factors

524288 0x0080000 Clear Response Factors for this Level

1048576 0x0100000 Print Response Factors

2097152 0x0200000 Average Replicates

4194304 0x0400000 Clear Replicates

8388608 0x0800000 Begin Loop

16777216 0x1000000 End Loop

ASCII action record

Action records relate to the previous Sequence Record only.

Form:

ACTION=a,b,c,d,e

a: CONDITION:

0 Any Condition

1 Calibration

2 QC

3 System Suitability

4 Hardware Status

5 Conc. Limit

b: RESULT:

0 Pass

1 Fail

2 Below Limit

3 Above Limit

c: ACTION:

0 Abort

1 Pause

2 Reinject

3 Run User Program

4 Run Shutdown

5 Alarm

6 Goto

7 Restart System Suit

d: PARAMETER 1:

For Reinject and Goto - Rep Count.

For Run User Program - Program Path and Name.

e: PARAMETER 2:

For Goto - Goto Record Number.

Notes: Regarding method name, file name, pretreat name and fraction collector file name: If these items do not have path names embedded, the appropriate path from the header will be used (fraction collector files are assumed to reside in the pretreatment file path). All elements of the record line MUST be present; however, any record element not of interest can be skipped by specifying nothing in-between the commas. If you are creating the ASCII file using Microsoft Excel, save the file in the *.CSV format. Sample ID must be in the same cell as RECORD= to prevent a comma after the (=). Method and data paths must be selected manually using Sequence Properties because the .CSV adds a comma to the path.

Example of ASCII sequence file

The following is an example of an ASCII Sequence file.

ASCII Sequence 1

CREATIONDATE=

LASTCHANGEDDATE=

METHODPATH = D:\System\Methods

PRINTREPORTS = NO

DATAPATH = D:\System\data

PRETREATPATH =

SUMMARYPATH =

DESCRIPTION = The description of this ASCII Sequence.

RECORD=Samp,MULTICAL.MET,Multical001.dat,0,1.2,2.91,1.1,1,12,,,,16384,1,,3

RECORD=Samp,MULTICAL.MET,Multical002.dat,0,1.2,2.91,1.1,2,12,,,,,2,Record Desc,3

RECORD=Samp,MULTICAL.MET,Multical003.dat,3,1.2,2.91,1.1,1,12,,,,16384,,,3

ACTION = 1,1,3,D:\CHROM\Program.EXE

ACTION = 1,0,2,4

RECORD=Samp,MULTICAL.MET,Multical004.dat,0,1.2,2.91,1.1,2,12,,,,,4,Record Desc,3

RECORD=Samp,MULTICAL.MET,Multical005.dat,0,1.2,2.91,1.1,1,12,,,,16384,,,3

ACTION = 3,1,6,7 ,2

ACTION = 3,0,2,4

RECORD=Samp,MULTICAL.MET,Multical006.dat,6,1.2,2.91,1.1,2,12,,,,16384,3,,3

RECORD=Samp,MULTICAL.MET,Multical007.dat,0,1.2,2.91,1.1,1,12,,,,,2,,3

RECORD=Samp,MULTICAL.MET,Multical008.dat,0,1.2,2.91,1.1,2,12,,,,76,,Record Desc,3

ACTION = 4,1,5

ACTION = 4,0,2,4

RECORD=Samp,MULTICAL.MET,Multical009.dat,9,1.2,2.91,1.1,1,12,,,,16384,1,,3

RECORD=Samp,MULTICAL.MET,Multical010.dat,0,1.2,2.91,1.1,2,12,,,,16384,2,,3

Example of ASCII dual tower sequence file

ASCII Sequence 1

CREATIONDATE=

LASTCHANGEDDATE=

METHODPATH = \\Qa-glisowski01\transfer

PRINTREPORTS =

NO DATAPATH = \\Qa-glisowski01\transfer\public

PRETREATPATH =

SUMMARYPATH =

DESCRIPTION = The description of this ASCII Sequence.

TOWER=0

RECORD=Front Samp 1,HP6890 FRONT

JL01.MET,FrontMultical001.dat,0,1.2,2.91,1.1,1,1,,,,16384,1,,3

RECORD=Front Samp 2,HP6890 FRONT

JL01.MET,FrontMultical002.dat,0,1.2,2.91,1.1,2,1,,,,,2,Record Desc,3

RECORD=Front Samp 3,HP6890 FRONT

JL01.MET,FrontMultical003.dat,3,1.2,2.91,1.1,3,1,,,,16384,,,3

ACTION = 1,1,3,D:\CHROM\Program.EXE

ACTION = 1,0,2,4

RECORD=Front Samp 4,HP6890 FRONT

JL01.MET,FrontMultical004.dat,0,1.2,2.91,1.1,4,1,,,,,4,Record Desc,3

RECORD=Front Samp 5,HP6890 FRONT

JL01.MET,FrontMultical005.dat,0,1.2,2.91,1.1,5,1,,,,16384,,,3

ACTION = 3,1,6,7 ,2

ACTION = 3,0,2,4

RECORD=Front Samp 6,HP6890 FRONT

JL01.MET,FrontMultical006.dat,6,1.2,2.91,1.1,6,1,,,,16384,3,,3

RECORD=Front Samp 7,HP6890 FRONT

JL01.MET,FrontMultical007.dat,0,1.2,2.91,1.1,7,1,,,,,2,,

RECORD=Front Samp 8,HP6890 FRONT

JL01.MET,FrontMultical008.dat,0,1.2,2.91,1.1,8,1,,,,76,,Record Desc,3

ACTION = 4,1,5,

ACTION = 4,0,2,4,

RECORD=Front Samp 9,HP6890 FRONT

JL01.MET,FrontMultical009.dat,9,1.2,2.91,1.1,9,1,,,,16384,1,,3,

RECORD=Front Samp 10,HP6890 FRONT
JL01.MET,FrontMultical010.dat,0,1.2,2.91,1.1,10,1,,,,16384,2,,3,

TOWER=1 ASCII Sequence 1

CREATIONDATE=

LASTCHANGEDDATE=

METHODPATH = \\Qa-glisowski01\transfer

PRINTREPORTS =

NO DATAPATH = \\Qa-glisowski01\transfer\public

PRETREATPATH =

SUMMARYPATH =

DESCRIPTION = The description of this ASCII Sequence.

RECORD=Rear Samp 1,REAR

JL01.MET,RearMultical001.dat,0,1.2,2.91,1.1,11,1,,,,16384,1,,3

RECORD=Rear Samp 2,HP6890 REAR

JL01.MET,RearMultical002.dat,0,1.2,2.91,1.1,12,1,,,,,2,Record Desc,3

RECORD=Rear Samp 3,HP6890 REAR

JL01.MET,RearMultical003.dat,3,1.2,2.91,1.1,13,1,,,,16384,,,3

ACTION = 1,1,3,D:\CHROM\Program.EXE

ACTION = 1,0,2,4

RECORD= Rear Samp 4,HP6890 REAR

JL01.MET,RearMultical004.dat,0,1.2,2.91,1.1,14,1,,,,,4,Record Desc,3

RECORD=Rear Samp 5,HP6890 REAR

JL01.MET,RearMultical005.dat,0,1.2,2.91,1.1,15,1,,,,16384,,,3

ACTION = 3,1,6,7 ,2

ACTION = 3,0,2,4

RECORD=Rear Samp 6,HP6890REAR

JL01.MET,RearMultical006.dat,6,1.2,2.91,1.1,16,1,,,,16384,3,,3

RECORD=Rear Samp 7,HP6890 REAR

JL01.MET,RearMultical007.dat,0,1.2,2.91,1.1,17,1,,,,,2,,3

RECORD=Rear Samp 8,HP6890 REAR

JL01.MET,RearMultical008.dat,0,1.2,2.91,1.1,18,1,,,,76,,Record Desc,3

ACTION = 4,1,5

ACTION = 4,0,2,4

RECORD= Rear Samp 9,HP6890 REAR

JL01.MET,RearMultical009.dat,9,1.2,2.91,1.1,19,1,,,,16384,1,,3

RECORD=Rear Samp 10,HP6890 REAR

JL01.MET,RearMultical010.dat,0,1.2,2.91,1.1,20,1,,,,16384,2,,3

Functional reference

Functions are used to define what data is displayed and the source of the data, as well as for application of mathematical formulas. Functions do not appear on the spreadsheet unless they are being edited. (To view the function in a cell, double-click on that cell.) The results of defined functions do not appear on the spreadsheet, but will appear in Print Preview or when the report is printed, provided the data is available for the function to work. (For example, sequence summary tables will not contain valid data until after a sequence has been acquired and processed or reprocessed.)

In cases where data is not available for the function to work on, an error may be displayed on your spreadsheet. If this happens, click **OK** to close the error, then click the **Print Preview** button. If the function is technically correct, but has no data available, no error messages will appear on the print preview. If an error message appears on the print preview, your function has not been entered correctly.

The following functions are available when creating advanced reports using the template editor.

Syntax Notes:

= All of the functions described here are placed in cells in the template reporting spreadsheet, and must begin with an '=' sign. For example, if a function were described as Custom.Func([Param A]), then the actual function would look something like =Custom.Func(Param A)

[] These brackets indicate optional parameters. The brackets themselves are not included in the actual parameters. For example, if a function were described as Custom.Func([Param A]), then the

actual function would look something like =Custom.Func(Param A)

<> These brackets indicate required parameters. The brackets themselves are not included in the actual parameters. For example, if a function were described as Custom.Func(<Param A>), then the actual function would look something like =Custom.Func(Param A)

"" Quotation marks shown are required. The quotation marks are included in the actual parameters. For example, if a function were described as Custom.Func(<"Param A">), then the actual function would look something like =Custom.Func("Param A")

See Also

Parameter Description

Datafile Functions

Extended Helper Functions

Group Functions

Instrument Functions

Peak Functions

Project Functions

Sequence Functions

Parameter description

The following describes the parameters that may be passed to template functions to describe the requested data file, peak, and group information.

'Run Info' may be one of the following:

RC	The current run or currently loaded data file.
R<x>	The sequence run specified by run <x>.

'Trace Info' may be one of the following:

T<x>	The trace specified by index <x>.

'Peak Info' may be one of the following:

P<x>; <peak type>	The peak with an index of <x> having the given peak type.

'Group Info' may be one of the following:

G<x>; <group type>	The group with an index of <x> having the given group type.

'Direction' may be one of the following:

0	The data will be repeated across the spreadsheet.
1	The data will be repeated down the spreadsheet.

'Peak Type' may be any combination of the following:

1	Report named peaks that were detected.
2	Report named peaks that were not detected.
4	Report unnamed peaks.

'Group Type' may be one of the following:

0	Report calibrated range groups that calculate concentrations for unnamed peaks in this group.
1	Report calibrated range groups that do not calculate concentrations for unnamed peaks in this group.
2	Report named peak groups.

Datafile functions

These functions return information about data files that have been collected and analyzed.

See Also

Data.AcquisitionDate

Data.AnalysisDate

Data.BCDValue

Data.Description

Data.Filename

Data.FullFilename

Data.InstrumentName

Data.ISTDAmount

Data.LastMethodFilename

Data.LastMethodFullFilename

Data.MultiplierFactor

Data.OriginalMethodFilename

Data.OriginalMethodFullFilename

Data.SampleAmount

Data.SampleID

Data.SystemWideParam

Data.SystemWideParamByName

Data.TraceName

Data.UserName

Data.Vial

Data.Volume

Data.AcquisitionDate

Returns date and time of acquisition for the specified data file.

Syntax

=Data.AcquisitionDate(<Run Info>)

Parameters

<Run Info> Describes the data file(s) that will be used to extract the value.

See the Parameter Description section for a description of the above parameter(s).

Return Type

Date/Time

Data.AnalysisDate

Returns date and time of the last analysis for the specified data file.

Syntax

=Data.AnalysisDate(<Run Info>)

Parameters

<Run Info> Describes the data file(s) that will be used to extract the value.

See the Parameter Description section for a description of the above parameter(s).

Return Type

Date/Time

Data.BCDValue

Returns BCD value of the specified data file.

Syntax

=Data.BCDValue(<Run Info>)

Parameters

<Run Info> Describes the data file(s) that will be used to extract the value.

See the Parameter Description section for a description of the above parameter(s).

Return Type

Number

Data.Description

Returns the description of the specified data file.

Syntax

=Data.Description(<Run Info>)

Parameters

<Run Info> Describes the data file(s) that will be used to extract the value.

See the Parameter Description section for a description of the above parameter(s).

Return Type

String

Data.Filename

Returns file name of the specified data file. Only the file name is returned the path information is not returned.

Syntax

=Data.Filename(<Run Info>)

Parameters

<Run Info> Describes the data file(s) that will be used to extract the value.

See the Parameter Description section for a description of the above parameter(s).

Return Type

String

Data.FullFilename

Returns full file name of the specified data file. The file name and path information is returned.

Syntax

=Data.FullFilename(<Run Info>)

Parameters

<Run Info> Describes the data file(s) that will be used to extract the value.

See the Parameter Description section for a description of the above parameter(s).

Return Type

String

Data.InstrumentName

Returns the name of the instrument that was used to acquire the specified data file.

Syntax

=Data.InstrumentName(<Run Info>)

Parameters

<Run Info> Describes the data file(s) that will be used to extract the value.

See the Parameter Description section for a description of the above parameter(s).

Return Type

String

Data.ISTDAmount

Returns ISTD amount of the specified data file.

Syntax

=Data.ISTDAmount(<Run Info>)

Parameters

<Run Info> Describes the data file(s) that will be used to extract the value.

See the Parameter Description section for a description of the above parameter(s).

Return Type

Number

Data.LastMethodFilename

Returns the name of the last method file that was used to analyze the specified data file.

Syntax

=Data.LastMethodFilename(<Run Info>)

Parameters

<Run Info> Describes the data file(s) that will be used to extract the value.

See the Parameter Description section for a description of the above parameter(s).

Return Type

String

Data.LastMethodFullFilename

Returns the full name and path of the last method file that was used to analyze the specified data file.

Syntax

=Data.LastMethodFullFileName(<Run Info>)

Parameters

<Run Info> Describes the data file(s) that will be used to extract the value.

See the Parameter Description section for a description of the above parameter(s).

Return Type

String

Data.MultiplierFactor

Returns multiplier factor of the specified data file.

Syntax

=Data.MultiplierFactor(<Run Info>)

Parameters

<Run Info> Describes the data file(s) that will be used to extract the value.

See the Parameter Description section for a description of the above parameter(s).

Return Type

Number

Data.OriginalMethodFilename

Returns the name of the method file that was used to acquire the specified data file.

Syntax

=Data.OriginalMethodFilename(<Run Info>)

Parameters

<Run Info> Describes the data file(s) that will be used to extract the value.

See the Parameter Description section for a description of the above parameter(s).

Return Type

String

Data.OriginalMethodFullFilename

Returns the full name and path of the method file that was used to acquire the specified data file.

Syntax

=Data.OriginalMethodFullFileName(<Run Info>)

Parameters

<Run Info> Describes the data file(s) that will be used to extract the value.

See the Parameter Description section for a description of the above parameter(s).

Return Type

String

Data.SampleAmount

Returns sample amount of the specified data file.

Syntax

=Data.SampleAmount(<Run Info>)

Parameters

<Run Info> Describes the data file(s) that will be used to extract the value.

See the Parameter Description section for a description of the above parameter(s).

Return Type

Number

Data.SampleID

Returns sample id of the specified data file.

Syntax

=Data.SampleID(<Run Info>)

Parameters
<Run Info> Describes the data file(s) that will be used to extract the value.
See the Parameter Description section for a description of the above parameter(s).

Return Type

String

Data.SystemWideParam

Returns a custom system wide result from the specified data file.

Syntax

=Data.SystemWideParam (<Param ID>, <Run Info>)

Parameters
<Param ID> A numeric identifier of the requested system wide custom parameter.
<Run Info> Describes the data file(s) that will be used to extract the value.
See the Parameter Description section for a description of the above parameter(s).

Return Type

String / Number

Data.SystemWideParamByName

Returns a custom system wide result from the specified data file.

Syntax

=Data.SystemWideParamByName (<Param Name>, <Run Info>)

Parameters
<Param ID> The name of the identifier of the requested system wide custom parameter.
<Run Info> Describes the data file(s) that will be used to extract the value.
See the Parameter Description section for a description of the above parameter(s).

Return Type

String / Number

Data.TraceName

Returns trace name for the specified index and data file.

Syntax

=Data.TraceName(<Trace Index>, <Run Info>)

Parameters

<Trace Index> A numeric index of the requested trace.

<Run Info> Describes the data file(s) that will be used to extract the value.

See the Parameter Description section for a description of the above parameter(s).

Return Type

String

Data.UserName

Returns the name of the user that acquired the specified data file.

Syntax

=Data.UserName(<Run Info>)

Parameters

<Run Info> Describes the data file(s) that will be used to extract the value.

See the Parameter Description section for a description of the above parameter(s).

Return Type

String

Data.Vial

Returns vial of the specified data file.

Syntax

=Data.Vial(<Run Info>)

Parameters

<Run Info> Describes the data file(s) that will be used to extract the value.

See the Parameter Description section for a description of the above parameter(s).

Return Type

Number

Data.Volume

Returns volume of the specified data file.

Syntax

=Data.Volume(<Run Info>)

Parameters

<Run Info> Describes the data file(s) that will be used to extract the value.

See the Parameter Description section for a description of the above parameter(s).

Return Type

Number

Extended helper functions

These functions are provided to make the user of other features in the spreadsheet easier to user.

See Also

Ex.D

Ex.R

Ex.D

Returns a cell range for a dynamic set of data. If data in a cell will be expanded dynamically, then this function can be used to create a reference to the cells that the data expands into.

Syntax

=Ex.D (<Cell>, [Range Direction])

Parameters
<Cell> Contains a reference to a cell that will be expanded for a dynamic data range. This is in the form of 'B5', 'C12', etc. There are no enclosing quotes on the cell reference.
[Range Direction] This is an optional numeric parameter that specifies the direction of the dynamic expansion to use. If data is being expanded in only one direction, then this parameter is not necessary. If data is being expanded both across and down, then this parameter can be used to control the range that will be used. The values of this parameter are as follows:
Not Used or 0 Use any dynamic range that is available. If the data expands both across and down, then a range will be generated that contains the entire expansion.
1 Only generate a range for dynamic data that expands across the spreadsheet.
2 Only generate a range for dynamic data that expands down the spreadsheet.
Return Type
Cell Range

Ex.R

This function can be used to repeat an enclosed spreadsheet formula over a series of cells, based on a dynamic data set. For example, this function could be used to produce a total field showing the sum of a set of peak areas for all peaks in a data file.

When using this function, the enclosed function must not have any run, trace, or peak information. For example, the formula to show the peak area for the first named peak from the current data file using the first trace would be:

=Peak.Area("RC", "T1", "P1;3")

However, when repeating the formula with the EX.R function to show the peak area for all named peaks from all runs of a sequence using

the first trace, the formula would look as follows:

=Ex.R(Peak.Area(), "RA;1;0", "T1", "PA;3;0;0")

Syntax

=Ex.R(<Spreadsheet Formula>, <Dynamic Run Info>, [Trace Info], [Dynamic Peak Info])

or

=Ex.R(<Spreadsheet Formula>, <Dynamic Run Info>, [Trace Info], [Dynamic Group Info])

Parameters

<Spreadsheet Formula> Contains any valid spreadsheet formula that will be expanded for a dynamic data range.

[Range Direction] This is an optional numeric parameter that specifies the direction to repeat the formula. If the referenced cell is being repeated in only one direction, then this parameter is not necessary. If the referenced cell is being repeated both across and down, then this parameter can be used to control the direction that will be used. The values of this parameter are as follows:

Not Used or 0 Repeat exactly like the referenced cell. If the referenced cell repeats both across and down, then this formula will be repeated both across and down.

1 Only repeat the formula across the spreadsheet as the referenced cell does.

2 Only repeat the formula down the spreadsheet as the referenced cell does.

<Dynamic Run Info> Used to determine the dynamic range to expand the formula over.

[Trace Info] This is an optional parameter that is used to determine the dynamic range to expand the formula over. See the Parameter Description section for a description of this parameter.

[Dynamic Peak Info] This is an optional parameter that is used to determine the dynamic range to expand the formula over.

Return Type

None

'Dynamic Run Info' may be one of the following:

RC	The current run or currently loaded data file.
R<x>	The sequence run specified by run <x>.
R<x-y>; <direction>; <separation>	The sequence runs specified by <x-y>. The runs will be repeated in the direction specified by <direction>, and will be separated by <separation> rows or columns.
RA; <direction>; <separation>	All sequence runs. The runs will be repeated in the direction specified by <direction>, and will be separated by <separation> rows or columns.

'Dynamic Peak Info' may be one of the following:

P<x>; <peak type>	The peak with an index of <x> having the given peak type.
P<x-y>; <peak type>; <direction>; <separation>	The peaks with an index in the range of <x-y> having the given peak type. The peaks will be repeated in the direction specified by <direction>, and will be separated by <separation> rows or columns.
PA; <peak type>; <direction>; <separation>	All peaks of the given peak type. The peaks will be repeated in the direction specified by <direction>, and will be separated by <separation> rows or columns.

'Dynamic Group Info' may be one of the following:

G<x>; <group type>	The group with an index of <x> having the given group type.
G<x-y>; <group type>; <direction>; <separation>	The groups with an index in the range of <x-y> having the given group type. The groups will be repeated in the direction specified by <direction>, and will be separated by <separation> rows or columns.
GA; <group type>; <direction>; <separation>	All groups of the given group type. The groups will be repeated in the direction specified by <direction>, and will be separated by <separation> rows or columns.

'Direction' may be one of the following:

0	The data will be repeated across the spreadsheet.
1	The data will be repeated down the spreadsheet.

'Peak Type' may be any combination of the following:

1	Report named peaks that were detected.
2	Report named peaks that were not detected.
4	Report unnamed peaks.

'Group Type' may be one of the following:

0	Report calibrated range groups that calculate concentrations for unnamed peaks in this group.
1	Report calibrated range groups that do not calculate concentrations for unnamed peaks in this group.
2	Report named peak groups.

Group functions

These functions return information about groups.

See Also

Group.Area

Group.AreaPercent

Group.ESTDConcentration

Group.Height

Group.HeightPercent

Group.ISTDConcentration

Group.Name

Group.NORMConcentration

Group.Number

Group.Quantitation

Group.ResponseFactor

Group.Units

Group.Area

Returns the area for the requested group(s).

Syntax

=Group.Area(<Run Info>, <Trace Info>, <Group Info>)

Parameters

<Run Info> Describes the data file(s) that will be used to extract the value.

<Trace Info> Describes the trace that will be used to extract the value.

<Group Info> Describes the group(s) to use for the value.

See the Parameter Description section for a description of the above parameter(s).

Return Type

Number

Group.AreaPercent

Returns the area percent for the requested group(s).

Syntax

=Group.AreaPercent(<Run Info>, <Trace Info>, <Group Info>)

Parameters

<Run Info> Describes the data file(s) that will be used to extract the value.

<Trace Info> Describes the trace that will be used to extract the value.

<Group Info> Describes the group(s) to use for the value.

See the Parameter Description section for a description of the above parameter(s).

Return Type

Number

Group.ESTDConcentration

Returns the ESTD concentration for the requested group(s).

Syntax

=Group.ESTDConcentration(<Run Info>, <Trace Info>, <Group Info>)

Parameters

<Run Info> Describes the data file(s) that will be used to extract the value.

<Trace Info> Describes the trace that will be used to extract the value.

<Group Info> Describes the group(s) to use for the value.

See the Parameter Description section for a description of the above parameter(s).

Return Type

Number

Group.Height

Returns the height for the requested group(s).

Syntax

=Group.Height(<Run Info>, <Trace Info>, <Group Info>)

Parameters

<Run Info> Describes the data file(s) that will be used to extract the value.

<Trace Info> Describes the trace that will be used to extract the value.

<Group Info> Describes the group(s) to use for the value.

See the Parameter Description section for a description of the above

parameter(s).

Return Type

Number

Group.HeightPercent

Returns the height percent for the requested group(s).

Syntax

=Group.HeightPercent(<Run Info>, <Trace Info>, <Group Info>)

Parameters

<Run Info> Describes the data file(s) that will be used to extract the value.

<Trace Info> Describes the trace that will be used to extract the value.

<Group Info> Describes the group(s) to use for the value.

See the Parameter Description section for a description of the above parameter(s).

Return Type

Number

Group.ISTDConcentration

Returns the ISTD concentration for the requested group(s).

Syntax

=Group.ISTDConcentration(<Run Info>, <Trace Info>, <Group Info>)

Parameters

<Run Info> Describes the data file(s) that will be used to extract the value.

<Trace Info> Describes the trace that will be used to extract the value.

<Group Info> Describes the group(s) to use for the value.

See the Parameter Description section for a description of the above parameter(s).

Return Type

Number

Group.Name

Returns the group name for the requested group(s).

Syntax

=Group.Name(<Run Info>, <Trace Info>, <Group Info>)

Parameters

<Run Info> Describes the data file(s) that will be used to extract the value.

<Trace Info> Describes the trace that will be used to extract the value.

<Group Info> Describes the group(s) to use for the value.

See the Parameter Description section for a description of the above parameter(s).

Return Type

String

Group.NORMConcentration

Returns the NORM concentration for the requested group(s).

Syntax

=Group.NORMConcentration(<Run Info>, <Trace Info>, <Group Info>)

Parameters

<Run Info> Describes the data file(s) that will be used to extract the value.

<Trace Info> Describes the trace that will be used to extract the value.

<Group Info> Describes the group(s) to use for the value.

See the Parameter Description section for a description of the above parameter(s).

Return Type

Number

Group.Number

Returns the group number for the requested group(s).

Syntax

=Group.Number(<Run Info>, <Trace Info>, <Group Info>)

Parameters

<Run Info> Describes the data file(s) that will be used to extract the value.

<Trace Info> Describes the trace that will be used to extract the value.

<Group Info> Describes the group(s) to use for the value.

See the Parameter Description section for a description of the above parameter(s).

Return Type

Number

Group.Quantitation

Returns the group quantitation for the requested group(s). This will return 'Area', 'Height', or 'Counts'.

Syntax

=Group.Quantitation (<Run Info>, <Trace Info>, <Group Info>)

Parameters

<Run Info> Describes the data file(s) that will be used to extract the value.

<Trace Info> Describes the trace that will be used to extract the value.

<Group Info> Describes the group(s) to use for the value.

See the Parameter Description section for a description of the above parameter(s).

Return Type

String

Group.ResponseFactor

Returns the response factor for the requested group(s).

Syntax

=Group.ResponseFactor(<Run Info>, <Trace Info>, <Group Info>)

Parameters

<Run Info> Describes the data file(s) that will be used to extract the value.

<Trace Info> Describes the trace that will be used to extract the value.

<Group Info> Describes the group(s) to use for the value.

See the Parameter Description section for a description of the above parameter(s).

Return Type

Number

Group.Units

Returns the units for the requested group(s).

Syntax

=Group.Units(<Run Info>, <Trace Info>, <Group Info>)

Parameters

<Run Info> Describes the data file(s) that will be used to extract the value.

<Trace Info> Describes the trace that will be used to extract the value.

<Group Info> Describes the group(s) to use for the value.

See the Parameter Description section for a description of the above parameter(s).

Return Type

String

Instrument Functions

These functions return information about the current instrument.

See Also

Instrument.ID

Instrument.Name

Instrument.UserName

Instrument.ID

Returns the internal instrument id of the current instrument.

Syntax

=Instrument.ID()

Parameters

None

Return Type

Number

Instrument.Name

Returns the instrument name of the current instrument.

Syntax

=Instrument.Name()

Parameters

None

Return Type

String

Instrument.UserName

Returns the name of the user logged into the current instrument.

Syntax

=Instrument.UserName()

Parameters

None

Return Type

String

Peak functions

These functions return information about detected and named peaks.

See Also

Peak.AOHResolution
Peak.AOHTheoreticalPlates
Peak.AOHTheoreticalPlatesPerMeter
Peak.Area
Peak.AreaPercent
Peak.Asymmetry
Peak.AsymmetryTenPercent
Peak.CapacityFactor
Peak.CurrentResponseFactor
Peak.CustomParam
Peak.CustomParamByName
Peak.DABResolution
Peak.DABTheoreticalPlates
Peak.DABTheoreticalPlatesPerMeter
Peak.JPTheoreticalPlates
Peak.TheoreticalPlatesPerMeter
Peak.Name
Peak.NORMConcentration
Peak.Number
Peak.Quantitation
Peak.RelativeRetentionTime
Peak.Resolution
Peak.ResolutionID
Peak.ResponseFactor
Peak.RetentionTime
Peak.StartTime
Peak.StopTime
Peak.TheoreticalPlates

Peak.AOHResolution

Returns the AOH resolution for the requested peak(s).

Syntax

=Peak.AOHResolution(<Run Info>, <Trace Info>, <Peak Info>)

Parameters

<Run Info> Describes the data file(s) that will be used to extract the value.

<Trace Info> Describes the trace that will be used to extract the value.

<Peak Info> Describes the peak(s) to use for the value.

See the Parameter Description section for a description of the above parameter(s).

Return Type

Number

Peak.AOHTheoreticalPlates

Returns the AOH theoretical plates for the requested peak(s).

Syntax

=Peak.AOHTheoreticalPlates(<Run Info>, <Trace Info>, <Peak Info>)

Parameters

<Run Info> Describes the data file(s) that will be used to extract the value.

<Trace Info> Describes the trace that will be used to extract the value.

<Peak Info> Describes the peak(s) to use for the value.

See the Parameter Description section for a description of the above parameter(s).

Return Type

Number

Peak.AOHTheoreticalPlatesPerMeter

Returns the AOH theoretical plates per meter for the requested peak(s).

Syntax

=Peak.AOHTheoreticalPlatesPerMeter(<Run Info>, <Trace Info>, <Peak Info>)

Parameters

<Run Info> Describes the data file(s) that will be used to extract the value.

<Trace Info> Describes the trace that will be used to extract the value.

<Peak Info> Describes the peak(s) to use for the value.

See the Parameter Description section for a description of the above parameter(s).

Return Type

Number

Peak.Area

Returns the area for the requested peak(s).

Syntax

=Peak.Area(<Run Info>, <Trace Info>, <Peak Info>)

Parameters

<Run Info> Describes the data file(s) that will be used to extract the value.

<Trace Info> Describes the trace that will be used to extract the value.

<Peak Info> Describes the peak(s) to use for the value.

See the Parameter Description section for a description of the above parameter(s).

Return Type

Number

Peak.AreaPercent

Returns the area percent for the requested peak(s).

Syntax

=Peak.AreaPercent(<Run Info>, <Trace Info>, <Peak Info>)

Parameters

<Run Info> Describes the data file(s) that will be used to extract the value.

<Trace Info> Describes the trace that will be used to extract the value.

<Peak Info> Describes the peak(s) to use for the value.

See the Parameter Description section for a description of the above parameter(s).

Return Type

Number

Peak.Asymmetry

Returns the asymmetry for the requested peak(s).

Syntax

=Peak.Asymmetry(<Run Info>, <Trace Info>, <Peak Info>)

Parameters

<Run Info> Describes the data file(s) that will be used to extract the value.

<Trace Info> Describes the trace that will be used to extract the value.

<Peak Info> Describes the peak(s) to use for the value.

See the Parameter Description section for a description of the above parameter(s).

Return Type

Number

Peak.AsymmetryTenPercent

Returns the asymmetry at 10% for the requested peak(s).

Syntax

=Peak.AsymmetryTenPercent(<Run Info>, <Trace Info>, <Peak Info>)

Parameters

<Run Info> Describes the data file(s) that will be used to extract the value.

<Trace Info> Describes the trace that will be used to extract the value.

<Peak Info> Describes the peak(s) to use for the value.

See the Parameter Description section for a description of the above parameter(s).

Return Type

Number

Peak.CapacityFactor

Returns the capacity factor for the requested peak(s).

Syntax

=Peak.CapacityFactor(<Run Info>, <Trace Info>, <Peak Info>)

Parameters

<Run Info> Describes the data file(s) that will be used to extract the value.

<Trace Info> Describes the trace that will be used to extract the value.

<Peak Info> Describes the peak(s) to use for the value.

See the Parameter Description section for a description of the above parameter(s).

Return Type

Number

Peak.CurrentResponseFactor

Returns the current response factor for the requested peak(s).

Syntax

=Peak.CurrentResponseFactor(<Run Info>, <Trace Info>, <Peak Info>)

Parameters

<Run Info> Describes the data file(s) that will be used to extract the value.

<Trace Info> Describes the trace that will be used to extract the value.

<Peak Info> Describes the peak(s) to use for the value.

See the Parameter Description section for a description of the above parameter(s).

Return Type

Number

Peak.CustomParam

Returns a custom peak result for the requested peaks.

Syntax

=Peak.CustomParam(<Param ID>, <Run Info>, <Trace Info>, <Peak Info>)

Parameters

<Param ID> A numeric identifier of the requested peak custom parameter.

<Run Info> Describes the data file(s) that will be used to extract the value.

<Trace Info> Describes the trace that will be used to extract the value.

<Peak Info> Describes the peak(s) to use for the value.

See the Parameter Description section for a description of the above parameter(s).

Return Type

String / Number

Peak.CustomParamByName

Returns a custom peak result for the requested peaks.

Syntax

=Peak.CustomParamByName(<Param Name>, <Run Info>, <Trace Info>, <Peak Info>)

Parameters

<Param ID> The name of the requested peak custom parameter.

<Run Info> Describes the data file(s) that will be used to extract the value.

<Trace Info> Describes the trace that will be used to extract the value.

<Peak Info> Describes the peak(s) to use for the value.

See the Parameter Description section for a description of the above parameter(s).

Return Type

String / Number

Peak.DABResolution

Returns the DAB resolution for the requested peak(s).

Syntax

=Peak.DABResolution(<Run Info>, <Trace Info>, <Peak Info>)

Parameters

<Run Info> Describes the data file(s) that will be used to extract the value.

<Trace Info> Describes the trace that will be used to extract the value.

<Peak Info> Describes the peak(s) to use for the value.

See the Parameter Description section for a description of the above parameter(s).

Return Type

Number

Peak.DABTheoreticalPlates

Returns the DAB theoretical plates for the requested peak(s).

Syntax

=Peak.DABTheoreticalPlates(<Run Info>, <Trace Info>, <Peak Info>)

Parameters

<Run Info> Describes the data file(s) that will be used to extract the value.

<Trace Info> Describes the trace that will be used to extract the value.

<Peak Info> Describes the peak(s) to use for the value.

See the Parameter Description section for a description of the above parameter(s).

Return Type

Number

Peak.DABTheoreticalPlatesPerMeter

Returns the DAB theoretical plates per meter for the requested

peak(s).

Syntax

=Peak.DABTheoreticalPlatesPerMeter(<Run Info>, <Trace Info>, <Peak Info>)

Parameters

<Run Info> Describes the data file(s) that will be used to extract the value.

<Trace Info> Describes the trace that will be used to extract the value.

<Peak Info> Describes the peak(s) to use for the value.

See the Parameter Description section for a description of the above parameter(s).

Return Type

Number

Peak.EMGResolution

Returns the EMG resolution for the requested peak(s).

Syntax

=Peak.EMGResolution(<Run Info>, <Trace Info>, <Peak Info>)

Parameters

<Run Info> Describes the data file(s) that will be used to extract the value.

<Trace Info> Describes the trace that will be used to extract the value.

<Peak Info> Describes the peak(s) to use for the value.

See the Parameter Description section for a description of the above parameter(s).

Return Type

Number

Peak.EMGTheoreticalPlates

Returns the EMG theoretical plates for the requested peak(s).

Syntax

=Peak.EMGTheoreticalPlates(<Run Info>, <Trace Info>, <Peak Info>)

Parameters

<Run Info> Describes the data file(s) that will be used to extract the

value.

<Trace Info> Describes the trace that will be used to extract the value.

<Peak Info> Describes the peak(s) to use for the value.

See the Parameter Description section for a description of the above parameter(s).

Return Type

Number

Peak.EMGTheoreticalPlatesPerMeter

Returns the EMG theoretical plates per meter for the requested peak(s).

Syntax

=Peak.EMGTheoreticalPlatesPerMeter(<Run Info>, <Trace Info>, <Peak Info>)

Parameters

<Run Info> Describes the data file(s) that will be used to extract the value.

<Trace Info> Describes the trace that will be used to extract the value.

<Peak Info> Describes the peak(s) to use for the value.

See the Parameter Description section for a description of the above parameter(s).

Return Type

Number

Peak.ESTDConcentration

Returns the ESTD concentration for the requested peak(s).

Syntax

=Peak.ESTDConcentration(<Run Info>, <Trace Info>, <Peak Info>)

Parameters

<Run Info> Describes the data file(s) that will be used to extract the value.

<Trace Info> Describes the trace that will be used to extract the value.

<Peak Info> Describes the peak(s) to use for the value.

See the Parameter Description section for a description of the above parameter(s).

Return Type

Number

Peak.ExpectedRetentionTime

Returns the expected retention time for the requested peak(s).

Syntax

=Peak.ExpectedRetentionTime(<Run Info>, <Trace Info>, <Peak Info>)

Parameters

<Run Info> Describes the data file(s) that will be used to extract the value.

<Trace Info> Describes the trace that will be used to extract the value.

<Peak Info> Describes the peak(s) to use for the value.

See the Parameter Description section for a description of the above parameter(s).

Return Type

Number

Peak.Height

Returns the height for the requested peak(s).

Syntax

=Peak.Height(<Run Info>, <Trace Info>, <Peak Info>)

Parameters

<Run Info> Describes the data file(s) that will be used to extract the value.

<Trace Info> Describes the trace that will be used to extract the value.

<Peak Info> Describes the peak(s) to use for the value.

See the Parameter Description section for a description of the above parameter(s).

Return Type

Number

Peak.HeightPercent

Returns the height percent for the requested peak(s).

Syntax

=Peak.HeightPercent(<Run Info>, <Trace Info>, <Peak Info>)

Parameters

<Run Info> Describes the data file(s) that will be used to extract the value.

<Trace Info> Describes the trace that will be used to extract the value.

<Peak Info> Describes the peak(s) to use for the value.

See the Parameter Description section for a description of the above parameter(s).

Return Type

Number

Peak.Index

Returns the peak index information for the requested named peak, based on its peak id. The returned information can be used in place of <Peak Info> for another function. For example, to find the peak name of a named peak with a peak id of 2 in the current data file, use the following formula: =Peak.Name("RC", "T1", Peak.Index(2, "RC", "T1"))

Syntax

=Peak.Index(<Peak ID>, <Run Info>, <Trace Info>)

Parameters

<Peak ID> A numeric identifier of the requested named peak. This number comes from the peak table.

<Run Info> Describes the data file(s) that will be used to extract the value.

<Trace Info> Describes the trace that will be used to extract the value.

See the Parameter Description section for a description of the above parameter(s).

Return Type

String

Peak.IntegrationCodes

Returns the integration codes for the requested peak(s).

Syntax

=Peak.IntegrationCodes(<Run Info>, <Trace Info>, <Peak Info>)

Parameters

<Run Info> Describes the data file(s) that will be used to extract the value.

<Trace Info> Describes the trace that will be used to extract the value.

<Peak Info> Describes the peak(s) to use for the value.

See the Parameter Description section for a description of the above parameter(s).

Return Type

String

Peak.ISTDConcentration

Returns the ISTD concentration for the requested peak(s).

Syntax

=Peak.ISTDConcentration(<Run Info>, <Trace Info>, <Peak Info>)

Parameters

<Run Info> Describes the data file(s) that will be used to extract the value.

<Trace Info> Describes the trace that will be used to extract the value.

<Peak Info> Describes the peak(s) to use for the value.

See the Parameter Description section for a description of the above parameter(s).

Return Type

Number

Peak.JPResolution

Returns the JP resolution for the requested peak(s).

Syntax

=Peak.JPResolution(<Run Info>, <Trace Info>, <Peak Info>)

Parameters

<Run Info> Describes the data file(s) that will be used to extract the value.

<Trace Info> Describes the trace that will be used to extract the value.

<Peak Info> Describes the peak(s) to use for the value.

See the Parameter Description section for a description of the above parameter(s).

Return Type

Number

Peak.JPTheoreticalPlates

Returns the JP theoretical plates for the requested peak(s).

Syntax

=Peak.JPTheoreticalPlates(<Run Info>, <Trace Info>, <Peak Info>)

Parameters

<Run Info> Describes the data file(s) that will be used to extract the value.

<Trace Info> Describes the trace that will be used to extract the value.

<Peak Info> Describes the peak(s) to use for the value.

See the Parameter Description section for a description of the above parameter(s).

Return Type

Number

Peak.JPTheoreticalPlatesPerMeter

Returns the JP theoretical plates per meter for the requested peak(s).

Syntax

=Peak.JPTheoreticalPlatesPerMeter(<Run Info>, <Trace Info>, <Peak Info>)

Parameters

<Run Info> Describes the data file(s) that will be used to extract the value.

<Trace Info> Describes the trace that will be used to extract the value.

<Peak Info> Describes the peak(s) to use for the value.

See the Parameter Description section for a description of the above parameter(s).

Return Type

Number

Peak.Name

Returns the peak name for the requested peak(s).

Syntax

=Peak.Name(<Run Info>, <Trace Info>, <Peak Info>)

Parameters

<Run Info> Describes the data file(s) that will be used to extract the value.

<Trace Info> Describes the trace that will be used to extract the value.

<Peak Info> Describes the peak(s) to use for the value.

See the Parameter Description section for a description of the above parameter(s).

Return Type

String

Peak.NORMConcentration

Returns the NORM concentration for the requested peak(s).

Syntax

=Peak.NORMConcentration(<Run Info>, <Trace Info>, <Peak Info>)

Parameters

<Run Info> Describes the data file(s) that will be used to extract the value.

<Trace Info> Describes the trace that will be used to extract the value.

<Peak Info> Describes the peak(s) to use for the value.

See the Parameter Description section for a description of the above parameter(s).

Return Type

Number

Peak.Number

Returns the detected peak number for the requested peak(s).

Syntax

=Peak.Number(<Run Info>, <Trace Info>, <Peak Info>)

Parameters

<Run Info> Describes the data file(s) that will be used to extract the value.

<Trace Info> Describes the trace that will be used to extract the value.

<Peak Info> Describes the peak(s) to use for the value.

See the Parameter Description section for a description of the above parameter(s).

Return Type

Number

Peak.Quantitation

Returns the peak quantitation for the requested peak(s). This will return 'Area', 'Height', or 'Counts'.

Syntax

=Peak.Quantitation (<Run Info>, <Trace Info>, <Peak Info>)

Parameters

<Run Info> Describes the data file(s) that will be used to extract the value.

<Trace Info> Describes the trace that will be used to extract the value.

<Peak Info> Describes the peak(s) to use for the value.

See the Parameter Description section for a description of the above parameter(s).

Return Type

String

Peak.RelativeRetentionTime

Returns the relative retention time for the requested peak(s).

Syntax

=Peak.RelativeRetentionTime(<Run Info>, <Trace Info>, <Peak Info>)

Parameters

<Run Info> Describes the data file(s) that will be used to extract the value.

<Trace Info> Describes the trace that will be used to extract the value.

<Peak Info> Describes the peak(s) to use for the value.

See the Parameter Description section for a description of the above parameter(s).

Return Type

Number

Peak.Resolution

Returns the resolution for the requested peak(s).

Syntax

=Peak.Resolution(<Run Info>, <Trace Info>, <Peak Info>)

Parameters

<Run Info> Describes the data file(s) that will be used to extract the value.

<Trace Info> Describes the trace that will be used to extract the value.

<Peak Info> Describes the peak(s) to use for the value.

See the Parameter Description section for a description of the above parameter(s).

Return Type

Number

Peak.ResolutionID

Returns the resolution ID for the requested peak(s).

Syntax

=Peak.ResolutionID(<Run Info>, <Trace Info>, <Peak Info>)

Parameters

<Run Info> Describes the data file(s) that will be used to extract the value.

<Trace Info> Describes the trace that will be used to extract the value.

<Peak Info> Describes the peak(s) to use for the value.

See the Parameter Description section for a description of the above

parameter(s).

Return Type

Number

Peak.ResponseFactor

Returns the response factor for the requested peak(s).

Syntax

=Peak.ResponseFactor(<Run Info>, <Trace Info>, <Peak Info>)

Parameters

<Run Info> Describes the data file(s) that will be used to extract the value.

<Trace Info> Describes the trace that will be used to extract the value.

<Peak Info> Describes the peak(s) to use for the value.

See the Parameter Description section for a description of the above parameter(s).

Return Type

Number

Peak.RetentionTime

Returns the retention time for the requested peak(s).

Syntax

=Peak.RetentionTime(<Run Info>, <Trace Info>, <Peak Info>)

Parameters

<Run Info> Describes the data file(s) that will be used to extract the value.

<Trace Info> Describes the trace that will be used to extract the value.

<Peak Info> Describes the peak(s) to use for the value.

See the Parameter Description section for a description of the above parameter(s).

Return Type

Number

Peak.StartTime

Returns the start time for the requested peak(s).

Syntax

=Peak.StartTime(<Run Info>, <Trace Info>, <Peak Info>)

Parameters

<Run Info> Describes the data file(s) that will be used to extract the value.

<Trace Info> Describes the trace that will be used to extract the value.

<Peak Info> Describes the peak(s) to use for the value.

See the Parameter Description section for a description of the above parameter(s).

Return Type

Number

Peak.StopTime

Returns the stop time for the requested peak(s).

Syntax

=Peak.StopTime(<Run Info>, <Trace Info>, <Peak Info>)

Parameters

<Run Info> Describes the data file(s) that will be used to extract the value.

<Trace Info> Describes the trace that will be used to extract the value.

<Peak Info> Describes the peak(s) to use for the value.

See the Parameter Description section for a description of the above parameter(s).

Return Type

Number

Peak.TheoreticalPlates

Returns the theoretical plates for the requested peak(s).

Syntax

=Peak.TheoreticalPlates(<Run Info>, <Trace Info>, <Peak Info>)

Parameters

<Run Info> Describes the data file(s) that will be used to extract the value.

<Trace Info> Describes the trace that will be used to extract the value.

<Peak Info> Describes the peak(s) to use for the value.

See the Parameter Description section for a description of the above parameter(s).

Return Type

Number

Peak.TheoreticalPlatesPerMeter

Returns the theoretical plates per meter for the requested peak(s).

Syntax

=Peak.TheoreticalPlatesPerMeter(<Run Info>, <Trace Info>, <Peak Info>)

Parameters

<Run Info> Describes the data file(s) that will be used to extract the value.

<Trace Info> Describes the trace that will be used to extract the value.

<Peak Info> Describes the peak(s) to use for the value.

See the Parameter Description section for a description of the above parameter(s).

Return Type

Number

Peak.Units

Returns the concentration units for the requested peak(s).

Syntax

=Peak.Units(<Run Info>, <Trace Info>, <Peak Info>)

Parameters

<Run Info> Describes the data file(s) that will be used to extract the value.

<Trace Info> Describes the trace that will be used to extract the value.

<Peak Info> Describes the peak(s) to use for the value.

See the Parameter Description section for a description of the above parameter(s).

Return Type

String

Peak.USPResolution

Returns the USP resolution for the requested peak(s).

Syntax

=Peak.USPResolution(<Run Info>, <Trace Info>, <Peak Info>)

Parameters

<Run Info> Describes the data file(s) that will be used to extract the value.

<Trace Info> Describes the trace that will be used to extract the value.

<Peak Info> Describes the peak(s) to use for the value.

See the Parameter Description section for a description of the above parameter(s).

Return Type

Number

Peak.USPTheoreticalPlates

Returns the USP theoretical plates for the requested peak(s).

Syntax

=Peak.USPTheoreticalPlates(<Run Info>, <Trace Info>, <Peak Info>)

Parameters

<Run Info> Describes the data file(s) that will be used to extract the value.

<Trace Info> Describes the trace that will be used to extract the value.

<Peak Info> Describes the peak(s) to use for the value.

See the Parameter Description section for a description of the above parameter(s).

Return Type

Number

Peak.USPTheoreticalPlatesPerMeter

Returns the USP theoretical plates per meter for the requested peak(s).

Syntax

=Peak.USPTheoreticalPlatesPerMeter(<Run Info>, <Trace Info>, <Peak Info>)

Parameters

<Run Info> Describes the data file(s) that will be used to extract the value.

<Trace Info> Describes the trace that will be used to extract the value.

<Peak Info> Describes the peak(s) to use for the value.

See the Parameter Description section for a description of the above parameter(s).

Return Type

Number

Peak.USPWidth

Returns the USP width for the requested peak(s).

Syntax

=Peak.USPWidth(<Run Info>, <Trace Info>, <Peak Info>)

Parameters

<Run Info> Describes the data file(s) that will be used to extract the value.

<Trace Info> Describes the trace that will be used to extract the value.

<Peak Info> Describes the peak(s) to use for the value.

See the Parameter Description section for a description of the above parameter(s).

Return Type

Number

Peak.Width

Returns the width for the requested peak(s).

Syntax

=Peak.Width(<Run Info>, <Trace Info>, <Peak Info>)

Parameters

<Run Info> Describes the data file(s) that will be used to extract the value.

<Trace Info> Describes the trace that will be used to extract the value.

<Peak Info> Describes the peak(s) to use for the value.

See the Parameter Description section for a description of the above parameter(s).

Return Type

Number

Peak.WidthFiftyPercent

Returns the width at 50% for the requested peak(s).

Syntax

=Peak.WidthFiftyPercent(<Run Info>, <Trace Info>, <Peak Info>)

Parameters

<Run Info> Describes the data file(s) that will be used to extract the value.

<Trace Info> Describes the trace that will be used to extract the value.

<Peak Info> Describes the peak(s) to use for the value.

See the Parameter Description section for a description of the above parameter(s).

Return Type

Number

Peak.WidthFivePercent

Returns the width at 5% for the requested peak(s).

Syntax

=Peak.WidthFivePercent(<Run Info>, <Trace Info>, <Peak Info>)

Parameters

<Run Info> Describes the data file(s) that will be used to extract the value.

<Trace Info> Describes the trace that will be used to extract the value.

<Peak Info> Describes the peak(s) to use for the value.

See the Parameter Description section for a description of the above parameter(s).

Return Type

Number

Peak.WidthTenPercent

Returns the width at 10% for the requested peak(s).

Syntax

=Peak.WidthTenPercent(<Run Info>, <Trace Info>, <Peak Info>)

Parameters

<Run Info> Describes the data file(s) that will be used to extract the value.

<Trace Info> Describes the trace that will be used to extract the value.

<Peak Info> Describes the peak(s) to use for the value.

See the Parameter Description section for a description of the above parameter(s).

Return Type

Number

Project Functions

These functions return information about the current project.

See Also

Project.DataPath

Project.Description

Project.MethodPath

Project.Name

Project.RootPath

Project.SequencePath

Project.TemplatePath

Project.DataPath

Returns the default path used to store data files in the current project.

Syntax

=Project.DataPath()

Parameters

None.

Return Type

String

Project.Description

Returns the description for the current project.

Syntax

=Project.Description()

Parameters

None.

Return Type

String

Project.MethodPath

Returns the default path used to store method files in the current project.

Syntax

=Project.MethodPath()

Parameters

None.

Return Type

String

Project.Name

Returns the name of the current project.

Syntax

=Project.Name()

Parameters

None.

Return Type

String

Project.RootPath

Returns the default root path for the current project.

Syntax

=Project.RootPath()

Parameters

None.

Return Type

String

Project.SequencePath

Returns the default path used to store sequence files in the current project.

Syntax

=Project.SequencePath()

Parameters

None.

Return Type

String

Project.TemplatePath

Returns the default path used to store report template files in the current project.

Syntax

=Project.TemplatePath()

Parameters

None.

Return Type

String

Sequence Functions

These functions return information about the sequence file that will be used for reporting purposes.

See Also

Sequence.Filename

Sequence.FullFilename

Sequence.RunNumber

Sequence.Filename

Returns file name of the sequence file that will be used for reporting. Only the file name is returned the path information is not returned.

Syntax

=Sequence.Filename()

Parameters

None.

Return Type

String

Sequence.FullFilename

Returns full file name of the sequence file that will be used for reporting. The file name and path information is returned.

Syntax

=Sequence.FullFilename()

Parameters

None.

Return Type

String

Sequence.RunNumber

Returns the run number of the specified sequence run. This function can be used in conjunction with the EX.R() formula to generate the run number of the runs in a sequence. For example, the following formula would generate run numbers for all runs of a sequence going down: =EX.R(SEQUENCE.RUNNUMBER(),"RA;1;0")

Syntax

=Sequence.RunNumber(<Run Info>)

Parameters

<Run Info> Describes the data file(s) that will be used to extract the value.

See the Parameter Description section for a description of the above parameter(s).

Return Type

Number

Advanced reporting formulas and Functions

This section gives details on formulas available in the spreadsheet engine used in the Advanced Reports feature.

See Also

1. Spreadsheet Formulas

2. Built-in Functions

3. Fnctions

4. Using Spreadsheet Built-in Functions

5. Spreadsheet Error Messages

1. Spreadsheet formulas

Formulas are the backbone of the spreadsheet, establishing and calculating mathematical relationships between elements of the spreadsheet. Whereas numeric entries remain the same until you change them, cells defined by formulas are automatically changed to reflect changes in referenced cells - even where there are complex interdependencies among cells.

Spreadsheet formulas can calculate with numbers, text, logical values, cell references, and other formulas. For example, you can easily calculate the sum of a series of cells, the total of values in a column, a minimum or maximum value within a range, the rounded result of another formula, or the absolute value of a cell entry. Formulas can express complex interdependencies among cells, and they can define constraints on the calculation, such as limits on acceptable values or specific conditions under which a calculation should take place.

Once entered in a cell, formulas are hidden behind the scenes, perform their work in the background, and display only the result of their calculation. To view the formula in a cell, simply select the cell. Spreadsheet also provides an option that lets you make all formula expression visible (via CGXGridParam::m_nDisplayExpression).

Spreadsheet also provides a wide array of functions that perform certain tasks. Functions can be used alone or in conjunction with formulas and other functions. Spreadsheet provides many specialized functions in addition to those that are found in typical financial spreadsheets.

See Also

Formula Syntax

Formula Values

Formula Operators

Referencing Other Cells in Formulas

Cell Referencing in Spreadsheet

Constraint Expressions

Explicit Dependency

1.1 Formula syntax

The general form of a Spreadsheet formula is:

= expression ; constraint expression // comment

where expression defines the calculations needed to generate the cell's value, constraint expression places limits on acceptable values or the circumstances under which the calculation should take place, and comment is any text you want to attach to the cell.

The expression part of Spreadsheet formulas looks just like an algebraic formula; it contains values and operators that define the relationships between values.

Spreadsheet uses the following conventions for formulas:

- A formula must begin with an equal (=) sign. When you begin typing into a cell, Spreadsheet automatically assumes that you are typing a formula if you start with one of the following characters:

  0 1 2 3 4 5 6 7 8 9 . - @ =+

- Formulas can have as many as 511 characters. You can type spaces if you wish, but the spreadsheet automatically removes them.

1.2 Formula values

Formulas can contain any or all of the following types of values:

Numbers, such as 123, -123, 12.3.

Addresses of single cells, such as A1, D5, Z100.

Addresses of cell ranges such as B12..G29, A1..D5.

Absolute cell references de**Note**d with dollar signs before the fixed coordinate (A1, $A1, or A$1), which will not be updated when the referencing cell is moved or copied.

Spreadsheet functions, such as @SUM or @RADIANS, with their arguments.

Text surrounded by double quotation marks, such as "The sum is " or "Total".

User-defined cell names or cell range names, such as **TOTALS** or **PROJECT1**

1.3 Formula operators

Spreadsheet supports all the arithmetic, boolean and logical operators available in the C programming language. It does not support the C address operators or the operators that have side effects, such as ++. Spreadsheet provides two operators, exponentiation (**) and percent (%), that are not available in the C language.

Spreadsheet Formulas can contain the following operators to define relationship between values.

Operator Precedence Definition

% 14 Unary percent

**** 13** Exponentiation

+ 12 Unary plus

- 12 Unary minus

~ 12 Bitwise complement (integer)

! 12 Logical not

*** 11** Multiplication

/ 11 Division

% 11 Remainder (integer)

+ 10 Addition

- 10 Subtraction

<< 9 Shift left (integer)

>> 9 Shift right (integer)

< 8 Less Than

> 8 Greater Than

<= 8 Less Than or Equal

= 8 Greater Than or Equal

== 7 Equal

!= 7 Not Equal

& 6 Bitwise And, or String Concatenation

^ 5 Bitwise Exclusive-Or (integer)

| 4 Bitwise Or

&& 3 Logical And

|| 2 Logical Or

?: 1 Conditional

In formulas with more than one operator, Spreadsheet evaluates operators in the order of precedence presented above, with highest precedence first. That is, AND/OR/NOT operators are evaluated after inequality operators in a logical expression, and multiplication/division operations are performed before subtraction/addition operations in an arithmetic expression. Operators at the same precedence level are evaluated from left to right.

The precedence of operators can be overridden by using parentheses to explicitly specify the order of evaluation.

Here are some special **Note**s about Spreadsheet operators:

- The operators marked ``(integer)'' on the table above automatically convert their operands to integers.

- The & operator performs double duty: as a bit-wise ``and'' if the operands are numbers or as a string concatenation operator joining two strings together if the operands are text.
- The % operator also performs double duty: as the ``percent'' operator when appended to a number or numeric expression, or as the C-style ``modulus'' operator when applied between two integer expressions.
- Operators that define equality/inequality relationships (such as == and <) can be used to compare text strings lexically (alphabetically). In comparing mixed strings lexically, Spreadsheet considers string operands to be lower than numeric operands.
- The conditional operator returns its second operand if its first operand evaluates True (non-zero) and returns its third operand if it evaluates False, (zero).
- In formulas with conditional operators, the second and third operands may be any type the spreadsheet supports, including ranges. For example, the expression

  =@SUM(A1 ? B1..C20 : C10..D15)

  returns the sum of B1..C20 if A1 evaluates to non-zero; otherwise it returns the sum of C10..D15.
- Spreadsheet accepts most arithmetic operators used in other spreadsheets like MS Excel, but there are a few differences in syntax and precedence.

1.4 Referencing other cells in formulas

The real power of Spreadsheet lies in its ability to calculate relationships among different cells in the spreadsheet by typing the row/column coordinates, or address, in the formula.

To reference a cell by address:

Type the row and column coordinates of the cell in the formula. For example, to reference Row 5 in Column D, type **D5**.

To reference a contiguous group of cells by address:

Type the row and column coordinates of two cells in opposite corners of the block to be referenced, with two periods (..) between the coordinates. For example, to reference the first five columns and the first five rows of the spreadsheet, type **A1..E5**.

1.5 Cell referencing in spreadsheet

Spreadsheet differentiates between relative, absolute, and indirect references. The latter is unique to Spreadsheet.

Relative Reference

Spreadsheet tracks the referenced cell by considering its position relative to the formula cell, not by its address. For example, if the formula in cell A1 references cell B2, Spreadsheet remembers that

the referenced cell is one row down and one column right. If you copy the formula in cell A1 to another location (e.g., D17), the formula will reference the cell one row down and one column right of the new location (e.g., E18).

Absolute Reference

Absolute references remain the same, no matter where you move or copy the original formula. For example, if the formula in cell A1 references cell B2, and you copy the formula in cell A1 to another location (e.g. D17), the formula still references cell B2. To specify an absolute cell address, insert a dollar sign (**$**) before the address coordinate to be fixed, or before both coordinates if the row and column coordinates are to be fixed. For example: **B2.**

To specify all or part of a cell address to be absolute, insert a dollar sign (**$**) before the address coordinate to remain fixed For example:

- **B$5** makes the complete address absolute.
- **$B5** makes the column coordinate (B) absolute, the row coordinate (5) relative.
- **B$5** makes the column coordinate (B) relative, the row coordinate (5) absolute.

Cell ranges are also relative, so when you move a cell range, references in formulas within that range are updated to reflect their new location.

To specify an absolute range reference, insert dollar signs (**$**) before the coordinates in the formula. For example, to make the range A1..D5 absolute, type the reference as **A1..D5**.

To specify part of a cell range to be absolute, insert dollar signs only before the coordinates to remain absolute. For example, **$A1..$D5** will fix the column coordinates of cell references but adjust the row coordinates to reflect the new location.

To reference a cell or range by name:

Type the pre-assigned name of the cell or cell block into the formula.

To assign a name to a cell or range of cells, use the **SetRangeName** command.

Current Cell Reference

Certain expressions within the context of Spreadsheet require a means to express the current cell.

Examples include the conditional statistical functions described in Built-In Worksheet Functions, and constraint expressions described in Section Constraint Expressions.

The current cell is identified in any expression with a pound sign (#). References to cells in the neighborhood of the current cell are made with offset values enclosed in braces ({}) following the #.

The offsets tell Spreadsheet where to look, in relation to the current cell, for the cell being referenced.

The format is as follows:

#{column offset, row offset}

- If you include only one value in the offset, Spreadsheet assumes that it is a column offset. For example, the offset reference #{-1} tells Spreadsheet to look to the column just left of the current cell.
- The offset values may be constants or expressions.

Examples:

- #{0,-1} refers to the cell above the current cell.
- #{-2} refers to the cell two columns left of the current cell.
- #{1} refers to the cell to the right of the current cell.
- #{0,1} refers to the cell below the current cell.
- @CSUM(C4..C100, #{-1} == "Joe") calculates the sum of all the values in the range C4..C100 for which the cell in the column to the left contains the string Joe.
- @CCOUNT(C4..C100, # #{0,-1}) counts all the cells in the range C4..C100 whose value is greater than the contents of the cell immediately above.
- @XVALUE("master.xs3", #) returns the value of the same cell reference in which this function is stored from the sheet indicated.
- /verb/#-1+2/ adds 2 to the cell value from the cell to the left.

1.6 Constraint expressions

Constraints are limitations or conditions placed on the variables in your spreadsheet. They are expressed as algebraic statements appended to formulas. You can attach a constraint expression to any formula, by typing a semicolon (**;**) and the constraint conditions after the formula.

Constraint expressions establish conditions under which a formula operates or boundaries for valid results of the formula. Constraint expressions may be simple equality/inequality relationships, or they can be arbitrary formulas. Any valid Spreadsheet expression which returns a numeric value is also a valid constraint expression. However, unlike the expression that defines a cell value, a constraint expression can reference the cell in which it resides, using the symbol **#**.

For example, the formula

=A1 + A2 ; #2 && #<=B5 || #==C7

means, ``the value of the current cell is the sum of cells A1 and A2, and that value must be either greater than 2 and less than or equal to the value of cell B5, or equal to the value of cell C7."

Constraint expressions are used for example in the conditional statistical functions.

The benefit of constraint expressions is maximized when combined

with current cell reference support (#) as indicated in the above example.

1.7 Explicit dependency

There may be instances where you need to force a recalculation when certain cell values change, when there is no implicit dependency in the formula that would trigger an automatic recalculation. This option is indicated by appending a backslash (\) to the end of the dependent formula. For example, the formula:

=@SUM(A1..A20)\D50

instructs Spreadsheet to recalculate @SUM(A1..A20) whenever the contents of D50 change. This feature is particularly important when you have a constraint expression containing an offset reference that produces a cell reference outside the cell range referenced in a dependent formula. Under these circumstances, Automatic Recalculation would not necessarily be triggered. Take for instance, the example from above:

@CCOUNT(C4..C100, # #{0,-1})

Counts all the cells in the range C4..C100 whose value is greater than the contents of the cell immediately above. In order for C4 to be evaluated, it must be compared to C3 - which is not part of the explicit range, C4..C100. Without indicating an explicit dependency, C4 would never be evaluated properly. So, in this case, we would indicate the dependency as follows:

@CCOUNT(C4..C100, # #{0,-1})\C3..C99

which tells Spreadsheet to recalculate whenever any cell in the range C3..C99 changes.

2 Built-in functions

Spreadsheet functions are predefined formulas supplied with the program. They offer a shortcut approach to accomplishing the work of long, complex formulas. Mathematical and statistical functions are often used to sum a column of numbers, compute an average, determine a minimum or maximum value, or round the results of a formula. Other functions are used for more specialized purposes such as computing the future value of an investment or the product of multiplying one cell range by another range. Some functions perform calculations that arithmetic operators cannot handle such as text-string manipulations.

See Also

Mathematical Functions

Statistical Functions

Conditional Statistical Functions

String Functions

Logic Functions

Digital Logic Functions

Financial Functions

Date and Time Functions

Miscellaneous Functions

Embedded Tools

2.1 Mathematical functions

Mathematical Functions perform calculations such as determining absolute value, finding the integer portion of a number, or establishing the value of a constant. Although you could accomplish these tasks with a formula, using a function saves time and trouble.

Spreadsheet also provides a full range of trigonometric functions including sine, cosine, tangent, arc sine, hyperbolic sine, hyperbolic arc sine as well as vector and matrix arithmetic and manipulation.

Mathematical functions perform calculations with numeric values as arguments, returning numeric values.

2.2 Statistical functions

Statistical Functions perform aggregation operations such as calculating means, minimums, maximums, and averages.

Spreadsheet also provides more sophisticated statistical test functions that perform operations on a group of values expressed as a list of arguments. These include the F-test, T-tests, correlation coefficient, deviations, and all common averages.

Statistical functions return numeric values.

2.3 Conditional statistical functions

Conditional Statistical Functions operate much like statistical aggregation functions, except that the last argument is a constraint expression that Spreadsheet evaluates for each cell in the argument list.

Only cells that meet constraint criteria are included in the calculation. The constraint expression may be any Spreadsheet expression that evaluates to a numeric result.

Conditional Statistical Functions return a numeric value.

2.4 String functions

String Functions manipulate and evaluate character strings. For example, string functions can return the length of a string, find the first occurrence of a string in a range, change a string from upper to lower-case and vice versa, or replace one string with another.

String functions return strings or numeric values.

2.5 Logic functions

Logic Functions return one value if an argument meets certain criteria, another value if it does not.

Logic functions are used as an adjunct to conditional statements.

Logic functions return the value 1, 0, or a value.

2.6 Digital logic functions

Digital Logic Functions perform digital logic operations such as AND, OR, NOT, etc.

Digital logic functions return the values 0, 1, or -1 (unknown). Any value whose integer portion is not equal to 0 or 1 is considered unknown. Unknown input values may cause unknown output values.

2.7 Financial functions

Financial Functions perform common financial calculations, such as calculating the future value of an annuity at a given interest rate, straight-line depreciation, double-declining depreciation, or the payment term for a given investment. The financial functions in Spreadsheet cover annuities, cash flows, assets. bonds, and Treasury Bills.

Financial functions are most useful for solving cash flow calculations where you know all but one variable. For example, if you know the present value of an investment, interest rate, and periodic payment, you can use the **@FV** function to calculate the future value of the investment. If you know the future value and other variables, but need to know the present value, you can use the **@PV** function.

Many financial functions require specifying a Day Count Basis. A Day Count Basis indicates the way in which the days in a month and the days in a year are to be counted. Most of the financial functions in securities involve 4 different Day Count Basis: 30/360, actual/actual, actual/360 and actual/365. 30/360 Day Count Basis assumes 30-day months and 360-day years (12 months x 30 days). Spreadsheet also follows the ``End-of-Month'' rule which assumes that a security pays interest on the last day of the month and will always make its interest on the last day of the month. Special rules are followed when calculating the days between two dates on 30/360 Day Count Basis.

For example, let Start_Date = D1/M1/Y1, End_Date = D2/M2/Y2.

1. If D1=31, Spreadsheet uses 30 for D1.

2. If D2=31, Spreadsheet uses 31, unless D1=30 or D1=31. In this case, Spreadsheet uses 30.

3. If D1 is the last day of February (D1=28 or 29 in a leap year), Spreadsheet uses 30 for D1.

4. If D2 is the last day of February (D2=28 or 29 in a leap year) and D1 is also the last day of

February, Spreadsheet uses 30 for D2.

The special arguments used by Spreadsheet financial functions are defined in Table TODO:

Financial functions use the arguments defined in Table **interest rate** The interest rate to be used in the calculations. The rate may be specified as annual, monthly or quarterly, but it must agree with the increment you use for periods. By default the interest rate is an annual rate.

- **Present value** The present value of an investment, representing the amount already received from or committed to an investment.
- **Period** The number of periods over which the loan, investment or depreciation is to be calculated. The periods may be defined in months, quarters or years, but must agree with the increment used to define interest rate.
- **Future value** The future value of an investment, given a certain present value, interest rate, and number of periods.
- **Cost** The original cost of a depreciable capital asset.
- **Salvage value** The remaining value of a capital asset after the depreciation period has expired.
- **Allowable life** The allowable life of a depreciable item.
- **Yield** The interest rate that will make the present value of the expected future cash flows equal to the price of the financial instrument.
- **Price** The present value of the expected future cash flows where the discount rate is equal to the yield of the financial instrument.
- **Coupon rate** The annual coupon rate of a security.
- **Frequency** The number of coupon payments in a year.
- **Basis** The day count basis to be used in calculation.

Functions related fixed income securities usually require special dates as arguments: issue date, settlement date, first coupon date, last coupon date, maturity date of a security. When specified, the following constraints should be followed:

- Issue settlement maturity
- Issue first coupon maturity
- Issue last coupon maturity

2.8 Date and time functions

Date and Time Functions return values corresponding to the specified date, month, year, hour, minute or second. You can also use date/time functions to enter the current system time and date in a cell.

These functions open up many possibilities for managing accounts receivable and calculating test times.

Spreadsheet internally stores date and time information using the same convention as other popular spreadsheet programs:

- Dates are represented as an integer equal to the number of days since December 31, 1899, so January 1, 1900 equals 1.
- Times are represented as fractions of a day, starting at midnight. For example, 6:00 AM is stored as 0.25 (a quarter of a 24-hour day).

Using this convention, date and time values may be used together. For example, the date/time value 1.25 corresponds to 6:00:00 AM, January 1, 1900.

2.9 Miscellaneous functions

Miscellaneous Functions perform a variety of calculations, such as returning a reference to specific cells or ranges or returning the Nth argument from a list of arguments.

2.10 Embedded tools

Embedded Tools are a powerful feature in Spreadsheet. Their power derives in part from their ability to return a set of data, not just a single value. This function makes non-scalar operations such as matrix multiplication and live recalculation as easy to use as an ordinary spreadsheet function.

Embedded tools store values in a group of adjacent cells. These adjacent cells are set to constant formulas with explicit dependencies on their neighboring cells. For example, an embedded tool in cell B2 might produce the formula =1.3459\B2 in cell B3. This formula indicates that the cell currently contains the constant 1.3459 but that its value depends on the contents of cell B2 (the cell containing the embedded tool).

This notion of explicit dependencies is important for recalculation. It

guarantees that any cell that references B3 will not be recalculated until after cell B2 is recalculated. This ensures that data generated by the embedded tool is always current.

Embedded tools look like normal functions, and they can be copied, moved and formatted just as any other formula in the spreadsheet. However, you must follow one important guideline: DO NOT combine embedded tools with other embedded tools in a single formula. For example the following formula is not allowed:

@INVERT(@MMUL(A1..C4,F1..I3))

3 Functions

See Also

Mathematical Functions

Statistical Functions

Conditional Statistical Functions

String Functions

Logic Functions

Financial Functions

Date and Time Functions

Miscellaneous Functions

Embedded Tools

3.1 Mathematical functions

@ABS(*X*) -The absolute value of *X*.

@ACOS(*X*) -The arc cosine of *X*.

@ASIN(*X*) -The arc sine of *X*.

@ATAN(*X*) -The 2-quadrant arc tangent of *X*.

@ATAN2(*X, Y*) -The 4-quadrant arc tangent of *Y/X*.

@CEIL(*X*) -The smallest integer greater than or equal to *X*.

@COS(*X*) -The cosine of *X*.

@COSH(*X*) -The hyperbolic cosine of *X*.

@DEGREES(*X*) -Converts the angle expressed in radians to degrees ( ).

@DET(*M*) -The determinant of the matrix range *M*, which must be a square matrix.

@DOT(*R1, R2*) -The dot product of the vectors *R1* and *R2*.

@EXP(*X*) -*e* raised to the *X* power.

@FACT(*N*) - The value of *N!*.

@FLOOR(*X*) -The largest integer less than or equal to *X*.

@FRAC(*X*) -The fractional portion of *X*.

@GAMMA(*X*) -The value of the gamma function evaluated at *X*.

@GRAND -A 12th-degree binomial approximation to a Gaussian random number with zero mean and unit variance.

@INT(*X*) -The integer portion of *X*.

@LN(*X*) -The natural log (base *e*) of *X*.

@LNGAMMA(*X*) -The log base *e* of the gamma function evaluated at *X*.

@LOG(*X*) -The log base 10 of *X*.

@LOG10(*X*) -The log base 10 of *X*.

@LOG2(*X*) -The log base 2 of *X*.

@MOD(*X, Y*) -The remainder of *X/Y*.

@MODULUS(*X, Y*) -The modulus of *X/Y*.

@PI -The value of p.

@POLY(*X, ...*) -The value of an *N*th-degree polynomial in *X*.

@PRODUCT(*X, ...*) -The product of all the numeric values in the argument list.

@RADIANS(*X*) -Converts the angle expressed in degrees to radians ( ).

@RAND -A uniform random number on the interval [0,1).

@ROUND(*X, n*) -*X* rounded to n number of decimal places (0 to 15).

@SIGMOID(*X*) -The value of the sigmoid function .

@SIN(*X*) -The sine of *X*.

@SINH(*X*) -The hyperbolic sine of *X*.

@SQRT(*X*) -The positive square root of *X*.

@SUMPRODUCT(*R1, R2*) -The dot product of the vectors *R1* and *R2*, where *R1* and *R2* are of equal dimension.

@TAN(*X*) -The tangent of *X*.

@TANH(*X*) -The hyperbolic tangent of *X*.

@TRANSPOSE(*M*) -The transpose of matrix *M*.

@VECLEN(...) -The square root of the sum of squares of its arguments.

3.2 Statistical functions

@AVG(...) -The average (arithmetic mean) of its arguments.

@CORR(*R1, R2*) -Pearson's product-moment correlation coefficient for the paired data in ranges *R1* and *R2*.

@COUNT(...) -A count of its non-blank arguments.

@F(*M, N, F*) -The integral of Snedecor's *F*-distribution with *M* and *N* degrees of freedom from minus infinity to *F*.

@ERF(*L[, U]*) -Error function integrated between 0 and *L*; if *U* specified, between *L* and *U*.

@ERFC(*L*) -Complementary error function integrated between *L* and infinity.

@FORECAST(...) -Predicted *Y* values for given *X*.

@FTEST(*R1, R2*) -The significance level ( ) of the two-sided *F*-test on the variances of the data specified by ranges *R1* and *R2*.

@GMEAN(...) -The geometric mean of its arguments.

@HMEAN(...) -The harmonic mean of its arguments.

@LARGE(*R, N*) -The *N*th largest value in range *R*.

@MAX(...) -The maximum of its arguments.

@MEDIAN(...) -The median (middle value) of the range *R1*.

@MIN(...) -The minimum of its arguments.

@MODE(...) - The mode, or most frequently occurring value.

@MSQ(...) -The mean of the squares of its arguments.

@PERCENTILE(*R, N*) -The value from the range *R* which is at the *N*th percentile in *R*.

@PERCENTRANK(*R, N*) -The percentile rank of the number *N* among the values in range *R*.

@PERMUT(*S, T*) -The number of *T* objects that can be chosen from the set *S*, where order is significant.

@PTTEST(*R1, R2*) -The significance level ( ) of the two-sided *T*-test for the paired samples contained in ranges *R1* and *R2*.

@QUARTILE(*R, Q*) -The quartile *Q* of the data in range *R*.

@RANK(*E, R[, O]*) -The rank of a numeric argument *E* in the range *R*.

@RMS(...) -The root of the mean of squares of its arguments.

@SMALL(*R, N*) -The *N*th smallest number in range *R*.

@SSE(...) -The sum squared error of its arguments. It is equivalent to @VAR(...) @COUNT(...).

@SSQ(...) -The sum of squares of its arguments.

@STD(...) -The population standard deviation (N weighting) of its

arguments.

@STDS(...) -The sample standard deviation (N-1 weighting) of its arguments.

@SUM(...) -The sum of its arguments.

@T(*N, T*) -The

integral of Student's *T*-distribution with *N* degrees of freedom from minus infinity to *T*.

@TTEST(*R, X*) -The significance level (of the two-sided single population *T*-test for the population samples contained in range *R*.

@TTEST2EV(*R1, R2*) -The significance level ( ) of the two-sided dual population *T*-test for ranges *R1* and *R2*, where the population variances are equal.

@TTEST2UV(*R1, R2*) -The significance level ( ) of the two-sided dual population *T*-test for ranges *R1* and *R2*, where the population variances are not equal.

@VAR(...) -The sample variance (N weighting) of its arguments.

@VARS(...) -The sample variance (N-1 weighting) of its arguments.

@VSUM(...) -The ``visual sum" of its arguments, using precision and rounding of formatted cell values.

3.3 Conditional statistical functions

@CAVG(..., C) – Conditional average.

@CCOUNT(..., C) – Conditional count.

@CMAX(..., C) – Conditional maximum.

@CMIN(..., C) – Conditional minimum.

@CSTD(..., C) – Conditional sample standard deviation (N weighting).

@CSTDS(..., C) – Conditional sample standard deviation (N-1 weighting).

@CSUM(..., C) – Conditional sum.

@CVAR(..., C) – Conditional population variance (N weighting).

@CVARS(..., C) – Conditional population variance (N-1 weighting).

3.4 String functions

@CHAR(*N*) -The character represented by the code *N*.

@CLEAN(*S*) -The string formed by removing all non-printing characters from the string *S*.

@CODE(*S*) -The ASCII code for the first character in string *S*.

@EXACT(*S1, S2*) -Returns true (1) if string *S1* exactly matches string *S2*, otherwise returns 0.

@FIND(*S1, S2, N*) -The index of the first occurrence of *S1* in *S2*.

@HEXTONUM(*S*) -The numeric value for the hexadecimal interpretation of *S*.

@LEFT(*S, N*) -The string composed of the leftmost *N* characters of *S*.

@LENGTH(*S*) -The number of characters in *S*.

@LOWER(*S*) -*S* converted to lower case.

@MID(*S, N1, N2*) -The string of length *N2* that starts at position *N1* in *S*.

@NUMTOHEX(*X*) - The hexadecimal representation of the integer portion of *X*.

@PROPER(*S*) -The string *S* with the first letter of each word capitalized.

@REGEX(*S1, S2*) -Returns true (1) if string *S1* exactly matches string *S2*; otherwise returns false (0). Allows ``wildcard'' comparisons by interpreting *S1* as a regular expression.

@REPEAT(*S, N*) -The string *S* repeated *N* times.

@REPLACE(*S1, N1, N2, S2*) -The string formed by replacing the *N2* characters starting at position *N1* in *S1* with string *S2*.

@RIGHT(*S, N*) -The string composed of the rightmost *N* characters of *S*.

@STRCAT(...) -The concatenation of all its arguments.

@STRING(*X, N*) -The string representing the numeric value of *X*, to *N* decimal places.

@STRLEN(...) -The total length of all strings in its arguments.

@TRIM(*S*) -The string formed by removing spaces from the string *S*.

@UPPER(*S*) -The string *S* converted to upper case.

@VALUE(*S*) -The numeric value represented by the string *S*; otherwise 0 if *S* does not represent a number.

3.5 Logic functions

@FALSE -The logical value 0.

@FILEEXISTS(*S*) -1 if file *S* can be opened for reading; otherwise 0.

@IF(*X, T, F*) -The value of *T* if *X* evaluates to on-zero, or *F* if *X* evaluates to zero.

@ISERROR(*X*) -Returns 1 if *X* ``contains'' an error, otherwise 0.

@ISNUMBER(*X*) -1 if *X* is a numeric value; otherwise 0.

@ISSTRING(*X*) -1 if *X* is a string value; otherwise 0.

@TRUE -The logical value 1.

Digital Logic Functions

@AND(...) -0 if any arguments are 0; 1 if all arguments are 1; otherwise -1.

@NAND(...) -0 if all arguments are 1; 1 if any arguments are 0; otherwise -1.

@NOR(...) -0 if any arguments are 1; 1 if all arguments are 0; otherwise -1.

@NOT(*X*) -0 if *X*=1; 1 if *X*=0; otherwise -1.

@OR(...) -0 if all arguments are 0; 1 if any arguments are 1; otherwise -1.

@XOR(...) - 1 if any of the arguments are not 0 or 1; otherwise 0 if the total number of arguments with the value 1 is even; 1 if the total number of arguments with the value 1 is odd.

3.6 Financial functions

@ACCRINT(I, Ft, S, R, P, F[, B]) -Accrued interest for a security that pays periodic interest.

@ACCRINTM(I, S, R, P[, B]) - Accrued interest for a security that pays interest at maturity.

@COUPDAYBS(S, M, F[, B]) -The number of days between the beginning of the coupon period to the settlement date.

@COUPDAYS(S, M, F[, B]) -The number of days in the coupon period that the settlement date is in.

@COUPDAYSNC(S, M, F[, B]) -The number of days between the settlement date and the next coupon date.

@COUPNCD(S, M, F[, B]) -The next coupon date after the settlement date.

@COUPNUM(S, M, F[, B]) -The number of coupon payments between the settlement date and maturity date.

@COUPPCD(S, M, F[, B]) -The previous (most recent) coupon date before the settlement date.

@CTERM(R, FV, PV) -The number of compounding periods for an investment.

@CUMIPMT(R, NP, PV, S, E, T) -The cumulative interest on a loan between start period S and end period E.

@CUMPRINC(R, NP, PV, S, E, T) -The cumulative principal paid on a loan between start period S and end period E.

@DB(C, S, L, P[, M]) -Fixed- declining depreciation allowance.

@DDB(C, S, L, N) -Double- declining depreciation allowance.

@DISC(S, M, P, R[, B]) -The discount rate for a security.

@DOLLARDE(FD, F) -Converts a dollar amount expressed as a fraction form into a decimal form.

@DOLLARFR(DD, F) -Converts a dollar amount expressed as a decimal form into a fraction form.

@DURATION(S, M, R, Y, F[, B]) -

The Macauley duration of a security assuming $100 face value.

@EFFECT(*NR, NP*) -Returns the effective annual interest rate.

@FV(*P, R, N*) -Future value of an annuity.

@FVSCHEDULE(*P, S*) -The future value of an initial investment after compounding a series of interest rates.

@INTRATE(*S, M, I, R[, B]*) -The interest rate for a fully invested security.

@IPMT(*R, P, NP, PV, FV[, T]*) -The interest payment for a specific period for an investment based on periodic, constant payments and a constant interest rate.

@IRR(*G, F*) -The internal rate of return on an investment. (See also @XIRR and @MIRR.)

@MDURATION(*S, M, R, Y, F[, B]*) -The modified Macauley duration of a security assuming $100 face value.

@MIRR(*CF, FR, RR*) -The modified internal rate of return for a series of periodic cash flows.

@NOMINAL(*ER, NP*) -The nominal annual interest rate.

@ODDFPRICE(*S, M, I, FC, R, Y, RD, F[, B]*) -The price per $100 face value of a security with an odd (short or long) first period.

@ODDFYIELD(*S, M, I, FC, R, PR, RD, F[, B]*) -The yield per of a security with an odd (short or long) first period.

@PMT(*PV, R, N*) -The periodic payment for a loan.

@PPMT(*R, P, NP, PV, FV, T*) -The payment on the principal for a specific period for an investment based on periodic, constant payments and a constant interest rate.

@PRICE(*S, M, R, Y, RD, F[, B]*) -The price per $100 face value of a security that pays periodic interest.

@PRICEDISC(*S, M, D, RD[, B]*) -The price per $100 face value of a discounted security.

@PRICEMAT(*S, M, I, R, Y[, B]*) -The price per $100 face value of a security that pays interest at maturity.

@PV(*P, R, N*) -The present value of an annuity

@RATE(*FV, PV, N*) -The interest rate required to reach future value *FV*.

@RECEIVED(*S, M, I, D, [, B]*) -The amount received at maturity for a fully vested security.

@SLN(*C, S, L*) -The straight-line depreciation allowance.

@SYD(*C, S, L, N*) -The ``sum-of-years-digits'' depreciation allowance.

@TBILLEQ(*S, M, D*) -The bond-equivalent yield (BEY) for a Treasury Bill.

@TBILLYIELD(*S, M, D*) -The yield on a Treasury bill.

@TERM(*P, R, FV*) -The number of payment periods for an investment.

@VDB(*C, S, L, S, E*) -Fixed- declining depreciation allowance between two periods.

@XIRR(*G, V, D*) -Internal rate of return for a series of cash flows with variable intervals.

@XNPV(*R, V, D*) -Returns the net present value for a series of cash flows with variable intervals.

@YIELD(*S, M, R, PR, RD, F[, B]*) -Yield of a security that pays periodic interest.

@YIELDMAT(*S, M, I, R, PR[, B]*) -Annual yield of a security which pays interest at maturity.

3.7 Date and time functions

@DATE(*Y, M, D*) -The date value for year *Y*, month *M*, and day *D*.

@DATEVALUE(*S*) -The corresponding date value for a given string *S*.

@DAYS360(*S, E*) -The number of days between two dates, based on a 30/360 day count system.

@DAY(*DT*) -The day number in the date/time value *DT*.

@EDATE(*S, M*) -The date/time value representing number of months (*M*) before or after start date (*S*).

@EOMONTH(*S, M*) -The date/time value representing the last day of the month *M* months after *S*, if M is positive, or *M* months before if *M* is negative.

@HOUR(*DT*) -The hour value (0-23) of date/time value *DT*.

@MINUTE(*DT*) -The minute value (0-59) of date/time value *DT*.

@MONTH(*DT*) -The number of the month in date/time value *DT*.

@NETWORKDAYS(*S, E[, H]*) -The number of whole working days, starting at *S* and going to *E*, excluding weekends and holidays.

@NOW -The date/time value of the current system date and time.

@SECOND(*DT*) -The seconds value (0-59) of the date/time value *DT*.

@TIME(*H, M, S*) -The time value for hour *H*, minute *M*, and second *S*.

@TIMEVALUE(*S*) -The corresponding time value for a given string value *S*.

@TODAY -The date value of the current system date.

@WEEKDAY(*D*) -The integer representing the day of the week on which the day *D* falls. 1 is Sunday, 7 is Saturday.

@WORKDAY(*S, D[, H]*) -The day that is *D* working days after *S*, if *D* is positive, or before *S*, if *D* is negative, excluding weekends and all holidays specified as dates in range *H*.

@YEAR(*DT*) -The year value of date/time value *DT*.

@YEARFRAC(*S, E[, B]*) -The portion of the year represented by the number of days between start date (*S*) and end date (*E*).

3.8 Miscellaneous functions

@CELLREF(*N1, N2*) -A reference to the cell in column *N1* and row *N2*.

@CHOOSE(*N, ...*) -The *N*th argument from the list.

@COL(*C*) -The column address of the cell referenced by *C*.

@COLS(*R*) -The number of columns in the specified range *R*.

@HLOOKUP(*X, S, R*) -The value of the cell in range *S* that is *R* number of rows beneath *X*.

@INIT(*X1, X2*) -The first argument on the first recalculation pass and the second argument on all subsequent recalculation passes when Spreadsheet is performing iterative calculations.

@INTERP2D(*R1, R2, N*) -The interpolation value for a 2-dimensional vector.

@INTERP3D(*R, X, Y*) -The interpolation value for a 3-dimensional vector.

@MATCH(*V, R[, T]*) -The relative position in range *R* of value *V* based on positioning criteria *T*.

@N(*R*) -The numeric value of the top left cell in range *R*.

@RANGEREF(*N1, N2, N3, N4*) -A reference to the range defined by coordinates *N1* through *N4*.

@ROW(*C*) -The row address of the cell referenced by *C*.

@ROWS(*R*) -The number of rows in the specified range *R*.

@S(*R*) -The string value of the top left cell in range *R*.

@VLOOKUP(*X, S, C*) -The value of the cell in range *S* that is *C* number of columns to the right of *X*.

IMPORTANT: Some Spreadsheet functions return a result that is a range or cell reference.

Spreadsheet does not include these indirect references in determining the pattern of recalculation.

Plan carefully before using these functions. See the section, Computed Cell References at the end of this chapter for more information.

3.9 Embedded tools

@DFT(*R*) -The Discrete Fourier Transform of the range *R*.

@EIGEN(*M*) -The eigenvalues of the matrix *M*.

@FFT(*R*) -The Discrete Fourier Transform of the range *R* using a fast Fourier Transform algorithm.

@FREQUENCY(*R, B*) -Returns a frequency distribution for values *R* with a set of intervals *B*.

@INVDFT(*R*) -The inverse of the Discrete Fourier Transform of the range *R*.

@INVERT(*M*) -The inverse of matrix *M*.

@INVFFT(*R*) -The inverse of the Discrete Fourier Transform of the range *R* using a fast Fourier Transform algorithm.

@LINFIT(*X, Y*) -The straight line least squares fit. This function is equivalent to @POLYFIT(*X, Y, 1*).

@LLS(*A, Y*) -The linear least squares solution *X* to the over-determined system of equations *AX=Y*.

@MMUL(*M1, M2*) -The product of multiplying matrix *M2* by matrix *M1*.

@PLS(*X, Y, d*) -Analyzes the least squares polynomial model *Y=P(X)*, where *P* is a polynomial of degree *d*.

@POLYCOEF(*X, Y, d*) -The least squares coefficients for the polynomial fit *Y=P(X)*, where *P* is a polynomial of degree *d*.

@TRANSPOSE(*M*) -The transpose of matrix *M*.

@TREND(*NX, KX, KY*) -The y values for new x values given existing x and y values.

Note

Embedded tools should not be contained within other functions or arithmetic operations in a single formula. You may, however, copy, move and format embedded tools just as any other function.

4 Using spreadsheet built-in functions

You enter a function in a cell in the same way you enter a formula or any other entry, with a few additional guidelines.

Type in the function name. Spreadsheet recognizes the string as a function. Function names are abbreviations that indicate what the function does. For instance, ABS computes absolute value, ROUND rounds to the specified number of places, and AVG computes the average of a list of arguments. Function names may be preceded with an '@' sign, but this is not required.

After typing the function name, enter arguments in parentheses. Most functions use one or more arguments to define the task to be performed. For example, the @AVG function averages the value of

two or more arguments. The @LENGTH function returns the length of an argument that is a character string.

Use only the arguments required by the function, in the exact order specified in the function syntax. If you enter other arguments or enter them in the wrong order, Spreadsheet will misinterpret their meaning or return an error message.

All the function names in this chapter are typed in uppercase letters, but you can enter them in upper or lower-case for your entries.

See Also

Arguments

Using Operators with Functions

Computed Cell References

4.1 Arguments

Arguments specify the values the function should use in its calculations. The number of arguments, their types, and their formats varies from one function to another. Arguments are usually numeric values, cell or range references, or string values. Most functions have at least one argument; a few have none.

The following chart shows different types of arguments used in Spreadsheet functions.

Argument Example

Numeric Value 123

Address of a cell A10

Address of a range F9..F99

String Value ``Quarterly Report''

4.2 Using operators with functions

The result of a function depends on the order in which Spreadsheet handles the calculations.

4.3 Computed cell references

Several Spreadsheet functions such as **@CELLREF** and **@RANGERE** return a result that is itself a cell reference or range reference. This is a powerful facility, but it must be used with caution because Spreadsheet can not take these indirect references into account when determining the order of recalculation. The same caution applies to constraint expressions used in conditional statistical functions. As a rule, cells that are indirectly referenced by a function are not automatically recalculated. Spreadsheet provides a special construct to force a recalculation, referred to as an explicit dependency.

Spreadsheet does not recalculate the spreadsheet unless explicit dependencies have been changed, so you may need to force recalculation if you change the value of a cell that is referenced only

indirectly through a function.

For example, suppose you want to count the numeric values in the range C3..J100 that fall within the limits specified in cells A1 and A2. The Spreadsheet formula to compute this is

@CCOUNT(C3..J100,#A1 && #<A2)

This formula will correctly count the numeric values in the range C3..J100. However, if you change the value in A1, Spreadsheet will not automatically recalculate the result, because A1 is referenced only indirectly through the constraint expression.

- To force Spreadsheet to recalculate the entire spreadsheet you should call the **Recalc()** command. You should also add **Recalculate** menu in your application that calls Recalc().
- You can also force Spreadsheet to do a partial recalculation with respect to that cell, edit the cell and append a blank and press the [**Return**] key on the cell containing the **@CCOUNT** formula.
- You can also use explicit dependencies to circumvent the limitation described above, if you entered the formula below in the form, the Spreadsheet would take into account the dependencies on A1 and A2 and update the spreadsheet just as you expect.

  @CCOUNT(C3..J100,#A1 && #<A2)\A1\A2
- Another approach is to construct the condition string with an expression that references the cells directly. In this example, A1 and A2 are directly referenced and thus will properly trigger recalculation. Explicit Dependency is described in more detail in Section Explicit Dependency.

  @CCOUNT(C3..J100, @STRCAT("#",A1,"&_<",A2))

5 Spreadsheet error messages

Spreadsheet checks for a variety of errors. Depending on the error type, the most recent error message is displayed either inside the affected cell(s), on the Message Line or is displayed inside the Spreadsheet Message dialog box.

See Also

Types of Errors

Summary of Error Messages

5.1 Types of errors

Errors in functions

Errors that occur inside functions are reported along with the name of the function in which the error occurred.

Formula syntax errors

These errors occur only when you are typing in a formula. When you

finish entering the formula, Spreadsheet will attempt to read the formula and convert it to an internal representation. If it is unable to do so, it continues to display the erroneous formula, switches into ``edit mode'', places the text cursor at the beginning of the text which it had difficulty parsing, and displays the error message.

The problem must be corrected before Spreadsheet can continue.

Formula evaluation errors

Formula evaluation error occurs when Spreadsheet reads in a formula and converts it into its internal formula representation, but is not able to evaluate the formula and produce a correct numeric or string formula. In some cases, the formula has been entered incorrectly, for example, an operand or parenthesis is missing. In other cases, an error has occurred as a result of computation that cannot be handled properly by the computer's floating point hardware, or there is an error condition in a cell or range that is referenced in the context of this formula. Errors can also occur in the evaluation of Spreadsheet built-in functions.

5.2 Summary of error messages

argument must be an integer

@FACT has been passed a non-integer argument.

argument not a cell or range

@@ has been passed an argument that is neither a cell nor a range.

argument out of range

An argument to a function is not within the correct range for the function and its other arguments.

arguments must be numeric

The function requires numeric arguments, which may be literal numbers, formulas which return numeric values, or references to cells containing numeric values.

arguments must be positive

The arguments in this function must be all positive values.

can not parse condition string

Spreadsheet has encountered a malformed conditional expression.

cannot find interpolation

@INTERP2D or @INTERP3D is unsuccessful in finding interpolated values.

cash flow series must be a range

@NPV and @MIRR require that their cash flow series must be a range, which must represent a single column or row.

cash flow series must be single column or row

@NPV and @MIRR require that their cash flow series must be a range, which must represent a single column or row.

cell operand contains error condition

A cell which is referenced from the cell in which the error occurs contains an error condition.

cell reference out of range

A cell reference has been made which is outside the range A1..FAN32767

coefficient matrix has linearly dependent columns

The existence of a unique solution to a linear least squares (@LLS) problem, Ax=b, requires that the columns of A are linearly independent.

column offset out of range

The third argument to the @VLOOKUP function specifies an offset that is less than 0 or is greater than the width of the range specified in the second argument.

constraint check not supported with ``As Needed"

Constraint checking is not supported when the recalculation is set to ``As Needed".

contains an error indicator

A cell in one or more of the data ranges for a graph contains an error condition. The error condition must be resolved before Spreadsheet can plot the graph.

could not find real root

@IRR could not find a real root. This suggests that the data given to @IRR is probably wrong.

count less than zero

User has passed a negative argument to a function which requires a count, for example, with @LEFT, it is impossible to take the -2 leftmost characters of a string.

data set size must be = 3

@LINFIT and @LINCOEF require a data set of size 3 or larger.

data set size must be = polynomial degree + 2

@PLS, @POLYFIT, and @POLYCOEF require that the data set size be greater than or equal to the polynomial degree + 2.

date series must be single column or row

@XIRR and @XNPV require the argument D (date series) to be a single column or single row.

decimal places out of range

@STRING only takes a decimal place argument between 0 and 15.

degrees of freedom must be 0

@F and @T require degrees of freedom greater than zero, as ``degrees of freedom'' is mathematically undefined for zero or less.

dimension must be power of 2

@FFT and @INVFFT require matrices whose dimensions are powers of two. The somewhat slower functions @DFT and @INVDFT, respectively, are equivalent functions which do not share this requirement.

divide by zero

An attempt has been made to divide by zero. **Note** that Spreadsheet considers cells which are empty or contain text strings to have the value zero in the context of a numerical calculation.

does not accept arguments

Several Spreadsheet functions, including @PI, @TRUE, @FALSE, @RAND, and @GRAND, do not accept any arguments.

domain is -1 < x < 1

@ATANH only takes arguments between -1 and 1, exclusive.

domain is -1 <= x <= 1

@ACOS and @ASIN only take arguments between -1 and 1, inclusive.

domain is 0 <= x <= 170

@FACT only takes arguments between 0 and 170, inclusive. (Most platforms)

domain is 0 <= x <= 33

@FACT only takes arguments between 0 and 33, inclusive. (VAX platforms)

domain is x 0

@LN, @LOG2, @LOG, @GAMMA, and @LNGAMMA only take arguments greater than zero.

domain is x = 1

@ACOSH only takes arguments greater than or equal to 1.

``End Period'' must be = 1

@CUMIPMT and @CUMPRINC require the argument E (end period) to be greater than or equal to 1.

``End Period'' must be = ``Start Period''

@CUMIPMT, @CUMPRINC and @VDB require the argument E (end period) to be greater than or equal to S (start period).

ending line with a

\

The \ is an escape sequence introducer, which should be followed by another character for interpretation, but the string ended prematurely.

ending line with a superscript command

When displaying text in the context of graphics, a **^** is a superscript introducer. Like y**^**2 means ``y squared." This message occurs when a **^** occurs at the end of the string.

ending line with subscript command

When displaying text in the context of graphics, an `_' is a subscript introducer. Like y_2 means ``y subscript 2." This message occurs when an `_' occurs at the end of the string.

error in regular expression

An error occurred while parsing the regular expression used in a search or extract operation, or while executing @REGEX or @MATCH.

expected the right hand side of a range here

The outer range reference is missing.

expected to find [*something*] here

There was a parsing error. The cursor will be placed in the edit window in edit mode. Read the documentation for the function and correct the error.

expecting a function

There is something wrong with the formula you have entered on the edit line. The parser was expecting to find a function name at the point indicated by the cursor position.

expecting an operand

There is something wrong with the formula you have entered on the edit line. The parser was expecting to find a function name at the point indicated by the cursor position.

expecting an operator

There is something wrong with the formula you have entered on the edit line. The parser was expecting to find a function name at the point indicated by the cursor position.

extraneous operands

There is something wrong with the formula you have entered on the edit line. The parser was expecting to find a function name at the point indicated by the cursor position.

F must be = 0

The third argument to @F must be greater than or equal to 0.

first argument must be numeric

@NPV and @CHOOSE require that their first argument be numeric.

floating exception

A floating-point arithmetic hardware exception occurred during the computation of the function or expression. This means that the calculations resulted in a number out of the range that the computer hardware is able to represent.

found something unexpected here

Spreadsheet has found something it doesn't understand in an expression.

``Fraction" must be = 1

@DOLLARDE and @DOLLARFR require the argument F (fraction) to be greater than and equal to 1.

``Frequency" must be 1, 2 or 4

The argument Frequency (number of coupon payment per year) in financial functions is limited to one of the following choices: 1, 2 or 4

function not installed

This error occurs when Spreadsheet encounters an ``@" followed by a function name which it does not recognize as one of its built-in functions, or one that has been installed by a connection program.

function stack overflow

This error occurs when functions are nested too deeply. Spreadsheet supports nesting of functions up to 50 levels deep.

hex number greater than 32 bits

Spreadsheet cannot convert a hex string to a number if the hex string is longer than 8 characters, which translates to 32 bits in the internal binary representation.

IEEE Floating Exception (Infinity or NaN)

This error means that the formula caused a computation to occur which could not be calculated properly by the computer's IEEE standard floating point hardware. Most likely, this means that the computation would produce an intermediate or final result outside the range +/-1.8e308.

illegal cell or range reference

It happens when a copy or move operation results in a cell or range reference that is outside the range A1..FAN32767.

illegal operand of ``operator"`

This error occurs when one or both of the operands of the specified ``operator" are not valid. Most likely, a range name was used as an operand in an arithmetic expression.

improper argument type

One or more arguments to the function are incompatible with the type of arguments required by the functions.

improper coefficient type

In the polynomial evaluation function (@POLY), one or more of the polynomial coefficients are non-numeric.

improper dimensions

Several Spreadsheet matrix functions and embedded tools have certain requirements on the dimensions of their matrix arguments. Check the reference manual if you are uncertain about those requirements.

incompatible matrix dimensions

In matrix multiplication (@MMUL), the number of columns in the first matrix must equal the number of rows in the second matrix.

incompatible range dimensions

The Spreadsheet dot product functions (@DOT) requires vectors of equal size. It will also compute the sum-of-products of any two ranges with equal dimensions.

index column contains empty cell

The first column in the lookup table referenced by @VLOOKUP must not contain empty cells.

index out of range

In @FIND, the third argument may not be larger than the length of the second argument. In @MID, the second argument may not be larger than the length of the first argument.

index row contains empty cell

The first row in the lookup table referenced by @HLOOKUP must not contain empty cells.

integer parameter out of range

An integer parameter greater than 4294967296 or less than -2147483649 has been entered.

interest rate should be 0

@EFFECT and @NOMINAL require that argument R (interest rate) to be greater than 0.

interest schedule must be a single column or row

The argument R (array of interest rates) in @FVSCHEDULE must be a single column or row.

invalid cell reference

User has tried to access a cell with a row which is negative, zero, or greater than 32767, or with a column which is negative or greater than FAN, or 4095.

invalid date

Spreadsheet could not understand the date format. Date values must be in the range 1-73,050, representing the dates January 1, 1900, to December 31, 2099, respectively. This error can also occur when the year, month, and day values passed to @DATE do not represent an actual date within this range (February 31, 1950, or January 1, 2589, for example).

invalid day count basis

The day count basis in financial functions should be one of the following choices: 0 (30/360), 1 (actual/actual), 2 (actual/360) or 3 (actual/365)

invalid range reference

User has tried to make a range reference that references cells beyond the range of the spreadsheet; that is, a row which is negative, zero, or greater than 32767, or a column which is negative or greater than FAN, or 4095.

invalid table

The table of reference points in @INTERP2D or @INTERP3D contains non-numeric values or blank cells.

invalid time

Spreadsheet cannot parse a time which the user has provided. Time values are fractional values from 0 to 1, representing fractions of a 24-hour period. When interpreting a number as a date/time value, Spreadsheet interprets the integer portion of the number as the date and the fractional portion as the time on that date. A negative value is invalid. Also, the @TIME function must have arguments in the range of 0-23 hours, 0-59 minutes, and 0-59 seconds. Any other values are invalid.

iterative calculation not supported with ``As Needed"

To avoid infinite looping, iterative (self-referential) calculations are not supported when the recalculation method is ``As Needed". To use iterative calculations, the user must choose manual recalculation.

less than 2 arguments

@POLY requires 2 or more arguments.

``Life" and ``Period" must be integers

@DDB requires that ``Life" and ``Period", arguments 3 and 4, respectively, be integers.

``Life" must be 0

@SLN and @SYD require that ``Life" is greater than 0.

lookup failed to produce a match

@HLOOKUP or @VLOOKUP failed to produce a match. This should only happen with an alphabetic lookup.

``Lower limit'' must be =0

The argument L (lower limit) should be greater than or equal to 0 in @ERF and @ERFC.

magnitude too large

@NUMTOHEX requires an argument between 2147483646 and -2147483647, inclusive.

matrix is singular

It is mathematically impossible to invert a singular matrix.

matrix must be square

It is impossible to invert, take the eigenvalue of, or take the determinant of a non-square matrix.

``Match Type'' must be 0 for string match

The argument T (type of match) must be 0 if argument V (value to be matched) is text in @MATCH.

matrix must be symmetric

@EIGEN requires a symmetric matrix.

modula divide by zero

Mod 0 is an undefined operation.

must be -15 to +15 places

@ROUND cannot round to greater than 15 places on either side of the decimal point.

must have ``Cost'' = ``Salvage'' = 0

@DDB, @SLN, @SYD, @DB, and @VDB require that the ``Cost'' argument be greater than or equal to the ``Salvage'' argument, which must be greater than or equal to 0.

must have issue < first coupon < maturity

The values of argument I (issue date), FC (first coupon date) and M (maturity date) must satisfy the following condition: I < FC < M

must have issue < last coupon < maturity

The values of argument I (issue date), LC (last coupon date) and M (maturity date) must satisfy the following condition: I < LC < M

must have ``Life'' = ``Period'' = 1

@DDB, @DB, and @VDB all require that the ``Life'' argument be greater than or equal to the ``Period'' argument, which must be greater than or equal to 1.

must have N 0, K 0 and N < K

The arguments N (number of objects to choose from) and K (Number of objects to be chosen) in @PERMUT must follow the following condition: N0, K0 and N <K.

need at least 2 cash flow values

A single data point does not a cash flow series make; it takes two to trend. Computing the internal rate of return (@IRR) is undefined for only one value.

no duplicate number found

The @MODE can not find the most frequently occurring number because all numbers appears only once in the argument list.

no match was found

@MATCH is unsuccessful in finding a match.

non hex digits in string

@HEXTONUM requires that its argument be a string containing only hex digits, 0-9 and a-f.

non-numeric operand

An expression of some sort has a non-numeric operand where a numeric operand is required, making the result of the expression undefined.

non-numeric value in ...

Doing arithmetic on alphabetic entities is undefined.

not enough arguments to function

User has entered too few arguments to the function.

``Number'' is not in the reference list

The number to be ranked is not in the reference list in @RANK.

number is too [large|small]

The number is at or beyond the limit of the ability of the computer to express, and is treated as if it were slightly within the limit.

number of compounding periods should be =1

@EFFECT and @NOMINAL require that argument C (number of compounding periods) to be greater than or equal to 1.

one argument must be non-zero

@ATAN2 requires that one of it's arguments be non-zero.

operand contains error condition

Some cell referenced by the operand is in an error condition, or contains a reference to a cell which is in an error condition, etc.

operand equal to 0

@HMEAN does not take arguments whose value is 0.

operand larger than 32 bits

Integers in Spreadsheet cannot take more than 32 bits to express. This restricts integers to the range 2147483647 to -2147483648, or

4294967295 to zero, depending on whether the operand is only positive or can be negative.

operand less than or equal to 0

@GMEAN does not take arguments which are 0 or negative.

operand out of range

@CHAR only takes integers between 1 and 255

operands of ``&" must be same type

The ``&" operator serves a dual purpose; if its operands are numeric, then it performs a bitwise AND operation; if its operands are text strings, then it concatenates the two strings. If the operands are neither numeric nor both strings, this error occurs.

operands of ``.." must be cell reference

The .. operator can only join two cell references to create a range. It cannot join integers to make a range of integers, or do anything else.

``Payment" and ``FV" must have the same sign

@TERM requires that Payment and Future Value have the same sign.

Payment`` must be non-zero

@TERM requires that Payment be non-zero.

``Period" must be = 0

@SYD requires that Period be greater than or equal to 0.

``Period" must be an integer 0

@FV, @PMT, @PV, and @RATE require that Period be an integer greater than 0.

polynomial degree must be between 1 and 10

@PLS, @POLYFIT, and @POLYCOEF require that the polynomial degree by between 1 and 10.

pooled sample size less than 3

@TTEST2EV requires a pooled sample size greater than 2 to be mathematically defined.

population less than 1

@CVAR, @CSTD, @SSE, @VAR, and @STD require a population greater than or equal to 1.

``PV" and ``FV" must be non-zero

@CTERM and @RATE require that Present and Future Values be non-zero by definition.

``PV" and ``FV" must have the same sign

@CTERM and @RATE require that Present and Future Values have the same sign.

ranges must be same dimensions

@PTTEST and @CORR require that both their arguments be ranges of equal dimensions, since they work with pairs of values, one value from each range.

``Rate'' must be greater than -1

@CTERM, @FV, @PMT, @PV, @TERM, @NPV, @XNPV, and @XIRR require that their Rate argument be greater than -1.

``Rate'' must be non-zero

@CTERM requires that its Rate argument be non-zero.

rate found is less than -1

@IRR has found a rate less than -1 after iterating the maximum number of times.

recursion too deep

This error will occur if Spreadsheet encounters ``a condition string within a condition string.'' For example, it happens with a conditional statistical formula whose condition string calls another conditional statistical function which in turn contains its own condition string.

result of expression is a range

Some Spreadsheet functions, such as @CELLREF and @RANGEREF, return cell references or range references as a result. Cell and range references can not be the final result of a formula.

resultant string too long

A string generated by a formula is too long (greater than 512 characters).

row offset out of range

The third argument to the @HLOOKUP function specifies an offset that is less than 0 or is greater than the depth of the range specified in the second argument.

sample missing from pair

The two input ranges to the paired t-test (@PTTEST) and Pearson product-moment correlation (@CORR) functions contain paired values. If a value appears at a given position in the first range, then there must also be a value in the corresponding position of the second range.

sample size less than 2

@CVARS, @CSTDS, @VARS, @STDS, @TTEST, @PTTEST, @TTEST2UV, and @FTEST require a sample size greater than 1.

searching NULL list

searching list with a NULL function.

selector out of range

The first argument to @CHOOSE must be 0 or more and be less than or equal to the number of the rest of the arguments - 1.

settlement date should be < maturity date

Settlement date should be earlier than maturity date in financial functions.

settlement date should be = issue date

Settlement date should not be earlier than the issue date.

showing NULL list

showing list with a NULL function

``Start Period" must be = 1

@CUMIPMT and @CUMPRINC require the argument S (start period) to be greater than or equal to 1.

starting date should be at beginning of ``Dates"

The number in argument D (dates) should not precede the starting date in @XIRR and @XNPV.

substring longer than string

@FIND cannot find an instance of the pattern string within a shorter target string, since it is impossible to embed a string in a string shorter than itself.

substring not found

@FIND could not find an instance of the pattern string in the target string.

token buffer overflow

This error can only occur when a formula is entered which is more complex than Spreadsheet can accept. Spreadsheet can accept up to 200 operators, numbers, function calls, and text strings in a single formula, which is more than any human can reasonably deal with.

too few arguments

The function requires more arguments.

too many arguments to function

User has provided too many arguments to the function. No function can take more than 100 arguments.

too many arguments

@NOT only takes one argument, unlike the rest of the digital logic functions. @ROW and @COL take 1 argument, @ANNOTATE takes 3-5 arguments.

Treasury Bill should not be outstanding more than 1 year

The period between the settlement date and maturity date of a Treasury bill should not exceed one year.

unable to parse extract filter

Happens when you are doing an Extract operation and you specify an invalid boolean expression; e.g., #==/5.

unable to parse search condition

Happens when you are doing a numeric search and you specify an invalid boolean expression; e.g., #==/5

undefined symbolic name

This error occurs when Spreadsheet encounters a symbolic range or cell reference which has not been defined. To use a symbolic name to refer to a cell or range, you must first define it using the SetRangeName command.

unexpected question mark

Spreadsheet supports C-language compatible condition expressions, which use the operator pair ``?'' and ``:''. If one of these operators appears without the other, an error occurs.

unresolved name in expression

A name which is not a valid function or named range has been used in the expression.

``Upper limit'' must be =0

The argument U (Upper limit) should be greater than or equal to 0 in @ERF.

``values'' and ``dates'' series must have the same dimension

@XIRR and @XNPV require the argument V (cash flow series) and the argument D (date series) to have the same dimension.

``Values'' must have at least one inflow and one outflow

@MIRR requires the value range contains at least one income (positive value) or one payment (negative value)

wrong number of arguments

The number of arguments passed to the function is incorrect. Check the reference manual to determine the correct number of arguments that the function expects.

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