ChromQuest 5.0

Chromatography Data System

Reference Guide

CHROM-97253 Revision A   March 2008

Thermo
SCIENTIFIC

Software Version: ChromQuest 5.0

For Research Use Only. Not regulated for medical or veterinary diagnostic use by U.S. Federal Drug Administration or other competent authorities.

C

Contents

Contents

Preface

Welcome to ChromQuest™ 5.0. The ChromQuest chromatography data system is a member of the Thermo Scientific family of LC data systems.

Whether you are a new ChromQuest user or are upgrading from a previous version of ChromQuest, we think you will find the features of ChromQuest 5.0 both powerful and well organized.

This *ChromQuest Chromatography Data System Reference Guide* contains technical details, such as how integration is performed and equations are used.

For instructions on how to use the ChromQuest chromatography data system to acquire and process data, refer to the *ChromQuest User Guide.*

Related Documentation

In addition to this guide, Thermo Fisher Scientific provides the following documents for the ChromQuest chromatography data system:

- *ChromQuest 5.0 Installation Guide* (PDF on the ChromQuest CD)

- *ChromQuest 5.0 Administrator Guide* (PDF on the ChromQuest CD)

- *ChromQuest 5.0 User Guide* (PDF on the ChromQuest CD)

- *ChromQuest 5.0 Quick Reference Guide* (laminated card)

New Features

The ChromQuest 5.0 chromatography data system provides these new features:

- A navigation bar has been added to the Instrument window.

- The Move Baseline Start and Stop integration timed events have been replaced by the Move Baseline integration timed event. See "Move Baseline " on page 25.

- A custom peak parameter has been added to the sequence table.

- A new Graphics Export function has been added. See "Graphics Export" on page 91.

- Overlaid traces are now normalized by default.

- A System Administration Report has been added.

- Users can be found by searching the Active Directory.

- System Administrators can now create pre-defined custom reasons for audit trails.

- Multi-level bracketed calibrations are now supported.

- A sequence print table is available for custom reports.

- A sequence run type, baseline file, has been added that enables you to subtract a baseline file from other runs in the sequence.

- A Stop Run option has been added: Stop sequence after current run completes.

- A configurable Filtered Method Report has been added.

- Run Type can be selected as a field in Advanced Reports.

- A user-configurable Sequence Contents Report is available.

- The available fields in the Method Custom Report have been updated to include User Acquiring the Data.

- Page break has been added to the custom report editor.

- In the PDA software, you can specify a wavelength to designate a chromatogram to be used as a baseline subtraction chromatogram for other chromatograms extracted from the 3D data. See "Multi-Chromatogram" on page 131.

Safety and Special Notices

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

Safety and special notices include the following:

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

Note Highlights information of general interest.

Tip Highlights helpful information that can make a task easier.

Contacting Us

There are several ways to contact Thermo Fisher Scientific for the information you need.

❖ **To contact Technical Support**

Phone	800-685-9535
Fax	561-688-8736
E-mail	TechSupport.C+MS@thermofisher.com
Knowledge base	www.thermokb.com

Find software updates and utilities to download at www.mssupport.thermo.com.

❖ **To contact Customer Service for ordering information**

Phone	800-532-4752
Fax	561-688-8731
Web site	www.thermo.com/ms

❖ **To copy manuals from the Internet**

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

❖ **To suggest changes to documentation or to Help**

- Fill out a reader survey online at www.thermo.com/lcms-techpubs.

- Send an e-mail message to the Technical Publications Editor at techpubs-lcms@thermofisher.com.

Examples of Integration Timed Events

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

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. For details on how to add an event to your method, refer to **Chapter 3: Method Development** of the *ChromQuest Chromatography Data System User Guide*.

Contents

- Integration Timed Events Tables
- Required Integration Timed Events
- Optional Integration Events
- Baseline Code Descriptions

Integration Timed Events Tables

ChromQuest has two tables where integration timed events are saved. It is important to understand the difference between these two tables. When you add an integration timed event graphically, a dialog box appears before it is added to the method, allowing you to choose whether you want to place the event in your method, and if so, in which integration timed events table the event is placed. The default table for each integration event is selected. An example of such a dialog is shown below.

Figure 1. Integration Off dialog box

If you select the **Add to Table** command, the timed event is inserted in either the **Integration Events Table**, or the **Manual Integration Fixes Table**, depending on which of these is selected.

Integration Events Table

When you add an integration event to the Integration Events Table, the integration changes is used on all subsequent samples analyzed using this method. (Assuming the method is saved.) These events should be setup to accurately analyze typical samples.

Figure 2. Integration Events table

The Integration Events Table contains all current Integration Timed Events for the current method channel. You can add an event manually by selecting the event from the drop-down list in the **Events** field, entering an appropriate Start and Stop time and a Value for the event (if required). To remove an event's effect from an analysis, yet keep the event in the table, click the check mark next to the event. Only events with a red check mark have an effect on subsequent analyses.

To remove an event entirely from the table, click the row number of the event, followed by the **Delete** key.

A right-hand mouse click anywhere in the table produces a menu of commands for manipulating cells and rows in the spreadsheet. The Insert Paste command is used to insert a line at the same time you paste to the location. The Insert Line command simply inserts a blank line where your cursor is located.

Manual Integration Fixes Table

When you add an integration event to the Manual Integration Fixes Table, it is applied only to this sample. Thus, Manual Integration Fixes are One-time integration events. These events are attached to individual files to accurately integrate an atypical sample. The results using these events are 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, click the Manual Integration Fixes Table button, or choose the **Data > Manual Integration Fixes** command from the menu bar.

Figure 3. Manual Integration Fixes table

The Manual Integration Fixes Table contains all current Manual Integration Fixes for the current data file. You can add an event manually by selecting the event from the drop-down list in the **Events** field, entering an appropriate Start and Stop time and a Value for the event (if required). To remove an event's effect from an analysis, yet keep the event in the table, click the check mark next to the event. Only events with a red check mark have an effect on subsequent analyses.

To remove an event entirely from the table, click the row number of the event, followed by the **Delete** key.

A right-hand mouse click anywhere in the table produces a menu of commands for manipulating cells and rows in the spreadsheet. The Insert Paste command is used to insert a line at the same time you paste to the location. The Insert Line command simply inserts a blank line where your cursor is located.

View Preferences for Integration Events

By default the integration events toolbar appears at the bottom of the Instrument window when you open a data file. If you prefer to access the integration tools from the shortcut menu and want to maximize the chromatogram display area, you can hide the integration events toolbar.

When you select an integration event, a blue dialog box appears with instructions for using the event. The same instructions appear in the Status bar.

Figure 4. Move Baseline instructions
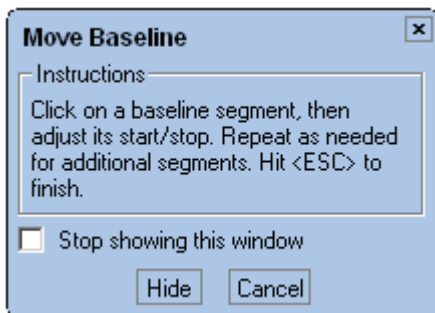
This section contains these procedures:

- Hiding the Integration Events Toolbar

- Hiding the Graphical Programming Tooltips

Hiding the Integration Events Toolbar

❖ **To hide the integration events toolbar**

1. Choose **View > Preferences**.

   The Preferences dialog box appears (see Figure 5).

   Figure 5. Preferences dialog box
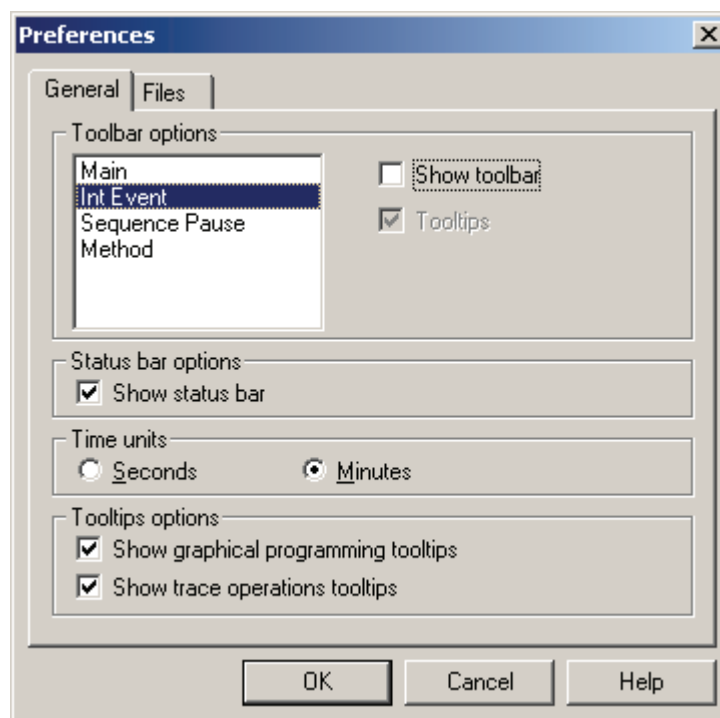
2. In the Toolbar options area, select **Int Event**, and then clear the **Show toolbar** check box.

3. Click **OK** to accept the change and close the dialog box.

Hiding the Graphical Programming Tooltips

❖ **To hide the graphical programming tooltips**

1. Choose **View > Preferences**.

   The Preferences dialog box appears (see Figure 6).

   Figure 6. Preferences dialog box
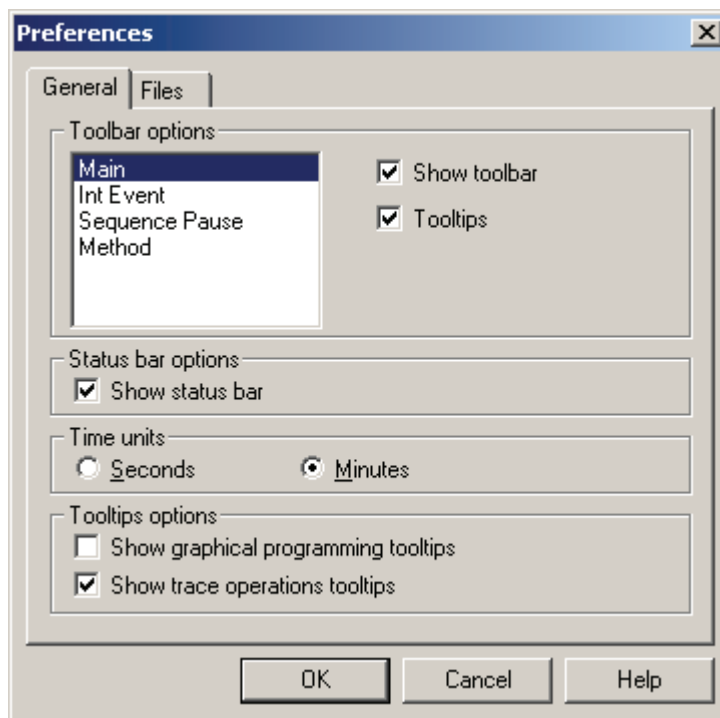
2. In the Tooltips options area, clear the **Show graphical programming tooltips** check box.

3. Click **OK** to accept the change and close the dialog box.

Required Integration Timed Events

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. When you create a new method, default values are entered automatically in the method. However, if you clear an Integration Event Table, you must be sure to enter these events again; otherwise you will get an error message when you analyze 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 (that is, the sampling frequency was too high), the **Width** parameter is 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.

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

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

> **Note** In most circumstances, an initial Width value based on the narrowest peak in the chromatogram is 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 affect the peak baseline.

Figure 7. Required integration events: Peak Width and Threshold

Fiber optic

| Peak width too narrow | Correct peak width | Peak width too large |
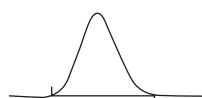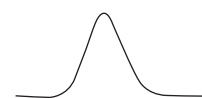
Fiber optic
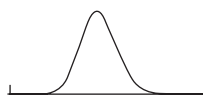
| Threshold value too small | Correct threshold value | Threshold value too large |
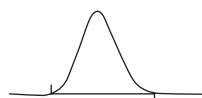
Note that extreme values of both Width and Threshold (too large or too small) can result in peaks not detected.

Optional Integration Events

The following integration timed events are available for you to program into your method to "customize" the integration of particular peaks or groups of peaks.

- Shoulder Sensitivity
- Integration Off
- Valley to Valley
- Horizontal Baseline
- Backward Horizontal Baseline
- Lowest Point Horizontal Baseline
- Tangent Skim
- Front Tangent Skim
- Minimum Area
- Negative Peak
- Disable End Peak Detection
- Reassign Peak
- Manual Baseline
- Manual Peak
- Split Peak
- Force Peak Start /Force Peak Stop
- Move Baseline
- Reset Baseline
- Reset Baseline At Valley
- Adjust Retention Time Window
- Adjust Group Range

Shoulder Sensitivity

This parameter is used to enable the detection of shoulders on larger peaks. A larger value decreases 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.

Figure 8. Shoulder Sensitivity dialog box
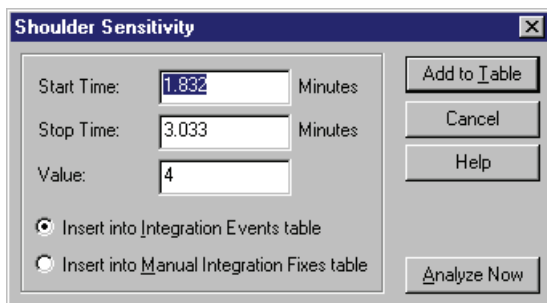
Click **Add to Table**, and the timed event is inserted in either the **Integration Events Table**, or the **Manual Integration Fixes Table**, depending on which of these you select. Click **Cancel** to ignore the timed event and cancel the operation. Click **Analyze now** to add the event to the table and analyze the chromatogram using the event.

Figure 9. Shoulder Sensitivity events
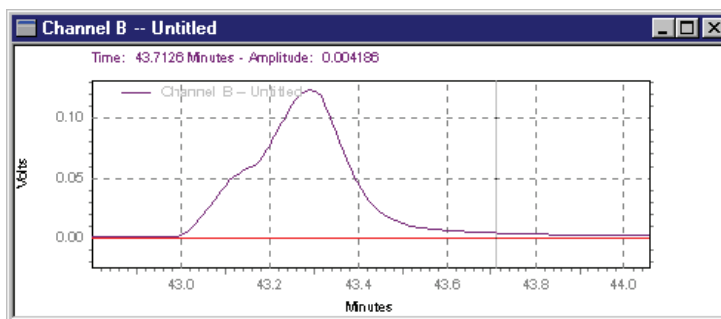
Shoulder Sensitivity value set too high

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.

Figure 10. Integration Off dialog box
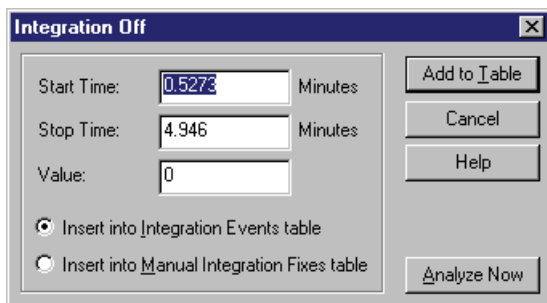
Click **Add to Table**, and the timed event is inserted in either the **Integration Events Table**, or the **Manual Integration Fixes Table**, depending on which of these you select. Click **Cancel** to ignore the timed event and cancel the operation. Click **Analyze Now** to add the event to the table and analyze the chromatogram using the event.

The following example chromatograms illustrate the effect of using the **Integration Off** event to turn integration off between 0 and 5 minutes.

Figure 11. Integration Off events
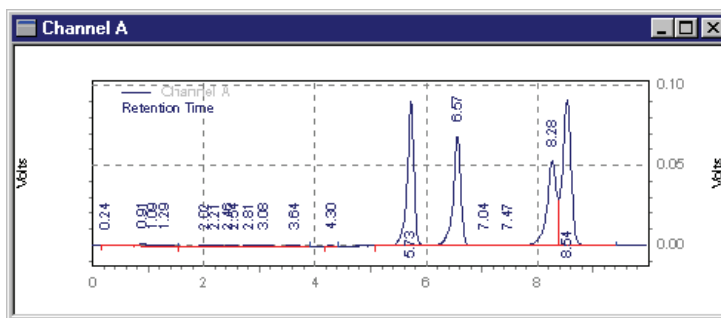
Default integration
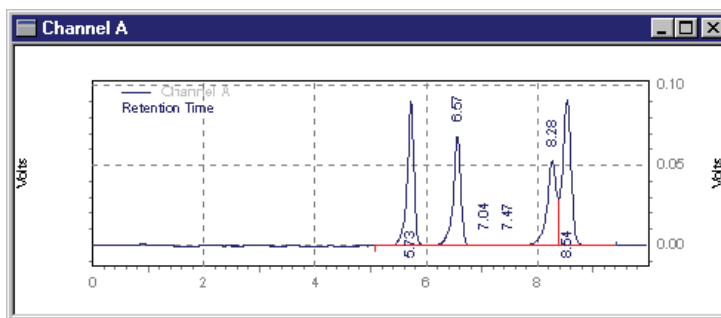
Integration Off event
from 0 to 5 minutes

Valley to Valley

This event causes the baselines of peaks that are not totally resolved (that is. 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 that do not reach baseline.

Figure 12. Valley to Valley dialog box
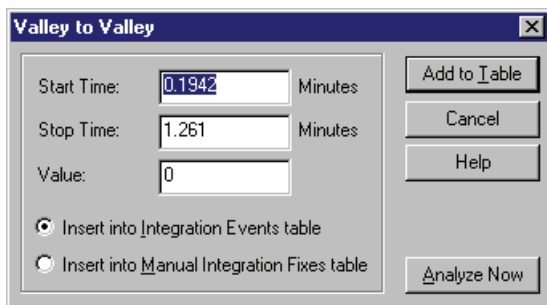
Click **Add to Table**, and the timed event is inserted in either the **Integration Events Table**, or the **Manual Integration Fixes Table**, depending on which of these you select. Click **Cancel** to ignore the timed event and cancel the operation. Click **Analyze Now** to add the event to the table and analyze the chromatogram using the event.

Figure 13. Valley to Valley events
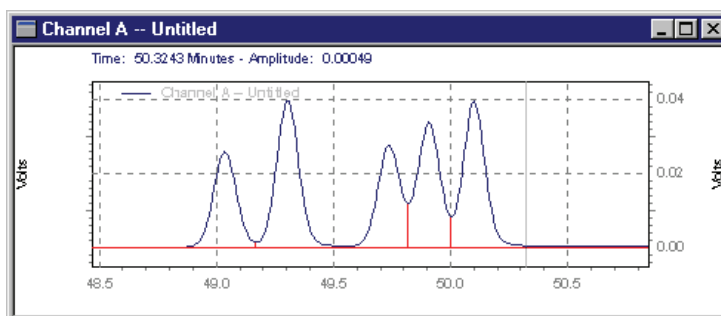
Default integration
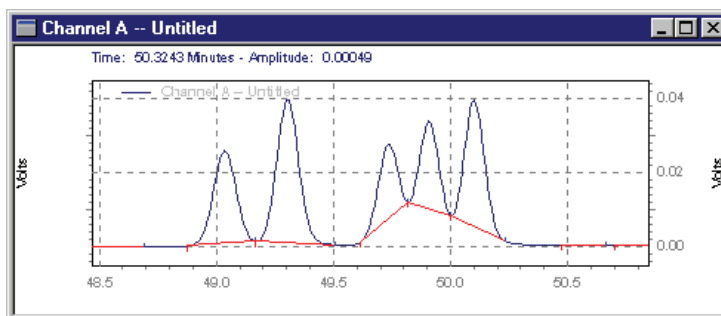
Integration with
Valley to Valley event

Horizontal Baseline

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

Figure 14. Horizontal Baseline dialog box
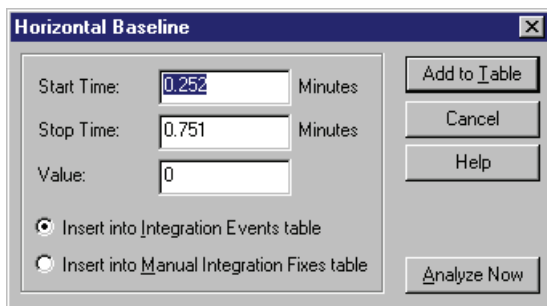
Click **Add to Table**, and the timed event is inserted in either the **Integration Events Table**, or the **Manual Integration Fixes Table**, depending on which of these you select. Click **Cancel** to ignore the timed event and cancel the operation. Click **Analyze Now** to add the event to the table and analyze the chromatogram using the event.

Figure 15. Horizontal Baseline events
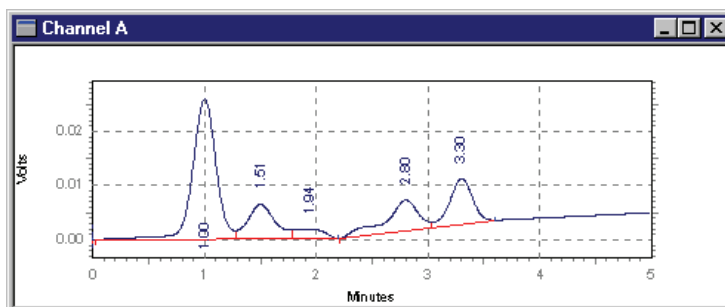
Integration without Horizontal Baseline event
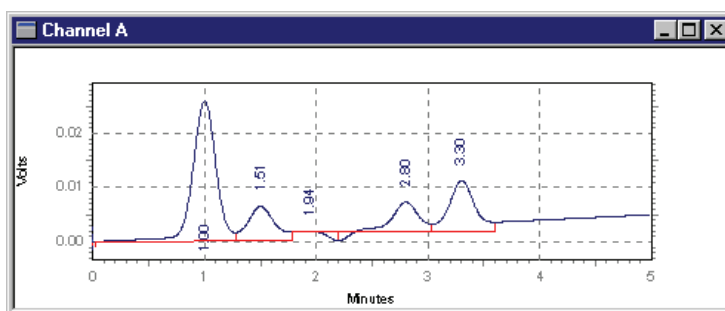
Integration with Horizontal Baseline between 1.8 and 3.6 minutes

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 is created between the times specified by the event.

Figure 16. Backward Horizontal Baseline dialog box
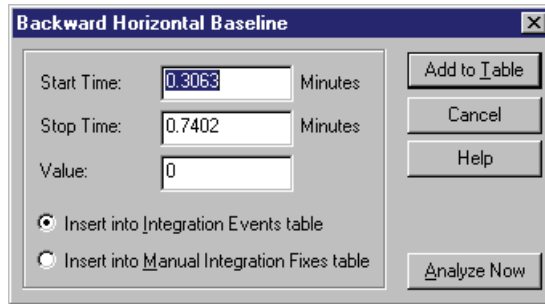
Click **Add to Table**, and the timed event is inserted in either the **Integration Events Table**, or the **Manual Integration Fixes Table**, depending on which of these you select. Click **Cancel** to ignore the timed event and cancel the operation. Click **Analyze Now** to add the event to the table and analyze the chromatogram using the event.

Figure 17. Backward Horizontal Baseline events
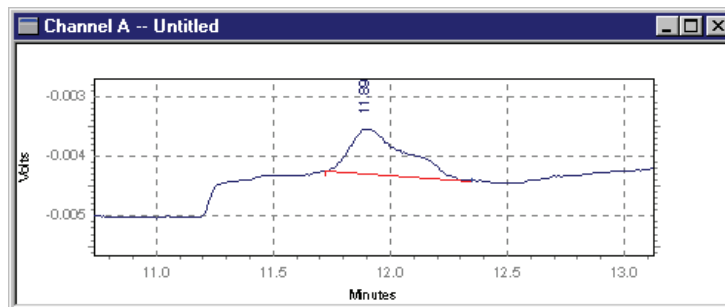
Default integration
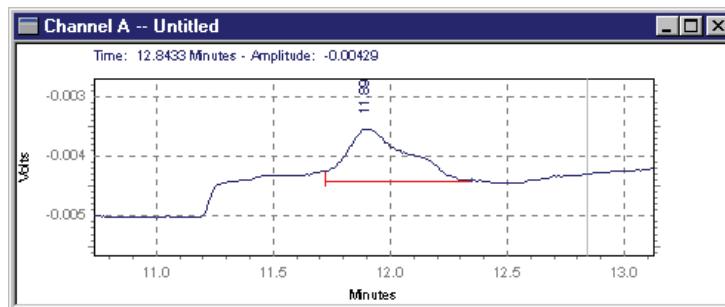
Integration after
Backward Horizontal Baseline
event

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 Start Time entered for this event is the point from which the software searches for the lowest point. The Stop Time is the time where the software stops searching for the lowest point.

Figure 18. Lowest Point Horizontal Baseline dialog box
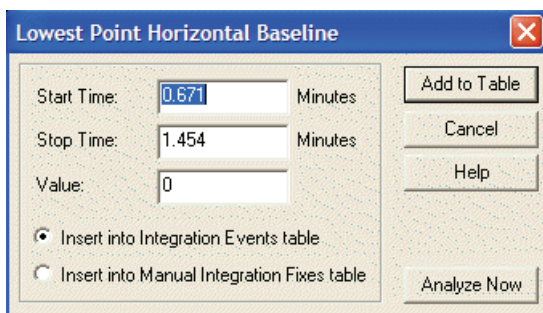
Click **Add to Table**, and the timed event is inserted in either the **Integration Events Table**, or the **Manual Integration Fixes Table**, depending on which of these you select. Click **Cancel** to ignore the timed event and cancel the operation. Click **Analyze Now** to add the event to the table and analyze the chromatogram using the event.

Figure 19. Lowest Point Horizontal Baseline events
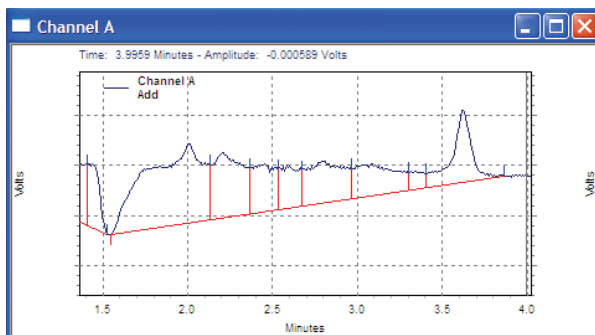
Integration before using Lowest Point Horizontal Baseline event
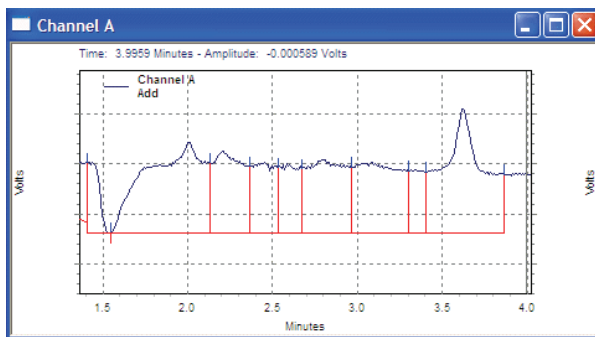
Integration after using Lowest Point Horizontal Baseline event

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.

Figure 20. Tangent Skim dialog box
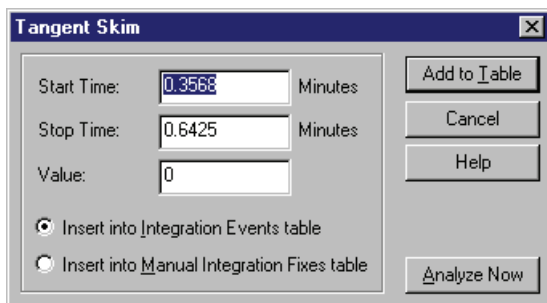
Click **Add to Table**, and the timed event is inserted in either the **Integration Events Table**, or the **Manual Integration Fixes Table**, depending on which of these you select. Click **Cancel** to ignore the timed event and cancel the operation. Click **Analyze Now** to add the event to the table and analyze the chromatogram using the event.

Figure 21. Tangent Skim events
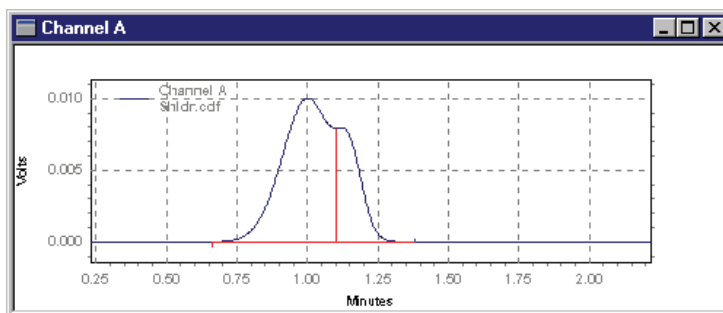
Integration without
Tangent Skim event

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.

Figure 22. Front Tangent Skim dialog box
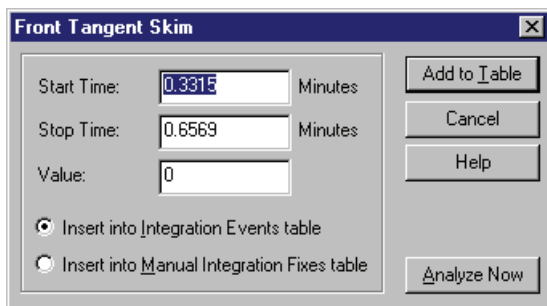
Click **Add to Table**, and the timed event is inserted in either the **Integration Events Table**, or the **Manual Integration Fixes Table**, depending on which of these you select. Click **Cancel** to ignore the timed event and cancel the operation. Click **Analyze Now** to add the event to the table and analyze the chromatogram using the event.

Figure 23. Front Tangent Skim events
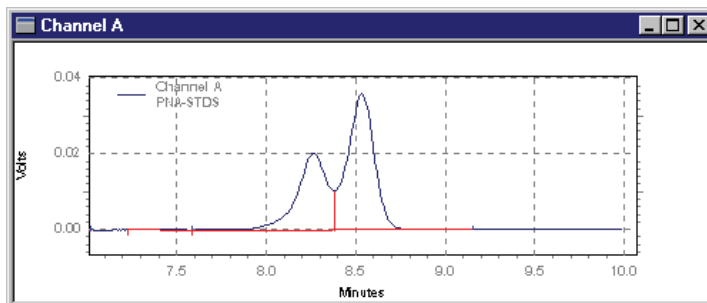
Before
Front Tangent Skim event

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 is not be integrated and reported as peaks. This event is useful for eliminating noise or contaminant peaks from your report.

Figure 24. Minimum Area dialog box
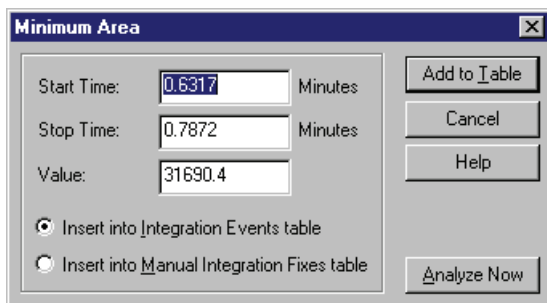
Click **Add to Table**, and the timed event is inserted in either the **Integration Events Table**, or the **Manual Integration Fixes Table**, depending on which of these you select. Click **Cancel** to ignore the timed event and cancel the operation. Click **Analyze Now** to add the event to the table and analyze the chromatogram using the event.

Figure 25. Minimum Area events
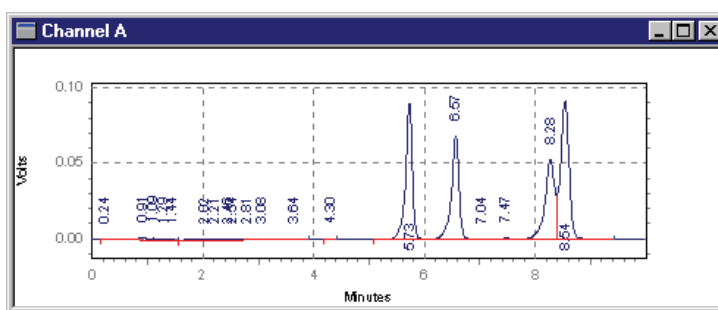
Integration without Minimum Area event
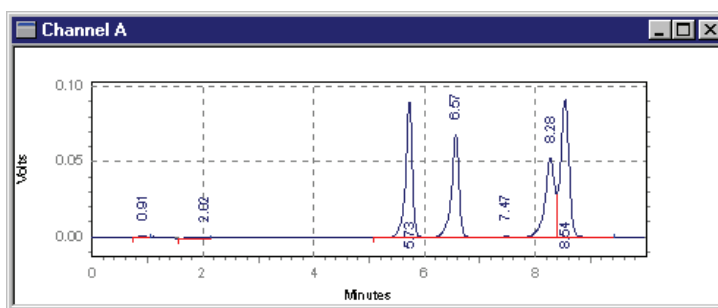
Integration with Minimum Area event

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 that give a negative response to certain compounds.
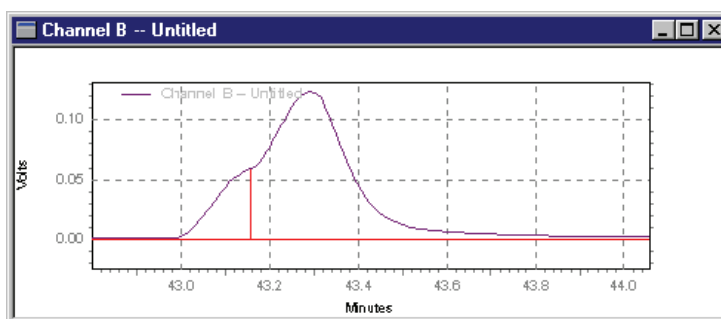
Figure 26. Negative Peak dialog box
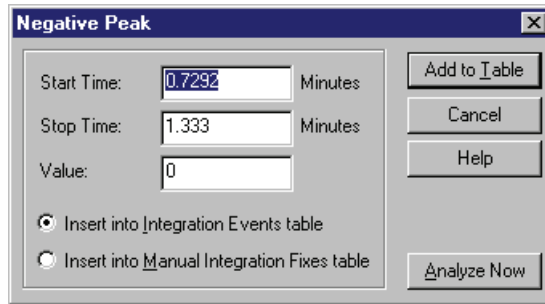
Click **Add to Table,** and the timed event is inserted in either the **Integration Events Table**, or the **Manual Integration Fixes Table**, depending on which of these you select. Click **Cancel** to ignore the timed event and cancel the operation. Click **Analyze Now** to add the event to the table and analyze the chromatogram using the event.

Figure 27. Negative Peak events
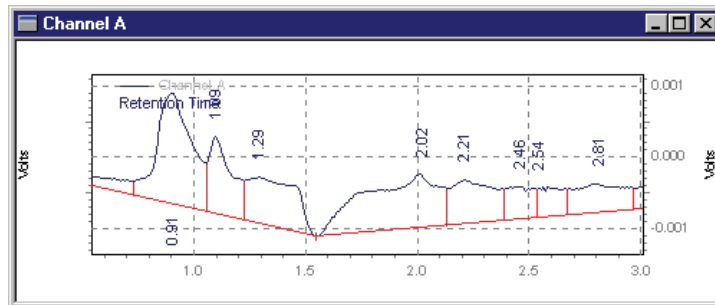
Default integration
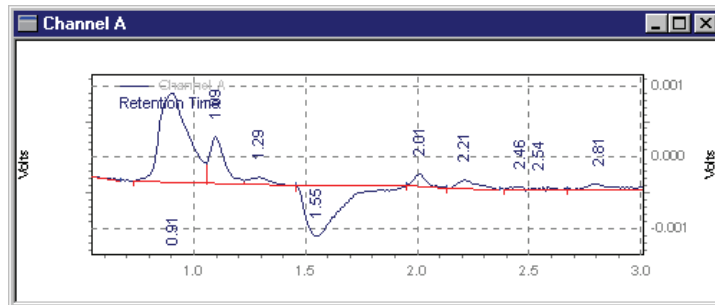
Integration with
Negative Peak event

Disable End 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 Peak Detection event.

Figure 28. Disable End Peak Detection dialog box
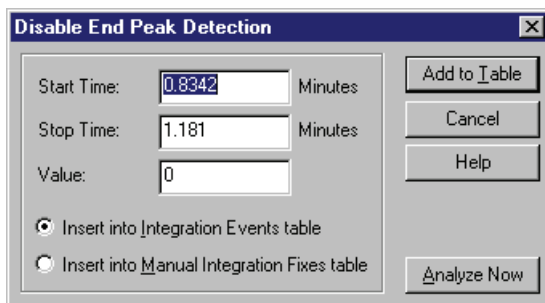
Click **Add to Table**, and the timed event is inserted in either the **Integration Events Table**, or the **Manual Integration Fixes Table**, depending on which of these you select. Click **Cancel** to ignore the timed event and cancel the operation. Click **Analyze Now** to add the event to the table and analyze the chromatogram using the event.

Figure 29. Disable End Peak Detection events
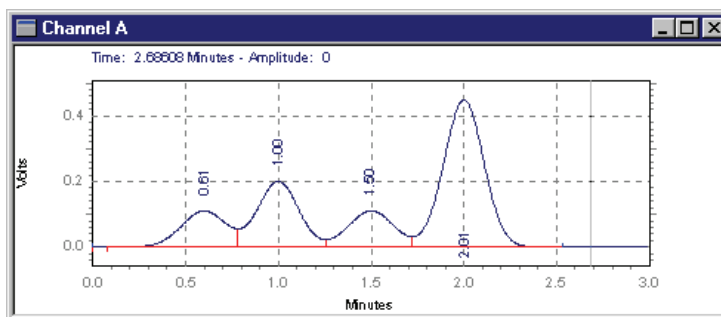
Default integration
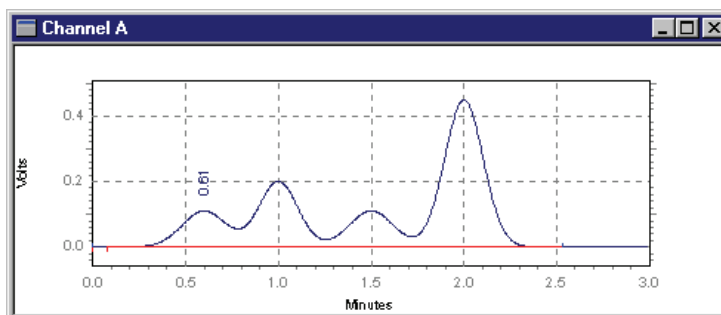
Disable End Peak Detection between 0.4 and 2.2 minutes

Reassign Peak

This event allows you to graphically designate a different peak as the calibrated peak in place of the peak that has been identified. When you use the Reassign event, the expected retention time of the named peak is adjusted in the Peak Table to the retention time of the designated peak.

Figure 30. Reassign Peak dialog box
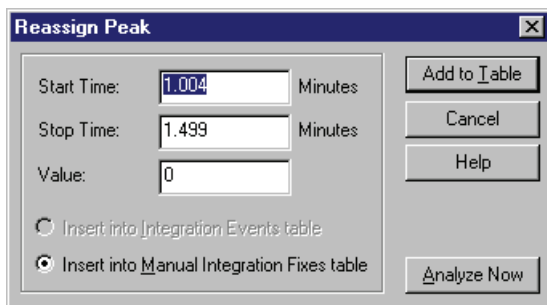
Click **Add to Table**, and the timed event is inserted in the **Manual Integration Fixes Table**. Click **Cancel** to ignore the timed event and cancel the operation. Click **Analyze Now** to add the event to the table and analyze the chromatogram using the event. In the following example, Peak 2 has been reassigned to a new peak.

Figure 31. Reassign Peak events
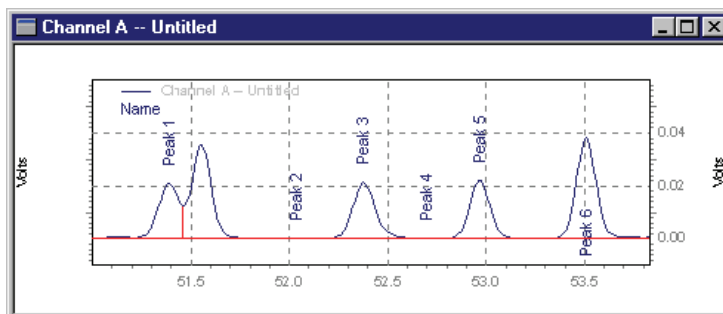
Before
Peak 2 reassignment
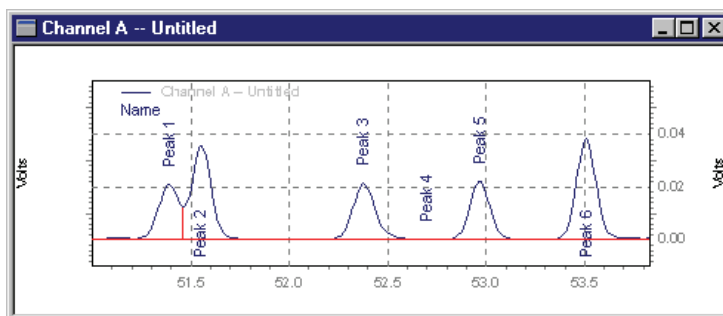
After
Peak 2 reassignment

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, choose the **Manual Baseline** command, and then click your mouse at the start of the desired baseline, and again at the end of the desired baseline.

Figure 32. Manual Baseline dialog box
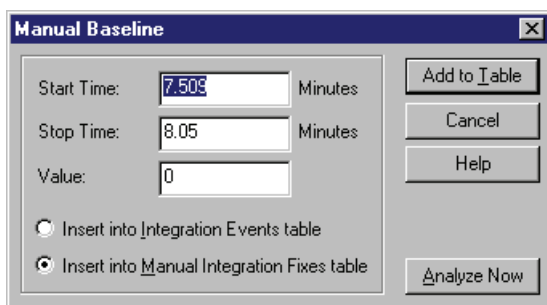
Click **Add to Table**, and the timed event is inserted in the **Manual Integration Fixes Table**. Click **Cancel** to ignore the timed event and cancel the operation. Click **Analyze Now** to add the event to the table and analyze the chromatogram using the event. **Manual Baseline** events are stored in the Manual Integration Fixes table by default.

Figure 33. Manual Baseline events
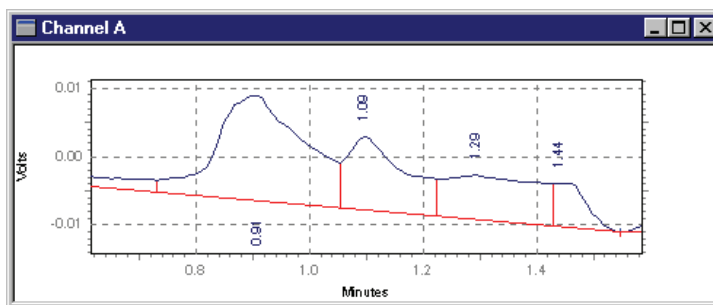
Default integration
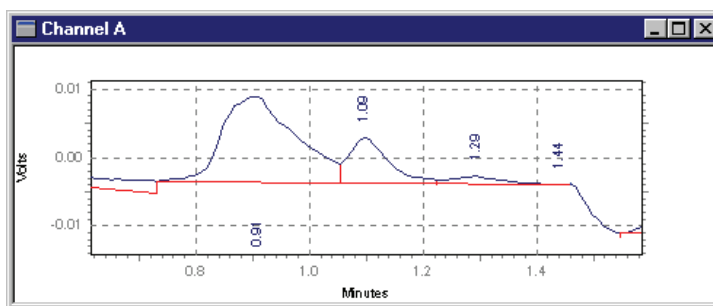
Integration with Manual Baseline between 0.765 and 1.43 minutes

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.

Figure 34. Manual Peak dialog box
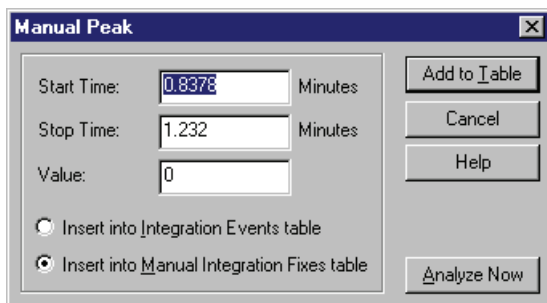
Click **Add to Table**, and the timed event is inserted in the **Manual Integration Fixes Table**. Click **Cancel** to ignore the timed event and cancel the operation. Click **Analyze Now** to add the event to the table and analyze the chromatogram using the event.

In the following example, the **Manual Peak** event was used to force the integration of the smaller peak on the right. To use this event, click the **Manual Peak** button from the Graphical Integration toolbar. Click once the start of the peak to be defined. Again, click the end of the peak to be defined. **Manual Peak** events are stored in the Manual Integration Fixes table by default.

Figure 35. Manual Peak events
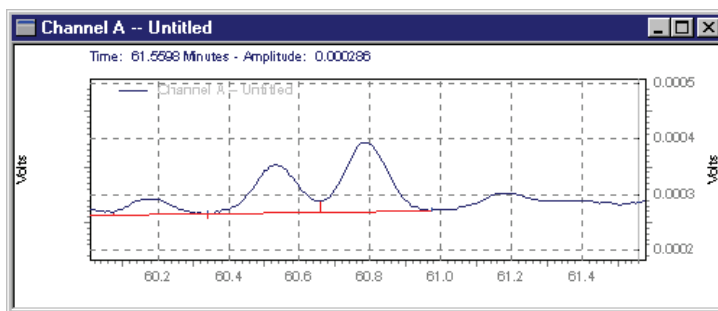
Default integration
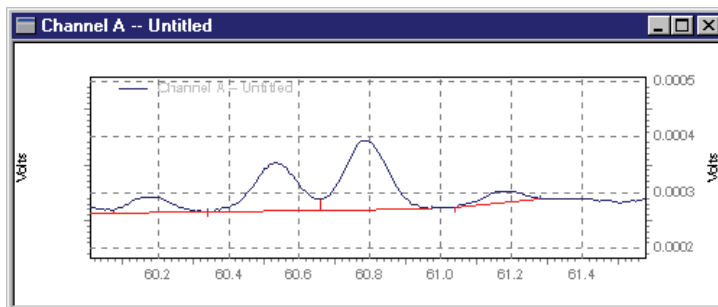
Small peak integration forced using Manual Peak event

Split Peak

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

Figure 36. Split Peak dialog box
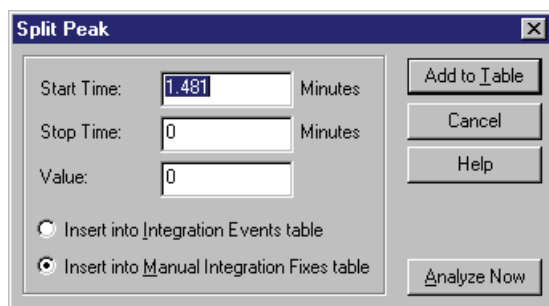
Click **Add to Table**, and the timed event is inserted in the **Manual Integration Fixes Table**. Click **Cancel** to ignore the timed event and cancel the operation. Click **Analyze Now** to add the event to the table and analyze the chromatogram using the event.

Figure 37. Split Peak events
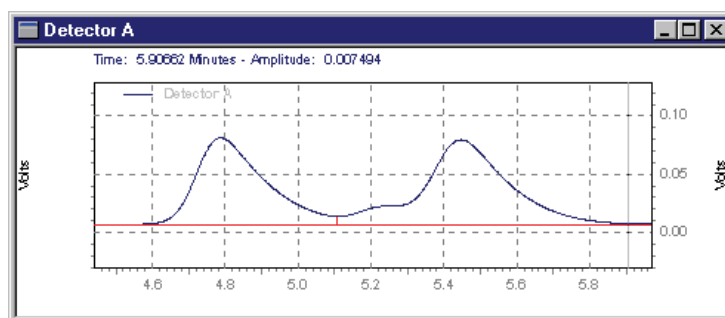
Integration before Split Peak event
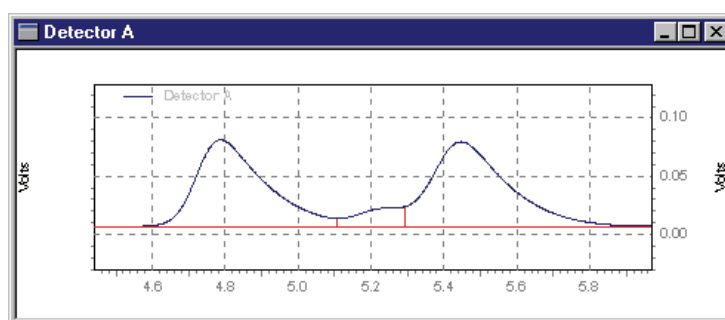
Integration after Split Peak added at 5.3 minutes

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

Force Peak Start /Force Peak Stop

These events are used to force the start or stop of the peak integration to a specific point. This event is stored in the Manual Integration Fixes table by default.

Figure 38. Force Peak Start dialog box
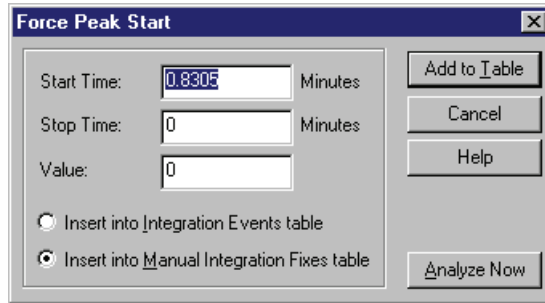
Click **Add to Table**, and the timed event is inserted in the **Manual Integration Fixes Table**. Click **Cancel** to ignore the timed event and cancel the operation. Click **Analyze Now** to add the event to the table and analyze the chromatogram using the event.

**Figure 39.** Force Peak Start events
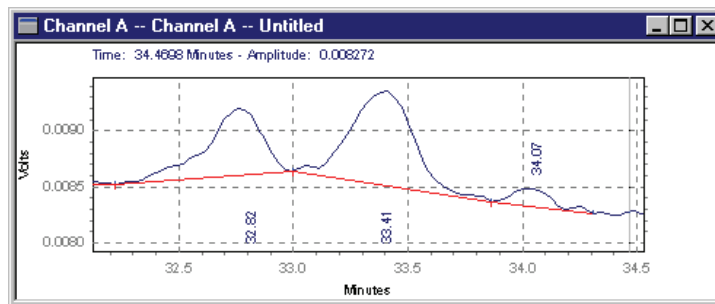
Default integration
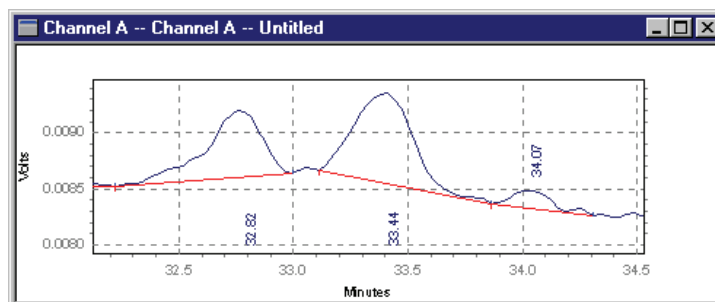
Integration after Force Peak Start to 33.1 minutes

Move Baseline

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

1. When you choose Move Baseline, you are prompted to click the baseline segment you want to modify. The start and end points of the baseline segment appears highlighted with boxes. See Figure 42.

2. When you move the cursor to a location within range of the start or stop point, it turns into an "anchor". Left-click and drag the baseline start-point to the new location, and then let go. Left-click and drag the baseline stop-point to a new location, and 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 box appears. See Figure 40.

Figure 40. Move BL Start dialog box
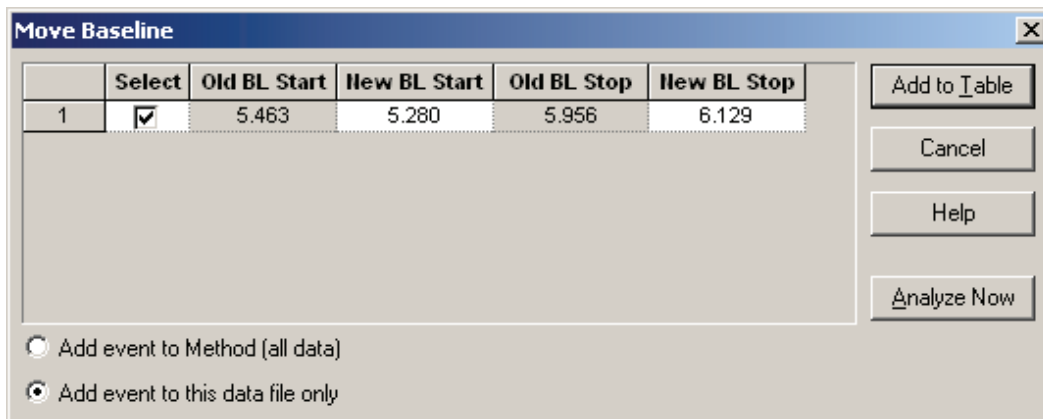
Click **Add to Table**, and the timed event is inserted in the **Manual Integration Fixes Table**. Click **Cancel** to ignore the timed event and cancel the operation. Click **Analyze Now** to add the event to the table and analyze the chromatogram using the event.

Figure 41 shows the initial start and stop times for a baseline segment (5.46 and 5.96 minutes). Figure 42 shows the selected baseline segment. Figure 43 shows the new baseline segment produced by dragging the start time to the left and the stop time to the right.

By default, the move baseline events are added to Manual Integration Fixes Table. See Figure 44

Figure 41. View of the initial start and stop times for a baseline segment
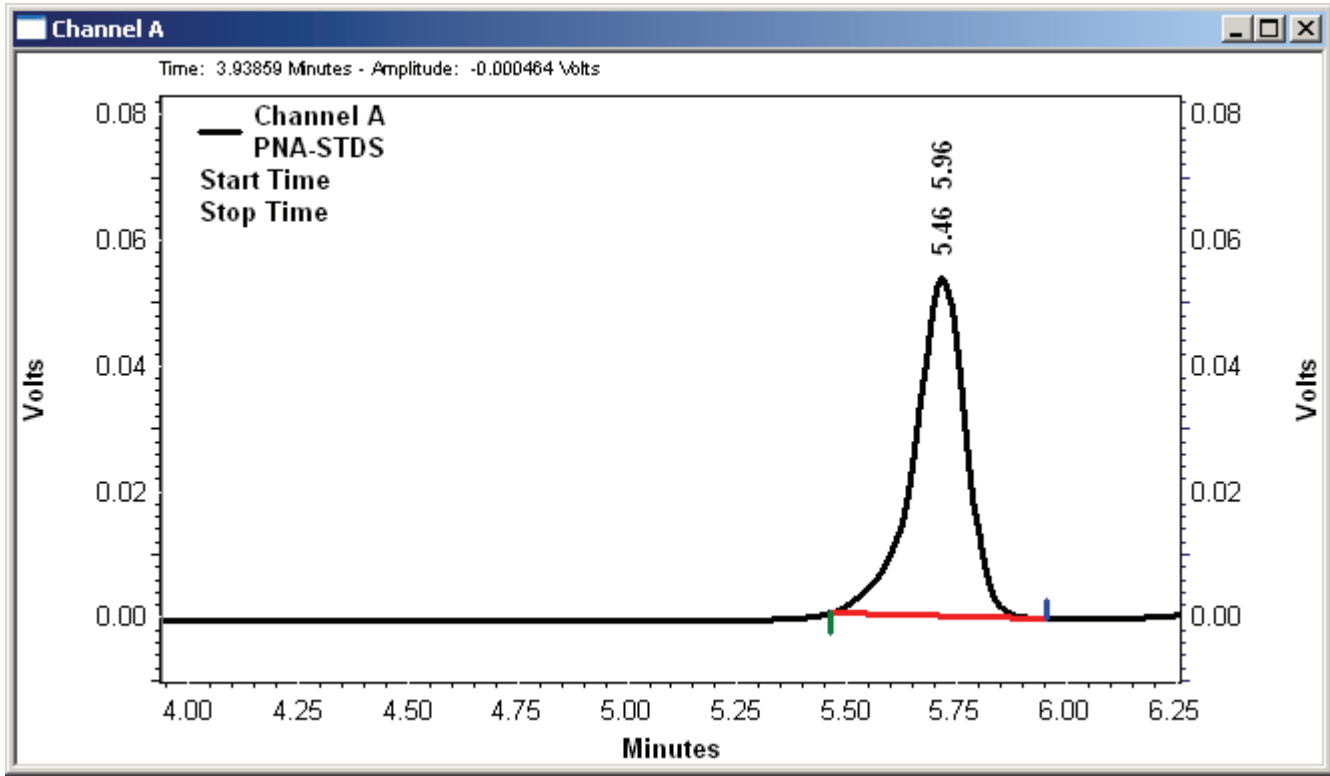
Figure 42. View of a selected baseline segment
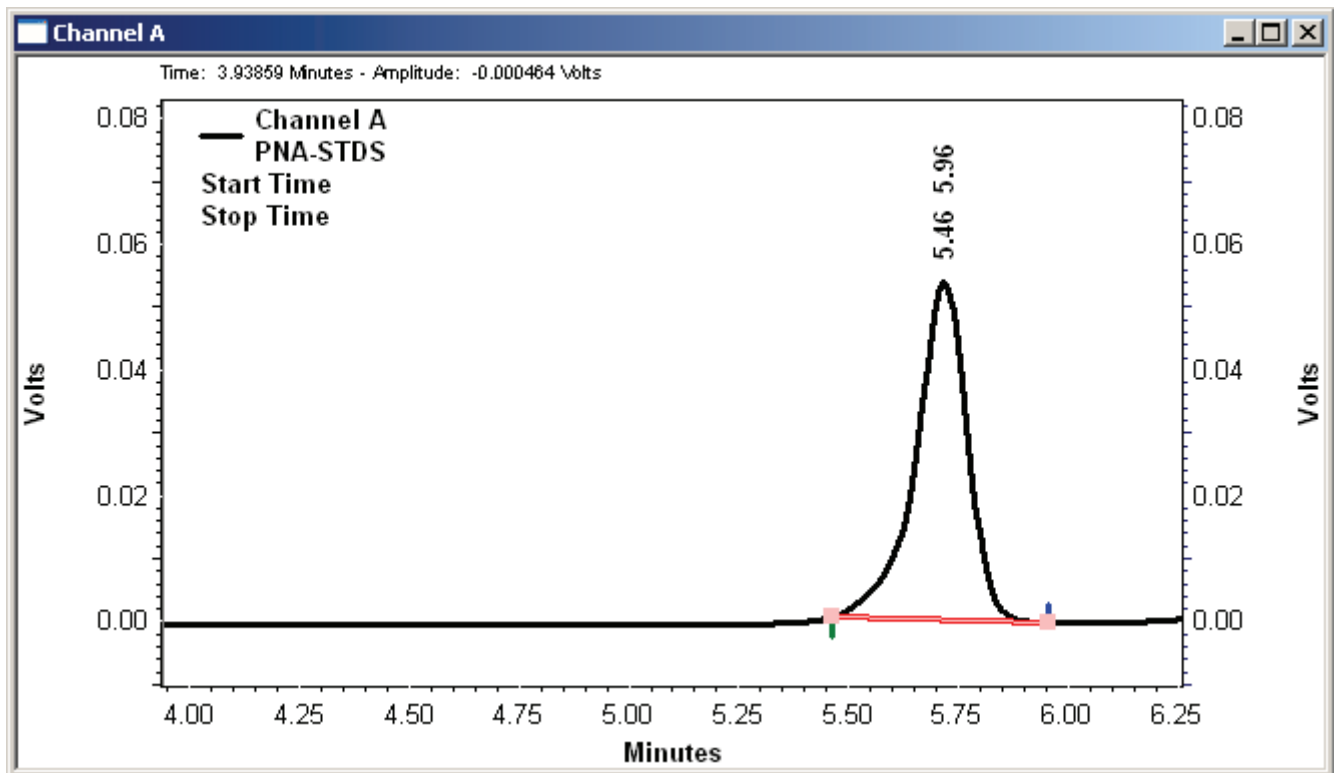
Figure 43.   View of the new baseline segment (after analyzing)
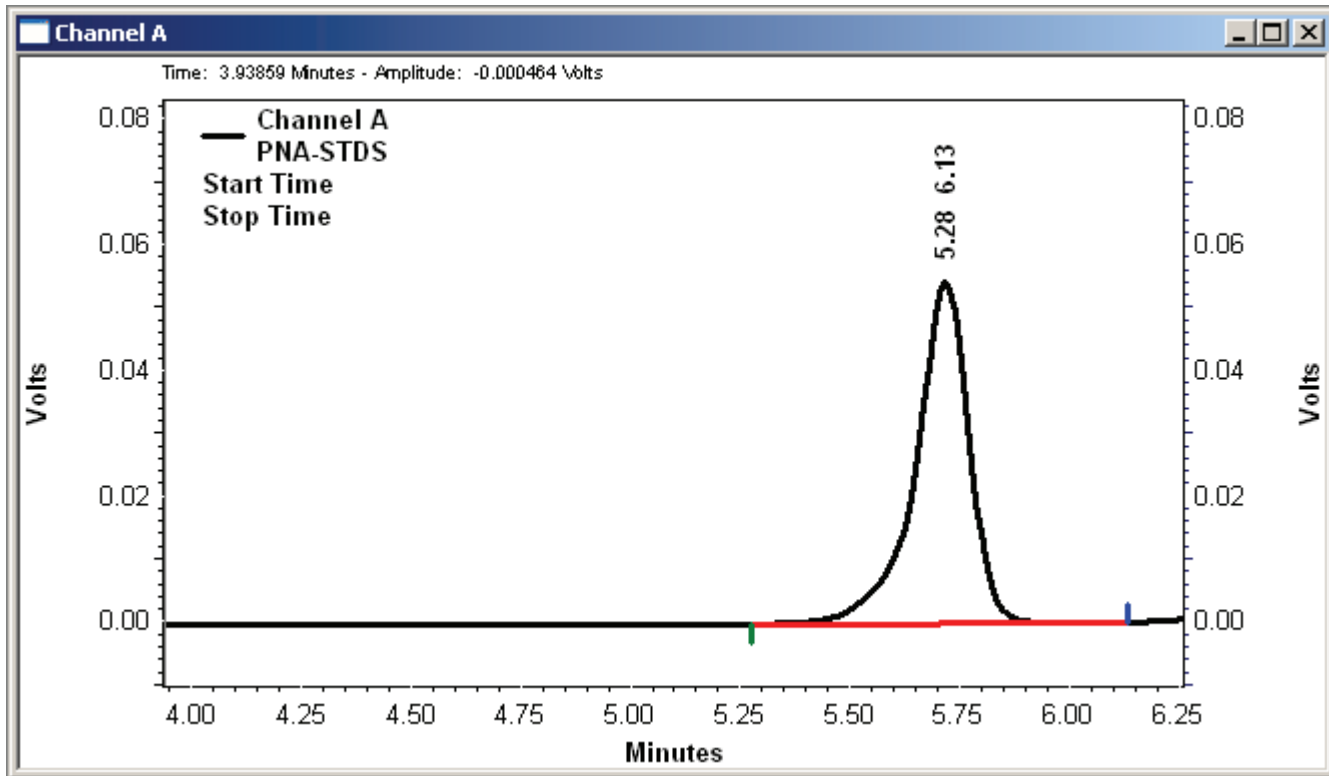
Figure 44.   Manual Integration Fixes table with the new baseline start and stop times

Reset Baseline

This event causes the baseline to be reset to the point you click. Baseline segments before this time point are not affected. This event is functionally equivalent to performing an Integration Off and Integration On event at the same time.
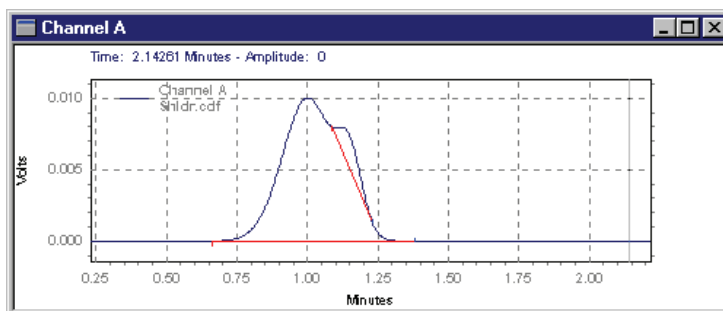
Figure 45. Reset Baseline dialog box
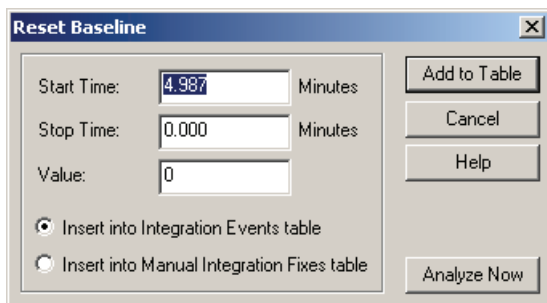
Click **Add to Table**, and the timed event is inserted in either the Integration Events Table, or the Manual Integration Fixes Table, depending on which of these you select. Click **Cancel** to ignore the timed event and cancel the operation. Click **Analyze Now** to add the event to the table and analyze the chromatogram using the event.

Reset Baseline At Valley

This event causes the baseline to be reset at the next valley detected after the event. To enter the event graphically, click the location you want to enter the event, and then click the Reset Baseline at Valley button at the bottom of the window.

> **Note** The event should be placed after the start of the peak first peak in the cluster; otherwise the start of the peak is identified as the valley
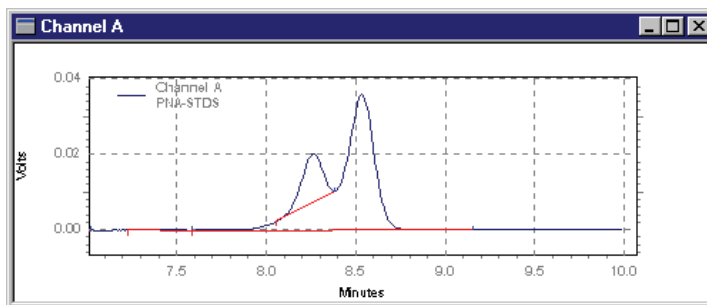
Figure 46. Reset Baseline at Valley dialog box
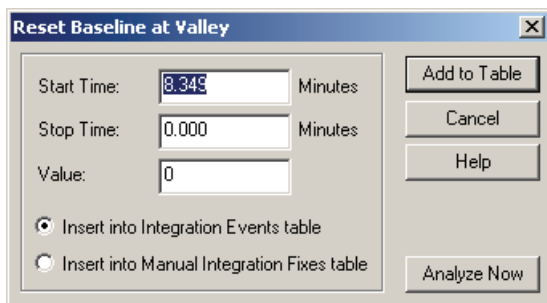
Click the **Add to Table** button, and the timed event is inserted in either the Integration Events Table, or the Manual Integration Fixes Table, depending on which of these you select. Click **Cancel** to ignore the timed event and cancel the operation. Click **Analyze Now** to add the event to the table and analyze the chromatogram using the event.

Figure 47 shows an example of this event.

Figure 47. Reset Baseline at Valley events
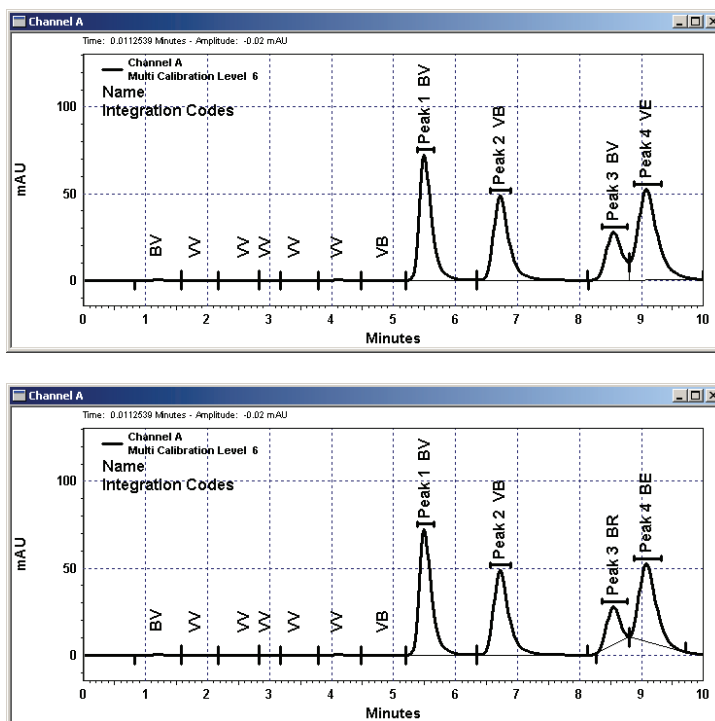
Baseline before Reset Baseline at Valley event

Baseline after Reset Baseline at Valley event

Adjust Retention Time Window

You can use this graphical integration tool to change the retention time and the retention time window for a peak. Before you can use this tool, you must add the Retention Time Window annotation to your chromatogram.

To add the Retention Time Window annotation to your chromatogram, right-click the chromatogram to open the shortcut menu. Then, choose **Annotations** to open the Trace Annotation Properties dialog box. In the Trace Annotation Properties dialog box, select the RT Window check box.

❖ **To use the Adj RT Window tool**

1. Click the Adjust Retention Time Window button in the integration toolbar. Alternatively, right-click the chromatogram to open the shortcut menu. Then, choose **Graphical Programming > Adjust Retention Time Window**.

   The following message appears in the Status box at the bottom of the screen: *Click an RT Window, then move/size it. Hit <ESC> to finish.*

   Figure 48. Adjust Retention Time Window
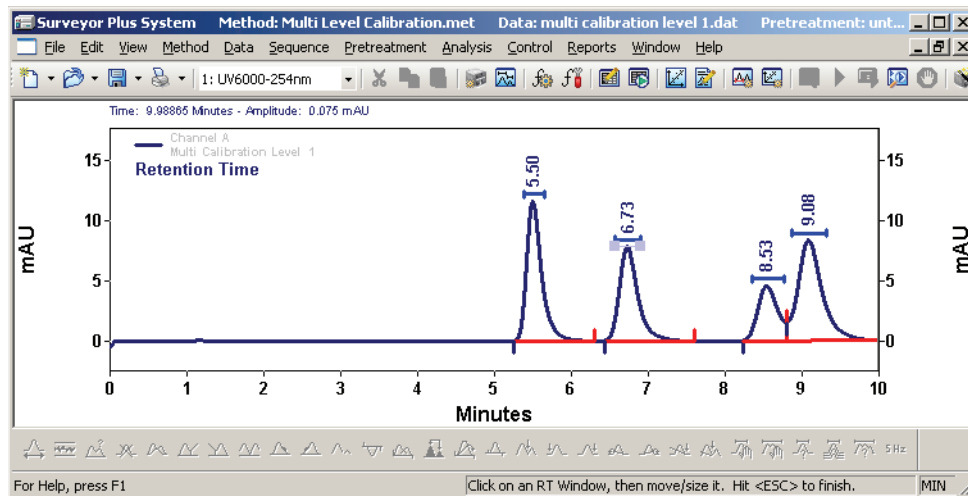
2. Click the RT Time Window that you want to adjust. Move it or resize it. Then, press ESC.

   The Adjust Retention Time Window dialog box appears.

   Figure 49. Adjust Retention Time Window dialog box
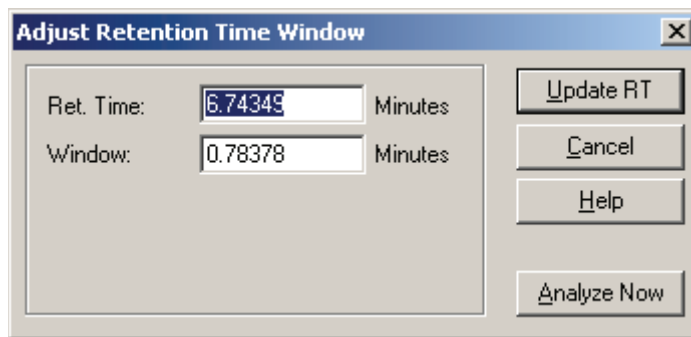
3. Verify the modified Retention Time Window. Then, do one of the following:

   • Click **Update RT** to update the Retention Time and Window for the selected peak in the peak table.

   • Click **Analyze Now** to add the event to the peak table and analyze the chromatogram using the updated Retention Time and Retention Time Window.

   • Click **Cancel** to ignore the operation.

Figure 50. Reset Retention Time window
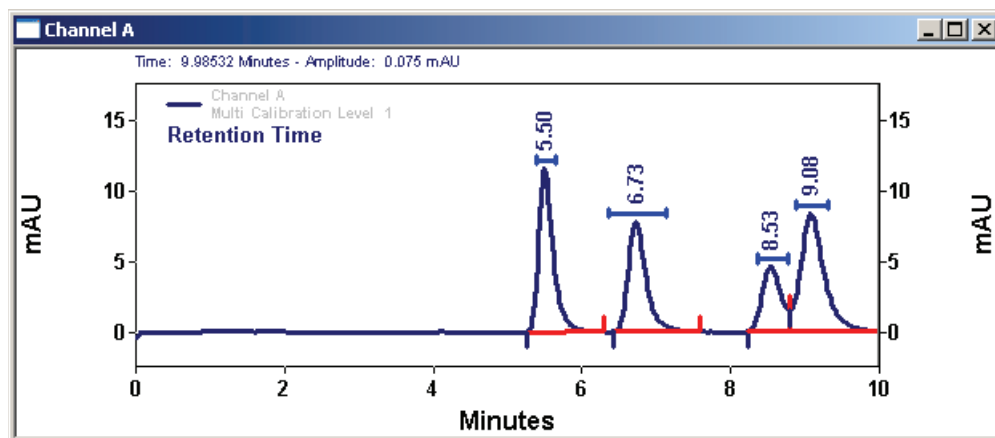
Adjust Group Range

This graphical integration feature allows you to adjust calibrated and uncalibrated group ranges from the Chromatogram window.

❖ **To adjust a group range**

1. Right-click a chromatogram to open the Trace Annotation Properties dialog box. Then, ensure that the Group Range check box is selected.

2. Click the Adjust Group button in the integration toolbar.

3. Click the group range annotation that you want to adjust. A grab bar appears.

4. Drag the bar to resize the Group Range definition.

5. Press ESC to finish. The Adjust Group Range dialog box appears. See Figure 51.

Figure 51. Adjust Group Range dialog box
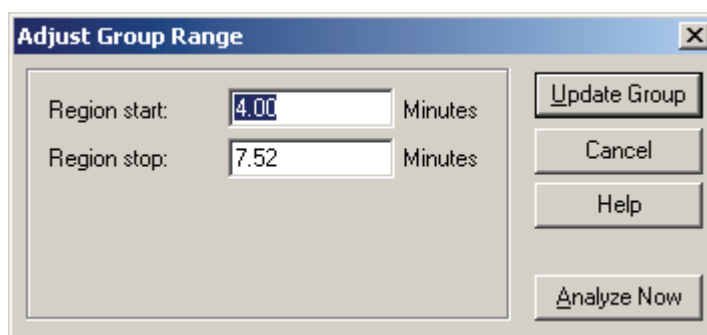
6. Verify the modified range. Then, do one of the following:

- Click **Update Group** to update the definition of the group range in the Peaks/Group table.

- Click **Analyze Now** to update the definition of the group range in the Peaks/Group table and to analyze the chromatogram using the updated group range.

- Click **Cancel** to ignore the operation.

Figure 52. Adjust Group Range dialog box events
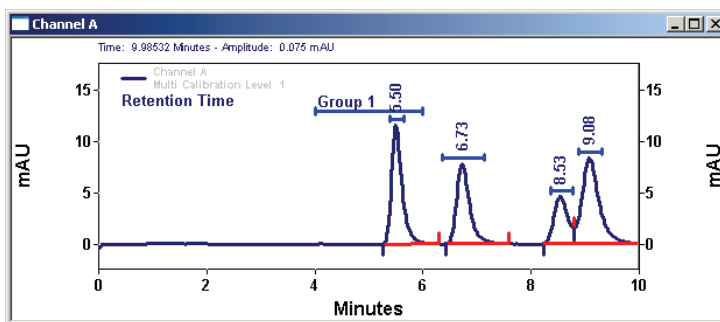
Group range before adjustment
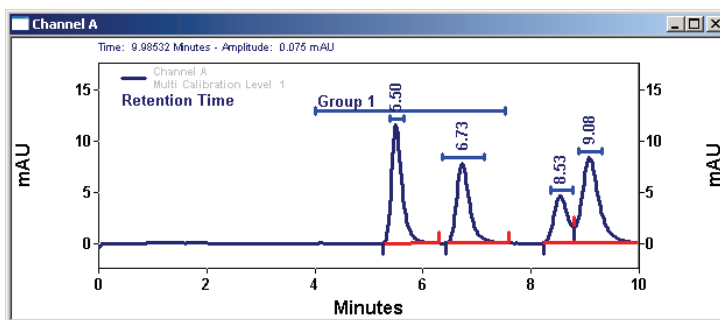
Group range after adjustment

Baseline Code Descriptions

Baseline codes can be included in custom reports, and 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.

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
LL	Lowest
RN	Reset Baseline at Next Valley
RB	Reset Baseline

Equations and Calculations

This chapter describes the equations that are used by ChromQuest 5.0 to create calibration curves and to calculate chromatographic performance.

Contents

- Calibration Curves
- Determining Concentrations for Uncalibrated Peaks
- Internal Standard Amounts
- Calibration Curve Calculations
- Report Calculations
- Performance Calculations

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). ChromQuest 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.

$$y \ = \ \int (x)$$

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

Response Factor Definition

In ChromQuest, you can select 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.

Area/Amount Response Factor Definition

If you select **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.) Figure 53 is an example calibration curve using **Area/Amount** response factor definition.

Figure 53. Calibration Curve with Area/Amount Response Factor Definition
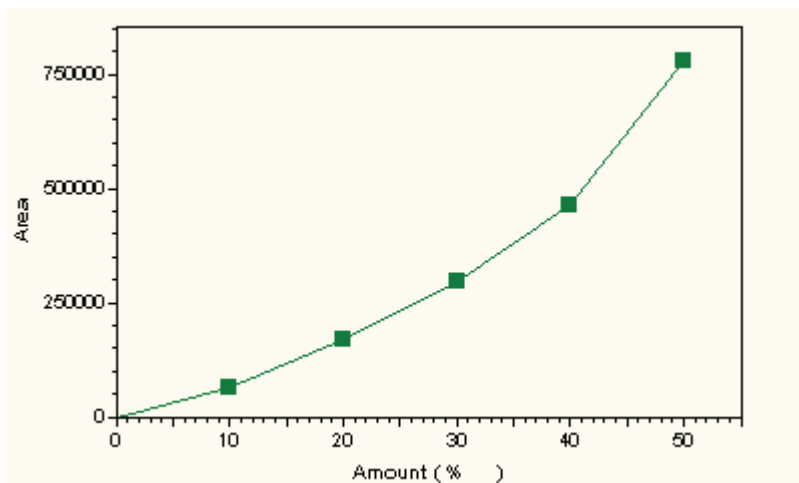
If you select **Amount/Area** for your response factor definition, the calibration curve (which can be viewed in **Review Calibration**) is defined where **y = area or height** and **x = amount**. (For internal standard calibrations, y = area or height ratio and x = amount ratio.) Figure 54 is an example calibration curve using **Amount/Area** response factor definition.

Figure 54. Calibration Curve with Amount/Area Response Factor Definition
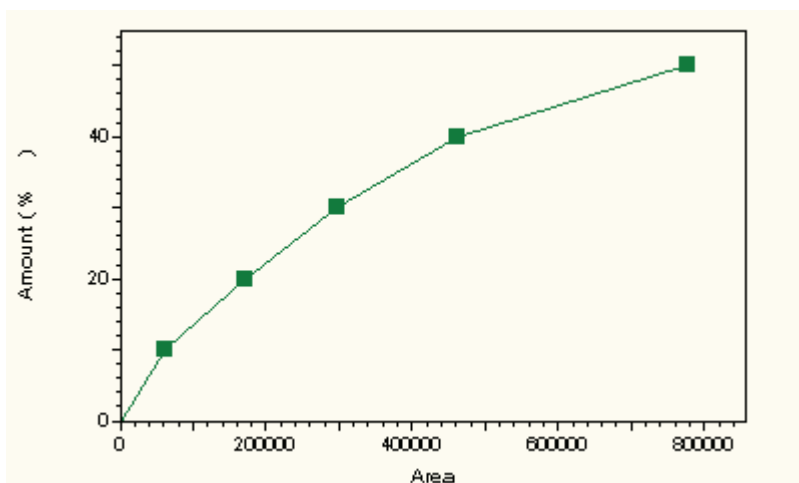
Internal Standard vs. External Standard and Normalization

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.

External Standard Calibration Curves

Figure 55 is an example of the External Standard and Normalization curve, the component Amount is plotted on the X-Axis and the component Area is plotted on the Y-Axis (Amount/Area Response Factor Definition):

Figure 55. External Standard Calibration Curve
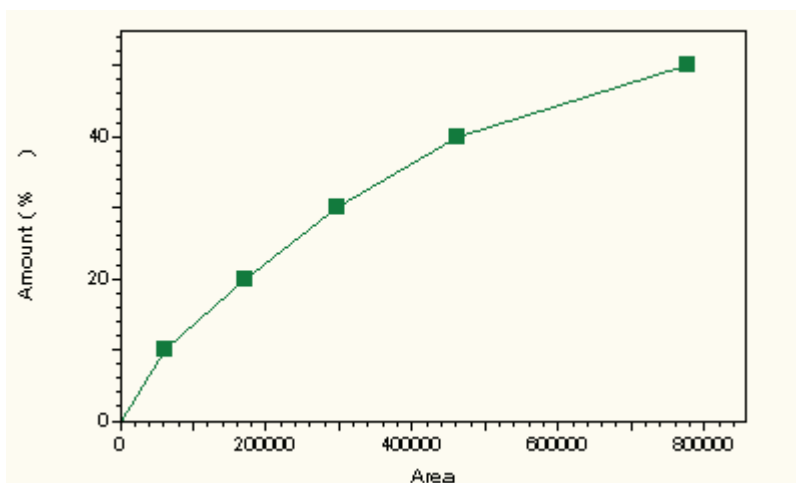
The external calibration curve (for Response Factor definition **Area/Amount**) is calculated as:

$$\text{Amt}_{cal} = \int (\text{Area}_{cal})$$

where

f = the equation of the calibration points according to the fit type you have selected (linear, quadratic, point to point, etc.)

Amt_{cal} = the amount of the calibration standard

Area_{cal} = the area of the calibration standard

Therefore the unknown is determined by:

$$Amt_{unk(u)} = \int (Area_{unk})$$

where

Amt$_{unk(u)}$ = the uncorrected amount of the unknown component

f = the equation of the calibration points according to the fit type you have selected

Area$_{unk}$ = the area of the unknown component

To calculate the concentration of the unknown sample:

$$Conc = \frac{Amt_{unk(u)}}{Sample\ Amt_u} \times MF$$

where

Conc = the concentration (in the same units used for calibration) of the unknown analyte of interest

Amt$_{unk(u)}$ = 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 = $M_1{}^*M_2{}^*M_3/D_1{}^*D_2{}^*D_3$

Internal Standards

Figure 56 is an example of an Internal Standard calculation, the **ratio** of component amount to Internal Standard amount is plotted on the X-Axis and the **ratio** of component area to Internal Standard area is plotted on the Y-Axis (Amount/Area Response Factor definition):

Figure 56. Internal Standard Calibration Curve
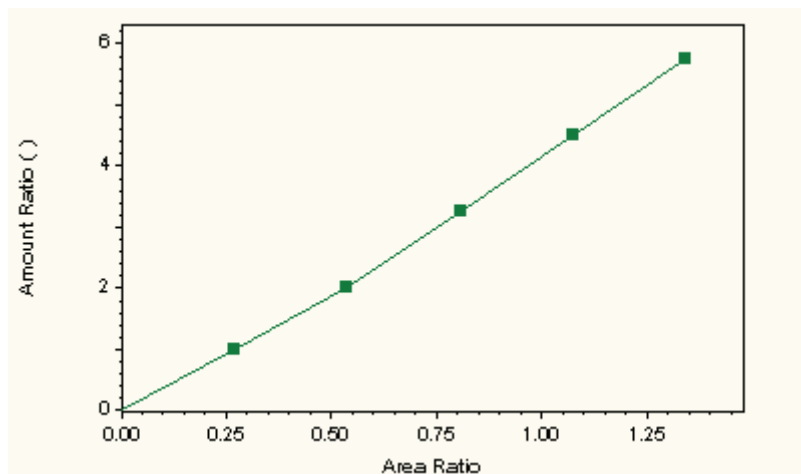
The calibration is calculated as:

$$\text{Amt Ratio}_{\text{ISCal}} = \int (\text{Area Ratio}_{\text{ISCal}})$$

where

Amt Ratio$_{\text{ISCal}}$ = amount ratio of the calibration standard

f = equation of the calibration points according to the fit type you have selected

Area Ratio$_{\text{ISCal}}$ = area ratio of the calibration standard

Therefore the unknown is determined by:

$$\text{Amt Ratio}_{\text{unk(u)}} = \int (\text{Area Ratio}_{\text{unk}})$$

where

Amt Ratio$_{\text{unk(u)}}$ = the uncorrected amount ratio of the unknown component

f = the equation of the calibration points according to the fit type you have selected

Area Ratio$_{\text{unk}}$ = the area ratio of the unknown component

The concentration of the unknown sample is calculated by:

$$\text{Conc}_u = \frac{\text{Amt}_{IS}}{\text{Sample Amt}_u} \times \text{MF} \times \text{Amt Ratio}_{unk}$$

where

Conc_u = Concentration (in the same units used for calibration) of the analyte of interest

Amt_{IS} = Amount of the internal standard

Sample Amt_u = Amount of the unknown sample from sequence or at start of single run

MF = multiplication and dilution factors applied = $M_1{}^*M_2{}^*M_3/D_1{}^*D_2{}^*D_3$ entered for the unknown sample

Amt Ratio_{unk} = Amount ratio value taken from the calibration curve at the given area ratio for the unknown sample

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 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.

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 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 (so it is not contribute to analyte concentration totals), enter a Manual RF value of zero for the internal standard components in the peak table.

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 as either 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.

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 is the same regardless of Response Factor definition. The equation for calculating the uncorrected amount is:

$$Y = aX + b$$

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

Internal Standard:

Y = Uncorrected Amount Ratio

a = Slope of the calibration line segment

$$X = \frac{\text{Component Area or Height}}{\text{Internal Standard Area or Height}}$$

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

Linear Fit

A linear calibration fit determines the best line (linear regression) for a series of calibration points. A minimum of two calibration points is required to determine a linear fit. The equation for calculating the uncorrected amount is:

$$Y = aX + b$$

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:

$$Y = \frac{\text{Component Area or Height}}{\text{Internal Standard Area or Height}}$$

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

$$X \ = \ \frac{\text{Component Area or Height}}{\text{Internal Standard Area or Height}}$$

b = Y-Axis intercept of the calibration line

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:

$$Y = \frac{\text{Component Area or Height}}{\text{Internal Standard Area or Height}}$$

a = Calibration Curve Coefficient

b = Calibration Curve Coefficient

c = Y-Axis intercept

X = Uncorrected Amount Ratio

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:

$$Y = aX^3 + bX^2 + cX + d$$

Note For cubic fits, only Response Factor definition of **Area/Amount** applies.

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

Internal Standard:

Y = Uncorrected Amount Ratio

a = Calibration Curve Coefficient

b = Calibration Curve Coefficient

c = Calibration Curve Coefficient

d = Y-Axis interceptt

$$X = \frac{\text{Component Area or Height}}{\text{Internal Standard Area or Height}}$$

Modified Least Squares Calculation

The following modified least squares formula is used to determine the calibration curve coefficients for linear fits:

$$\begin{vmatrix} a \\ b \end{vmatrix} = \begin{vmatrix} \Sigma WX & \Sigma W \\ \Sigma WX^2 & \Sigma WX \end{vmatrix}^{-1} \times \begin{vmatrix} \Sigma WY \\ \Sigma WXY \end{vmatrix}$$

where

a = the slope of the calibration line

b = the Y-Axis intercept of the calibration linet

W is the weighting term $= \dfrac{1}{X}$ or $\dfrac{1}{X^2}$ or 1 if no weighting is used,

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 C_u.

Y is the corrected relative area $= \dfrac{\text{peak area}}{\text{int std area}}$

For External Standard calculations, X is the uncorrected amount of the component of interest in the calibration sample C_u.

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:

$$
\begin{vmatrix} a \\ b \\ c \end{vmatrix} = \begin{vmatrix} \sum WX^2 & \sum WX & \sum W \\ \sum WX^3 & \sum WX^2 & \sum WX \\ \sum WX^4 & \sum WX^3 & \sum WX^2 \end{vmatrix}^{-1} \times \begin{vmatrix} \sum WY \\ \sum WXY \\ \sum WX^2Y \end{vmatrix}
$$

The following formula is used to determine the R-squared value for a series of values:

$$
R^2 = 1 - \frac{\displaystyle\sum_{i=1}^{n} (Yi - \hat{Y}i)^2}{\displaystyle\sum_{i=1}^{n} (Yi - \bar{Y})^2}
$$

where

Y is an ordinate of the least squares line.

$$
\bar{Y} = \frac{\sum Y}{n}
$$

Yi is the observed value of Y.

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:

$$y \; = \; ax^2 + bx + c$$

For a series of amount/area pairs (x, y) representing calibration points (or averaged calibration points):

$$(x_1, y_1) \; (x_2, y_2) \; (x_3, y_3).....(x_n, y_n)$$

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,

$$Y \; = \; M \bullet Z$$

To ensure a square matrix, the equation is multiplied by M^T to become

$$M^T \, Y \; = \; M^T \, M \, Z$$

where

M^T is matrix **M** transposed

$$\begin{bmatrix} x_1^2 & x_2^2 & \ldots & x_n^2 \\ x_1 & x_2 & \ldots & x_n \\ 1 & 1 & \ldots & 1 \end{bmatrix}$$

then

$$\mathbf{Z} \; = \; (M^T \, M)^{-1} \, M^T \, Y$$

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.

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:

$$\text{Conc}_{\text{Unknown}} \ = \ (\text{Average RF}) * \text{Area}_{\text{Unknown}}$$

where

C_u = Area/RF if Response Factor is set to Area/Amount

C_u = Area * RF if Response Factor is set to Amount/Area

The slope of each calibration line is calculated as follows:

C_u = 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

$$Y \ = \ \frac{\text{Component Area or Height}}{\text{Internal Standard Area or Height}}$$

Weighting and Scaling

There are a number ways to do averaging and weighting in ChromQuest. The following table summarizes the differences between these selections.

Selection	Located In	Effect or Use
Calib Flag (Replace/WtAverage)	Peak Table	If Replace, each new calibration area replaces previous calibration area in the method. If WtAverage, replicates is averaged. Weighted average using Calib Weight is calculated if method contains a Last Area. If Auto Averaging is also ON, calibration replicates is 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.
Weighting 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.

Calibration Averages

The **Replace/Wt Average** Calib Flags in the Peak Table allow you to select whether or not calibration the calibration area is averaged with previous replicates (Last Area). In general, when **Replace** is selected, the current calibration area replaces 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 (I_n)	Component Replicate Area (U_n)
$I_1 = 100$	$U_1 = 210$
$I_2 = 99$	$U_2 = 215$
$I_3 = 104$	$U_3 = 212$

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, and 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.

Automatic Averaging

When you have the Automatic Averaging turned On for your method (in Method Properties), averaging takes place for all peaks designated with the WtAverage flag in the peak table. Replicates continues to save in the method until a new level is calibrated for the method. When a new level is encountered, the replicates for the previous level is cleared, and the average at that point is 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.

Calib Weight

You can designate a "Calib Weight" in the Peak Table for the average of 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 in ChromQuest using the following equation:

$$A_w = (X_c * W) + [X_o * (1 - W)]$$

where

A_w is the weighted average result

X_c is the true average of replicates (if any) with current run area/height

W is the Calib Weight / 100

X_o is the "Last area" from the method

A weighted average is calculated for the following method as follows:

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.

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/X
- $1/X^2$
- ln[X]
- 1/ln[X]
- sqrt[X]
- x^2

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. The following figures are examples of LSQ weighting.

Figure 57. Linear fit with No LSQ Weighting
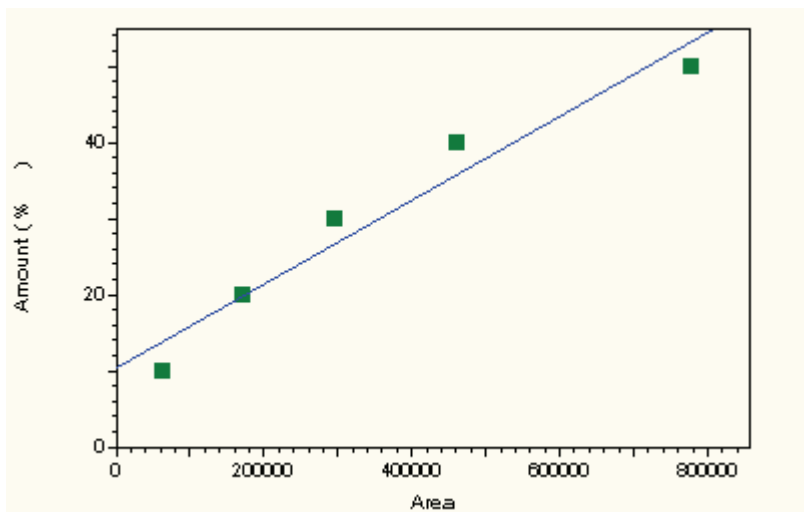
Figure 58. Linear Fit with 1/x LSQ Weighting
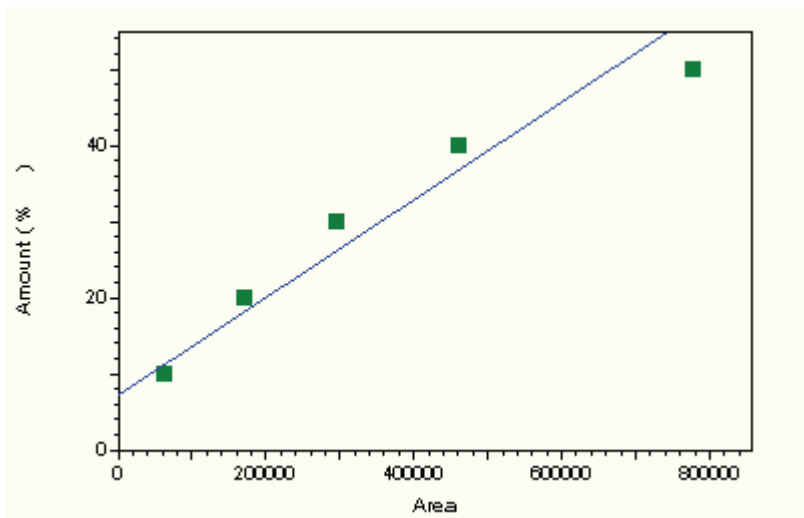
Figure 59. Linear Fit with $1/X^2$ LSQ Weighting
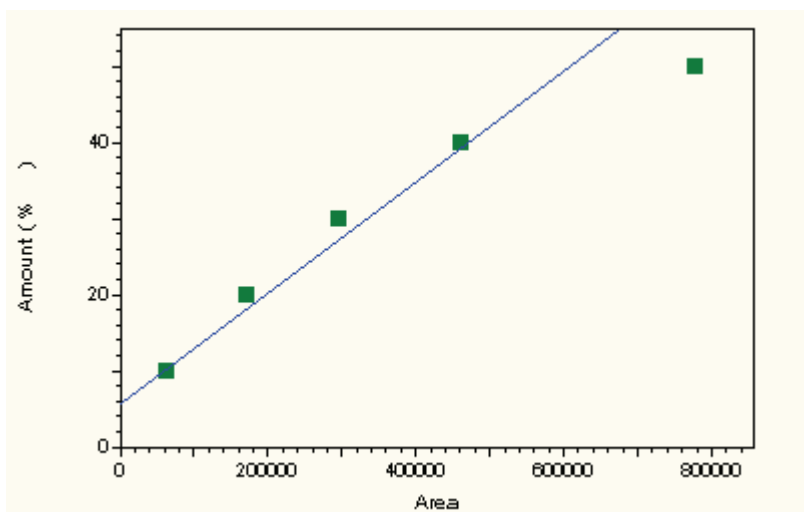
Report Calculations

The following calculations are used to determine the concentrations reported.

Area % Report

$$\text{Area\%} = \frac{\text{Area of peak} * 100}{\text{Sum of all peak areas}}$$

Normalization Report

$$\text{Conc} = \frac{C_u * 100}{\text{Sum of } C_u \text{ for named peaks} + \text{Sum}_{CR}}$$

where

Conc = Corrected Amount of component

C_u = Uncorrected Amount of component

Sum_{CR} = Sum of calibrated range groups

External Standard Report

$$\text{Conc} = \frac{C_u}{\text{Samp. Amt}} * MF$$

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 Report

$$\text{Conc} = \frac{C_u}{(\text{Sample Amt.})} * ISTD_u * MF$$

where

Conc = Corrected Amount of component

$ISTD_u$ = Amount of Internal Standard

Sample 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

Performance Calculations

ChromQuest calculates the following values 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.

Figure 60 shows the parameters used to calculate these system performance values for the separation of two chromatographic components.

Figure 60. Separation of Two Chromatographic Components
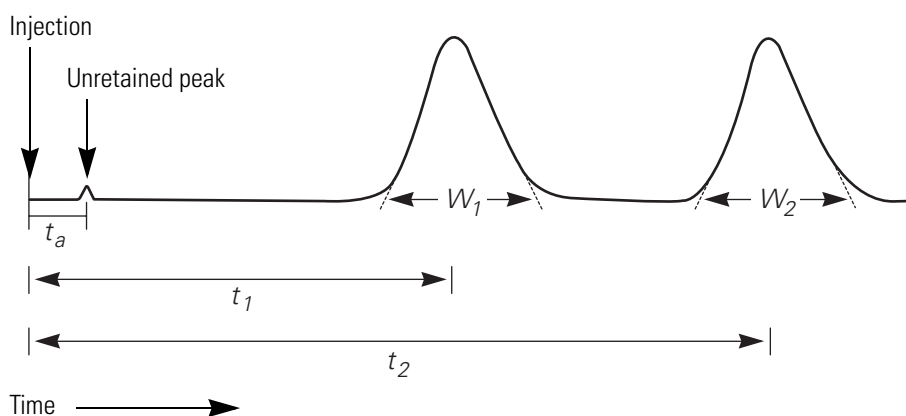
Note To accurately calculate suitability values, the sampling frequency (set in Acquisition Setup) must be set to provide at least 20 data points for the narrowest peak of interest.

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.

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.

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.

Noise Test (rms noise)

The rms noise is the standard deviation of the signal derived from n measurements.

$$\text{rms noise} = \left[\frac{\sum\limits_{i=1}^{n} (Ei - \bar{E})^2}{n-1} \right]^{1/2}$$

where

Ei = individual voltage readings

$\bar{E}$ = the average of n measurements

Drift Test

The drift test measures the change in voltage over a given period.

$$\text{drift} = \frac{y_2 - y_1}{x_2 - x_1}$$

where

y_2 = voltage (μv) at time x_2 (drift test start time in minutes)

y_1 = voltage (μv) at time x_1 (drift test stop time in minutes)

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.

Figure 61. Asymmetric Peak
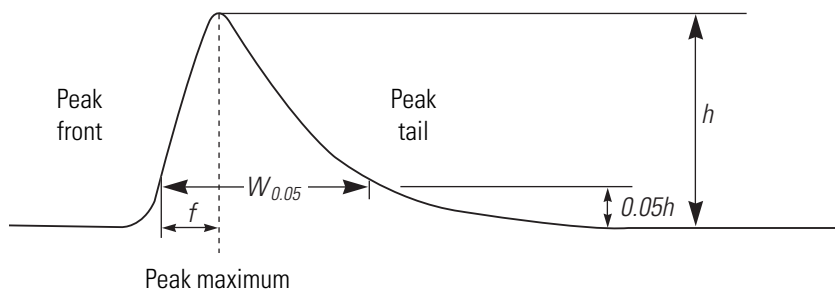
Resolution

$$R = \frac{2(t_2 - t_1)}{W_2 + W_1}$$

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_2 = The width of the base of the component peak 2

W_1 = The width of the base of the component peak 1

EMG (Exponential Modified Gaussian) Calculation Method

Theoretical Plates

$$N = 41.7 \times \frac{\left[\dfrac{t}{W_{0.1}}\right]^2}{\dfrac{b_{0.1}}{a_{0.1}} + 1.25}$$

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

Note 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

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

> **Note** 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 = 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

Japanese Pharmacopoeia (JP) Calculation Method

Theoretical Plates

$$N = 5.55 \times \left[\frac{t}{W_{0.5}} \right]^2$$

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

Note 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 = 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

Area/Height Calculation Method

Theoretical Plates

$$N = 16 \times \left[\frac{t}{W}\right]^2$$

where

N = theoretical plates

t = The retention time of the component

W = The width of the base of the component peak.

W = 4 × σ

$$\sigma = \frac{1}{\sqrt{2\pi}} \times \left[\frac{A}{H}\right]$$

$$= 0.399 \times \left[\frac{A}{H}\right]$$

where

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

> **Note** For peak asymmetry at 10%, the values for W and *f* are measured at 10% of peak height.

Resolution

$$R = \frac{2(t_2 - t_1)}{W_2 + W_1}$$

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_2 = The width of the base of the component peak 2

W_1 = The width of the base of the component peak 1

6-Sigma rms Noise Method

$$Signal\text{-}to\text{-}Noise = \frac{Peak\ Height}{rms\ Noise}$$

where

Peak Height = the standard peak height determined during integration.

Noise = the standard deviation of the signal derived from n measurements.

$$Noise = 6 \times \left[\frac{\sum_{i=1}^{n} (E_i - \int (E_i))^2}{n-1} \right]^{1/2}$$

where

E_i = data point

$f(E_i)$ = the point on the linear regression line of all the data points.

The n measurements are made between the time limits entered.

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.

$$SN_M = H/N_D$$

$$LOD = C * SN/SN_M$$

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

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 is the peak being evaluated is within the Limits of Quantitation as previously determined experimentally for that Method.

$$SN = H/N_D$$

$$LOQ = C * SN/SN_M$$

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

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.

$$\frac{a_1 f_1 + a_2 f_2 + \ldots a_9 f_9}{norm} \, , \, \frac{a_2 f_1 + a_3 f_2 + \ldots a_{10} f_9}{norm} \, , \, \frac{a_3 f_1 + a_4 f_2 + \ldots a_{11} f_9}{norm}$$

where

$a_1 \ldots a_x$ = the data points

$f_1 \ldots f_x$ = the filtering factors

$norm$ = 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.

User Programs and Custom Parameters

User Programs and Custom Parameters are available to provide a seamless link between ChromQuest and user-provided programs that do specific calculations and applications that may be required by the laboratory.

Contents

- User Programs
- Custom Parameter Programs

User Programs

User Programs are programs that are run before an acquisition, or before or after an analysis. These programs are meant to synchronize actions between ChromQuest 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.

Because ChromQuest runs in the Windows 2000/Windows XP environment, if the User Program is an executable (.exe) program, the program is launched by ChromQuest, and ChromQuest waits until the program is finished. No data is passed to an executable program.

If the User Program is a .DLL, it has access to all data and parameters of ChromQuest. This is the recommended method for User Programs. A User Program .DLL should implement the "RunUserProg" function.

Custom Parameter Programs

Custom Parameters are used to calculate specific values that are of interest to you, but are not normally calculated by ChromQuest. This feature gives you access to the entire database of named and detected peaks for a ChromQuest application (Method Development, Instrument 1, etc.). Custom parameters programs are called *after* all other analysis is finished.

Because ChromQuest runs in the Windows 2000/Windows XP environment, the Custom Parameter Program **must** be a .DLL, and should implement the "EvaluateCustomParam" function. Custom Parameter .DLL's have access to all data and parameters of ChromQuest.

Data and Graphics Export

ChromQuest allows you to export a wide variety of information for use in other applications. Data export involves two steps. First, you must choose what information you want to export and assign a destination for the exported data. Second, you must turn on the data export option in your method so that the data is exported as the method is used.

Contents

- Data Export
- Automatic Export to Microsoft Excel
- ODBC Export to Microsoft Access
- Graphics Export

Data Export

The **Method > Advanced Method Options > Export** function allows you to save results automatically in an ASCII file after each analysis is completed. You select the type of data to export: Peaks, Groups, Standard Reports, or Chromatogram. For Peaks and Groups, you can choose the parameters you want to export. When you export Standard Reports, only the contents of the report is exported.

When you choose the **Method > Advanced > Export** tab, a dialog box appears. You then select what type of data export you want.

Figure 62. Advanced Method Options dialog box
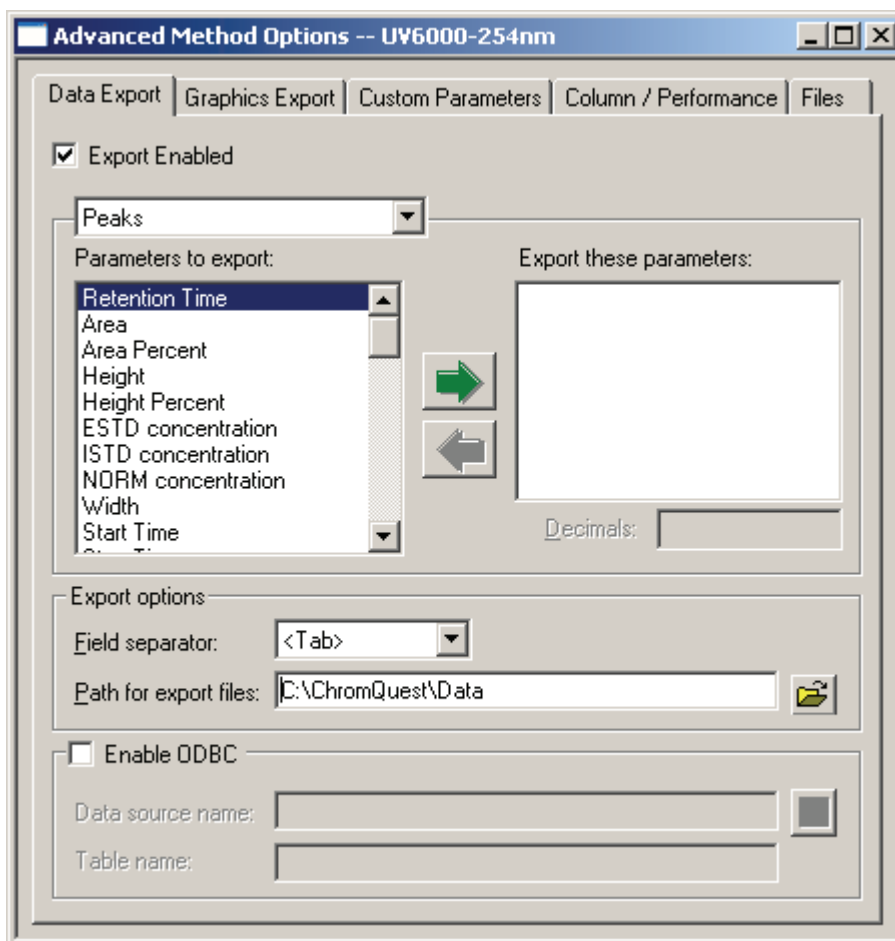
Export Enabled

Select the Export Enabled checkbox to turn data export on for the method. While this option is enabled, data export occurs after each Analysis of the data. Since the export of data occurs when the data is analyzed automatically at the end of a run and each time the data is manually analyzed, you should turn this option off while you are developing methods.

Select the type of information to export from the drop-down list. For each type of export chosen, you can select parameters for export. If you have defined any Custom Parameters, they appear in the appropriate list of items you can choose to export.

Exporting Peaks

When you select Peaks to be exported, a list of available peak export parameters is displayed. 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-hand box. To remove an item from the export box, highlight it, and then click the Red (bottom) arrow button.

Exporting Groups

If you select Groups for export, a list of group parameters is presented in the left-hand box. To select an item for export, double-click it, or click it to highlight it, then click the Green (Top) arrow. To remove an item from the export list, highlight it, and then click the Red (Bottom) arrow.

Exporting Standard Reports

When you choose to export Standard Reports, a list of available standard reports is displayed. Choose a report to export by double-clicking it, or highlighting it with the mouse, then clicking the Green (Top) arrow button.

Exporting Chromatograms

If you select Chromatograms to be exported, you are given the option to export in either/or **AIA (*.CDF)** file format, or in **ASCII** format.

Selecting the **AIA** option causes ChromQuest 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 ChromQuest results to be read by other chromatography data systems.

> **Note** AIA Level 2 support is for export only. Import of AIA files is supported only at Level 1 (raw data).

Export Options

- Field Separator

  Select the type of separator you want to include between data fields in your export file. Choices include Tab, Space, and Comma. Your choice is determined by what you wish to do with your exported file. If you want to import the file into a Microsoft Excel spreadsheet, for example, choose Tab.

- Path for export files

  Enter 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.

ODBC Enabled

Select this box 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. ODBC drivers use the standard Structured Query Language (SQL) to gain access to data.

> **Note** Microsoft Data Access Components (MDAC) 2.5 or higher is required for ODBC export. A version of this is on the ChromQuest CD-ROM under \Updates.

Data source name

Enter the name of the database you are using. To select the name from a list of available sources, click **Open**. The SQL Data Sources dialog box appears where you can select the data source for your export.

Figure 63. SQL Data Sources dialog box
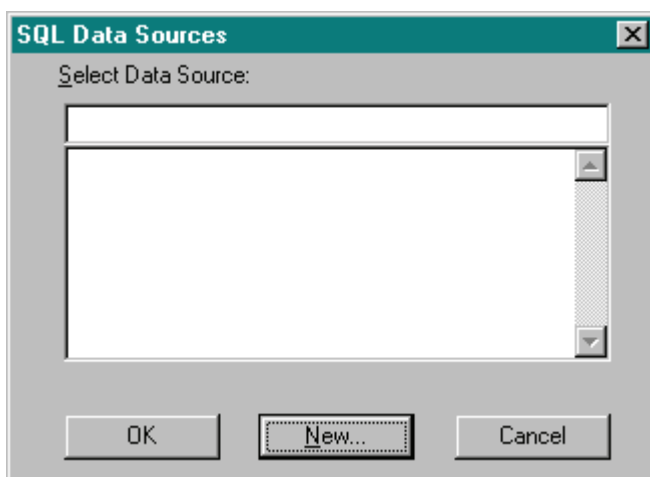
To create a new data source, click **New**. The Add Data Source dialog box appears.

Figure 64. Add Data Sources dialog box
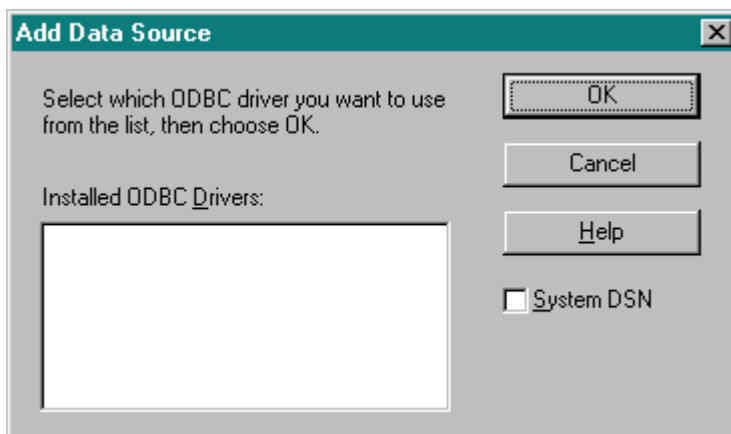
Table name

Enter the name of the table you wish to use for your data export.

Export Files

Data exported using ChromQuest 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, Figure 65 is an example of a file created for export of area for five runs.

Figure 65. Export file

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	c:\system\m	cathi	63088	52014	49749
5/9/92	20:49:09	STDS	c:\system\c	c:\system\m	cathi	170789	142665	136661
5/9/92	20:49:21	STDS	c:\system\c	c:\system\m	cathi	298854	251660	241049
5/9/92	20:49:34	STDS	c:\system\c	c:\system\m	cathi	461695	394081	376339
5/9/92	20:51:56	STDS	c:\system\c	c:\system\m	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 might occur when ChromQuest 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.

Figure 66 shows an example of a file created for Standard Export of an External Standard report.

Figure 66. Standard Export of an External Standard report

Report	Channel	# Peaks	Date	Time	Sample Id	File	Method	User
ESTD	A	4	5/9/92	0:48:53	STDS	C:\system\c	c:\system\m	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			

File Extensions Used for Data Export

ChromQuest automatically names the files used to save exported data. Each data export option uses a specific file naming convention, as follows.

Peak and Group Parameter Export Files

Filename = [method name]-[channel name].[short parameter name]

Example:

> Method Name - multi level.met
>
> Data File - calib std 3.dat
>
> Channel - TCD

Custom Export Option	Custom Export Filename
	(Uses the method filename followed by the extension.)
Retention Time	multi level-tcd.apex
Area	multi level-tcd.area
Area %	multi level-tcd.areaperc
Height	multi level-tcd.height
Height %	multi level-tcd.heightperc
ESTD	multi level-tcd.estdconc
ISTD	multi level-tcd.istdconc
NORM	multi level-tcd.normconc
Width	multi level-tcd.width
Relative RT	multi level-tcd.relativert
Theoretical Plates	multi level-tcd.TPlates
Plates / Meter	multi level-tcd.TPlatesPerMeter
Capacity Factor	multi level-tcd.capacity
Resolution	multi level-tcd.resolution
Peak Asymmetry	multi level-tcd.asymmetry
Custom Parameters	multi level-tcd.custom parameter1..x

Note For Group export files, the file naming convention is as described above, except that each file begins with a "G". In the example above, the group export file for NORM becomes **Gmulti level-tcd.normconc**.

Standard Report Export Files

Filename = [data file name][data file extension]-[channel name].[data type]

Example:

>Method Name - multi level.met

>Data File - calib std 3.dat

>Channel - TCD

Standard Export Option	Standard Export Filename
	(Uses the data filename followed by the extension.)
Area%	calib std 3 dat-tcd.are
ESTD	calib std 3 dat-tcd.ESD
ISTD	calib std 3 dat-tcd.ISD
NORM	calib std 3 dat-tcd.NOM
Performance	calib std 3 dat-tcd.PER

Chromatogram Export	
AIA	calib std 3 dat-tcd.CDF
ASCII	calib std 3.dat.ASC

The following is an example of the format for an exported chromatogram file. The numbers at the end of the file are the individual data points from the chromatogram, with channel 1 data first, followed in order by data from additional channels if present.

Figure 67. Format for an exported chromatogram file

```
Sample ID:  Tutor.001
Vial Number : -1000
Data File:  C:\System\Chrom\Tutor.dat
Method:  C:\System\Methods\Tutor.met
User Name:  J.W.
Acquisition Date and Time:          Dec. 19, 1991          10:19:43
Sampling Rate :          0.559          1          1          1 Hz
Total Data Points :          2648          0          0          0 Pts.
X Axis Title :          Minutes    Minutes    Minutes    Minutes
Y Axis Title :          Volts      Volts      Volts      Volts
X Axis Multiplier :     0.016667        0          0          0
Y Axis Multiplier :     0.000001        0          0          0
                 103
                 108
                 124
                 115
                 110
                  82
```

The format for ASCII data files to be imported into ChromQuest must follow the example shown above. If data from more than one channel are involved, they are appended to the string. In this example, channel B starts at data point 2649.

Automatic Export to Microsoft Excel

ChromQuest provides a user program, *ExcelExport.dll* that can be used to open a user-supplied Excel worksheet and run a user-supplied macro within that worksheet. The macro can be written by the user to open an exported file from ChromQuest and perform operations on the content. To set up and use this program, follow the directions outlined below.

Select Parameters to Export

Select the parameters to export by choosing the **Method > Advanced Method Options** command, and then the **Data Export** tab. Make sure the Export Enabled checkbox is selected, and then designate the parameters you want to export by double-clicking on each desired parameter listed in the left-hand box. The selected parameters appears in the right-hand box.

The **Field Separator** must be set to **Tab**, and the **Path for export files** must contain a valid path. Figure 68 shows an example for exporting "Area" and "Area Percent" parameters.

Figure 68. Data Export page of the Advanced Method Options dialog box
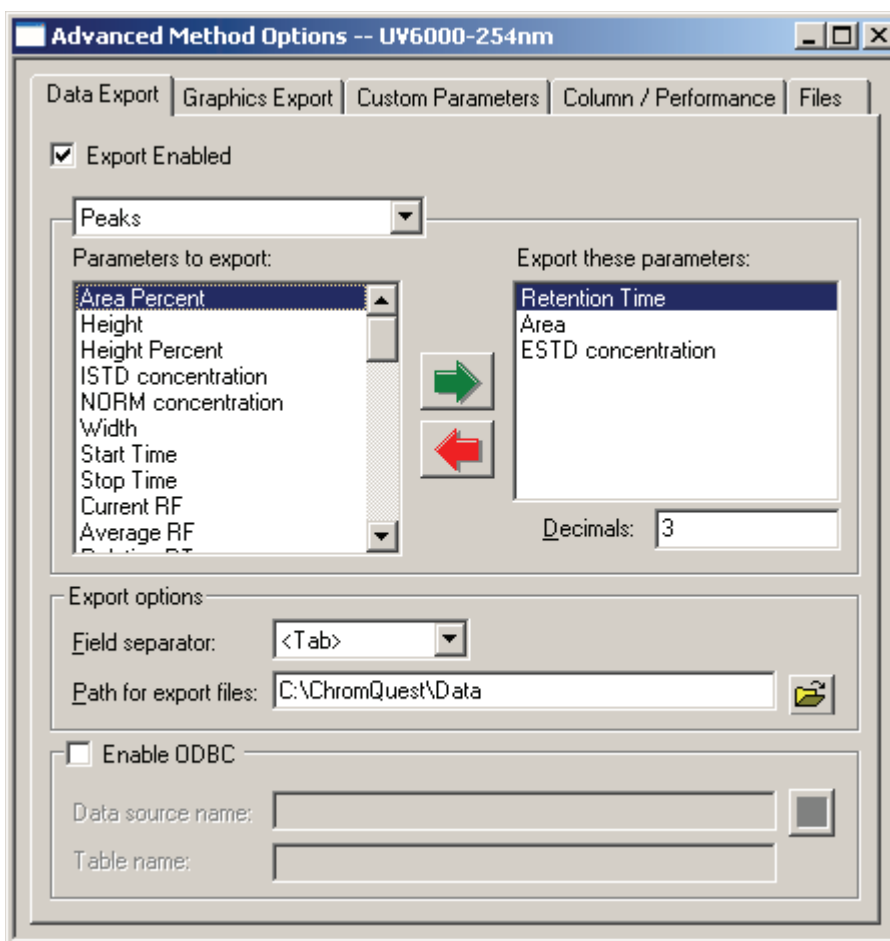
Set up Excel Export User Program

Next, you must set up the user program to run. From the Advanced Method Options dialog box, select the Files tab. Select the After analysis box, then select the **ExcelExport.dll** program. The ExcelExport.dll is located in the ChromQuest program folder.

The Additional Parameters field must contain entries that specify the following items (in the order specified), each in quotation marks, separated by a comma:

- Path of exported ChromQuest data

- Parameter Name

- Excel Macro File

- Excel Macro Name

Figure 69. Files page of the Advanced Method Options dialog box
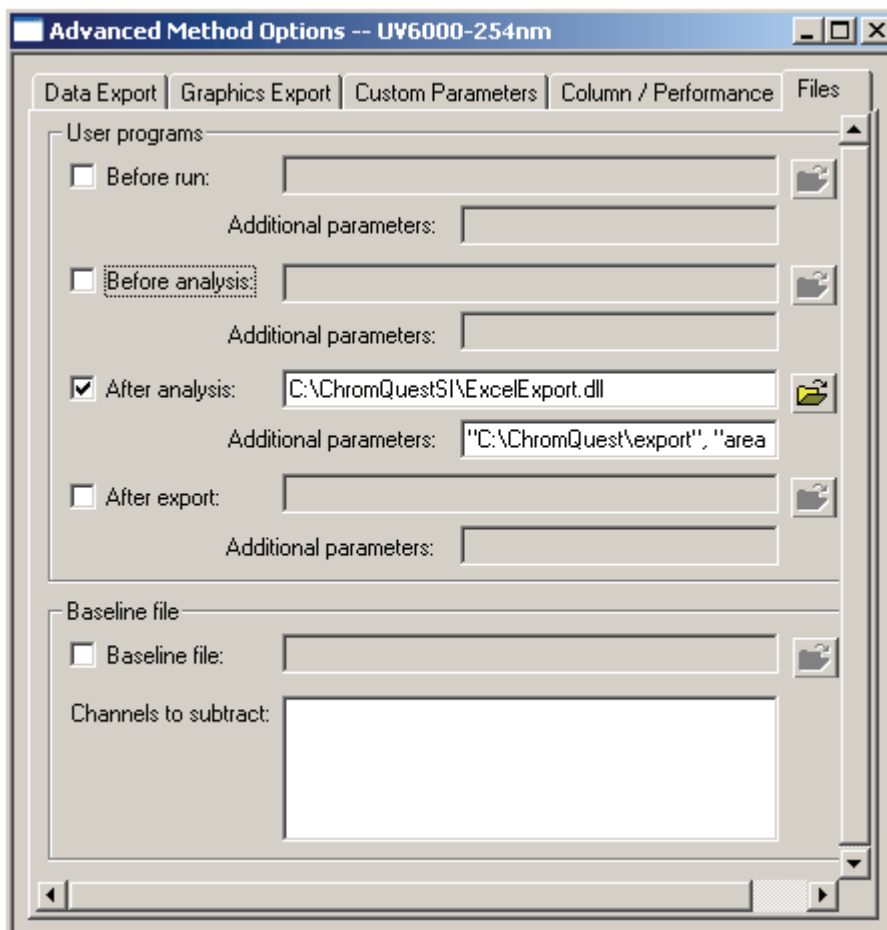
Figure 70. Location of ExcelExport.dll file
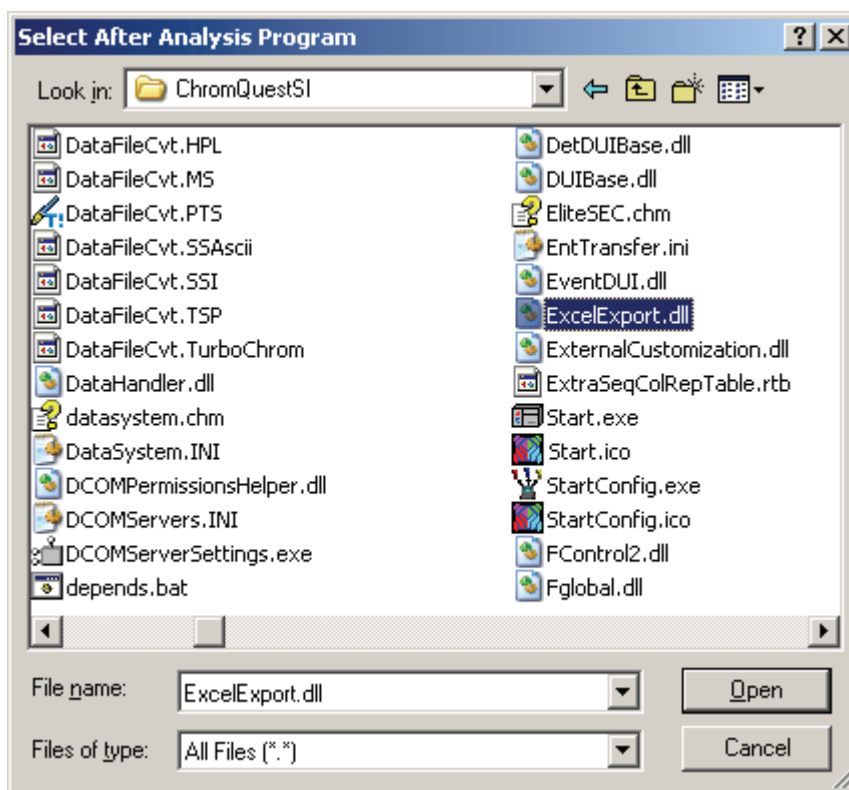
The **Parameter Name** entry may be repeated to specify additional parameters. All parameters must be enclosed in quotes, and must be separated by spaces and/or commas. For example, to export "Area" and "Area Percent" from the C:\ChromQuest\Export directory, and then run the "FormatData" macro from the C:\excel\xlstart\personal.xls spreadsheet, the entry would look like the following:

"C:\ChromQuest\export","Area","AreaPerc","C:\excel\xlstart\personal.xls","Form atData"

> **Note** The names of the parameters are not the same as the names shown on the Export tab. Instead, the names used must be the same as the name used for the file extension for the exported parameter file. For example, "Area Percent" becomes "AreaPerc". For a list of these file extensions see **File Extensions Used for Data Export** in help or in the "File Extensions Used for Data Export" on page 77 of the manual.

The data is organized in excel as follows: each parameter is in a separate Excel workbook and each wavelength channel of a parameter is in a separate sheet of a workbook.

ODBC Export to Microsoft Access

❖ **To export data to a Microsoft Access database**

Note Microsoft Data Access Components (MDAC) 2.5 or higher is required for ODBC export. A version of this is on the ChromQuest CD-ROM under Updates.

1. Install Microsoft Access on your Windows 2000/XP Server.

2. Update the Data Access components drivers on your Server by running the mdac_typ.exe, which is located in the *Updates\MDAC* directory on the ChromQuest CD-ROM.

3. On the Server, open Microsoft Access.

4. Create a new database:

   a. Select the Blank Database option button, then click **OK** to open the File New Database dialog box.

   Figure 71. Microsoft Access dialog box
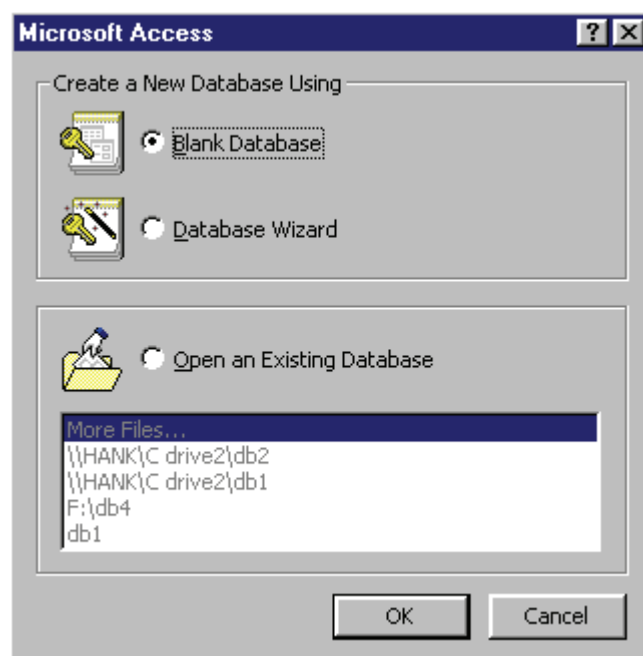
Figure 72. File New Database dialog box
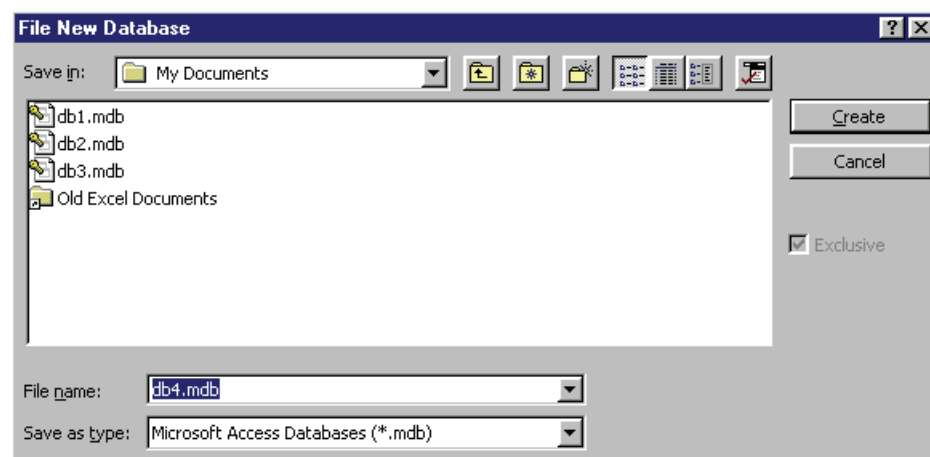
Access automatically creates a database file named *db*.mdb*, but you can enter your own database name if you prefer.

b. In the File New Database dialog box, click **Create**.

Access creates a new blank database and display the following screen.

Figure 73. Microsoft Access – Blank database window
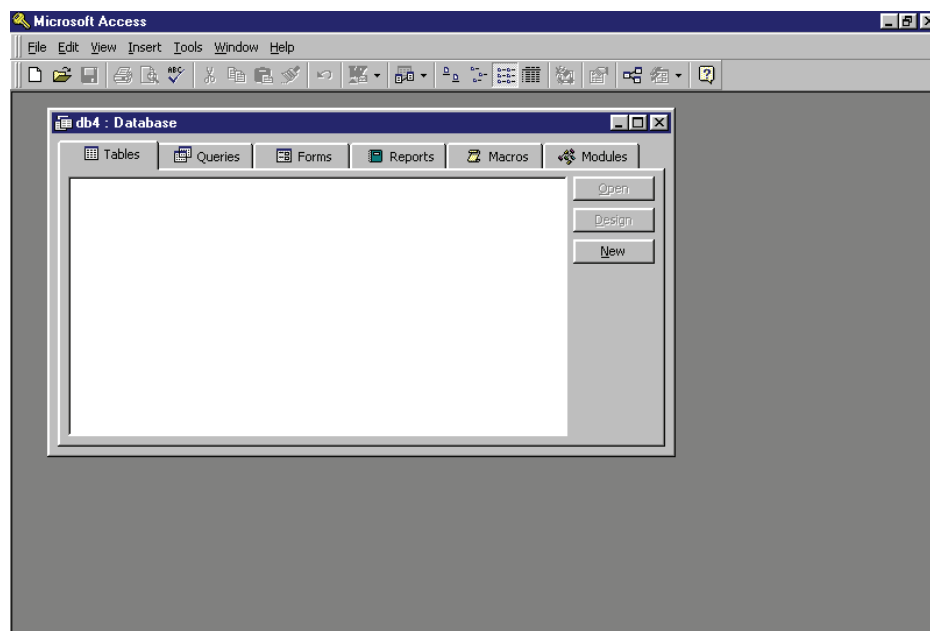
c. Close the new database and exit Microsoft Access.

5. On the Server, set up the ODBC protocol:

a. From the Control Panel, double-click the **32bitODBC** icon to open the ODBC Data Source Administrator.

Figure 74. Control Panel window
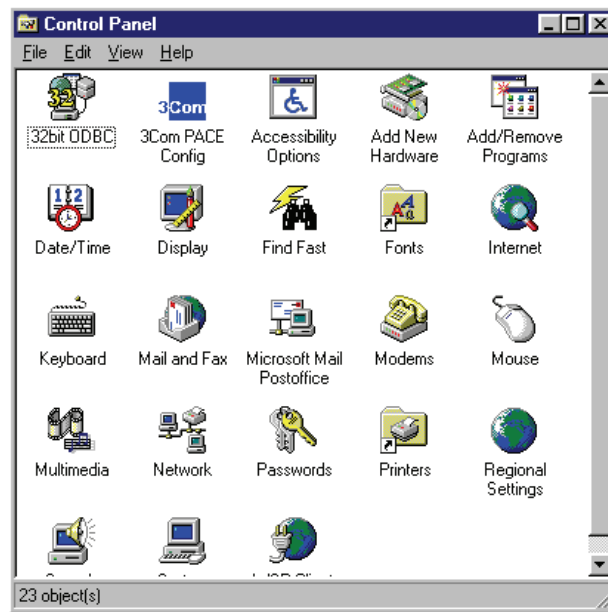
b. From the ODBC Data Source Administrator dialog box, click the System Data Source Name (DSN) tab.

Figure 75. ODBC Data Source Administrator – System DSN dialog box
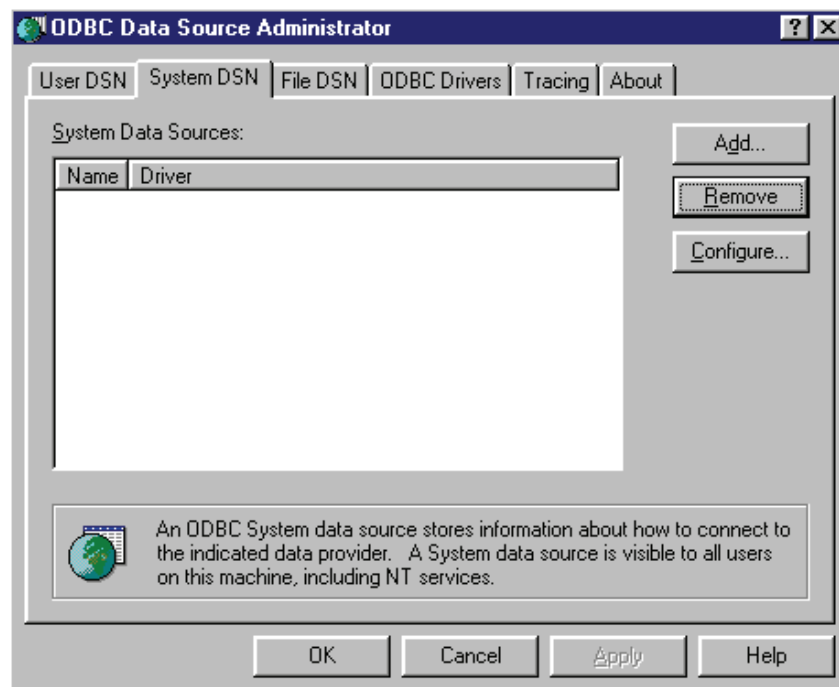
c. In the System DSN page, click **Add** to open the Create New Data Source dialog box.

d. From the Create New Data Source list box, select the *Microsoft Access Driver*. Then, click **Finish.**

The ODBC Microsoft Access Setup dialog box opens.

Figure 76. Create New Data Source dialog box
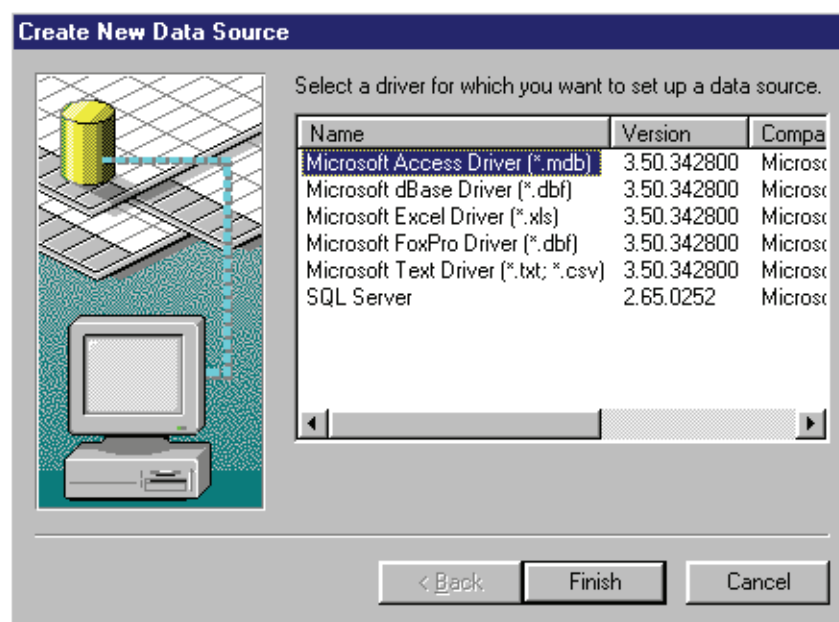
e. In the ODBC Microsoft Access Setup dialog box, type a unique Data Source Name in the Data Source Name text box.

Figure 77. ODBC Microsoft Access 97 Setup dialog box
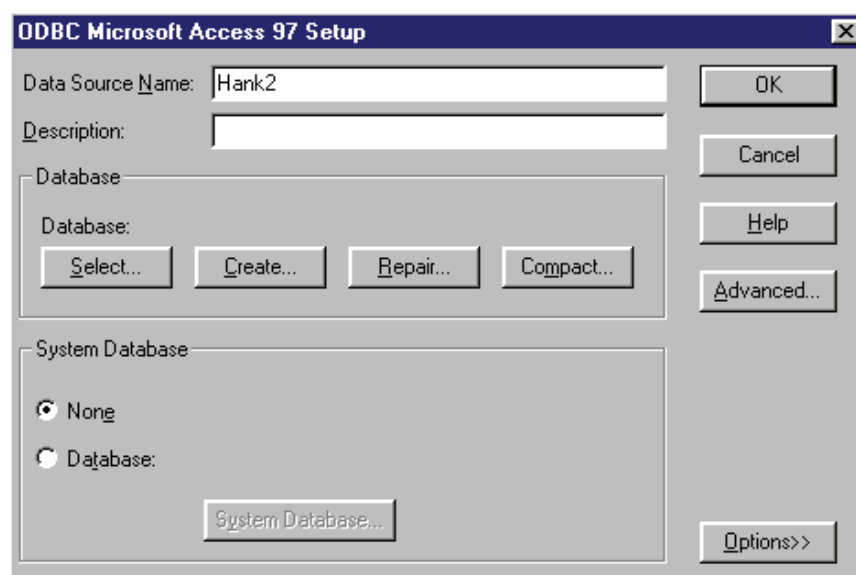
f.   Click **Select** to open the Select Database dialog box.

Figure 78.   ODBC Microsoft Access 97 Setup dialog box
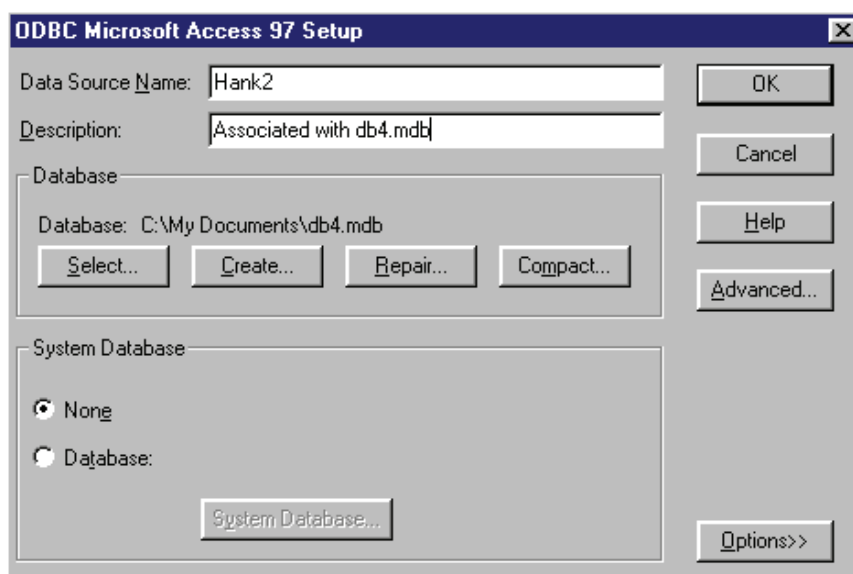
g.   In the Select Database dialog box, select the .mdb file that you created earlier. Then, click **OK** to return to the ODBC Microsoft Access Setup dialog box.

Figure 79.   Select Database dialog box
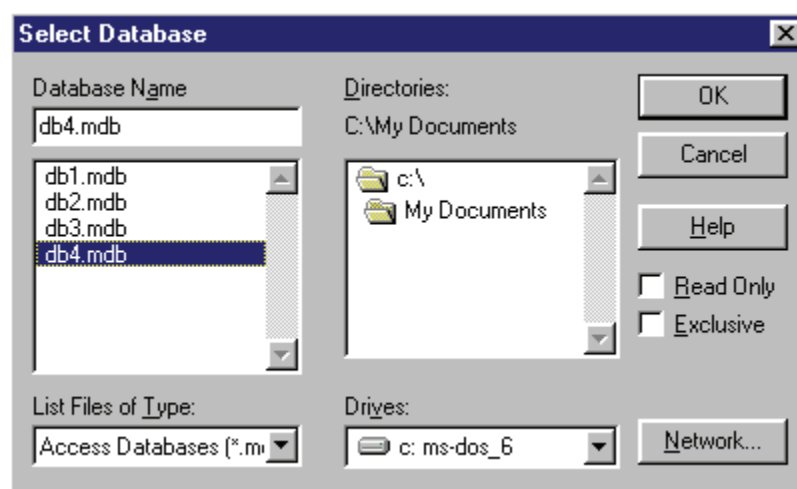
h. Enter a description, if desired, (helpful for later use), and click **OK** to return to the System DSN page of the set up.

Figure 80. ODBC Microsoft Access 97 Setup dialog box
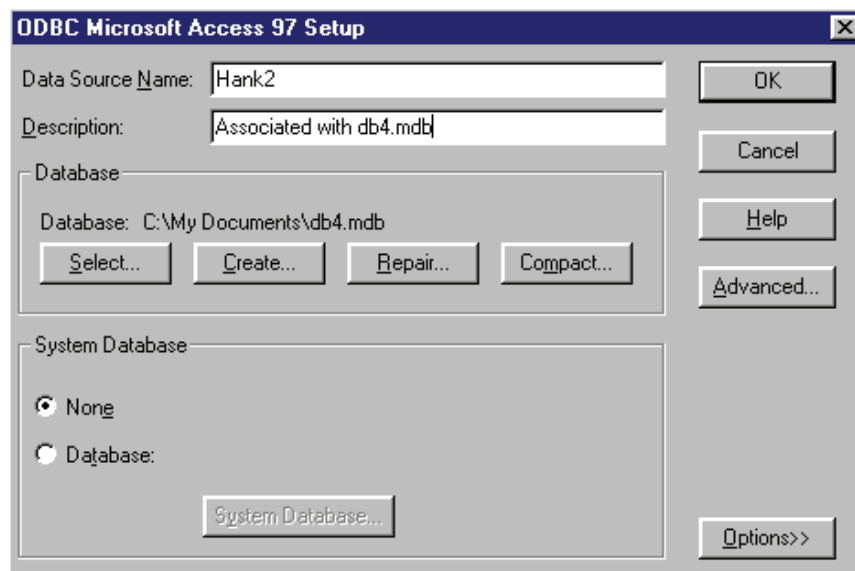
Figure 81. ODBC Data Source Administrator dialog box
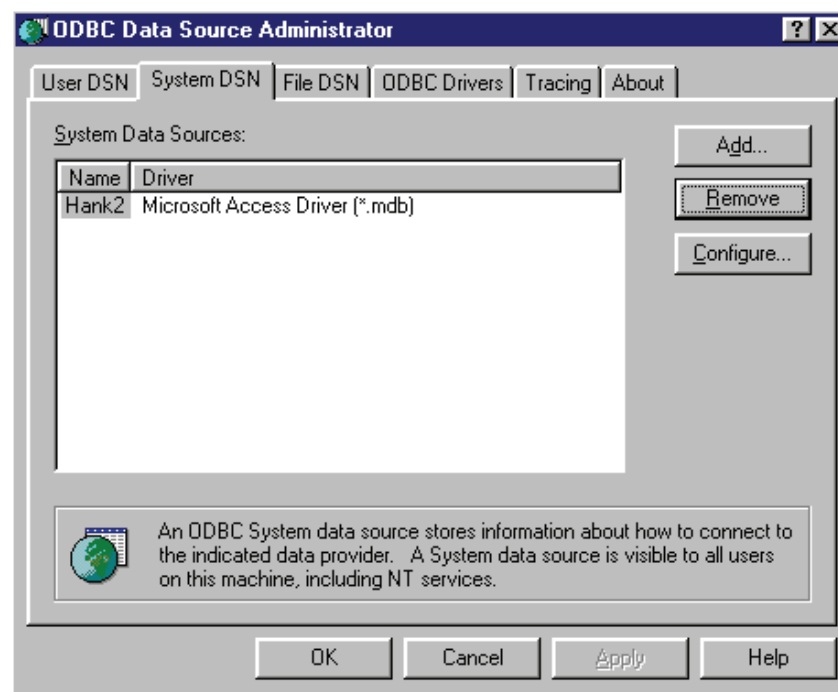
The New System Data source has now been created, and appears in the list of System Data Sources in the System DSN page.

i. In the System DSN page, click **OK** to exit the ODBC setup on the Server.

6. On the client PC, launch ChromQuest. Then, open the instrument that is networked to the above Server.

7. Create a method that exports data to Microsoft Access:

a. From the Instrument window, choose **Method > Peaks/Groups** and ensure that the method has a peak table.

b. Choose **Method > Advanced**, and then click the **Data Export** tab.

c. In the Export page, select the Export Enabled checkbox.

d. Select your export parameters.

e. In the Path for Export Files list box, browse to the appropriate directory on your Server. The Server name is listed in the Instrument Configuration.

f. Select the Enable ODBC checkbox.

g. Select the Data Source Name that you created on the Server in step 5.

h. Type a name in the Table Name text box where you want the export parameters to be entered.

If this table does not exist in your database, it is created during export. For details, see the "ODBC Export to Microsoft Access" on page 82 and Help.

Figure 82.   Data Export page of the Advanced Method Options dialog box
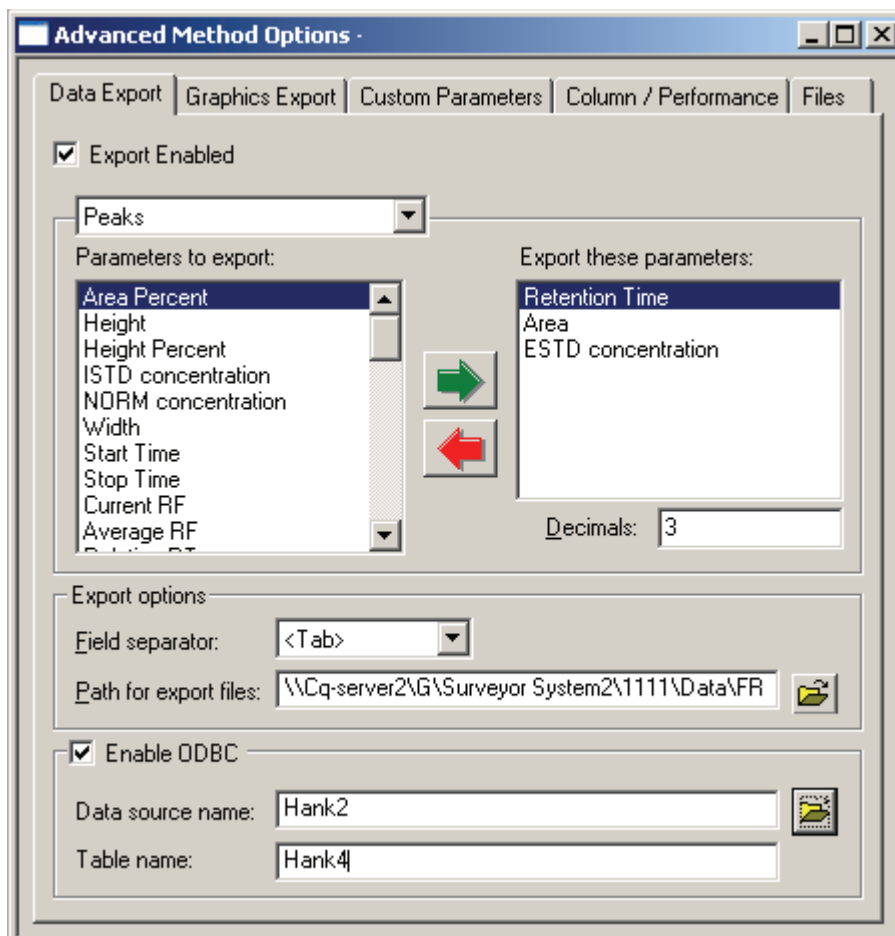
Once you save the method, each time you analyze a data file using this method, the parameters specified is automatically exported to your Access database.

8. To view the exported parameters after the data file has been analyzed:

a. Open Microsoft Access.

b. Use Explorer to locate the appropriate folder.

c. Locate the *.mdb file you selected for Data Source Name. (In the above example, this is db4.mdb, associated with Data Source Name Hank 2.)

d. Open this database file.

Figure 83. Microsoft Access – Database window
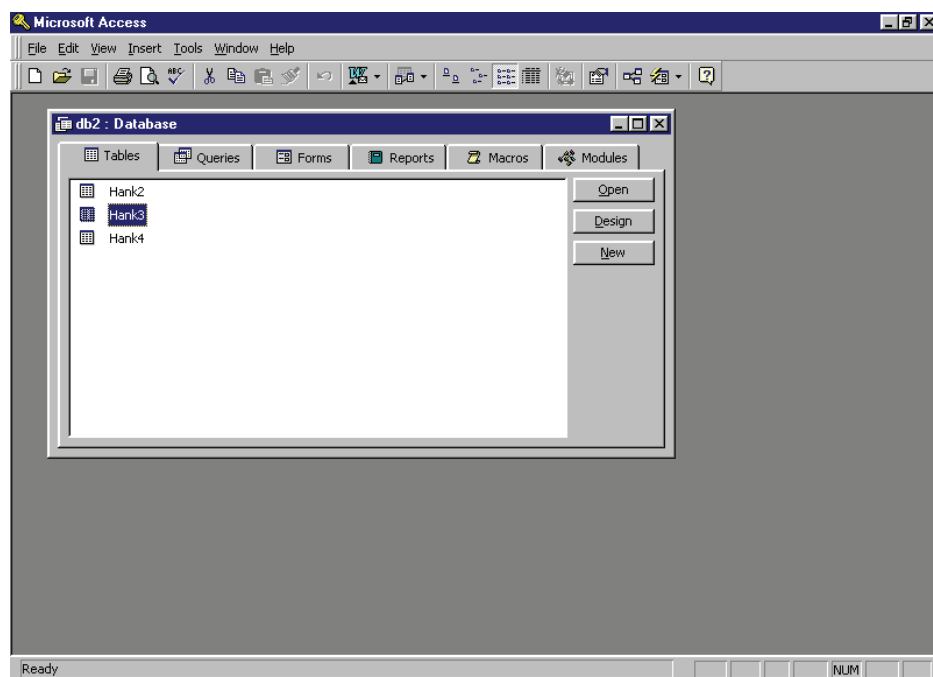
A list of existing tables in your database appears. In Figure 83, **Hank4** was the table name used to export parameters.

e. Select the appropriate table, and then click **Open** to view the exported parameters.

Figure 84. Microsoft Access – Table window
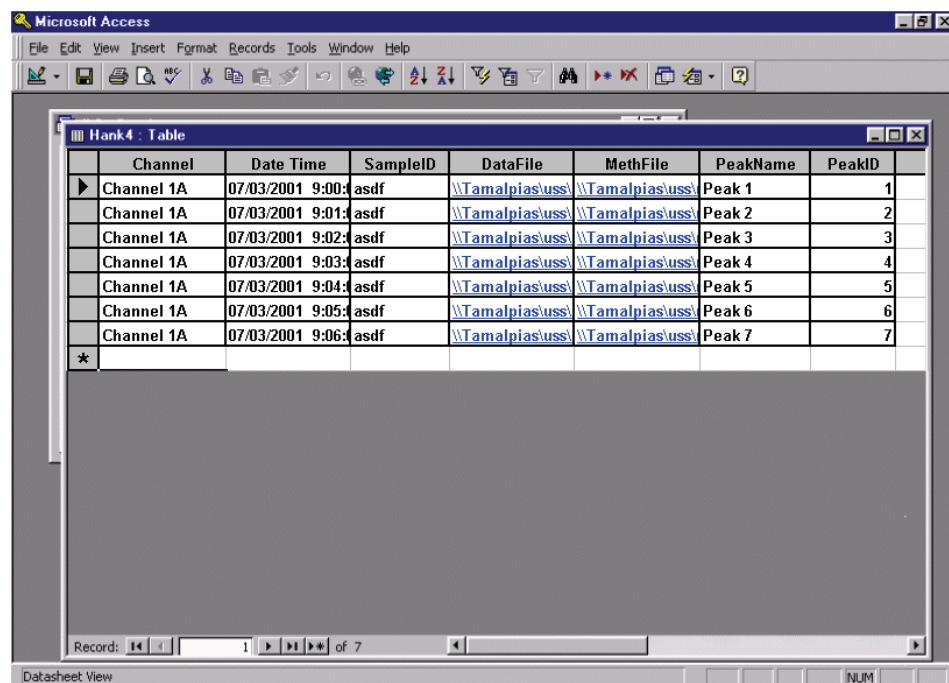
Graphics Export

Graphics export is a new feature provided in ChromQuest 5.0. Using this feature, you can export images of

❖ **To export graphics**

1. In the Instrument window, choose **Method > Advanced**. Then click the **Graphics Export** tab.

2. The Graphics Export page appears. See Figure 85.

Figure 85. Graphics Export page of the Advanced Method Options dialog box
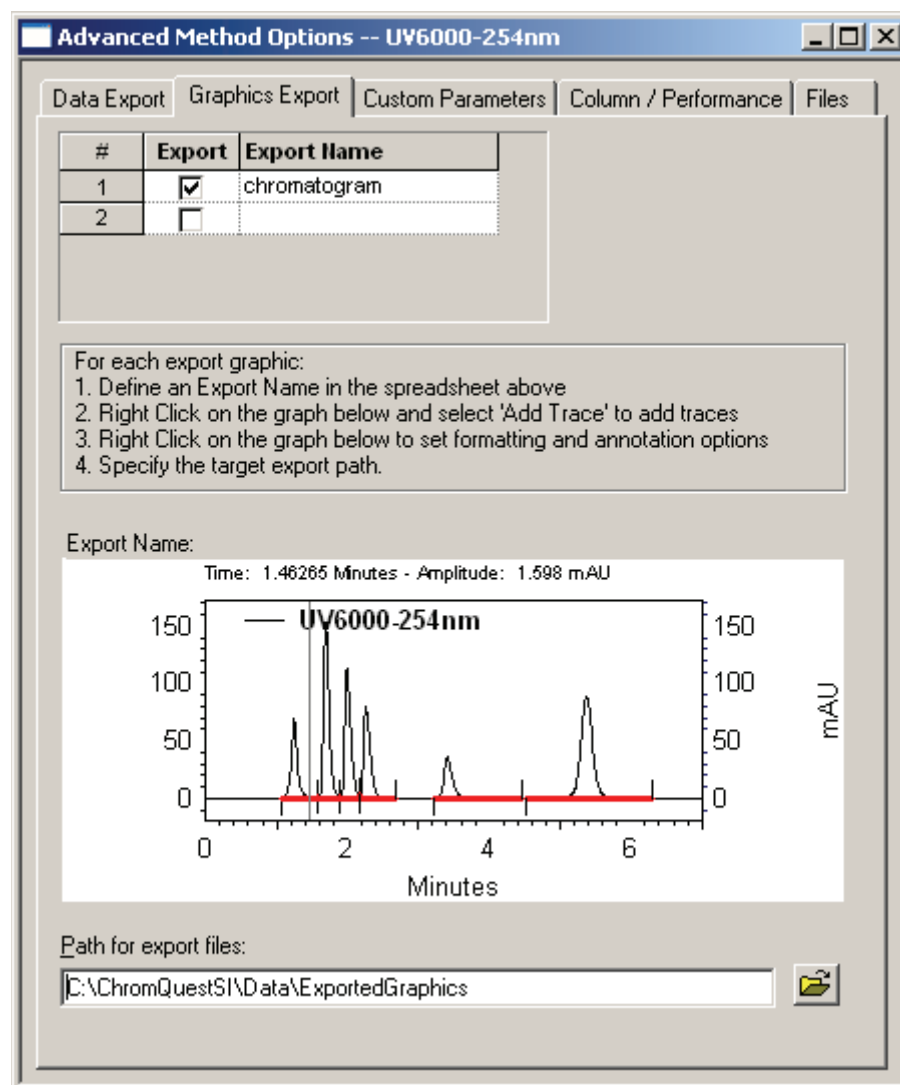
3. Select the traces to be exported as WMF files each time a data file is analyzed with the method.

    a. In the spreadsheet, select the Export check box and then type the filename to be used for the export.

    b. Follow the instructions below the spreadsheet.

        The graphics window displays the current graphic for export. To change the graphic, right-click the window and make a selection from the shortcut menu.

4. Select the path to be used for export of the graphics file.

    ChromQuest saves the exported graphics with the file name <Data file name> + " _ " + <Export Name> + ".wmf". See Figure 86.

Figure 86. Viewing the WMF file
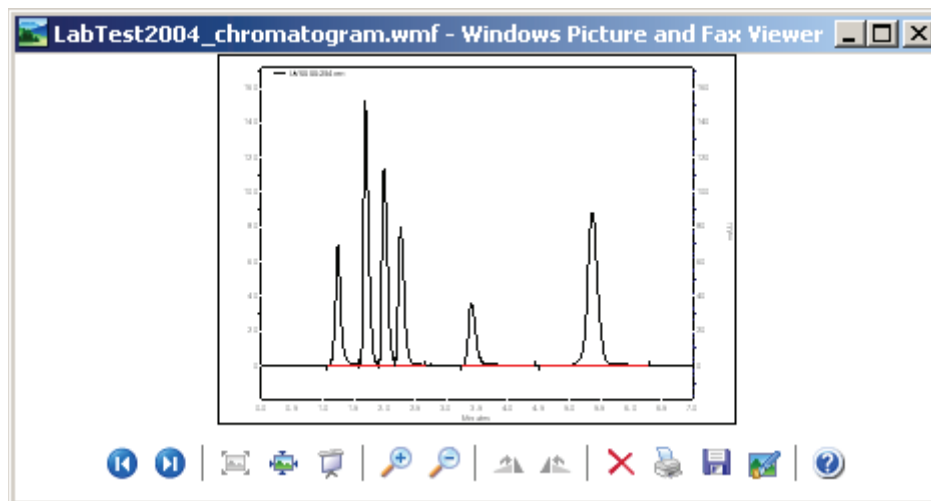
ASCII Sequence File Format

An ASCII sequence suitable for importing into ChromQuest 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".

Contents

- Sequence Header

- Sequence Records

- Action Record

- Example of ASCII Sequence File

- Example of ASCII Dual Tower Sequence File

Sequence Header

The next part of the text file contains sequence "header" information of the form:

<keyword>=<value>

For example:

DATAPATH=C:\CHROMQUEST\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 is used.

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.

Record Elements

The records contain comma-delimited elements detailing the operation of that line of the sequence. These lines are of the form:

RECORD = a,b,c,d,e,f,g,h,i,j,k,l,m,n,o,p

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   = Dilution factor (a.k.a. "Mult."; 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 "Run Types" on page 96)

n   = Action (Leave blank. Not used in ChromQuest)

o   = Run description

p   = Repetitions per vial (1 - 9)

Note If you wish to use a delimiter other than the comma, set the List Separator field in the International settings in the Control Panel to the character that you wish to use. This setting is consulted before the ASCII sequence is read in. You may only specify a single character, such as the semicolon or the dash. You may use the space or tab character, but remember that any character that is used for the separator can not be recognized as a record element.

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

Action Record

Action records relate to the previous Sequence Record only. Form:

ACTION=a,b,c,d,e

where

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

Note 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 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

The following is an example of an 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

ChromQuest System Suitability

ChromQuest provides a System Suitability module that allows you to automatically calculate suitability parameters as a part of your general data acquisition and processing tasks.

Contents

- System Suitability Overview
- ChromQuest System Suitability Module
- System Suitability Setup
- Running a Suitability Test
- Suitability Reports

System Suitability Overview

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. While system suitability testing is not the same as method validation, they are often used to provide a complete picture of laboratory quality and reproducibility of results.

System suitability basically involves running a mixture containing the analytes you are running in your samples and examining various parameters that describe the ability of the chromatograph and column to separate those analytes. The chromatographer, based on the method and analysis to be performed, must determine the importance or need to examine any given parameter. Some important suitability parameters are described briefly below. Calculations used in the system suitability test are given at the end of this manual.

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.

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.

Peak asymmetry (Tailing)

The quantitative values for peak asymmetry are important, especially when dealing with trace components. In addition, since asymmetry can vary through the life of a column, it can be important to track this data on an ongoing basis.

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.

Noise and Drift

Particularly important to trace analyses, the noise and drift values for your chromatograph indicate the limits of detection and quantification. Three types of noise calculations are available: RMS noise, ASTM noise, and 6-sigma noise.

ChromQuest System Suitability Module

ChromQuest System Suitability module includes the ability to do automatic System Suitability calculations for experimental variables such as efficiency, capacity, resolution, and reproducibility. The package includes four choices of calculation methods, including USP (United States Pharmacopia), EMG (Exponential Modified Gaussian), Area/Height method, and DAB (German Pharmacopia). DAB calculation is also used for JP (Japanese Pharmacopia), BP (British Pharmacopia), and EP (European Pharmacopia). The user can set acceptance ranges for each peak individually. Suitability Test can be programmed as part of a sequence of runs, with automatic printout of System Suitability Report indicating pass/fail on a per-peak and per-run basis.

❖   **To run a suitability test**

1. Complete the **System Suitability Setup** dialog. For each peak of interest, select one or more **Parameters**, and set Min, Max, and % RSD values for each. Additionally, set Noise test and/or Drift test, enter start and end times for the test, along with threshold values.

2. Enter values for parameters such as Unretained Peak Time, required for calculation of performance options. Select a method for calculation of the performance values. This is done by choosing the **Method > Advanced Method Options > Performance** command. Select **Calculate Performance Parameters** to enable the suitability calculations.

3. Create and run a sequence where system suitability standards are included at the beginning of the sequence. For example, following USP protocols, 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 ChromQuest generates a system suitability report.

System Suitability Setup

Before ChromQuest can make System Suitability calculations, you must enter the required acceptance ranges for the peaks of interest information about your chromatographic column.

This section contains the following topics:

- Setting Up a System Suitability Report

- Entering the Performance Parameters

Setting Up a System Suitability Report

There is one System Suitability Setup dialog box for each detector in your instrument configuration.

> **Note** If you are performing a multi-wavelength analysis with one detector (UV2000, UV3000, UV6000, Surveyor PDA, or Surveyor PDA Plus), you might want to label your peaks (in the Peak Table) with additional information pertaining to their analysis channels.

❖ **To set up a system suitability report**

1. Choose the **Method > System Suitability** command to open the System Suitability Setup dialog.

Figure 87. System Suitability Setup dialog box
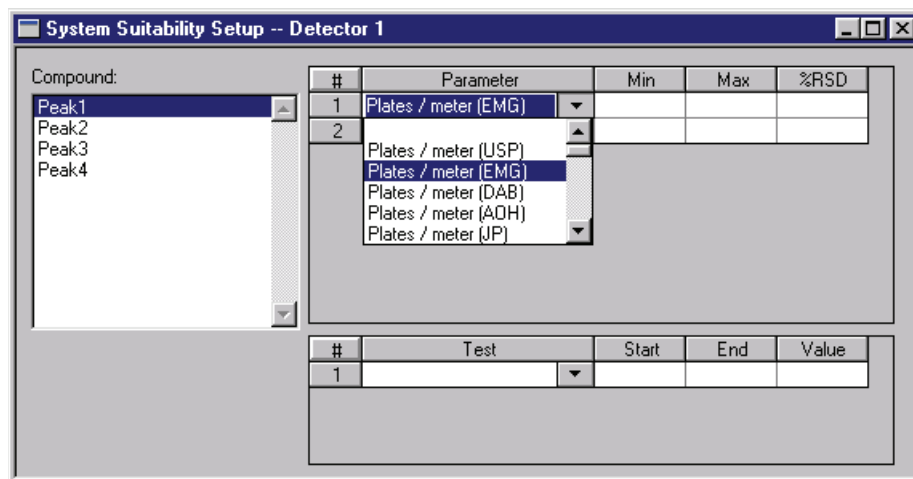
2. Select the first peak to be used for calculations by highlighting it with the mouse in the **Compound** list.

3. In the adjacent spreadsheet click the first field in the **Parameter** column. A drop-down list of available parameters is displayed. 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. (for example, Plates/Meter (JP) indicates Plates/Meter calculated using the Japanese Pharmacopoeia calculation.) For details on these calculations, see the equations section.

4. For each parameter selected, enter a minimum value (**Min**), maximum value (**Max**), and maximum allowed percent relative standard deviation (**%RSD**).

5. If you want a noise test to be performed, click the lower spreadsheet in the column labeled **Test**. Select one of the noise calculations **Noise (rms)/ ASTM Noise (rms)**, or **6-sigma Noise (rms)** from the drop-down list. If you select this box, you must enter a **Start** and **Stop** time for the test, and a **Threshold** value to determine acceptable limit. The RMS noise value for the portion of chromatogram between the Start and Stop times are 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.

6. If you want a drift test to be performed, click the lower spreadsheet in the column labeled **Test**. Select **Drift (mV/min)** from the drop-down list. If you select this box, you must enter a **Start** and **Stop** time for the test, and a **Threshold** value (in $\mu V/Min$) for the acceptable limit.

7. After highlighting sections of the spreadsheet that you want to copy, press:

- CTRL+C to copy the highlighted section of the spreadsheet to the clipboard.

- SHIFT+INSERT to paste the clipboard item to where the cell is highlighted.

- SHIFT+ARROWS highlights the spreadsheet cells, and can move them.

8. When you have completed the System Suitability Setup, close the dialog box.

Entering the Performance Parameters

System Suitability calculations require information about your chromatography column. These parameters are entered in the **Method > Advanced > Performance** dialog box. The information in this dialog box pertains to one detector. If you are performing a multi-detector analysis, select an Analysis Channel, and then enter the appropriate information for the selected detector.

❖ **To enter your column parameters**

1. Choose **Method > Advanced**. Click the **Performance** tab to open the Column/Performance page.

2. Enter your column information.

Figure 88. Column/Performance page of the Advanced Method Options dialog box
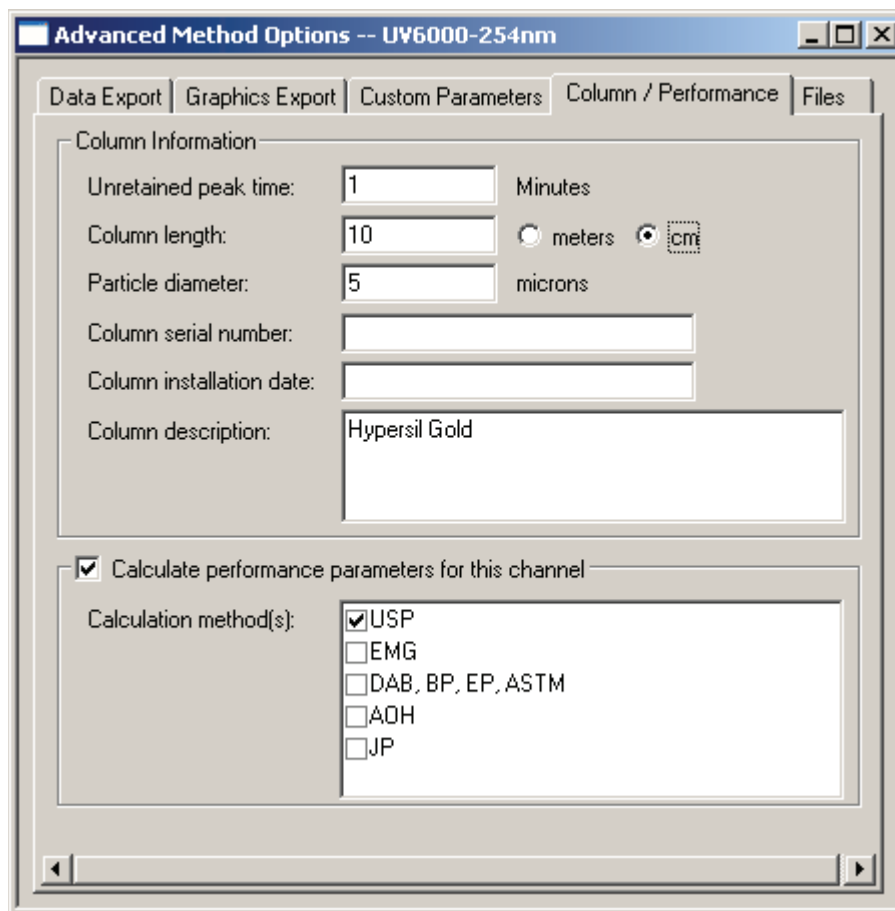
3. Select the **Calculate performance parameters for this channel** check box to enable the suitability calculations for the method.

> **Note** If you are performing a multi-detector analysis, you can select a different calculation method for each detector.

4. Select a method for the calculation of the performance values.

   Choices include **USP, EMG** (Exponential Modified Gaussian), **DAB, JP,** and **AOH (Area/Height)** method. The calculations used are given in the equations section. For BP, EP, and ASTM methods, choose DAB.
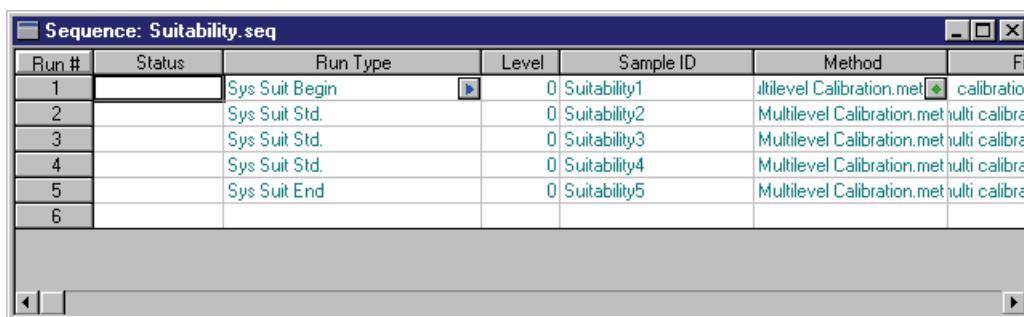
5. When you have completed the dialog box, exit to accept the parameters.

Running a Suitability Test

After completing the **System Suitability Setup** and **Performance** dialogs, 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. If you want the System Suitability Report to print automatically at the end of the sequence, you must also select the **Print Sequence Reports** option from the **Sequence Properties** dialog box.

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 ChromQuest generates a system suitability report.

Figure 89. Sequence Suitability report

Run Type is selected by clicking on the **Run Type** field, then selecting the appropriate sample type from the choices provided.

Figure 90. Sample Run Type(s) dialog box
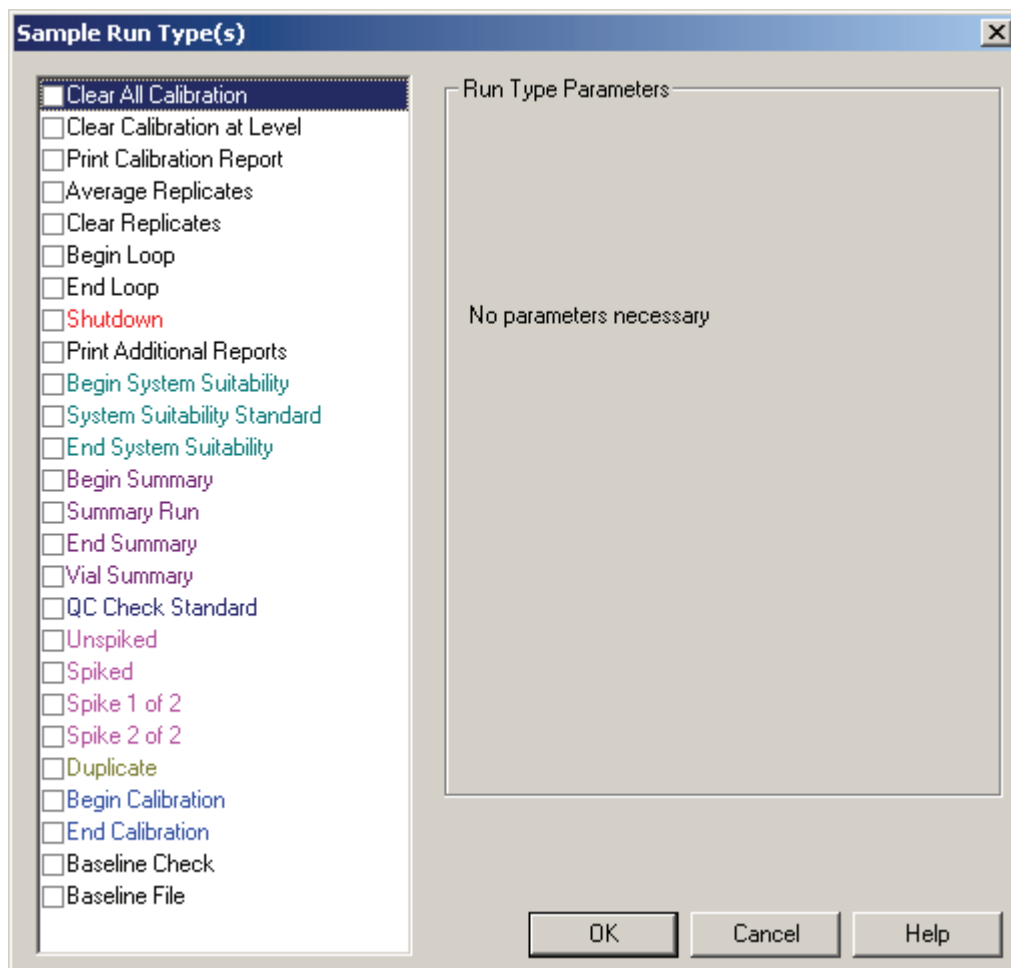
The first sample in your suitability set should be designated as **Begin System Suitability**. Additional suitability standards should be designated as **System Suitability Standards**, and the final sample in your suitability set should be designated as **End System Suitability**. Multiple run types can be selected for a given sample.

A System Suitability Report is generated at the end of the set of suitability standards when the sequence is run.

To view the Suitability Report on screen, choose **Reports > View > Sequence Custom Report** from the menu bar. The System Suitability Report appears in a list of available Sequence Custom Reports.

To print the Suitability Report, choose **Reports > Print > Sequence Custom Report**, and select the **System Suitability Report** choice. Note that 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.

Suitability Reports

ChromQuest provides a default suitability report template. This report template can be used as-is, or it can be customized in the Sequence Custom Report editor.

Figure 91. Default suitability report

Standard Reports

ChromQuest has a very powerful custom report editor. However, it is not necessary to create a custom report in order to print results. The following standard report templates are provided with the system to enable you to print any type of report you wish. However, these report templates can be modified by the user from the Custom Report editor.

Contents

- Error Condition Flags
- Area % Report
- External Standard Report
- Internal Standard Report
- Normalization Report
- Summary Report
- Calibration Report
- QC Check Standard Report
- Duplicate Report
- Spike 1 Report
- Spike 2 Report
- System Suitability Report

Error Condition Flags

Whenever 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.

Area % Report

This is an example of the Area % (**Area%.srp**) report template output.

Area % Report   Page 1 of 1

Method Name: C:\ChromQuest \methods\Multilevel Calibration.met
Data: C:\ChromQuest \Data\Multi Calibration Level 5.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	

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:\ChromQuest\METHODS\Test.met
Data: C:\ChromQuest\Data\Multi Calibration Level 5.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**

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:\ChromQuest\METHODS\Istd.met
Data: C:\ChromQuest\DATA\multi calibration level 3.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**

Normalization Report

This is an example of the Normalized Report (**Normalization.Srp**) template output.

Normalization Report   Page 1 of 1

Method Name: C:\ChromQuest\METHODS\untitled.met
Data: C:\ChromQuest\Data\Multi Calibration Level 5.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

Summary Report

This is an example of a Sequence Summary (**Summary.brp**) report template output. This template is included for compatibility with ChromQuest 2.x versions only.

Sequence Summary Report   Page 1 of 1

Sequence :   C:\Chromquest\sequence\multilevel calibration.seq
User :   System
Printed :   4/10/97 11:13:46 AM

ESTD concentration	Channel A			
Sample ID	Multilevel Calibration Level 1	Multilevel Calibration Level 2	Multilevel Calibration Level 3	Multilevel Calibration Level 4
Filename	C:\ChromQuest\ data\multi calibration level 1.dat	C:\ChromQuest\ data\multi calibration level 2.dat	C:\ChromQuest\ data\multi calibration level 3.dat	C:\ChromQuest\ data\multi calibration level 4.dat
Date	11/26/90 8:48:53 PM	11/26/90 8:49:09 PM	11/26/90 8:49:21 PM	11/26/90 8:49:34 PM
Peak1	10.000	20.086	30.095	40.034
Peak2	5.000	6.017	7.014	8.015
Peak3	15.002	20.035	25.001	30.017
Peak4	10.001	20.025	30.003	40.007

Calibration Report

This is an example of the Calibration (**Calibration .brp**) report template output.

Calibration Report   Page 1 of 1

Sequence :   C:\ChromQuest\SEQUENCE\multilevel calibration.seq
User :   System
Printed :   4/10/97 11:27:25 AM

Channel A

Compound	Old RT (Min)	New RT (Min)	RF Average	RF %RSD	RF %RSD Limit	Status
Peak1	5.739	5.729	10405.544	33.4551	0.00	Passed
Peak2	6.587	6.568	38653.028	63.3824	0.00	Passed
Peak3	8.303	8.273	10020.500	56.8338	0.00	Passed
Peak4	8.569	8.540	13135.420	34.2093	0.00	Passed

QC Check Standard Report

This is an example of the Check Standard (**QC Check Std.brp**) template output.

File	Sample ID	Acquired
c:\ChromQuest\data\multi calibration level 2.dat	Multilevel Calibration Level 2	2/18/97 12:58:38 PM

Channel A

Compound	Expected Conc.	Actual Conc.	%RD Actual	%RD Limit	Status
Peak1	25.000	20.000	20.000	25.000	Passed
Peak2	15.000	6.000	60.000	25.000	FAILED
Peak3	25.000	20.000	20.000	25.000	Passed
Peak4	25.000	20.000	20.000	25.000	Passed

Duplicate Report

This is an example of the Duplicate (**Duplicate.brp**) report template output.

Type	File	Sample ID	Acquired
Dup 1	c:\ChromQuest\data\multi calibration level 1.dat	Multilevel Calibration Level 1	11/26/90 8:48:53 PM
Dup 2	c:\ChromQuest\data\multi calibration level 2.dat	Multilevel Calibration Level 2	11/26/90 8:49:09 PM

Channel A

Compound	Dup 1 Conc.	Dup 2 Conc.	Mean Conc.	%RD Actual	Dup %RD Limit	Status
Peak1	10.000	20.000	15.000	66.667	50.000	FAILED
Peak2	5.000	6.000	5.500	18.182	60.000	Passed
Peak3	15.000	20.000	17.500	28.571	50.000	Passed
Peak4	10.000	20.000	15.000	66.667	50.000	FAILED

Spike 1 Report

This is an example of the Spike/Unspike (**Spike 1.brp**) report template output.

Type	File	Sample ID	Acquired
UnSpiked	c:\ChromQuest\data\multi calibration level 3.dat	Multilevel Calibration Level 3	11/26/90 8:49:21 PM
Spiked	c:\ChromQuest\data\multi calibration level 4.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 2 Report

This is an example of the Spike 2 of 2 (**Spike 2.brp**) report template output.

Type	File	Sample ID	Acquired
UnSpiked	c:\ChromQuest\data\multi calibration1level 3.dat	Multilevel Calibration Level 3	11/26/90 8:49:21 PM
Spike 1	c:\ChromQuest\data\multi calibration1level 4.dat	Multilevel Calibration Level 4	11/26/90 8:49:34 PM
Spike 2	c:\ChromQuest\data\multi calibration1level 5.dat	Multilevel Calibration Level 5	11/26/90 8:51:56 PM

Channel A

Compound	Unspiked Conc.	Spike1 Amount	Spike1 Conc.	Spike1 Recovery	Spike2 Amount	Spike2 Conc.	Spike2 Recovery	Relative Diff.	Mean Recovery	Low Limit	High Limit	Status
Peak1	30.000	10.000	40.000	100.000	20.000	50.000	100.000	0.000	100.000	90.000	110.000	OK
Peak2	7.000	1.500	8.000	66.667	2.000	9.000	100.000	0.400	83.333	75.000	125.000	OK
Peak3	25.000	4.500	30.000	111.111	10.000	35.000	100.000	0.105	105.556	90.000	110.000	OK
Peak4	30.000	10.000	40.000	100.000	21.000	50.000	95.238	0.049	97.619	90.000	110.000	OK

System Suitability Report

This is an example of the System Suitability (**SysSuit.brp**) report template output.

System Suitability Report   Page 1 of 1

Sequence : C:\Chromquest\SEQUENCE\multilevel calibration.seq
User : System
Printed : 4/10/97 11:52:08 AM

System is Suitable

Channel A	Compound	Parameter	Min	Max	%RSD	
	Peak1	rt	5.600	5.800		

Sample ID	Compound	Parameter	Average	Low	High	%RSD	Status
	Peak1	rt	5.719	5.710	5.739	0.244	
Multilevel Calibration Level 1		5.739					Passed
Multilevel Calibration Level 2		5.710					Passed
Multilevel Calibration Level 3		5.710					Passed
Multilevel Calibration Level 4		5.719					Passed

Spectral Options

ChromQuest provides special features to optimize your chromatographic analyses when collecting UV-Visible scanning data from the UV3000 high-speed scanning detector, the UV6000LP photodiode array detector (PDA), the Surveyor PDA, or the Surveyor PDA Plus detector. The features are collectively referred to as Spectral Analysis. These features include peak purity assessment for determining the presence of co-eluting impurities and spectral library searches for confirming the identity of an analyte.

With a standard UV-Vis detector, the absorbance is measured at one wavelength (or sometimes two wavelengths). The two-dimensional array of data plotted as absorbance versus time is commonly called a chromatogram. The UV3000 scanning detector measures the absorbance at multiple wavelengths in a fraction of a second. The photodiode array detectors measure the absorbance at multiple wavelengths, simultaneously. Therefore, these detectors can produce a 3-dimensional plot of absorbance versus time and wavelength.

Contents

- Spectral Method Setup
- Spectral Views
- Custom Report
- Peak Table
- Spectral Analysis and Calculations
- Library Search Calculations
- Ratio Chromatogram Calculation
- Similarity Calculations
- Lambda Max/Min Calculations
- Peak Purity Calculations

Spectral Method Setup

In addition to the instrument control parameters that control the operation of your scanning detector, the method contains spectral options for the scan data. These include setting up libraries, spectral filtering, defining multiple wavelengths for multi-wavelength display and calibration, and setting up the Ratio view. These options are available from the Instrument window by choosing **Method > Spectral Options** to open the Spectral Options dialog box. The Spectral Options dialog box contains the following pages:

- Library

- Purity

- Spectrum

- Multi-Chromatogram

- Ratio

Library

On the Library page of the Spectral Options dialog box, you can enter library parameters for the spectral library searches that is performed automatically as part of your method. When you perform a spectral library search "using method parameters", these parameters are used.

Figure 92. Spectral Options – Library dialog box

Parameter	Description
Library/Enabled	Enter the spectral library to be searched or select from available libraries by clicking the Library field followed by clicking on the file button ⬇. You can select more than one library. To enable the library for searching, select the **Enabled** checkbox. If this list is empty, or no library is enabled, no hits are returned when a search is performed.
Search parameters	Enter the parameters to use for the search.
Wavelength range	Enter the wavelength range to search.
Wavelength step	Enter a step number for the search. Larger numbers makes the search faster, but if you use too large of a step, spectral details might not be picked up. Because the spectral comparison program compares spectra on a per wavelength basis, it is best to collect the library spectra with a step size of one.
Max hits	Specify the number of hits that are reported in the results of a library search. Note that this works in conjunction with the *Similarity Threshold* parameter to limit the number of hits reported.
Similarity threshold	Enter a number for threshold of similarity. The library search results only displays matches whose similarity to the unknown exceeds this value. The options in this group allow you to specify search pre-filters that is performed on library spectra prior to the test for similarity. All pre-filters are optional.
Pre-filters	
Retention time range	When values are entered in these fields, ChromQuest limits its search to library spectra obtained from peaks whose apex are within the specified retention time range. This pre-filter is optional and may be left blank.
Lambda max	When one or more of these values is specified, library search is restricted to those library entries containing lambda max value(s) within 5nm of all of the specified values. Entries without matching lambda max value(s) are automatically excluded from the search (no similarity calculation is made). Entering values for lambda max is optional.
Compound name filter	If you are searching only for spectra that contain a certain name, enter the name here. Only spectra containing that name is searched.

Purity

The Purity page allows you to set the parameters necessary to perform manual peak purity calculations and peak purity calculations that occur automatically as part of analysis.

Figure 93. Spectral Options – Purity dialog box

Parameter	Description
Purity calculations	The Purity calculations group box contains the following parameters:
Wavelength range	Specify the wavelength range over which the purity calculations is performed, for example, from 200nm to 400nm.
Wavelength step	Specify the wavelength spacing (in nm) used for purity calculations.
Scan threshold	This value is the minimum absorbance value that a spectrum must have to be included in the purity calculations
Peak coverage	The Peak Coverage parameter indicates the fraction of the peak used for purity calculations. It is possible to allow the calculation to be done over the entire width of the peak (100%), which ensures the greatest possibility of detecting an impurity. However, this has the disadvantage of including data that has a relatively low signal to noise ratio, and for which spurious results might be calculated. The default value is a peak coverage of 95%.
Background compensation	Selecting this checkbox causes spectra to be corrected for background baseline absorbance using the peak baseline prior to being used in the calculation of purity.
Per-peak spectrum calculations	The result of these calculations is available in reports and as chromatogram annotations. Deselecting these checkboxes speeds up analysis. If a checkbox is not selected and the field appears in a run report, it is reported as zero.
Total purity	Selecting this checkbox causes total peak purity to be calculated on a per-peak basis during analysis. The result of this calculation is available in reports and as chromatogram annotations. If this box is not selected and a report contains the field, a value of zero is reported.
3 point purity	Checking this box causes 3-point peak purity to be calculated on a per-peak basis during analysis. The result of this calculation is available in reports and as chromatogram annotations. If this box is unchecked and a report contains the field, a zero is reported.

Spectrum

The Spectrum page allows you to specify the types of filtering and processing to be performed on spectra that are extracted from the 3D data during analysis as well as to spectra displayed in the Spectrum View.

Note The processing specified on this page is performed prior to any use of the spectra in the software, including display, searching and reporting.

Figure 94. Spectral Options – Spectrum dialog box

Parameter	Description
Spectral filtering	In this group box, you designate how spectral filtering is performed.
Filtering type	Select the type of filtering for the spectral plot. Choices are: None, Smooth, 1st Derivative, and 2nd Derivative.
Background correction	If this checkbox is selected, a correction for the spectral background is made, for the following features: • Library search • Adding a spectrum from the current file to a library • Per-peak similarity calculations • Spectral confirm The background correction is accomplished as follows: 1. The spectra from the baseline start and baseline stop times for the peak are extracted from the data. 2. For each spectrum in the peak, a corresponding background spectrum is generated by linear interpolation between the baseline start and baseline stop spectra. 3. This background spectrum is subtracted from the original spectrum. **Note** The baseline start and stop times that are used in calculating background compensation are based on the detected peaks for the channel currently selected.
Interpolate spectra	Select this check box to automatically perform 10:1 interpolation of spectra displayed in the spectrum window using a cubic spline curve fit. This interpolation is performed after the applying any spectral filtering option (1st derivative, 2nd derivative or smooth) to the display spectrum. **Note** Interpolated spectra may not be stored or added to a library.
The peak spectrum is defined as	The parameters contained in this group box specify if and how spectra extracted from the 3D data are averaged before being exported or used in the Spectrum Report.
The peak apex spectrum	When this checkbox is selected, the spectrum at the apex of the peak is used, without averaging.
The avg. of the upslope, apex and downslope spectra	When this checkbox is selected, three spectra (the spectra at the upslope inflection point, the apex and the downslope inflection point) are averaged.
The avg. of every n spectra across the peak	When this checkbox is selected. Every nth spectrum from the peak is extracted, beginning at the start of the peak and continuing to the end of the peak. These extracted spectra are averaged and become the spectrum that is reported or exported.

Parameter	Description
Per-peak spectrum calculations	Selecting any of these checkboxes allows the indicated value to be calculated on a per-peak basis during analysis. The result of this calculation is then available in reports and as chromatogram annotations.

Deselecting options that are not of interest speeds up analysis. If a checkbox is not selected and the field appears in a run report, it is reported as zero |
| Similarity | Checking this box causes the Peak Apex Similarity to the reference spectrum to be calculated on a per-peak basis during analysis. The result of this calculation is then available in reports and as chromatogram annotations. If this box is unchecked and a report contains the field, a zero is reported.

Peak Apex Similarity applies only to named peaks and its use requires that a reference spectrum be included in the peak table. |
Up slope similarity	Checking this box causes upslope similarity to be calculated on a per-peak basis during analysis. Upslope similarity compares the peak apex spectrum to the spectrum at the peak inflection point on the upslope side (to the left of the apex). The result of this calculation is then available in reports and as chromatogram annotations. If this box is unchecked and a report contains the field, a zero is reported.
Down slope similarity	Checking this box causes downslope similarity to be calculated on a per-peak basis during analysis. Downslope similarity compares the peak apex spectrum to the spectrum at the peak inflection point on the downslope side (to the right of the apex). The result of this calculation is then available in reports and as chromatogram annotations. If this box is unchecked and a report contains the field, a zero is reported.
Lambda max	Checking this box indicates causes the lambda max (wavelength at which the highest absorbance occurs) to be computed for each peak of each multi-chromatogram extracted from the 3D data during analysis. The result of this calculation is then available in reports and as chromatogram annotations. If this box is unchecked and a report contains the field, a zero is reported.

Multi-Chromatogram

The Multi-Chromatogram page allows you to specify wavelength channels within the 3D data for integration and quantitation. In addition, it allows you to select wavelengths to display in the Multi-Chromatogram view. To create a Multi-Chromatogram channel, select an Enabled checkbox. Then, type a wavelength in the Wavelength text box and a bandwidth in the Bandwidth text box. The wavelength must be part of the scan data. After you have set up a multi-chromatogram channel, you can disable it temporarily by deselecting the Enabled checkbox. Choosing **View > Spectral View > Multi-Chromatogram** displays The Multi-Chromatogram view. The Multi-Chromatogram view is not functional unless one or more valid wavelengths are enabled in the Multi-Chromatogram Definition tab.

Figure 95. Spectral Options – Multi-Chromatogram dialog box
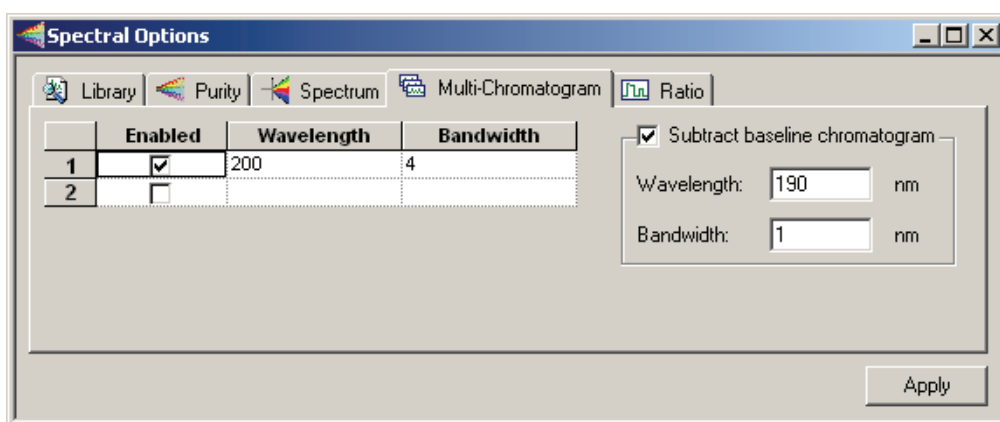
Parameter	Description
Enabled	To enable a wavelength, click the checkbox. To disable a wavelength, click the checkbox again to remove the checkmark. Only enabled wavelengths appears in the multi-chromatogram view.
Wavelength	Enter the wavelength you want to view or use as an analysis channel or both.
Bandwidth	Specify the nm range to be averaged in generating the analog signal for each channel.
Subtract baseline chromatogram	To enable baseline subtraction, select this check box, and then type a baseline wavelength in the Wavelength box and a bandwidth for this wavelength in the Bandwidth box.

The multi-chromatogram data is an average of the absorbances monitored at each wavelength in the wavelength range. The wavelength range is equal to the selected wavelength +/- one half of the bandwidth.

Ratio

The Ratio page allows you to set the displays of the Ratio Plot View. The Ratio View displays two PDA wavelength channels and the ratio of those two channels. These may be viewed during real-time acquisition as well as during post-run analysis. The flat tops on the ratio peaks are a preliminary indication of peak purity.

Figure 96. Spectral Options – Ratio dialog box

Parameter	Description
Ratio plot	These controls specify the wavelength of the ratio multi-chromatogram channels. The extracted chromatograms is centered about the specified wavelength.
Channel 1, Channel 2	• Wavelength Enter the wavelength of the chromatogram channel. • Bandwidth Enter the nm range to be averaged in generating the chromatogram channel.
Threshold	Enter the ratio threshold. The threshold is the minimum absorbance value required in the chromatograms of both channels for calculation of the ratio. It is a method of eliminating ratio calculation at low absorbance values to prevent calculation for baseline noise. If the threshold value is not met, the ratio plot is zero.
Max Plot Lambda Max Range	This allows the user to restrict the wavelength range over which the Spectrum Max Plot is calculated. The default is the detector acquisition range.

Spectral Views

The Spectral Views menu provides a variety of ways to view the scan data. This menu is accessed by choosing **View > Spectral View** from the Instrument window menu, or by clicking on **Views** in the Spectral View window menu bar. A right-mouse click within any of the view windows provides a unique menu of options for that view. The following views are available:

- Mixed View

- Chromatogram View

- Max Plot

- Multi-Chromatogram View

- Spectrum View

- Ratio View

- 3D View

- Contour View

Mixed View

This first, second, and third quadrants of this view display the Contour, Chromatogram, and Spectrum views, respectively. By default, the fourth quadrant of this view displays the peak purity view. You can change the view in the fourth pane by choosing a view from the Options menu that is accessed by clicking on **Options** in the Mixed View toolbar.

Figure 97. Spectral View – Mixed View window
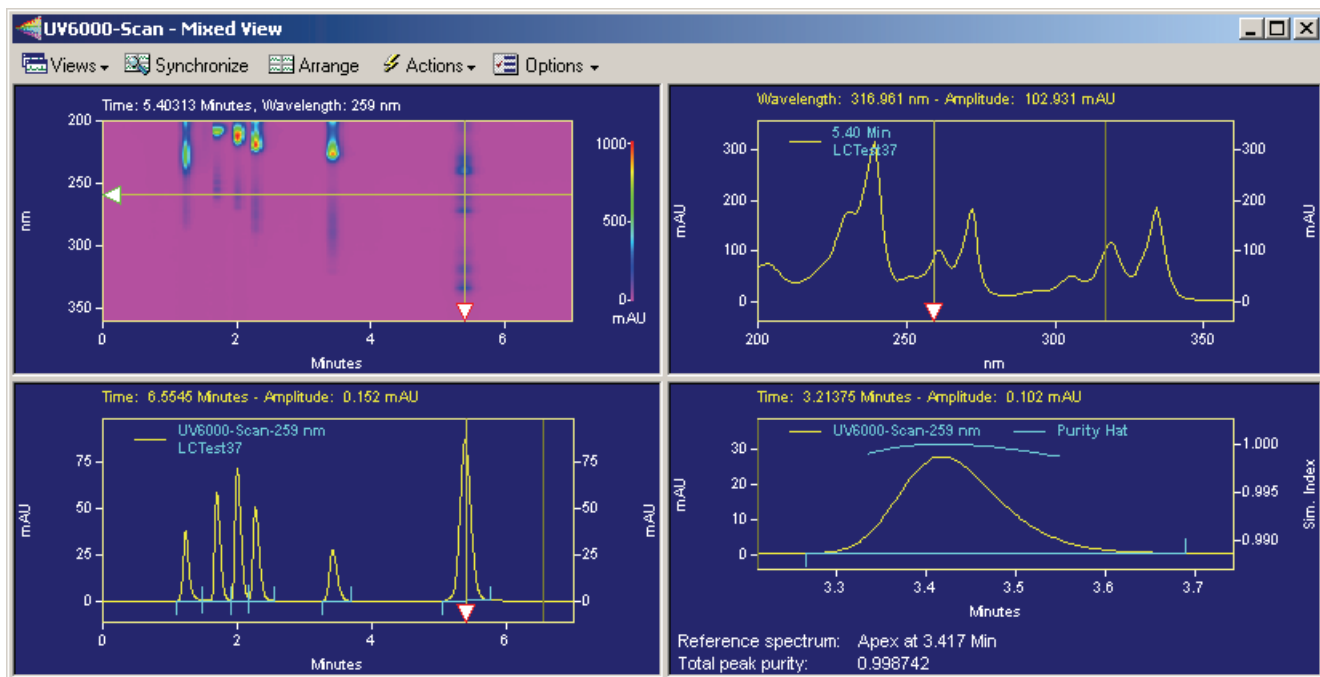
To zoom in on a portion of the contour plot, chromatogram or spectrum, hold the left mouse button down, move the mouse over the plot until the area of interest is highlighted, and release the mouse button.

To quickly move to the previous level of zoom, double-click the plot.

To unzoom to the full plot after multiple zooming operations, use CTRL+Z, or use SHIFT + double-click in the window, or click the right-mouse button anywhere in the window and select Full Unzoom from the pop-up menu.

Mixed View Synchronize Button

You can synchronize the axis and zoom limits with the other two plots using the Synchronize button on the Spectral toolbar. When the contour plot is zoomed, the time range of the chromatogram and the wavelength range of the spectrum plot are automatically adjusted to the same range as the contour. When synchronized zooming has been performed, the x-axis plot limits for the chromatogram and spectrum plot are changed. To unzoom these plots to the limits of the data, you must select Full Unzoom from the contour plot context menu.

Mixed View Actions Button

Figure 98. Mixed View – Actions button
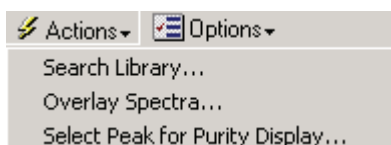
This button presents the following actions:

- Search Library

  Opens the Spectral Library Search window.

- Overlay Spectra

  Allows you to select a spectrum to overlay in the Spectrum view pane.

- Select Peak for Purity Display

  Enables you to select a peak for display in the Purity view pane.

Mixed View Options Button

Figure 99. Mixed View – Options button
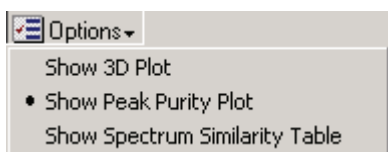
This button presents options that enable you to toggle the view for the lower right pane of the mixed view.

Spectral Peak Purity Plot

The peak purity plot appears when you choose the **Mixed View**. A peak purity plot only appears if the method Spectral options have specified purity information, and the data has been analyzed.

Select Peak

To select the reference spectrum for the purity calculation, make sure the data has been analyzed. (If you are not sure, click the analyze button on the toolbar.) Then, click **Actions > Select Peak for Similarity / Purity Display** from the Mixed View toolbar. A dialog appears that instructs you to select a peak by holding down the Ctrl button and then clicking on a peak on the Contour Plot or the Chromatogram view. The retention time of the reference spectrum is displayed along with a value indicating peak purity.

Figure 100. Select Peak for Similarity / Purity Display dialog box
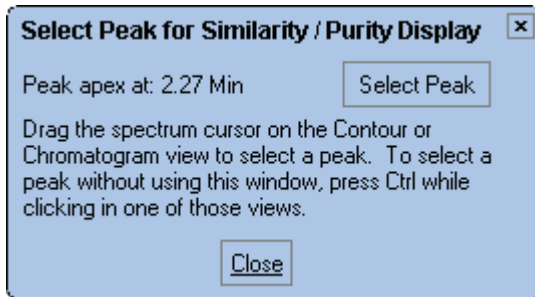
You can continue to select or change the peak. When you are finished, click **Close**.

The Peak Purity view displays the purity profile for a chromatogram extracted from the 3D data. The view displays purity information for the peak that has been chosen as well as the peak data itself. The shape of the purity profile ("hat") indicates the presence or absence of impurity in the peak of interest. For example, the less flat the profile is the more likely there is an impurity present. However, a symmetrical profile, mostly flat in the middle, but steeply falling off at the edges can indicate a fairly pure peak. The fall off at the edges is due to the lower signal-to noise ratio of the spectra there. The pane is blank until the data has been analyzed, and a peak has been selected for the purity calculation.

Figure 101. Peak Purity view
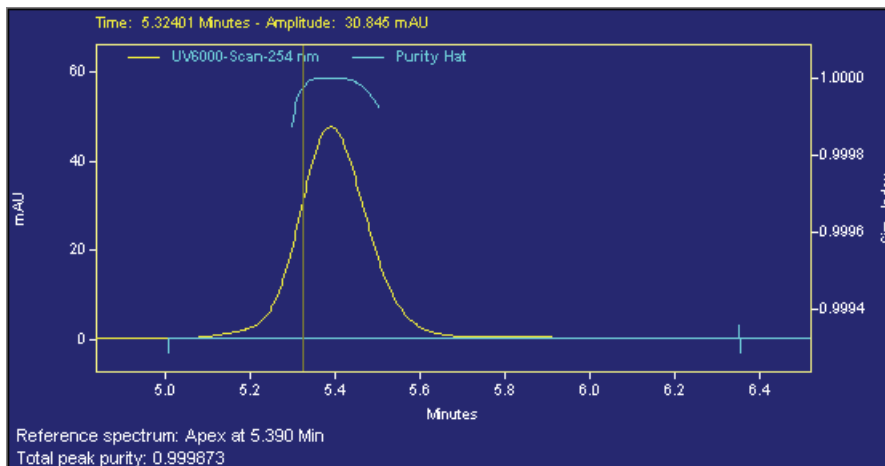
Chromatogram View

The Chromatogram View can be displayed alone or as part of the Mixed View display. Generate a chromatogram from the Contour plot as described in the section on contour plot.

Right-click within the chromatogram window to display the pop-up menu. This menu contains the same options as the basic chromatogram window for all detector types, and in addition enables you to overlay chromatograms from different wavelengths and change the Gallery view.

Overlay Chromatograms

When this option is available when you have a chromatogram view and a contour plot displayed simultaneously (Mixed View). Select **Overlay Chromatograms** to add chromatograms from different wavelengths to the view whenever you slide the wavelength selection cursor on the contour plot to a new wavelength.

Max Plot

A Max Plot is a chromatogram with each point plotted at its maximum absorbance. This plot gives an indication of the appearance of the chromatogram when the wavelengths are optimized for each peak.

Figure 102. Max Plot view
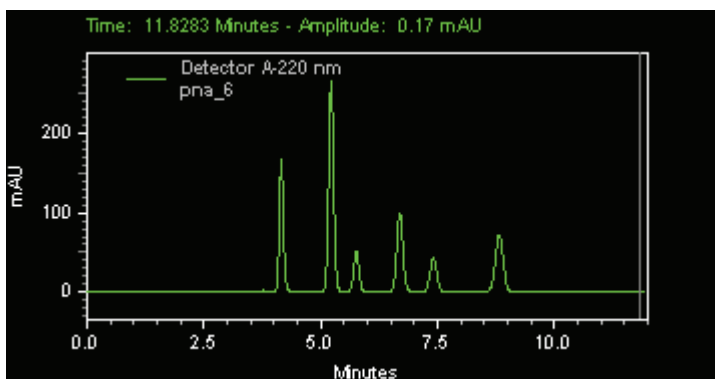
Multi-Chromatogram View

This displays multiple chromatographic plots of absorbance versus time, each at a different wavelength. Maximize the Spectral display and choose **View > Spectral Views > Multi-Chromatogram** (or use the Spectral toolbar/Views) to display all of the chromatograms in their respective channels that were specified in the **Method > Spectral Options > Multi-Chromatogram** tab.

Right-click within the window to display the pop-up context menu.

Figure 103. Multi-Chromatogram view
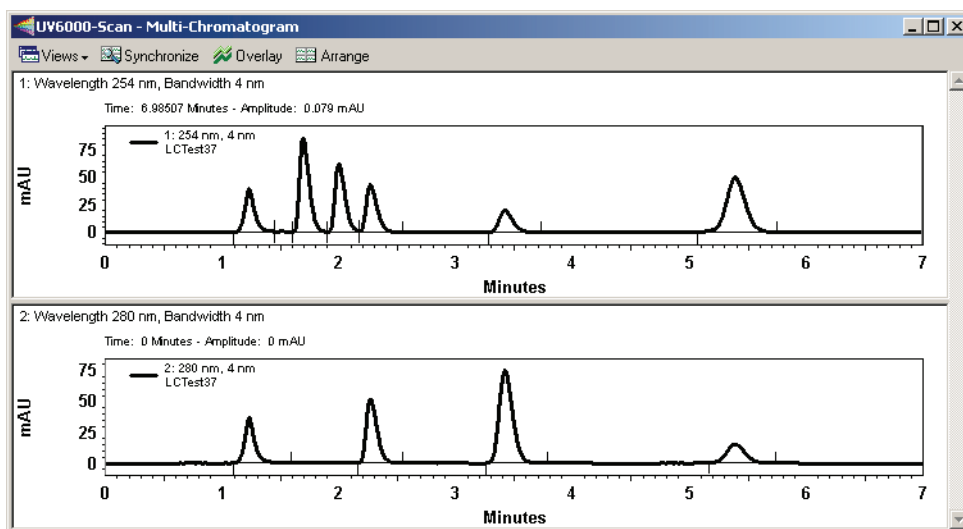
Spectrum View

This view displays the spectrum associated with a time point on the chromatogram. The spectrum displayed can be changed from the Mixed View by dragging the X-axis handle across the Contour plot.

Figure 104. Spectrum view
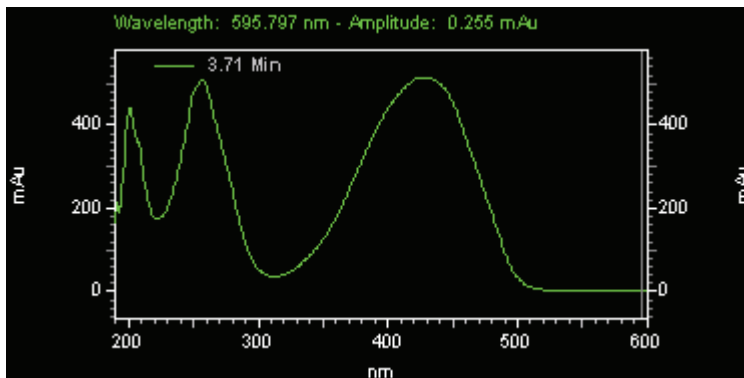
Right-clicking in the Spectrum view opens a shortcut menu that includes the following options:

- Spectrum Properties

  Right-click in the Spectrum view to display a shortcut menu. Then, choose properties to access the Data Graph Properties dialog box. The Data Graph Properties dialog box enables you to add another trace to the view, or change scaling. It also lets you selectively remove overlaid traces from the view.

- Spectrum Background Correction

  Select the right mouse click/Operations menu item to toggle the background correction on and off.

  If the current spectrum has been extracted from an integrated peak, select this option to correct the displayed spectrum for background based on the working chromatogram. Refer to the **"Spectral Analysis and Calculations"** on page 168 for details on how this calculation is performed.

  Background Correction may only be performed once on a spectrum. If a second background correction is attempted on an already corrected spectrum, a message box is displayed and the operation ignored.

  If the current spectrum has not been extracted from an integrated peak of the working chromatogram, selecting this menu item will have no effect on the spectrum.

  Background subtraction must always be the first operation performed on a spectrum. If a background correction is attempted on a spectrum after another operation has already been performed (including operation specified in the *Spectrum* tab of *Spectral Options*), a message box is displayed and the background correction request ignored.

- Interpolate Spectrum

  Select the **right-mouse click > Operations** menu item to toggle the interpolate option on and off.

  Selecting this menu item causes a 10:1 interpolation to be performed on the spectrum. Refer to the "Spectral Analysis and Calculations" on page 168 for details on how the values are computed.

- Export

  Selecting this menu item will display a *File Save As* dialog. When a valid filename is entered and Ok is pressed, the currently displayed spectrum is exported as an ASCII data file. Refer to Chapter 4, "Data and Graphics Export," for details on the data file format.

- Overlay Spectra

  You can overlay spectra using the **Actions > Overlay Spectra** command from the Mixed View toolbar. When you select this option, a dialog appears where you can enter the retention time from which you want to extract a spectrum. You can also overlay

spectra quickly by moving the wavelength cursor in the Contour or Chromatogram view to the desired wavelength. To remove the spectra you have added to the view, use the **Clear Overlays** command from the right mouse click menu in the Spectrum view. You can also clear selected spectra using the Trace Setup dialog accessed by doing a right mouse click in the view and then selecting Properties.

Figure 105. Overlay Spectra dialog box
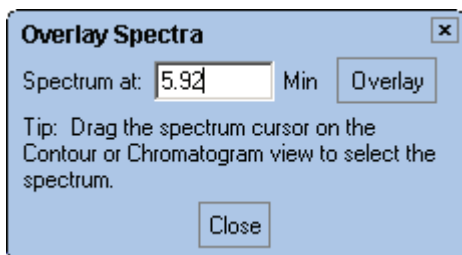
Ratio View

The Ratio view displays two spectral wavelength channels and the ratio of those two channels. These may be viewed during real-time acquisition as well as during post-run analysis. The flat tops on the ratio peaks are a preliminary indication of peak purity. The ratio wavelengths and parameters are set in the **Method >Spectral Options > Ratio** tab.

The Y-axis of the ratio chromatogram is auto-scaled to 1.

Figure 106. Ratio Plot view
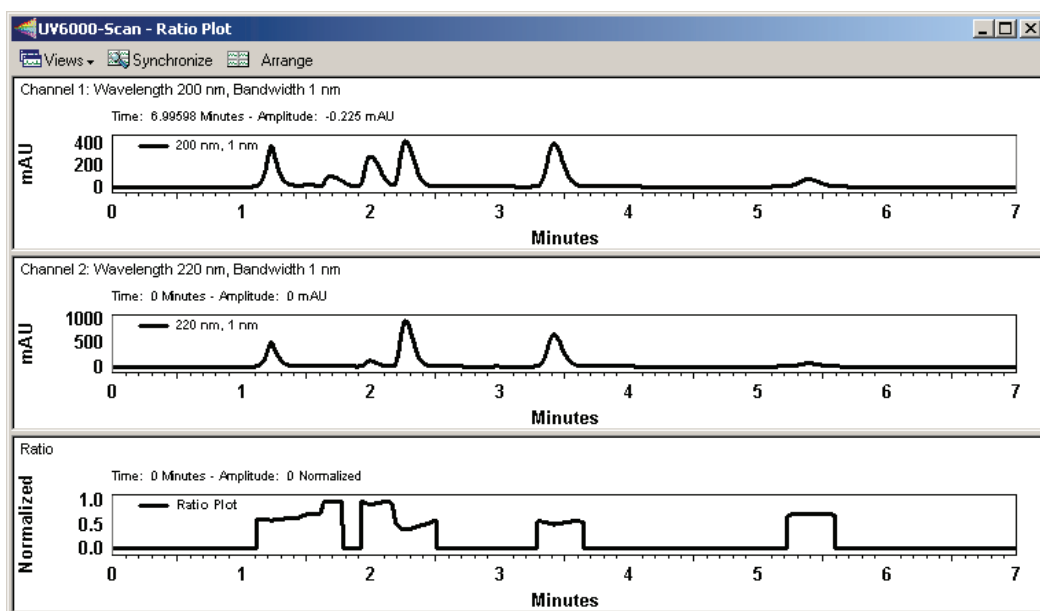
Right-click within the window to display the pop-up context menu. The context menu is the same as for a standard chromatogram graph window.

3D View

The 3D View provides a three-dimensional view of absorbance versus time and wavelength. Wavelengths of appreciable absorbance and interference, which may be invisible in a single wavelength plot, are easy to locate with the 3D View. The plot can be elevated and rotated around its axis for display from any angle.

Figure 107. 3D view
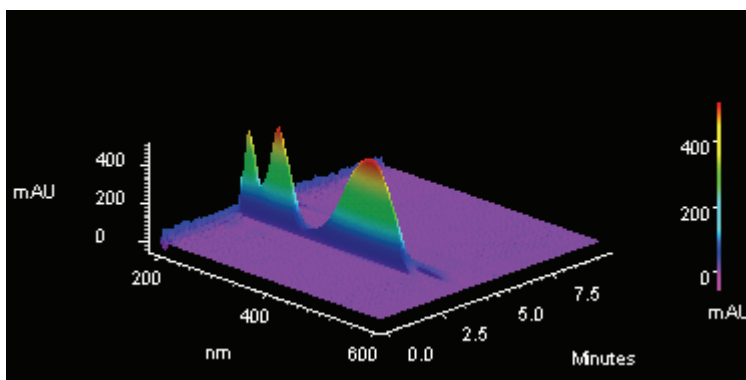
> **Note** During a run, the user must manually refresh this display. It does not update automatically.

Right-click inside the 3D view to display the pop-up menu that gives you access to plot rotation and axis setup features.

3D Plot movement selections

Click the type of plot movement you wish to use (elevate, roll, rotate, rotate XYZ, or spin). A checkmark appears next to the selected movement option. Once you have selected one of the options, you is returned to the plot and the cursor indicates the type of movement selected.

Figure 108. 3D Plot view
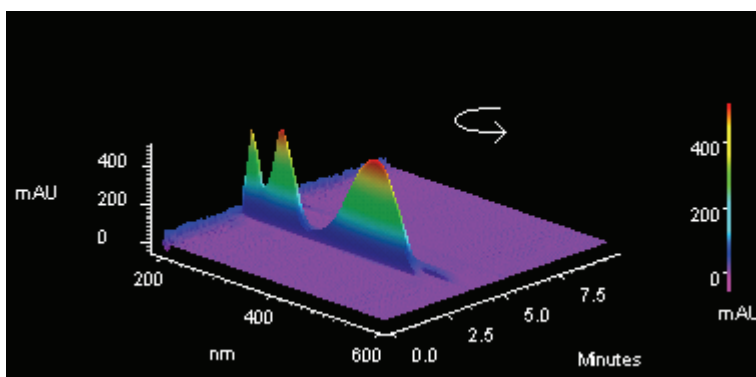
Hold down the left mouse button and move the cursor in the direction you wish to move the plot. The plot moves as you move the cursor. The movement option remains in effect until you turn it off. When finished, click the right mouse button, and de-select the movement option. If you wish to return to the original view, select the **Reset** command.

Note These values can be viewed or changed using the **3D > Properties** dialog.

3D Properties

This dialog allows you to set the properties of the 3D plot.

Figure 109. 3D Data Graphic Properties – General dialog box

Parameter	Description
Style	
Color or Grayscale	Select **Color** or **Grayscale** for the plot.
Wire Mesh	Checking the Wire Mesh box causes the data to be rendered as a wire frame plot, rather than as a solid fill plot.
Colors	
Range	Select how you want the coloration on the plot to appear. When **Light & Dark Range** is selected, alternating light and dark bands are used. When **Full Spectrum** is selected, then a continuous color spectrum is used.
Background	Select the color for the background of the plot.
Axes	Select the color for the plot axes.
Display	This specifies the relative quality of the displayed contour plot. Lower Display Detail results in faster drawing of the plot.
Print	This specifies the relative quality of the printed contour plot. Lower Print Quality results in faster printing.
Viewing	Use these fields to view current rotation settings, or to set them manually.
Light source	Selecting this option causes the plot to be shaded as if an external light source were shining upon it.
Rotation	This reports the current level of rotation (front to back) in the aspect position of the plot. When a new value is entered, the plot is redrawn to reflect the new value upon exiting the dialog.
Elevation	This reports the current level of tilt (forward or backward) in the aspect position of the plot. When a new value is entered, the plot is redrawn to reflect the new value upon exiting the dialog.
Roll	This reports the current level of roll (side to side) in the aspect position of the plot. When a new value is entered, the plot is redrawn to reflect the new value upon exiting the dialog.
Zoom	This reports the current level of magnification in the plot. When a new value is entered, the plot is redrawn to reflect the new value upon exiting the dialog.
Performance	
Use zoom/rotate bounding box	When this box is checked, the plot is temporarily replaced by a box during zoom and rotation operation. When the operation is completed, the plot is redrawn. Checking this box increases performance on computers with slower graphic subsystems.

Figure 110. 3D Properties – Zoom/rotate bounding box
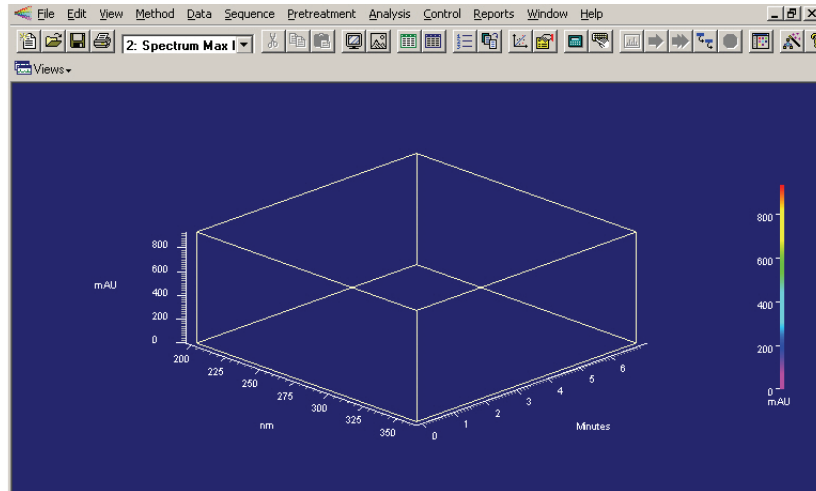
3D Properties Axis

This dialog lets you set up axis limits for your 3D plot.

Figure 111. 3D Data Graphic Properties – Axis Setup dialog box
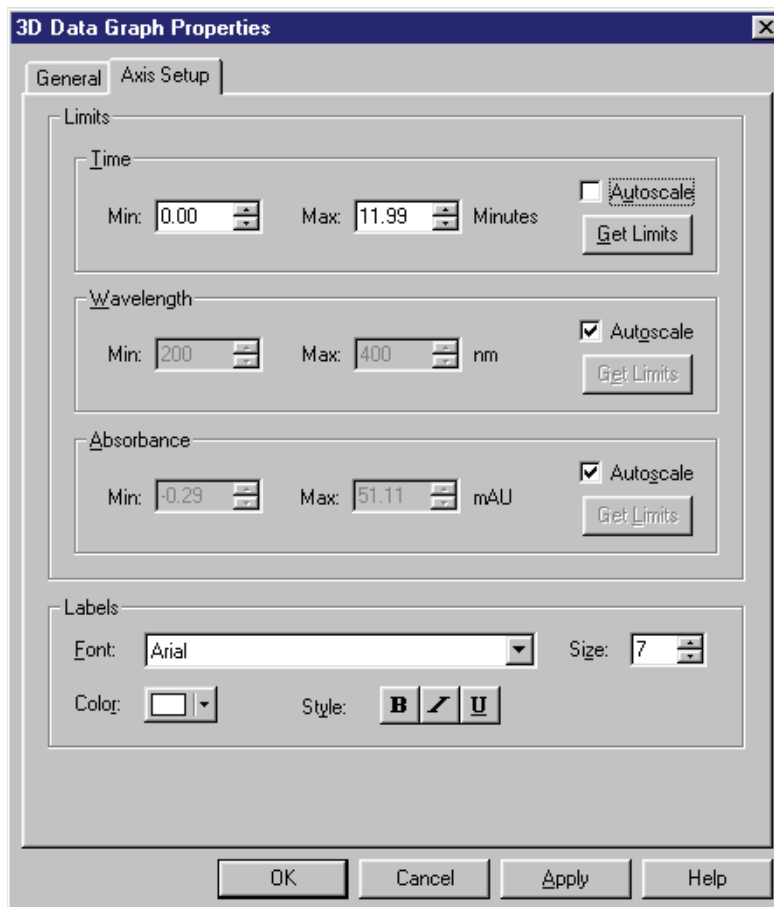
Parameter	Description
Limits	Enter the limits for the 3D plot.
Time	Select the **Autoscale** checkbox if you want to have the software automatically scale the time axis to the maximum values. To enter a manual range, de-select the **autoscale** box, and add your own limits, or click the **Get Limits** button to enter the limits displayed on the current 3D graph.
Wavelength	Select the **Autoscale** checkbox if you want to have the software automatically scale the wavelength axis to the maximum values. To enter a manual range, de-select the **autoscale** box, and add your own limits, or click the **Get Limits** button to enter the limits displayed on the current 3D graph.
Absorbance	Select the **Autoscale** checkbox if you want to have the software automatically scale the absorbance axis to the maximum values. To enter a manual range, de-select the **autoscale** box, and add your own limits, or click the **Get Limits** button to enter the limits displayed on the current 3D graph.
Labels	You can customize the labeling of the 3D plot using the parameters in this area. You can select font, size, color and style using the selections provided.

3D Plot Rotation Options

A right-click the 3d plot provides a menu containing various rotation options. When you select one of these rotation options, a checkmark appears next to the option and that rotation option becomes active on the plot.

Figure 112. 3D Plot Rotation Options menu

The cursor changes to indicate the option is in effect.

Figure 113. 3D Plot rotation
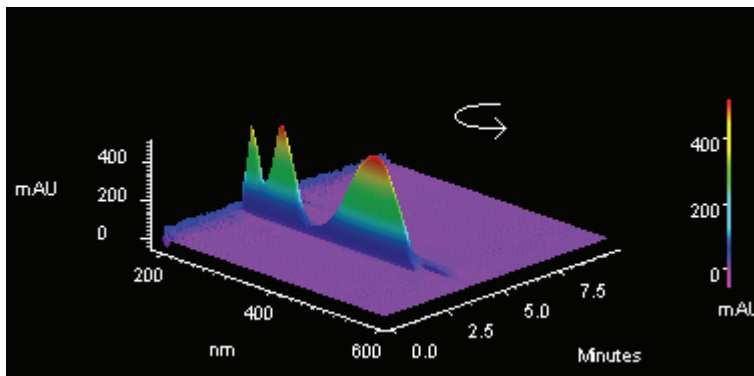
While the option is active, you can move the plot in the designated way by holding down the left mouse button and moving the mouse in the desired direction on the plot. When you have the plot in the desired position, click the right mouse button and turn off the option by selecting it again (checkmark removed). If you want to return to the original plot view, click the right mouse button and select **Reset**.

Contour View

The Contour Plot (also referred to as an Isoabsorbance Plot) provides an aerial view of the absorbance of the sample at each wavelength versus time. The contour view supplies quick and easy-to-assimilate information about those wavelengths at which the sample exhibits appreciable absorbance. With contour view, it is also possible to generate a Chromatogram View for an individual wavelength and a Spectrum View for a given point in time.

Figure 114. Contour view
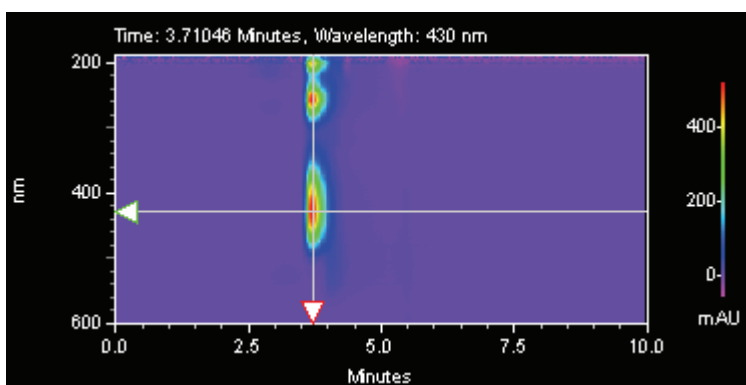
Right-click inside the window to display the pop-up menu. Select Properties to display the Contour Properties dialog box.

❖ **To generate a chromatogram view from contour view of Mixed View or Mixed View w/ 3D**

1. Choose **View > Spectral Views > Mixed View** to display the Contour Map, Chromatogram, and Spectrum.

2. Move the cursor to the triangle-shaped handle located on the left- hand wavelength axis of the Contour Map and press the left mouse button.

3. Drag the cursor up or down to the desired wavelength and release the mouse button.

4. The chromatogram associated with the specified wavelength is displayed in the Chromatogram View.

❖ **To generate a spectrum view from contour view of Mixed View or Mixed View w/ 3D**

1. Choose **View > Spectral Views > Mixed View** to display the Contour Map, Chromatogram, and Spectrum.

2. Move the cursor to the triangle-shaped handle located on the time axis of the Contour Map and press the left mouse button.

3. Drag the cursor to the desired peak and release the mouse button.

The Spectrum associated with the specified retention time value is displayed in the Spectrum View.

Contour Properties

A right mouse click anywhere on the contour plot, followed by selecting the **Properties** button displays a dialog where you can select the way the contour plot is displayed.

Figure 115. Contour Graph – General dialog box

Parameter	Description
Style	Select how you want the plot to appear, **Grayscale** or **Color**.
Colors	
Range	Use this to select how the coloration of the plot is to be displayed. When **Light & Dark Range** is selected, alternating light and dark bands are used. When **Full Spectrum** is selected, then a continuous color spectrum is used.
Background	Select the color to be used for the background of the plot.
Display	
Detail	This specifies the relative quality of the displayed contour plot. Less Display Detail results in faster rendering of the plot.
Print	
Quality	This specifies the relative quality of the printed contour plot. Coarse Print Quality results in faster printing.
Cursors	The values in these boxes reflect the current contour cursor positions. When you change the values, the cursors on the plot is changed when you exit the dialog or when you click the Apply button.
Time	This specifies the time position (X Value) of the cursor. When a value is entered, the X cursor is updated to the new position upon exiting the dialog.
Wavelength	This specifies the wavelength position (Y Value) of the cursor. When a value is entered, the Y cursor is updated to the new position upon exiting the dialog.
Bandwidth	This control specifies the wavelength band that is averaged when a chromatogram is extracted from the contour plot. The extracted chromatogram is an average of the absorbances at each wavelength in the wavelength band. The wavelength band is equal to the selected wavelength (see above) +/- one half of the bandwidth.

Contour Axis Setup

You can change the setup of the axes for the contour plot using this dialog. If the Autoscale box is selected, the software automatically sets the axis parameter. If you want to enter the parameter manually, de-select the Autoscale box, then enter the range values, or click the Get Limits button to bring in the limits from the current view.

Figure 116. Contour Graph – Axis Setup dialog box

Parameter	Description
Limits	
Time	Select the **Autoscale** checkbox if you want to have the software automatically scale the time axis to the maximum values. To enter a manual range, de-select the **autoscale** box, and add your own limits, or click the **Get Limits** button to enter the limits displayed on the current contour graph.
Wavelength	Select the **Autoscale** checkbox if you want to have the software automatically scale the wavelength axis to the maximum values. To Contour Axis Setup
Absorbance	Select the **Autoscale** checkbox if you want to have the software automatically scale the absorbance axis to the maximum values. To enter a manual range, de-select the **autoscale** box, and add your own limits, or click the **Get Limits** button to enter the limits displayed on the current contour graph.
Labels	You can customize the labeling of the contour plot using the parameters in this area. You can select font, size, color and style using the selections provided.

Spectral Utilities

The Utilities menu allows displayed spectra to be printed, copied, saved or exported. The Utilities menu is available from the right mouse click menus of various Spectral views.

- Print

  Select Print to automatically print the currently displayed spectra.

- Copy to Clipboard

  Select Copy to Clipboard to copy the displayed spectra to the Clipboard. The contents of the Clipboard may then be pasted into other software.

- Save trace

  Select Save trace to save the spectrum to a file with an .spc extension for later inclusion in a library or report.

Spectrum Similarity Table

The Spectrum Similarity table is displayed in the PDA Mixed View when the Options Mode is set to Show Spectrum Similarity Table. Spectra are automatically added to and deleted from this table whenever a spectrum is added to and deleted from the Spectrum pane of the Mixed View.

Figure 117. Spectrum Similarity table

Parameter	Description
Spectrum Name	This column displays identifications for each of the spectra added to the table. For spectra extracted from the 3D data, the identification includes the time. For spectra extracted from a chromatogram based on a peak name, the identification includes the peak name. For spectra loaded from a file, the identification includes the retention time. A check mark next to the colored line for a spectrum indicates that the spectrum serves as the Reference Spectrum for the similarity calculation. Spectra may be added to the table in the Mixed View by selecting the **Add to Similarity Table** from the **Actions** button menu.
Similarity	This column displays the similarity of the spectrum on that row relative to the Reference Spectrum. The Reference Spectrum is determined by double-clicking on a row of the table or by highlighting a row and pressing the 'Set Reference' button. Until a reference spectrum has been selected the similarity for all spectra in the table is zero. Refer to the **"Spectral Analysis and Calculations"** on page 168 for details on how this calculation is performed.

Parameter	Description
Spectrum Source	This column displays the source of the spectrum. (Current Data) refers to working spectra extracted form the current 3D data. When spectra come form a stored data file, this column displays the source filename.
Set Reference	Pressing this button designates the spectrum in the currently highlighted row of the table as the new reference spectrum. The similarities for all of the rows is recalculated based on the new reference spectrum.
Print	Pressing this button outputs a simple text report representation of the table to the default printer.
Properties	Pressing this button displays a dialog with parameters related to the calculation of similarity.

Similarity Table Properties

Enter the wavelength range and data point spacing (in nm) for similarity calculations.

Figure 118. Similarity Table Properties dialog box
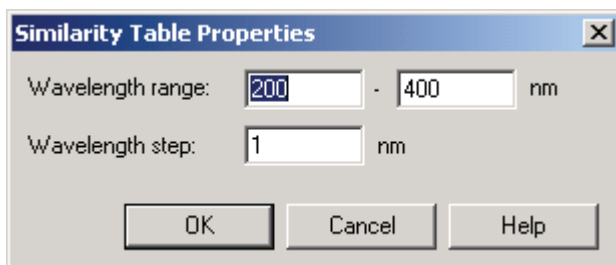
Note During analysis, it is possible that a portion of this wavelength range is outside the range of the acquired data. In that case, the wavelength range is truncated to the limits of the acquired data.

Spectral Library Definition

This window appears when you choose the **File > Spectral Library > New** command. It is used to define a spectral library that can be used with the Library Search option. In order to define a library, you must have spectrum files (.spc) on your datasystem PC or you can create a library from the spectra obtained during the current run.

Figure 119. Spectral Library Definition dialog box

Parameter	Description
Spectrum Data Source	Click the arrow ⬇ in this field to select **Current Data, Spectrum File**, or **Named Peak**.
	To add a spectrum from a spectrum file, the spectrum must have been previously saved as a file with an .spc extension. You can create spectrum files from your current data file by choosing the **Utilities > Save Trace** command from the pop-up menu in the Spectrum pane.
	If you chose to enter a spectrum from the current data file, a dialog appears where you must type the retention time from which you want the spectrum extracted.
Component Name	Enter the chemical name or description of the spectrum. This field is used for display and search pre-filter purposes.
Lambda Max From ... To	The wavelength range of the spectrum over which the software calculates the lambda (absorbance) max value is displayed in these columns.
Retention time	When the spectrum was extracted from a chromatographic run, the software automatically identifies the retention time of the spectrum and enters the value in this field. When desired, the value in this field may be edited. This field can also be used as a search pre-filter.
Comment	Enter any descriptive information desired related to the spectrum. This field is used only for display and documentation purposes.
Library notes	This field is used to document relevant information about the library as a whole, e.g., documentation about run conditions or general sample information.

Note Fields in existing library entries may be edited by selecting the fields with the cursor. Right-click a row in the library table to display a pop-up menu used to cut, paste, copy, and insert and delete lines from the library as necessary.

Spectrum Information

If you chose to enter a spectrum into your library from the current data file, this dialog appears where you must select the retention time at which you wish to select the spectrum.

Figure 120. Spectrum Information – Spectrum at Retention Time dialog box
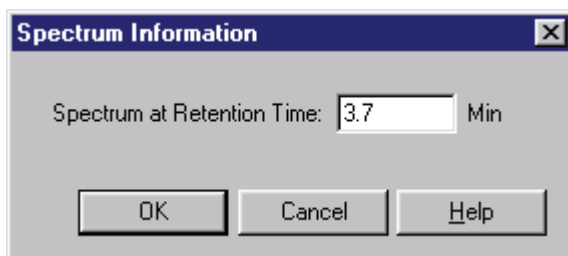
Figure 121. Spectrum Information – Named peak dialog box
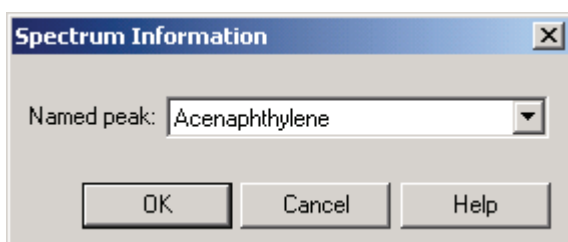
How to Collect Spectra for a Library

❖ **To collect spectra for a library**

1. Perform an acquisition using a sample with known components or standards to be placed in the library.

2. Perform an analysis using the appropriate integration parameters. (Ideally, Spectral Background Correction would be checked in the **Method > Spectral Options > Spectrum** tab.)

3. Using the contour plot in the Mixed View window, drag the vertical cursor to the apex of a peak to display the corresponding spectrum in the spectrum view (Figure 122). See also "Contour View" on page 146.

4. Right-click within the spectrum view to display the Spectrum pop-up menu, choose **Utilities > Save Trace,** and enter a file name in the dialog box. Repeat this procedure for each spectrum to be added to the library. Files are saved automatically with the .spc extension.

Note To add the 1st or 2nd Derivative of a spectrum to the library, select the appropriate filter in the **Method > Spectral Options > Spectrum** tab and repeat steps 3 and 4.

How to Add Spectra to a Library

❖ **To add spectra to a library**

1. When all of the spectra are saved as .spc files, choose **File > Library > New** to display the Library Definition dialog box and create a new library. Alternatively, choose **File > Library > Open** to add spectra to an existing library.

2. Click in the Spectrum File cell of row 1 to display the Open dialog box. Double-click the appropriate .spc file in the list box. The .spc file name is entered into that cell and the associated spectrum is simultaneously displayed. A component name and comment may be entered in the appropriate columns. Repeat this procedure with subsequent rows in the table until all spectrum files are entered into the library.

3. **Choose File > Library > Save As** and enter a name for the library. The .lib extension is automatically appended.

How to Perform a Manual Library Search

❖ **To perform a manual library search**

1. In the Contour map of the Mixed View window, drag the vertical cursor to the apex of the peak of interest to display the corresponding spectrum in the spectrum pane.

2. Choose **Actions > Search library.** Click either **Method** to use the library parameters from the method, or **Quick** to enable you to modify the search parameters. Before you do the search, make sure you have either selected a library in your method, or have opened a library to do a quick search.

   Click **Search Now** to display the Library Search Results window, showing the three closest matches in the specified library. When appropriate, click the **>>** or **<<** button to display additional matches.

Spectral Library Search

This window appears when you choose the **Actions > Search Library** command from the Mixed View window. It allows you to perform a library search on a spectrum you have selected in the contour map, and also lets you select a spectrum from the current data or stored spectrum file to search.

Figure 122. Spectral Library Search – Params dialog box
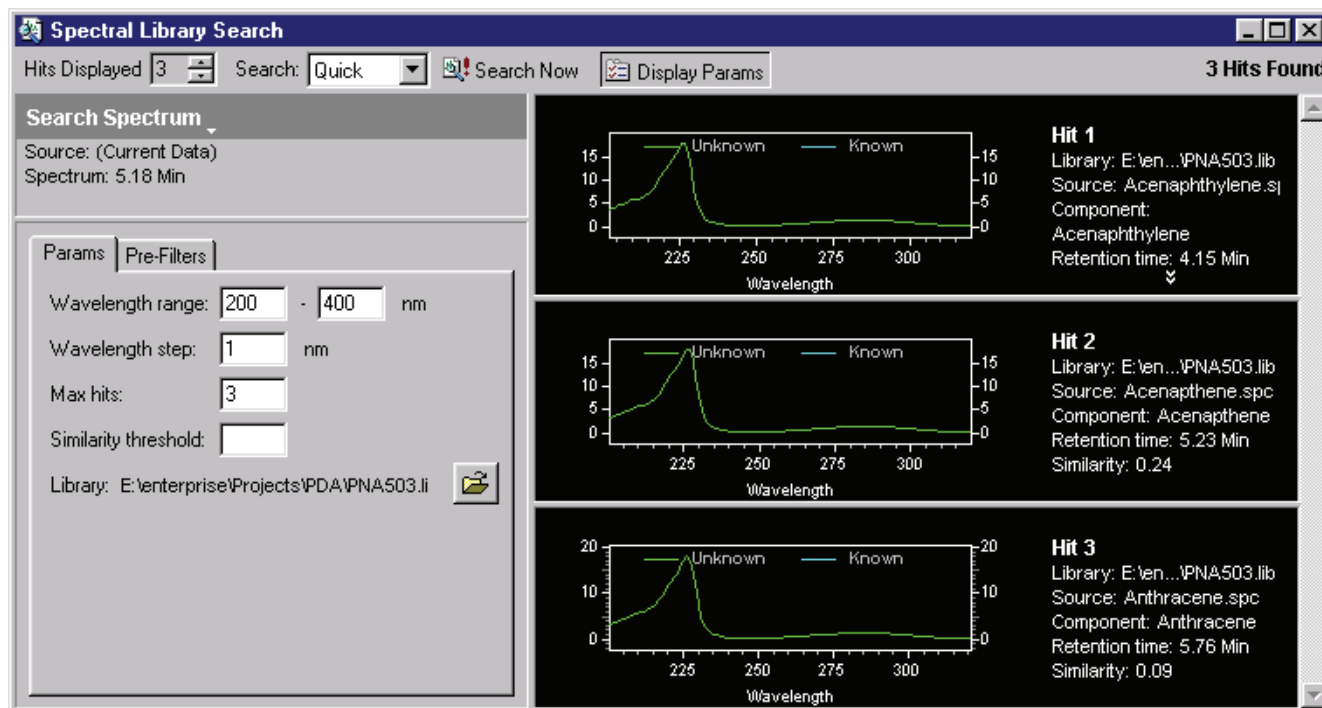
Parameter	Description
Hits Displayed	Select the number of hits you wish to display. Hits is displayed in order of similarity.
Search	Select **Method** if you want to use the parameters from the current method for your search. Select **Quick** if you want to enter or change the parameters yourself before the search.
Search Now	When you click this button, a library search is performed on the selected spectra using the parameters, and the number of hits requested is displayed.
Display Parameters	Click this button if you want to display the parameters. If you always use the method parameters, you may not wish to display them when you search.
Search Spectrum	Click the arrow to select a new spectrum to search on. You can choose from the current data, or from a stored spectrum file. The current spectra source is displayed.

Parameter	Description
Search Parameters	This tab contains search parameters. If you have elected to use the Method search parameters, the parameters displayed are those in your current method in the **Spectral Options > Library** tab. If you have elected to do a Quick search, the parameters are default parameters. • Wavelength range These specify the wavelength range over which the library search is performed. • Wavelength step This specifies the data point spacing to be used when a library search is performed. • Max hits This specifies the number of hits that is reported in the results of a library search. Note that this works in conjunction with the *Similarity Threshold* parameter to limit the number of hits reported. • Similarity threshold Specifying a value for this control will cause the library search results to only display matches whose similarity to the unknown exceeds this value. Note that this control works in conjunction with the *Max Hits* parameter to limit the number of hits reported. • Library Displays the library from the method or for Quick enables you to select a library to be used.

Parameter	Description
Pre-Filters	When *Quick* is selected as the *Search* Mode, the items on this tab allow the user to specify search pre-filters that is performed on library spectra prior to the test for similarity. All pre-filters are optional. If *Method* is selected as the *Search* Mode, the items on this tab are read-only and reflect the parameters values on the *Library* tab of *Spectral Options*.

- Retention time range

  When a Retention Time Range is specified, library search is restricted to those library entries whose retention time is within the specified range. Entries outside this range are automatically excluded from the search (no similarity calculation is made). Entering a value for this is optional.

- Lambda max

  When one or more of these values is specified, library search is restricted to those library entries containing a lambda max within 5 nm of one of the specified values. Entries without a matching lambda max are automatically excluded from the search (no similarity calculation is made). Entering values for this is optional.

- Compound name filter

  When a Compound Name Filter is specified, library search is restricted to those library entries whose name contains the specified string as a case-insensitive sub-string. Entries without a matching sub-string are automatically excluded from the search (no similarity calculation is made). Entering a value for this is optional.

Custom Report

A variety of spectral information can be placed in a custom report. These items are inserted in the report by placing the cursor at the location where you want to insert the item, then do a right mouse click to access the custom report menus.

Spectral Insert Graph Items

The Insert Graph menu has the following additional items available when the Spectral Option is enabled: 3D Data Graph, and Contour Graph.

3D Data Graph

The 3D View provides a three-dimensional view of absorbance versus time and wavelength. Wavelengths of appreciable absorbance and interferences, which may be invisible in a single wavelength plot, are easy to locate with the 3D View. Select this function to automatically enter the 3D map into the report. Click the right-mouse button within the 3D map and select Properties to display the 3D Properties dialog box and enter appropriate changes

The 3D map can be elevated and rotated around its axis for display from any angle. These functions work the same as in the 3D view window.

Insert Contour Graph

A data file containing Spectral data may include a Contour Plot in a custom report. The contour view (also referred to as Isoabsorbance plot) provides an aerial view of the absorbance of the sample at each wavelength vs. time. The contour view supplies quick and easy-to-assimilate information about those wavelengths at which the sample exhibits appreciable absorbance.

Changing parameters for the contour graph in a custom report works exactly as in the Contour view.

Spectral Insert Report Items

When the Spectral option is enabled, the following report items are available to insert into a custom report: Library Search Report, Purity Report, and Spectrum Report.

Library Search Report

To insert a Library Search Report, right-click in the custom report. Then choose **Insert Report > Library Search Report** from the popup menu. This command inserts a table of library search results in your custom report.

To modify the parameters of the report, right-click in the Library Search Report table, and select **Properties**. Figure 123 is an example of the dialog box that appears.

Figure 123. Library Search Report Properties dialog box

Parameter	Description
Search Libraries for	This specifies what peaks should be searched for the report.
Apex spectra of peaks	When selected, the Specific Spectrum button is disabled.
	• Detected on
	This allows the user to select the channel or channels from which peaks are detected.
	• Limit to named peaks only
	This allows the user to restrict the peak selection (made above) to a time range. When checked, only peaks within the specified time range is searched When this box is unchecked, the Time Range edit fields are disabled.
	• Limit to time range
	This allows the user to restrict the peak selection (made above) to a time range. When checked, only peaks within the specified time range is searched. When this box is unchecked, the Time Range edit fields are disabled.
	• Time range
	This allows the user to restrict the peak selection (made above) to a time range. When the *Limit to time range* box is unchecked, these fields are disabled.
A specific spectrum	When selected, the other controls of this group are disabled.
	Pressing this button displays a menu allowing the user to specify the spectrum to be searched. The menu allows you to specify a spectrum based on one of the following choices: Current Data, Named File, or Spectrum Peak.
Spectral display	The in this group specify the layout of the search results graphs.
Graph height	This specifies the relative height of a search results graph. A value of 100% corresponds to a standard sized graph. A larger value may be selected to provide more a detailed plot.
Graph Properties	Pressing this button displays the graph properties dialog as found on the standard Spectrum graph.

Library Definition Report

Selecting this option inserts a Library Definition Report into your custom report. To specify parameters for the report, do a right-click in the report table, and then select **Properties**. Figure 124 is an example of the dialog box that appears.

Figure 124. Library Definition Report Properties dialog box
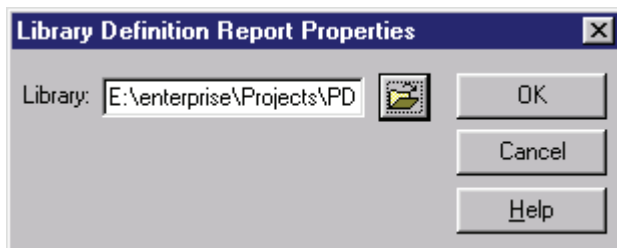
Enter or select the library you wish to include in the report, and then click **OK**.

Purity Report

Selecting this option inserts a Purity Report into your custom report. To specify parameters for the report, do a right-click in the report table, and then choose **Properties**. Figure 125 is an example of the dialog box that appears.

Figure 125. Purity Report Properties dialog box
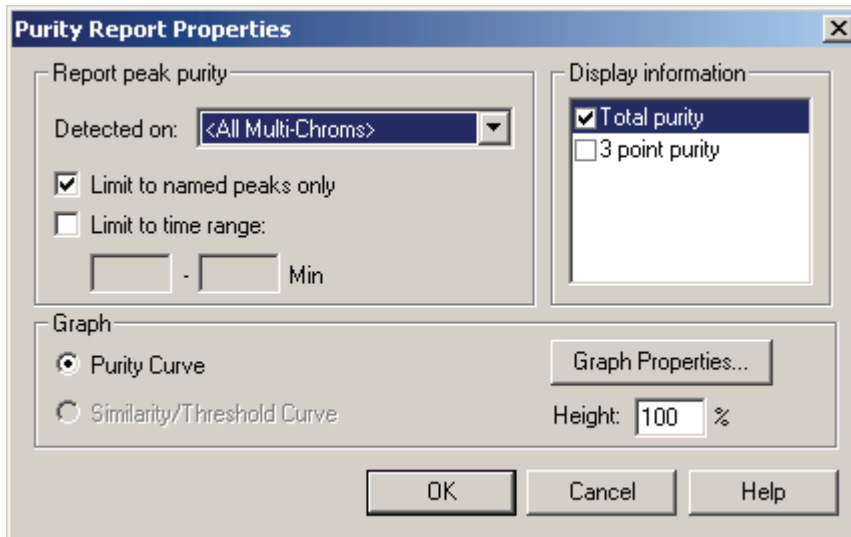
Parameter	Description
Report peak purity	
Detected on	This allows you to select the channel or channels from which peaks are detected.
Limit to named peaks only	This allows you to restrict the peak selection (made above) to a time range. When checked, only peaks within the specified time range is searched When this box is unchecked, the Time Range edit fields are disabled.
Limit to time range	This allows the user to restrict the peak selection (made above) to a time range. When checked, only peaks within the specified time range is searched. When this box is unchecked, the Time Range edit fields are disabled.
Time range	This allows the user to restrict the peak selection (made above) to a time range. When the *Limit to time range* box is unchecked, these fields are disabled.
Graph	
Graph Properties	Pressing this button displays the graph properties dialog as found on the standard graph.
Height	This specifies the relative height of a search results graph. A value of 100% corresponds to a standard sized graph. A larger value may be selected to provide more a detailed plot.

Spectrum Report

The Spectrum report displays a table showing spectra extracted from peaks of the chromatogram. Based on the selection on the *Spectrum* tab of *Spectral Options*, the report contains either the apex spectrum, an average of the upslope, apex and downslope spectra, or several averaged spectra. To set parameters for this report, right-click the table. Then, choose **Properties**. Figure 126 is an example of the dialog box that appears.

Figure 126. Spectrum Report Properties dialog box
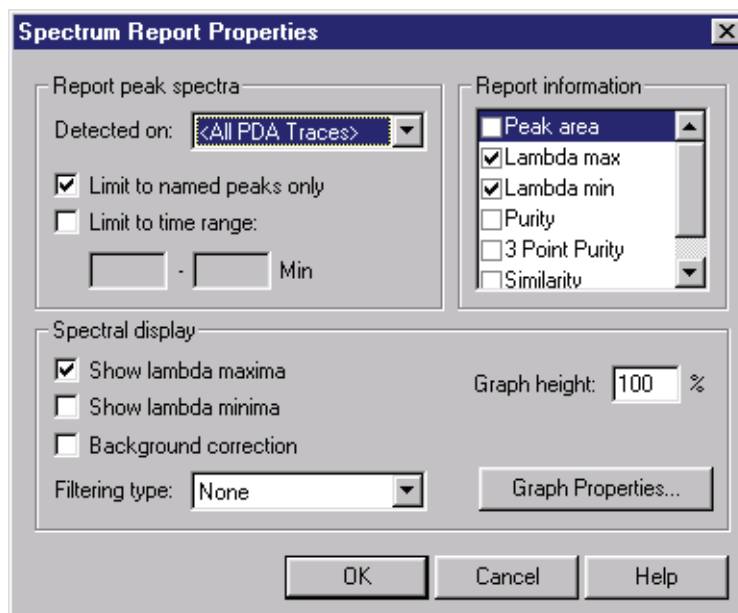
Parameter	Description
Report peak spectra	
Detected on	This allows you to select the channel or channels from which peaks are detected.
Limit to named peaks only	This allows you to restrict the peak selection (made above) to a time range. When checked, only peaks within the specified time range is searched When this box is unchecked, the Time Range edit fields are disabled.
Limit to time range	This allows the user to restrict the peak selection (made above) to a time range. When checked, only peaks within the specified time range is searched. When this box is unchecked, the Time Range edit fields are disabled.
Time range	This allows the user to restrict the peak selection (made above) to a time range. When the *Limit to time range* box is unchecked, these fields are disabled.

Parameter	Description
Report information	Checking any of these controls indicates that the indicated value is calculated and printed to the right of the graph. Deselecting options that are not of interest speeds up analysis.
Peak area	Checking this indicates that the peak area should be printed to the right of the spectrum graph.
Lambda max	Checking this indicates that the three largest lambda max values should be printed to the right of the spectrum graph.
Lambda min	Checking this indicates that the three largest lambda min values should be printed to the right of the spectrum graph.
Purity	Checking this indicates that total peak purity should be printed to the right of the spectrum graph.
3 Point Purity	Checking this indicates that 3-point peak purity should be printed to the right of the spectrum graph.
Similarity	Checking this indicates that peak apex similarity to the reference spectrum should be printed to the right of the spectrum graph. The use of this value requires that a reference spectrum be included in the peak table. See Spectral Analysis and Calculations for details.
Spectral display	The controls in this group specify the content and labeling of the spectrum graphs.
Show lambda maxima	Checking this box annotates each spectrum graph with the three largest lambda max absorbance.
Show lambda minima	Checking this box annotates each spectrum graph with the three largest lambda minima absorbance.
Background correction	Checking this option causes each apex spectrum to be corrected for background using the chromatographic baseline prior to being used elsewhere in analysis. Refer to "Spectral Analysis and Calculations" on page 168 for details on the formula used.
Filtering type	This allows the user to specify a mathematical filtering function to be performed on all spectra extracted from the 3D data during analysis. Refer to "Spectral Analysis and Calculations" on page 168 for details on the formula used for each filter.
Graph height	This specifies the relative height of the spectrum graph. A value of 100% corresponds to a standard sized graph. A larger value may be selected to provide more a detailed plot.
Graph properties	Pressing this button displays the graph properties dialog as found on the standard Spectrum graph.

Peak Table

When using the Spectral option, certain columns are added to the peak table that enable you to analyze peaks from the PDA or scanning detector.

There is one Peak/Group Table per detector. To analyze a peak at multiple wavelengths, you must enter the peak multiple times in the Peak Table, and then select the appropriate Analysis Channel for each entry.

For convenience, you might want to label each entry for a peak with a distinguishing label that helps you identify its associated Analysis Channel.

Figure 127. Peak table

Parameter	Description
Detection	Select the basis for the identification of the peak. If you select **Ret Time**, only the retention time is used for identification of the peak. If you select **Ret Time with Spectral Confirm**, the Similarity of the peak's spectrum to that of a designated reference spectrum is 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 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.

Parameter	Description
Analysis Channel	Specify which wavelength channel is to be used for analysis of the peak. The choices are those specified in method for the detector and shown in the Analysis Channel list box. For the PDA detectors, you can analyze data on any of the multi-chromatogram channels within the scan range, as well as the three discrete channels.
	The following detectors are capable of performing scans:
	• SpectraSYSTEM UV3000 scanning detector
	• SpectraSYSTEM UV6000 photo-diode array detector
	• Surveyor PDA detector
	• Surveyor PDA Plus detector

Spectral Analysis and Calculations

This section describes the various types of calculations that are related to spectral data and how the data is analyzed.

General

In order to maintain accuracy during the application of multiple operations, all calculations are performed using double-precision floating-point numbers.

Chromatograms Extracted from the 3D Data

Two types of chromatograms may be extracted from the 3D data:

• Multi-Chromatogram Channels

  One or more chromatograms defined on the *Multi-Chromatogram* tab of *Spectral Options*.

• Working Chromatogram

  A single chromatogram extracted from the Contour plot on the *Mixed View* display. (This chromatogram is displayed in the *Chromatogram* View).

Specific Analysis-related capabilities for these chromatograms are detailed below.

Multi-Chromatogram Channels

The following apply to multi-chromatogram channels:

- In the Channel Selection drop down list, each multi-chromatogram channel has a unique identifier that includes the wavelength and bandwidth of the channel.

- Each Multi-Chromatogram Channel has a separate Integration Events Table and Manual Integration Fixes Table associated with it.

- All Multi-Chromatogram Channels and discrete channels share a common peak and group table, a common Export tab, and a common Column/Performance tab. Within the peak and group tables, any channel can be selected as the analysis channel for quantitative information.

- When an analysis is performed, all multi-chromatogram channels are automatically analyzed.

- Each multi-chromatogram channel is an average of the absorbances monitored at each wavelength in the wavelength range. The wavelength range is equal to the selected wavelength +/- one half of the bandwidth.

Working Chromatogram

The following apply to the working chromatogram:

- In the Channel Selection drop down list, a single entry is added that identifies the channel as applying to the working chromatogram.

- This channel has a separate Integration Events Table and Manual Integration Fixes Table.

- When an analysis is performed, the working chromatogram is automatically analyzed.

- The working chromatogram is an average of the absorbances monitored at each wavelength in the wavelength range. The wavelength range is equal to the selected wavelength +/- one half of the bandwidth.

- The working chromatogram is not available as a trace in Custom Reports.

Spectra Extracted from the 3D Data

Two types of spectra may be extracted from the 3D data:

- Analysis Spectra

  One or more spectra automatically extracted from the 3D data during analysis and used for peak identification, similarity and/or library search.

- Working Spectrum

  A spectrum extracted from the Contour plot on the *Mixed View* display. (This chromatogram is displayed in the *Spectrum* View)

Specific Analysis-related capabilities are for these spectra are detailed below.

Analysis Spectra

The following applies to the analysis spectra:

Prior to being used elsewhere, all spectra extracted from the 3D data are filtered according to the settings on the *Spectrum* tab of *Spectral Options*.

Working Spectrum

The following apply to the working spectrum:

Working spectra extracted from the 3D data are never filtered according to the settings on the *Spectrum* tab of *Spectral Options*.

The working Spectrum is not available as a trace in Custom Reports.

Spectrum Operations

The following table describes what operations can be done on what type of spectra.

Available Operations	Raw Spectra (no filtering or operations)	Smoothed, 1st Derivative and 2nd Derivative Spectra	Interpolated Spectra
Search against Libraries	Yes		
Similarity	Yes		
Peak Identification using spectral confirmation	Yes, but generate an error if the operations that were performed on the reference spectrum do not match the current method.		
Appear in Reports	Yes	Yes, but label must include what operations were performed	
Purity	Yes	No	
Add to Spectrum Library	Yes		No

Background Correction

Background Correction may only be performed on a spectrum by using the settings on the *Spectrum* tab of *Spectral Options*, or the settings on the *Purity* tab of *Spectral Options*, by selecting **Operations > Background Correction** from the Spectrum View context menu or by setting the properties of the Spectrum Report.

Background subtraction is always the first operation performed on a spectrum. If a background correction is attempted on a spectrum after another operation has already been performed (including an operation specified in the *Spectrum* tab of *Spectral Options*), a message box is displayed and the background correction request ignored.

Background subtraction can only be performed once on a spectrum. If a second background correction is attempted on a spectrum after the operation has already been performed (including the operation specified in the *Spectrum* tab of *Spectral Options*), a message box is displayed and the background correction request ignored.

❖   **To perform background correction**

1. The spectra from the baseline start and baseline stop times for the peak are extracted from the 3D data. The Max Plot is used to determine the peak that is used.

2. For each spectrum in the peak, a corresponding background spectrum is generated by linear interpolation between the baseline start and baseline stop spectra.

3. These background spectra are subtracted from the original spectra.

Spectrum Interpolation

Spectrum interpolation can be performed on a spectrum by choosing the appropriate settings on the *Spectrum* tab of *Spectral Options* or by choosing **Operations > Interpolate** from the Spectrum View context menu.

Interpolation can only be performed once on a spectrum. If a second interpolation is attempted on a spectrum after the operation has already been performed (including the operation specified in the *Spectrum* tab of *Spectral Options*), a message box is displayed and the interpolation request is ignored.

Interpolated spectra can not be stored in spectrum libraries.

The calculation is performed by doing a 10:1 interpolation of the spectrum data points using a cubic spline curve fit. This interpolation is performed after the applying any spectral filtering option (1st derivative, 2nd derivative or smooth) to the spectrum.

Spectrum Smoothing

Spectrum smoothing can be performed on a spectrum by choosing the appropriate settings on the *Spectrum* tab of *Spectral Options* or by choosing **Operations > Smooth** from the Spectrum View context menu.

Interpolation can be performed repeatedly on a spectrum.

The calculation is performed by doing a 9-point Savitsky-Golay smooth on the spectrum data points.

Spectrum Derivatives

Calculation of the 1st and 2nd derivatives of a spectrum can be performed on a spectrum by choosing the appropriate settings on the *Spectrum* tab of *Spectral Options* or by choosing **Operations > Smooth** from the Spectrum View context menu.

Derivatives can be computed repeatedly on a spectrum.

The absorbance values of the 1st derivative of a spectrum are computed by calculating the differences between adjacent absorbance values to create a new spectrum. The 2nd derivative of a spectrum is defined as the 1st derivative of the 1st derivative of the spectrum.

Upslope and Downslope Spectra

The upslope and downslope spectra of a peak are identified by calculating the second derivative of the portion of the chromatogram containing the peak. The two times at which the second derivative plot crosses zero are known as the inflection points. For normal peaks (i.e. non-Negative peaks), the Upslope Spectrum is the spectrum at the time represented by the first inflection point, while the Downslope Spectrum is the spectrum at the time represented by the second inflection point.

Library Search Calculations

General

During analysis, if one or more search libraries are defined on the *Library* tab of *Spectral Options*, then an automated library search is performed on every integrated peak of every spectral analysis channel.

> **Note** Unless a *Library Search Results* object is part of the method custom report, no automated library searching will done when analysis is performed.

In this section, a *Query Spectrum* is defined the unknown spectrum that is being searched. A *Reference Spectrum* is defined as a spectrum from a spectrum library file.

During a search, the apex spectrum of the peak (the query spectrum) is compared to each spectrum contained in the libraries (reference spectra) to determine the similarity of the query spectrum to the reference spectrum. The similarity is quantified through the calculation of a Similarity Index for each query/reference pair. The Similarity Indices are used to generate a hit list of the best matching entries. A perfect match will have a Similarity Index of 1.0000. Similarity indices less than 1 indicate differences in the spectral patterns.

If the query spectrum and the reference spectrum have different wavelength ranges, then the intersection of the two ranges is used in the similarity calculation.

If the query spectrum and the reference spectrum have different wavelength steps, then the higher resolution spectrum is de-resolved to match the other spectrum before being used in the similarity calculation.

Pre-Filters

A pre-filter is a criterion on a reference spectrum that must be met before that spectrum is used in similarity calculations. One or more pre-filters may be specified in the search parameters. When multiple pre-filters are specified, a reference spectrum must meet all of the individual pre-filters in order to be considered for similarity calculations.

Reference spectra that do not meet all of the pre-filter criteria are automatically excluded from calculations and from being a candidate for a hit list. No similarity calculation is performed on these spectra.

The following pre-filters are supported:

- Retention Time Range

  When a Retention Time Range is specified, a reference spectrum is excluded unless the retention time for the spectrum in the library is within the specified range.

- Lambda Max

  Up to three Lambda Max values may be specified. When one or more Lambda Max values are specified, a reference spectrum is excluded unless all of the specified maxima are within 5 nm of a maxima for the spectrum in the library.

- Compound Name

  When a Compound Name is specified, a reference spectrum is excluded unless the specified string is a case-insensitive sub-string of the compound name for the spectrum in the library.

Ratio Chromatogram Calculation

The ratio chromatogram plot consists of data points calculated as follows:

$$\text{Ratio Pt.} = abs_1 \,/\, \text{sqrt}\,(abs_1 * abs_1 + abs_2 * abs_2)$$

where

abs_1 = the absorbance in chromatogram 1 at this wavelength

abs_2 = the absorbance in chromatogram 2 at this wavelength

If the absorbance of any point in chromatogram 1or chromatogram 2 is less than the threshold, the Ratio Pt. for that wavelength is set to 0.

Similarity Calculations

The Similarity Index (SI) compares two spectra across the wavelength range defined in **Method > Spectral Options > Library**. A Library Search is performed using the Similarity Index, determined as follows:

$$\text{Similarity} \; = \; \text{Sum}(C_i * C'_i) \; / \; (n-1)$$

where

$$C_i = (S_i - \text{Avg}(S)) / \text{StdDev}(S)$$

$$C'_i = (S'_i - \text{Avg}(S')) / \text{StdDev}(S')$$

n is the number of points, **S** is one of the spectra, and **S'** is the other spectrum.

Note that each spectral data point is first reduced by the amount of the average of all data points in the spectrum. This is called mean-centering. Each data point is also divided by the standard deviation of all data points in the spectrum, which has the effect of normalizing the resulting values (scaling them to the range of zero to one). So, in the above equations, **C** and **C'** are the *normalized mean-centered spectra*.

Lambda Max/Min Calculations

A lambda max (min) is defined as a local maximum (minimum) of the absorbance values of a spectrum. The user must define the wavelength range over which the calculation should be performed.

To compute *n* lambda max (min) values for a spectrum, the software finds the *n* local maxima (minima) with the largest (smallest) absorbance values.

Peak Purity Calculations

The purity of a peak is calculated by comparing the every spectrum to the apex spectra using the similarity calculation. Only those spectra that meet the Threshold and Peak Coverage criteria selected in the settings on the *Purity* tab of *Spectral Options* is used for the calculation of peak purity. The lowest value is reported as the peak purity value.

If the peak is pure, or at least homogenous, all spectra across the peak should be identical after normalization. In this case, the peak purity value would be 1.000. Normally "pure" peaks have a peak purity value of 0.990 to 1.000, but this is only a probability as the purity value depends on a number of factors. These factors include the similarity of the spectra of the compound of interest and any impurity, the concentration levels of each impurity, the resolution between possible peak components and the accuracy of the integration as well as the relative molar absorbtivity of between the compound and each impurity.

Peaks with purity values below 0.950 have a high probability of being impure. Peaks with values between 0.950 and 0.990 can be suspected of being impure, but more experiments are needed. Peaks with values above 0.990 are probably pure, subject to the limitations of the technique.

Background Correction

Background Correction may only be performed on a spectrum by using the settings on the *Spectrum* tab of *Spectral Options*, or the settings on the *Purity* tab of *Spectral Options*, by selecting **Operations > Background Correction** from the Spectrum View context menu or by setting the properties of the Spectrum Report.

Background subtraction is always the first operation performed on a spectrum. If a background correction is attempted on a spectrum after another operation has already been performed (including an operation specified in the *Spectrum* tab of *Spectral Options*), a message box is displayed and the background correction request ignored.

Background subtraction may only be performed once on a spectrum. If a second background correction is attempted on a spectrum after the operation has already been performed (including the operation specified in the *Spectrum* tab of *Spectral Options*), a message box is displayed and the background correction request ignored.

❖ **To perform background correction**

1. The spectra from the baseline start and baseline stop times for the peak are extracted from the 3D data. The Max Plot is used to determine the peak that is used, if there is on other relevant trace. For the Spectrum view, the peaks are taken from the current working chromatogram that appears in the Chromatogram pane. For the Spectrum Report, the trace that is specified in the report properties is used.

2. For each spectrum in the peak, a corresponding background spectrum is generated by linear interpolation between the baseline start and baseline stop spectra.

3. These background spectra are subtracted from the original spectra.

Note While compensation for background provides more precise purity calculations, it can slow down re-analysis of large data files.

Calculating Total Purity

❖ **To calculate total purity**

1. Each spectrum in the peak is evaluated to see if it meets the peak threshold and peak coverage criteria.

2. A similarity index is calculated on all the spectra that pass step 1 compared to the apex spectraum.

3. The lowest similarity index value is determined.

4. That value is reported as the purity index.

5. The purity index has a range of between 0.000000 and 1.000000

Three Point Purity

Three Point Purity is calculated by comparing the spectrum at the apex of a peak (**Point 1**) with the spectra at the up-slope (**Point 2**) and down-slope (**Point 3**) of the peak. The up-slope spectrum is defined as the spectrum located 20% of the peak width from the peak start. The down-slope spectrum is defined as the spectrum located 20% of the peak width from the peak end.

$$\text{Time}_{up} = \text{Time}_{start} + (\text{Time}_{apex} - \text{Time}_{start}) * 1/5$$

$$\text{Time}_{down} = \text{Time}_{apex} + (\text{Time}_{end} - \text{Time}_{apex}) * 4/5$$

Similarity indices are generated for the up-slope and down-slope spectra, relative to the apex. Since spectra taken at different points along a pure peak will look identical, they will have high similarity indices. The closer the Similarity Index is to 1.0000, the more similar or more pure the peak is deemed to be.

Converting PC1000 Archive Files to ChromQuest Files

In every PC1000 sequence (either one injection or more than one), there is a result file (.res), which is basically a pointer file which denotes the files which contain the actual data for the sequence.

These files are as follows:

- Acquisition method file (.aqm)

- Aalculation method file (.cam)

- Report method file (.rpm)

- Acquisition result file (raw data) for each injection (.aqr)

- Calculation result file for each injection (.car)

- and possibly a spectra library file (.slb)

When the PC1000 data is archived into an .arc file, all these various files are put inside one large file, for ease in transporting the data.

By contrast in ChromQuest, the data files (.dat) is associated with only one injection, and the conditions used to collect the data are also embedded in the file. Additionally, there are method files (.met) and spectral library files (.lib); the library files contain spectral files (.spc).

This organizational difference requires you to specify a particular PC1000 injection within the .arc archive file, when you perform the data conversion to ChromQuest.

Contents

Data Conversion

To convert the original discrete channel and scan data (located in an .aqr file located inside the PC1000 .arc-file), to a ChromQuest .dat file, simply go to the **Open Data** dialog box, select the desired archive file, and click Open. The **Select Injections** dialog box appears showing all available injections in the selected archive file.

You may highlight an item, double click it or press the **Select** button. ChromQuest displays acquisition results of the chosen injection. The figure shown below in ChromQuest is the converted data of an injection (one .aqr file) with scan data on the top and data from discrete channels displaying at the bottom. If your original .aqr file has only scan or discrete data, then only the data you have in the file, scan or discrete, are converted and displayed.

Figure 128. Select Injections dialog box
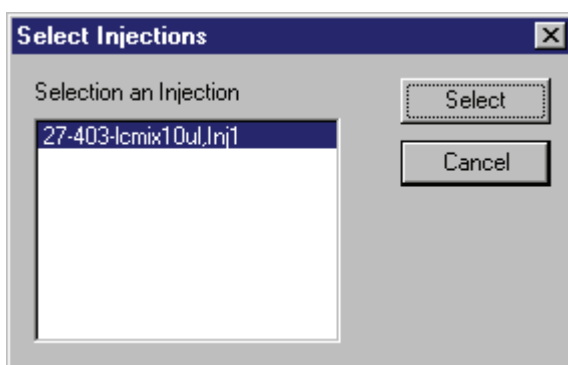
Data Conversion with Calculation Result

If you open an archive file with **Original Results** selected in the **Open Data** dialog box, then chromatograms from the sequentially selected injection are opened with original PC1000 calculation results (located in .car file), such as peak names, retention times, etc

Method Conversion

To access your calculation and acquisition method developed with PC1000, go to the **Open Data** dialog box (not the Open Method dialog box), select the archive file which contains the method, and check the **Open with Method** check box. You may select any injection from the **Select Injections** dialog box. Your original calculation method (in .cam file), such as peak names and expected retention times are displayed in **Peak / Group Tables**. The instrument setup (in .aqm file) is merged into the **Instrument Setup** property sheets.

> **Note** If your LC system configuration does not have all the modules in your acquisition method, you will see the following type of message box.

Figure 129. Instrument Setup property sheet
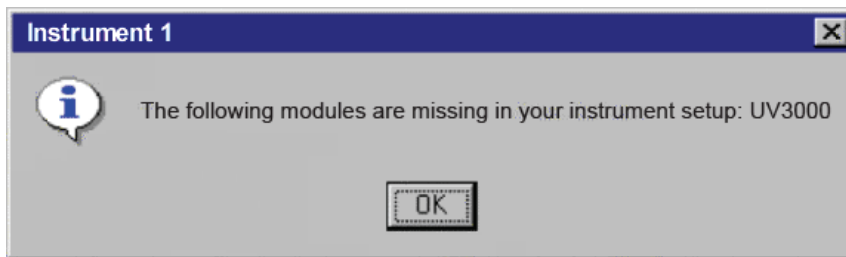
Consequently, the portion of the method which is associated with those missing modules, will not be opened. To complete your acquisition method conversion, you need to reconfigure your LC system by adding the missing modules. Once you are satisfied with the opened method, make sure to save it as a ChromQuest method (.met) file for future use.

Spectra Library Conversion

To convert a spectra library (located in .slb file), go to the **Open Library** dialog box, select the archive file which contains a spectral library. The spectral library are displayed. When you save it in ChromQuest library format (.lib), your original library name is suggested as the default name.

However, if the selected archive file has no spectra library in it, you will see the following message boxes:

Figure 130. Spectra Library Conversion - Missing message
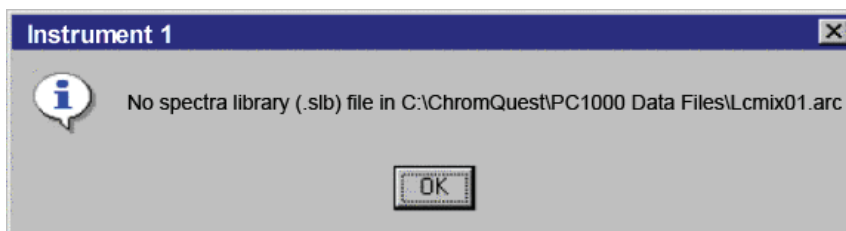
Figure 131. Spectra Library Conversion - Invalid version message
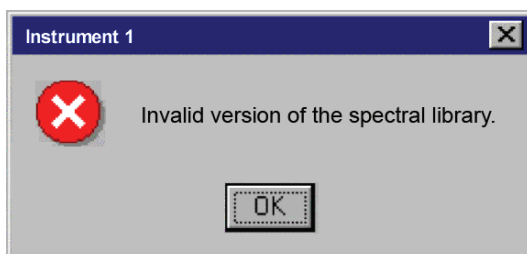
PC1000 Archive File Run-Time Exception Handling

When you try to convert a problematic archive file, ChromQuest informs you with message boxes reporting errors it has encountered when reading the archive.

You can continue to work on other tasks, for instance, convert another PC1000 archive, after these error messages.

Important Note on Data Conversion

The intention of this conversion routine is for PC1000 users to view and then convert their data, methods, and libraries to ChromQuest format. If you only want to see what an archive file contains, simply open, examine, and close it without saving. However, if you wish to manipulate your data, such as add traces from another data file and so on, you need to save your file into ChromQuest format and then work on the new file. The conversion covers archives generated with PC1000 releases version from the current version (PC1000 Ver 3.5.1) back to version PC1000 Ver 2.5.

Advanced Reporting Formulas

This chapter gives details on formulas available in the spreadsheet engine used in the Advanced Reports of ChromQuest.

Contents

- Spreadsheet Formulas
- Built-in Functions
- Quick-Reference Guide to Built-in Functions
- Using Spreadsheet Built-in Functions
- Spreadsheet Error Messages

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.

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.

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 denoted with dollar signs before the fixed coordinate (A1, $A1, or A$1), which is not 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**

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 notes 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.

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.

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 fixes 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.

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 combine with current cell reference support

(#) as indicated in the above example.

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.

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.

Spreadsheet functions fall into the following categories:

- Mathematical
- Statistical
- Conditional Statistical
- String
- Logic
- Digital Logic
- Financial
- Date and Time
- Miscellaneous
- Embedded Tools

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.

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.

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.

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.

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.

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.

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 makes 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

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.

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.

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 is not 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 formula

@INVERT(@MMUL(A1..C4,F1..I3))

is not allowed.

Quick-Reference Guide to Built-in Functions

Mathematical Functions

Formula	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.

Formula	Functions
@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.

Statistical Functions

Formula	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*.

Formula	Functions
@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.

Conditional Statistical Functions

Formula	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).

String Functions

Formula	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.

Logic Functions

Formula	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

Formula	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.

Financial Functions

Formula	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.

Formula	Functions
@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

Formula	Functions
@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.

Date and Time Functions

Formula	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*).

Miscellaneous Functions

Formula	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.

Embedded Tools

Formula	Functions
@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.

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 misinterprets 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.

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''

Using Operators with Functions

The result of a function depends on the order in which Spreadsheet handles the calculations. Please see Chapter Calculations, for more information on operators and their precedence.

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 correctly counts the numeric values in the range C3..J100. However, if you change the value in A1, Spreadsheet does 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

> **@CCOUNT(C3..J100,#A1 && #<A2)\A1\A2**

Spreadsheet would take into account the dependencies on A1 and A2 and update the spreadsheet just as you expect.

- Another approach is to construct the condition string with an expression that references the cells directly. For example,

> **@CCOUNT(C3..J100, @STRCAT("#",A1,"&_<",A2))**

In this example, A1 and A2 are directly referenced and thus properly triggers recalculation.

Explicit Dependency is described in more detail in Section Explicit Dependency.

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.

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 attempts 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.

Summary of Error Messages

Error Message	Description
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.

Error Message	Description
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.

Error Message	Description
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 is 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.

Error Message	Description
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.

Error Message	Description
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.

Error Message	Description
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.

Error Message	Description
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.

Error Message	Description
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.

Error Message	Description
"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 occurs 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.

Error Message	Description
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.

Error Message	Description
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.

Advanced Report Templates

This chapter describes the functionality available for creating advanced reports with the template editor.

Contents

- Functional Reference
- Datafile Functions
- Extended Helper Functions
- Group Functions
- Instrument Functions
- Peak Functions
- Project Functions
- Sequence Functions
- Summary

Functional Reference

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")

Datafile Functions

These functions return information about data files that have been collected and analyzed.

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 are used to extract the value.

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 are used to extract the value.

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 are used to extract the value.

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 are used to extract the value.

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 are used to extract the value.

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 are used to extract the value.

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 are used to extract the value.

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 are used to extract the value.

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 are used to extract the value.

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 are used to extract the value.

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 are used to extract the value.

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 are used to extract the value.

Return Type

String

Data.OriginalMethodFull Filename

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 are used to extract the value.

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 are used to extract the value.

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 are used to extract the value.

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 are used to extract the value.

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 are used to extract the value.

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 are used to extract the value.

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 are used to extract the value.

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 are used to extract the value.

Return Type

Number

Extended Helper Functions

These functions are provided to make the user of other features in the spreadsheet easier to user.

Ex.D

Returns a cell range for a dynamic set of data. If data in a cell is 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 is 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 is 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 is 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 the EX.R 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 is 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 is 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 is 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 appendix 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 are repeated in the direction specified by <direction>, and are separated by <separation> rows or columns.
"RA; <direction>; <separation>"	All sequence runs. The runs are repeated in the direction specified by <direction>, and are 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 are repeated in the direction specified by <direction>, and are separated by <separation> rows or columns.
"PA; <peak type>; <direction>; <separation>"	All peaks of the given peak type. The peaks are repeated in the direction specified by <direction>, and are 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 are repeated in the direction specified by <direction>, and are separated by <separation> rows or columns.
"GA; <group type>; <direction>; <separation>"	All groups of the given group type. The groups are repeated in the direction specified by <direction>, and are separated by <separation> rows or columns.

Direction may be one of the following:

0   The data is repeated across the spreadsheet.

1   The data is 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.

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 are used to extract the value.

<Trace Info>   Describes the trace that is used to extract the value.

<Group Info>   Describes the group(s) to use for the value.

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 are used to extract the value.
<Trace Info>	Describes the trace that is used to extract the value.
<Group Info>	Describes the group(s) to use for the value.

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 are used to extract the value.
<Trace Info>	Describes the trace that is used to extract the value.
<Group Info>	Describes the group(s) to use for the value.

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 are used to extract the value.
<Trace Info>	Describes the trace that is used to extract the value.
<Group Info>	Describes the group(s) to use for the value.

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 are used to extract the value.

<Trace Info>   Describes the trace that is used to extract the value.

<Group Info>   Describes the group(s) to use for the value.

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 are used to extract the value.

<Trace Info>   Describes the trace that is used to extract the value.

<Group Info>   Describes the group(s) to use for the value.

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 are used to extract the value.

<Trace Info>   Describes the trace that is used to extract the value.

<Group Info>   Describes the group(s) to use for the value.

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 are used to extract the value.

<Trace Info>   Describes the trace that is used to extract the value.

<Group Info>   Describes the group(s) to use for the value.

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 are used to extract the value.

<Trace Info>   Describes the trace that is used to extract the value.

<Group Info>   Describes the group(s) to use for the value.

Return Type

Number

Group.Quantitation

Returns the group quantitation for the requested group(s). This returns 'Area', 'Height', or 'Counts'.

Syntax

=Group.Quantitation (<Run Info>, <Trace Info>, <Group Info>)

Parameters

<Run Info>   Describes the data file(s) that are used to extract the value.

<Trace Info>   Describes the trace that is used to extract the value.

<Group Info>   Describes the group(s) to use for the value.

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 are used to extract the value.

<Trace Info>   Describes the trace that is used to extract the value.

<Group Info>   Describes the group(s) to use for the value.

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 are used to extract the value.

<Trace Info>   Describes the trace that is used to extract the value.

<Group Info>   Describes the group(s) to use for the value.

Return Type

String

Instrument Functions

These functions return information about the current instrument.

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.

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 are used to extract the value.

<Trace Info>   Describes the trace that is used to extract the value.

<Peak Info>   Describes the peak(s) to use for the value.

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 are used to extract the value.
<Trace Info>	Describes the trace that is used to extract the value.
<Peak Info>	Describes the peak(s) to use for the value.

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 are used to extract the value.
<Trace Info>	Describes the trace that is used to extract the value.
<Peak Info>	Describes the peak(s) to use for the value.

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 are used to extract the value.
<Trace Info>	Describes the trace that is used to extract the value.
<Peak Info>	Describes the peak(s) to use for the value.

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 are used to extract the value.
<Trace Info>	Describes the trace that is used to extract the value.
<Peak Info>	Describes the peak(s) to use for the value.

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 are used to extract the value.
<Trace Info>	Describes the trace that is used to extract the value.
<Peak Info>	Describes the peak(s) to use for the value.

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 are used to extract the value.
<Trace Info>	Describes the trace that is used to extract the value.
<Peak Info>	Describes the peak(s) to use for the value.

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 are used to extract the value.

<Trace Info>   Describes the trace that is used to extract the value.

<Peak Info>   Describes the peak(s) to use for the value.

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 are used to extract the value.

<Trace Info>   Describes the trace that is used to extract the value.

<Peak Info>   Describes the peak(s) to use for the value.

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 are used to extract the value.
<Trace Info>	Describes the trace that is used to extract the value.
<Peak Info>	Describes the peak(s) to use for the value.

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 are used to extract the value.
<Trace Info>	Describes the trace that is used to extract the value.
<Peak Info>	Describes the peak(s) to use for the value.

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 are used to extract the value.

<Trace Info>   Describes the trace that is used to extract the value.

<Peak Info>   Describes the peak(s) to use for the value.

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 are used to extract the value.

<Trace Info>   Describes the trace that is used to extract the value.

<Peak Info>   Describes the peak(s) to use for the value.

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 are used to extract the value.

<Trace Info>   Describes the trace that is used to extract the value.

<Peak Info>   Describes the peak(s) to use for the value.

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 are used to extract the value.
<Trace Info>	Describes the trace that is used to extract the value.
<Peak Info>	Describes the peak(s) to use for the value.

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 are used to extract the value.
<Trace Info>	Describes the trace that is used to extract the value.
<Peak Info>	Describes the peak(s) to use for the value.

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 are used to extract the value.
<Trace Info>	Describes the trace that is used to extract the value.
<Peak Info>	Describes the peak(s) to use for the value.

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 are used to extract the value.
<Trace Info>	Describes the trace that is used to extract the value.
<Peak Info>	Describes the peak(s) to use for the value.

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 are used to extract the value.
<Trace Info>	Describes the trace that is used to extract the value.
<Peak Info>	Describes the peak(s) to use for the value.

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 are used to extract the value.
<Trace Info>	Describes the trace that is used to extract the value.
<Peak Info>	Describes the peak(s) to use for the value.

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 are used to extract the value.
<Trace Info>	Describes the trace that is used to extract the value.

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 are used to extract the value.
<Trace Info>	Describes the trace that is used to extract the value.
<Peak Info>	Describes the peak(s) to use for the value.

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 are used to extract the value.
<Trace Info>	Describes the trace that is used to extract the value.
<Peak Info>	Describes the peak(s) to use for the value.

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 are used to extract the value.
<Trace Info>	Describes the trace that is used to extract the value.
<Peak Info>	Describes the peak(s) to use for the value.

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 are used to extract the value.
<Trace Info>	Describes the trace that is used to extract the value.
<Peak Info>	Describes the peak(s) to use for the value.

Return Type

Number

Peak.JPTheoreticalPlatesPer Meter

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 are used to extract the value.

<Trace Info>   Describes the trace that is used to extract the value.

<Peak Info>   Describes the peak(s) to use for the value.

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 are used to extract the value.

<Trace Info>   Describes the trace that is used to extract the value.

<Peak Info>   Describes the peak(s) to use for the value.

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 are used to extract the value.

<Trace Info>   Describes the trace that is used to extract the value.

<Peak Info>   Describes the peak(s) to use for the value.

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 are used to extract the value.
<Trace Info>	Describes the trace that is used to extract the value.
<Peak Info>	Describes the peak(s) to use for the value.

Return Type

Number

Peak.Quantitation

Returns the peak quantitation for the requested peak(s). This returns 'Area', 'Height', or 'Counts'.

Syntax

=Peak.Quantitation (<Run Info>, <Trace Info>, <Peak Info>)

Parameters

<Run Info>	Describes the data file(s) that are used to extract the value.
<Trace Info>	Describes the trace that is used to extract the value.
<Peak Info>	Describes the peak(s) to use for the value.

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 are used to extract the value.

<Trace Info>   Describes the trace that is used to extract the value.

<Peak Info>   Describes the peak(s) to use for the value.

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 are used to extract the value.

<Trace Info>   Describes the trace that is used to extract the value.

<Peak Info>   Describes the peak(s) to use for the value.

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 are used to extract the value.

<Trace Info>   Describes the trace that is used to extract the value.

<Peak Info>   Describes the peak(s) to use for the value.

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 are used to extract the value.

<Trace Info>   Describes the trace that is used to extract the value.

<Peak Info>   Describes the peak(s) to use for the value.

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 are used to extract the value.

<Trace Info>   Describes the trace that is used to extract the value.

<Peak Info>   Describes the peak(s) to use for the value.

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 are used to extract the value.

<Trace Info>   Describes the trace that is used to extract the value.

<Peak Info>   Describes the peak(s) to use for the value.

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 are used to extract the value.
<Trace Info>	Describes the trace that is used to extract the value.
<Peak Info>	Describes the peak(s) to use for the value.

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 are used to extract the value.
<Trace Info>	Describes the trace that is used to extract the value.
<Peak Info>	Describes the peak(s) to use for the value.

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 are used to extract the value.
<Trace Info>	Describes the trace that is used to extract the value.
<Peak Info>	Describes the peak(s) to use for the value.

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 are used to extract the value.

<Trace Info>   Describes the trace that is used to extract the value.

<Peak Info>   Describes the peak(s) to use for the value.

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 are used to extract the value.

<Trace Info>   Describes the trace that is used to extract the value.

<Peak Info>   Describes the peak(s) to use for the value.

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 are used to extract the value.

<Trace Info>   Describes the trace that is used to extract the value.

<Peak Info>   Describes the peak(s) to use for the value.

Return Type

Number

Peak.USPTheoreticalPlatesPer Meter

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 are used to extract the value.

<Trace Info>   Describes the trace that is used to extract the value.

<Peak Info>   Describes the peak(s) to use for the value.

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 are used to extract the value.

<Trace Info>   Describes the trace that is used to extract the value.

<Peak Info>   Describes the peak(s) to use for the value.

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 are used to extract the value.

<Trace Info>   Describes the trace that is used to extract the value.

<Peak Info>   Describes the peak(s) to use for the value.

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 are used to extract the value.

<Trace Info>   Describes the trace that is used to extract the value.

<Peak Info>   Describes the peak(s) to use for the value.

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 are used to extract the value.

<Trace Info>   Describes the trace that is used to extract the value.

<Peak Info>   Describes the peak(s) to use for the value.

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 are used to extract the value.

<Trace Info>   Describes the trace that is used to extract the value.

<Peak Info>   Describes the peak(s) to use for the value.

Return Type

Number

Project Functions

These functions return information about the current project.

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 is used for reporting purposes.

Sequence.Filename

Returns file name of the sequence file that is 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 is 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 are used to extract the value.

                          See the appendix for a description of the above parameter(s).

Return Type

Number

Summary

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   The peak with an index of <x> having the given peak type.
type>"

Group Info may be one of the following:

"G<x>; <group   The group with an index of <x> having the given group type.
type>"

Direction may be one of the following:

0   The data is repeated across the spreadsheet.

1   The data is 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.

Index

T

U

V

W