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Star Chromatography Workstation Version 6

Data Handling and Reports

Operation Manual



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Getting Started

About this Manual

This manual contains information about how to perform automated and interactive data handling, how to perform calibrated results calculations, how to generate reports, and how to use the suite of advanced applications included with your Star Chromatography Workstation. Use this manual in conjunction with the other Operation Manuals supplied with the Star Chromatography Workstation.

Additional Manuals

Other sources of information are available to help you get the most from this product.

Data Acquisition Manuals



Several variations of the Data Acquisition Manual exist. Choose the one that matches your Star Workstation configuration. These manuals contain information about instrument setup, sample injection, and Method editing.

Data Handling and Reports Tutorials



This manual contains step by step tutorials guiding you through common Data Handling and Reporting tasks.

Optional Post-Run Software Manuals

Refer to the manuals corresponding to the optional post-run software that you own. These manuals cover the use of these products with the Star Workstation.

Interactive Graphics and Data Handling

Viewing Chromatograms in Interactive Graphics

Interactive Graphics is the Star Workstation application that allows you to review chromatograms, edit Data Handling Method parameters, and recalculate results. Interactive Graphics may be launched from the Star Toolbar.



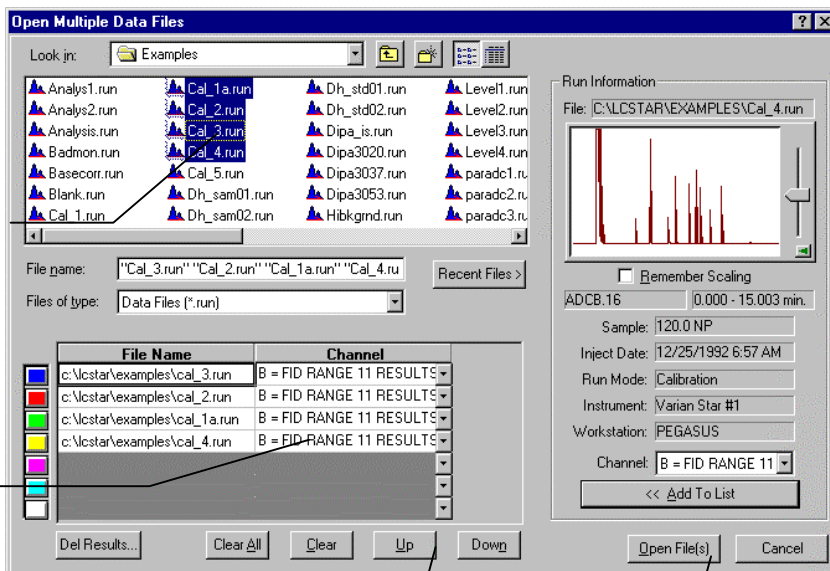
Click on the Interactive Graphics / Data Handling button.

If the Data File you wish to view appears in a QuickLink button, select View/Edit Chromatogram from the menu.

If you did not select View/Edit Chromatogram from a QuickLink menu, you are prompted for up to seven Data Files to open when Interactive Graphics starts.

Select files to open by double-clicking on the file name, or select the filename and click on the Add To List button, or drag and drop the files anywhere in the dialog box.

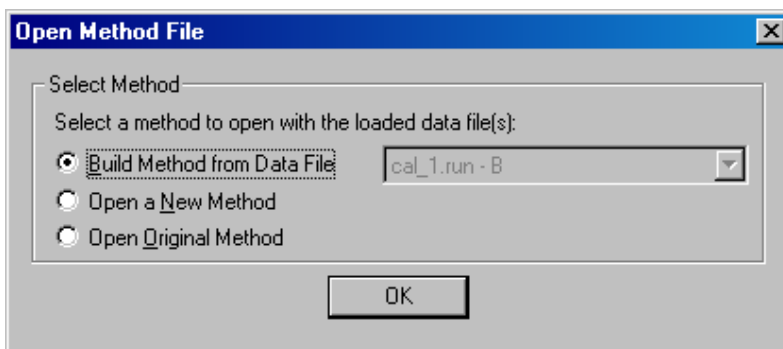
If necessary, change the detector channel.



You may re-order the files.

Click on Open Files to view the files.

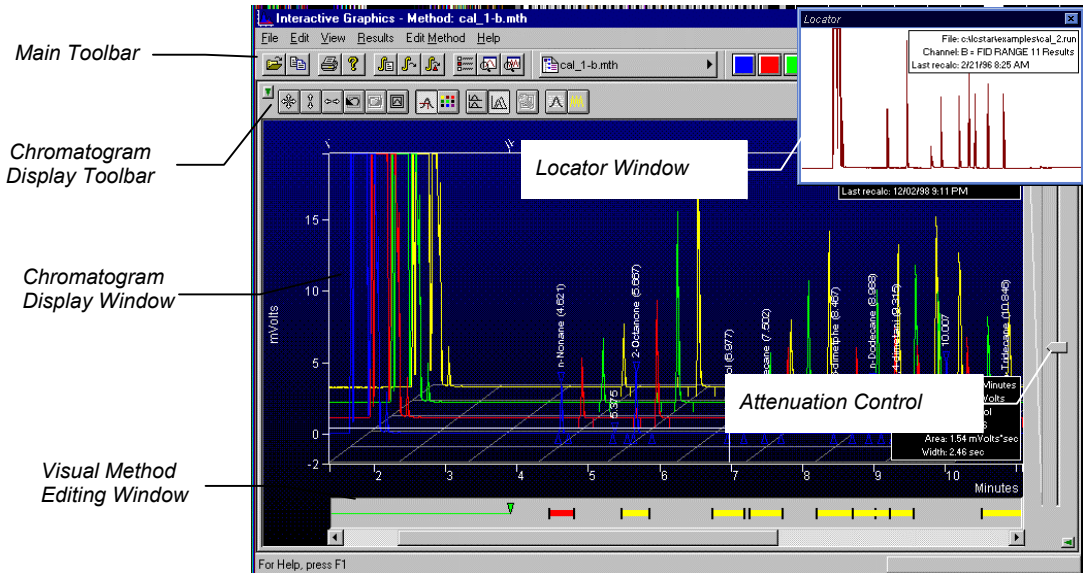
After you click on *Open File(s)*, you will be asked which method you would like to open with this data file. If you choose to build a method from the data file, a temporary method will be created from the information in the .RUN file.



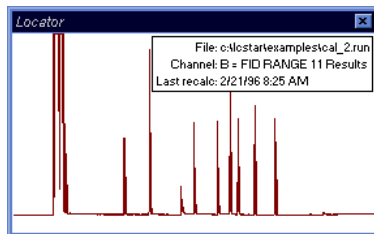
If you have opened several chromatograms and select "Build Method from Data File," you will build a new temporary method for each of those files.

Elements of the Interactive Graphics Window

Once you have selected the file or files to view, they are displayed in the Interactive Graphics window.



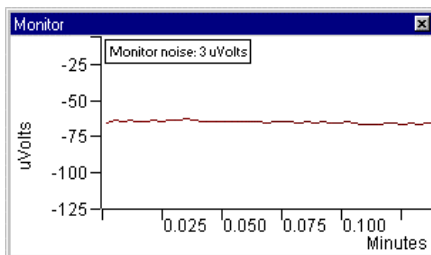
The Locator Window



The Locator Window shows the active chromatogram in full scale. Click and drag in this window to view a portion of the chromatogram. When you do, the Chromatogram Display Window is updated and the Locator Window shows the zoomed area as a highlighted rectangle. Double-click in this window to return the display to full scale.

You can size and position the Locator Window anywhere on the screen. The Locator Window can be closed by clicking on the button in the upper right corner, by toggling the Locator Display button in the main toolbar, or by deselecting the Locator Window menu item in the View menu. The display state and position of the Locator Window is retained the next time you start Interactive Graphics.

The Monitor Window



The Monitor Window shows the noise monitor signal. Click and drag in this window to zoom the noise monitor trace. Double-click in this window to return the noise monitor display to full scale.

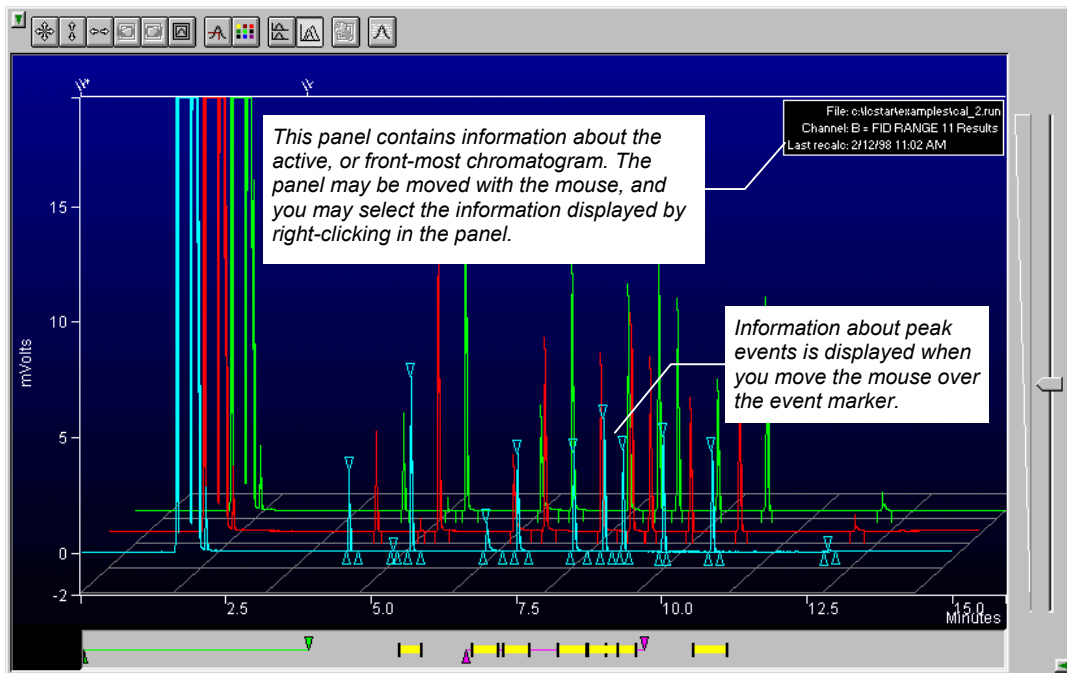
You can size and position the Monitor Window anywhere on the screen. The Monitor Window can be closed by clicking on the button in the upper right corner, by toggling the Monitor Display button in the main toolbar, or by deselecting the Monitor Window menu item in the View menu. The display state and position of the Monitor Window is retained the next time you start Interactive Graphics.

The Chromatogram Display Window

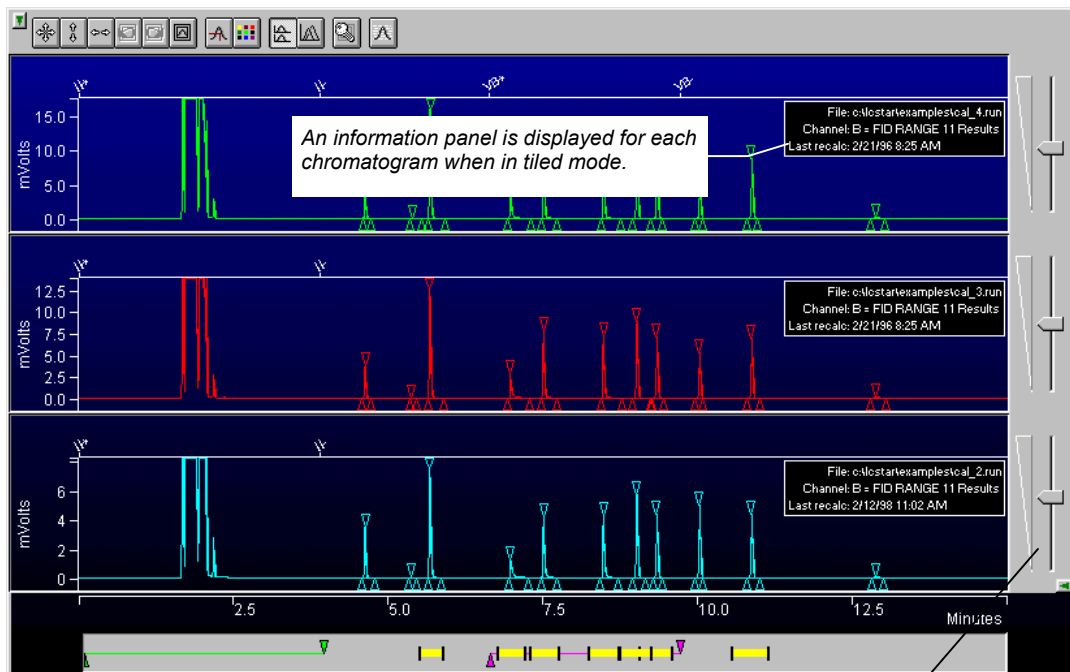
The Chromatogram Display Window shows any portion of chromatograms that you have opened. Click and drag to zoom on a specific area, or click and hold the mouse button down to continuously zoom on the area beneath the mouse cursor. Hold the control key down while continuously zooming to reverse the zooming direction. If the Locator Window is displayed, it is updated to show the zoom area on

the full scale chromatogram trace. Double-click in the Chromatogram Display Window to restore the display to full scale.

If you have opened multiple chromatograms, they may be displayed in overlaid or tiled modes. When overlaid, all chromatograms are shown on the same time and amplitude axes. By default, the chromatogram traces are offset both in time and amplitude to facilitate viewing. The offset amounts can be adjusted; refer to [Changing Viewing Options on page 11](#) for details.



When tiled, each chromatogram trace is displayed separately. All panels share the same time axis, but each trace can be independently scaled in the amplitude axis.

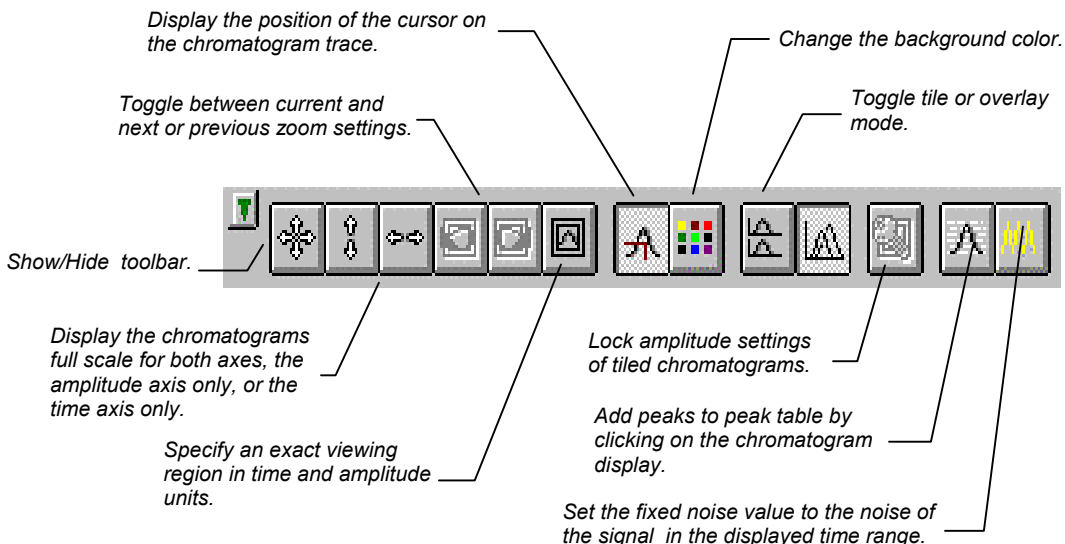


A separate attenuation control appears for each chromatogram.

When you right click on a chromatogram trace, either in overlay or tiled mode, you are presented with a popup menu containing options for that chromatogram. Included in these options are report generation and viewing, along with the ability to remove the chromatogram, or bring the chromatogram to the *active*. When in overlay mode, the active chromatogram is in the front-most position. When in tiled mode, the active chromatogram is on the bottom.

The Chromatogram Display Toolbar

The toolbar at the top of the Chromatogram Display Window allows you to adjust the chromatogram display settings.



The Attenuation Control

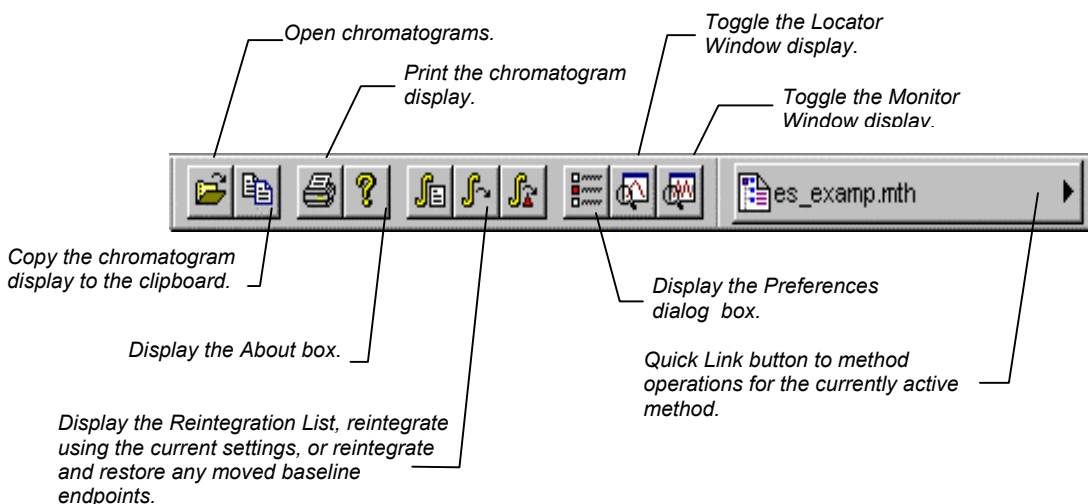
Located on the right side of the chromatogram display is an attenuation control, similar to a scrollbar, that allows you to adjust the scaling of the amplitude of the chromatogram trace. As you move the thumb tab up, the vertical scale is magnified.

The Visual Method Editing Panel

The area beneath the Chromatogram Display Window is the Visual Method Editing Panel. Timed integration events and peak table entries are graphically displayed in this panel. New events can be added by right clicking in the panel and selecting the desired event from the popup menu. Once inserted, events can be moved in time and their duration can be edited by dragging their endpoints with the mouse.

The Main Toolbar

At the top of the Interactive Graphics window is the application's main toolbar. This toolbar provides shortcuts to frequently used functions that are also available as menu items. The main toolbar and the Method Quick Link button can each be repositioned in the window or "undocked" and displayed as a floating window by clicking in an empty area in the toolbar and dragging with the mouse.



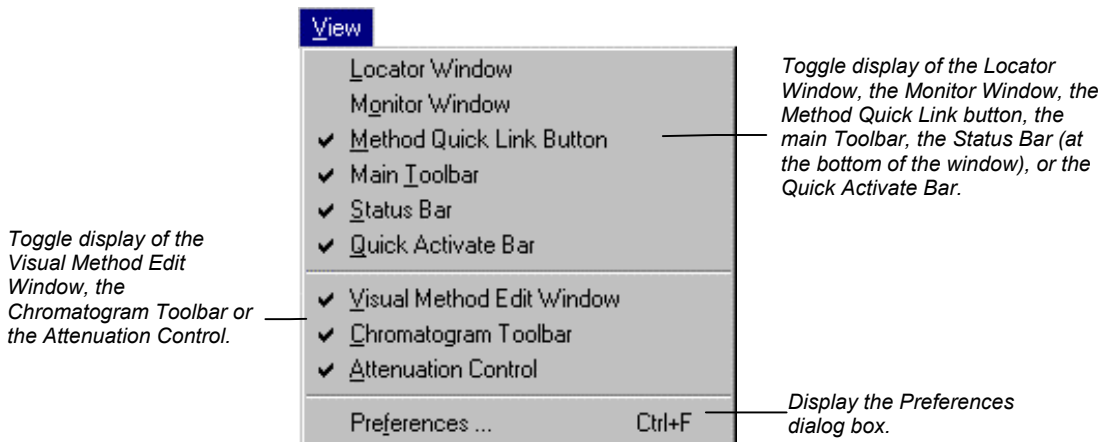
The Quick Activate Toolbar

The Quick Activate Toolbar provides a quick way to reorder the displayed chromatograms. Click on the button with the same color as the chromatogram trace you want in order to activate the chromatogram. In overlay mode, this brings the trace to the front of all loaded chromatograms. In tile mode, this makes the chromatogram panel to bottom most panel. Tool tips show the name of the run file. When followed by an asterisk this indicates the run file is the active chromatogram.



Changing Viewing Options

There are many options available for the way chromatograms are displayed in the Interactive Graphics window. Pull down the View menu to display the options.

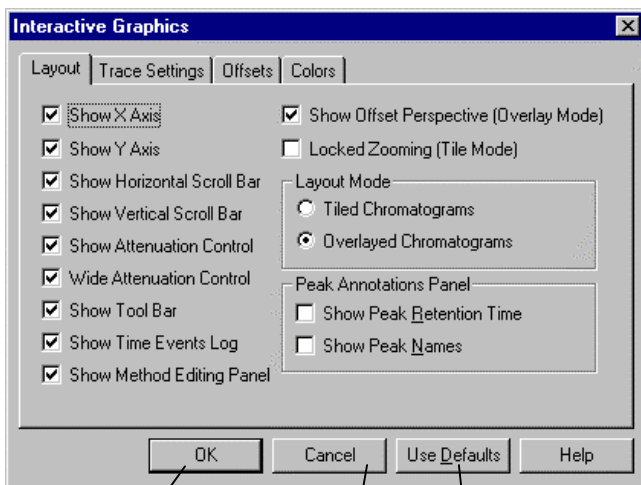


The Preferences Dialog Box

Select *Preferences...* from the View menu to display the Preferences dialog box. The dialog box contains four tabs at the top, each corresponding to a different category of preferences. As you make changes in the Preferences dialog box, the Interactive Graphics display is immediately updated so that you can preview the change. Refer to the on-line help in Interactive Graphics for a complete description of all of the fields in the Preferences dialog box.

Layout

The layout preferences determine the appearance and behavior of all elements in the Chromatogram Display Window other than the chromatogram trace itself.



Accept the changes and close the dialog box.

Use the previously saved preferences.

Return all preferences to default values.

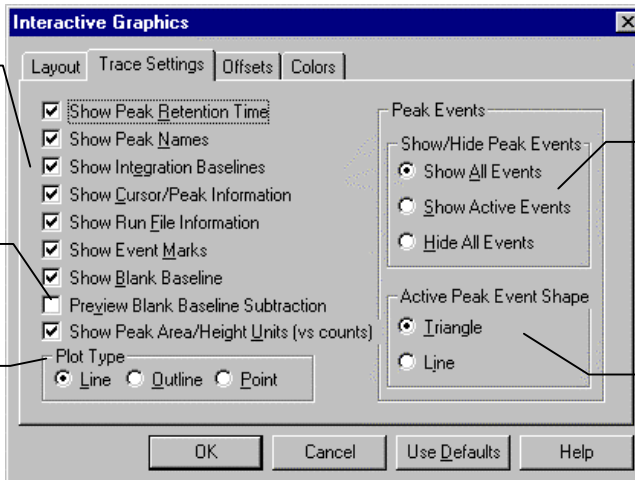
Trace Settings

The Trace Settings preferences determine the appearance of the chromatogram trace in the Chromatogram Display Window.

These settings affect what additional information is displayed with the chromatogram.

See the explanation of this option below.

These settings affect the way the chromatogram traces are drawn.



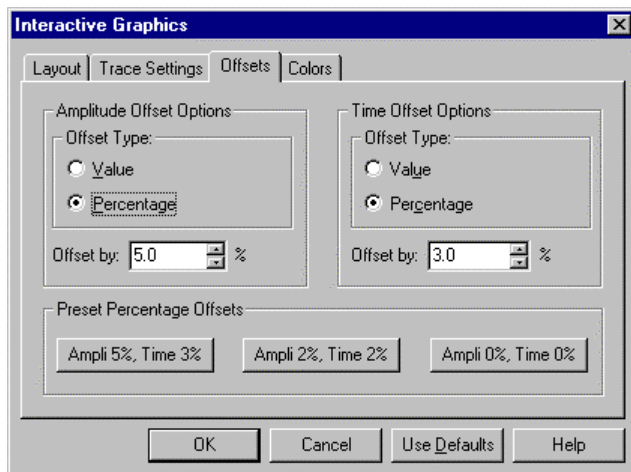
These settings determine whether peak start, end and apex events are drawn on all chromatograms, only the active chromatogram, or no chromatograms.

These settings affect the display of peak start, end and apex points.

When *Preview Blank Baseline Subtraction* is selected, the blank baseline stored in the Method can be edited by clicking and dragging points with the mouse. The chromatogram is drawn as if the baseline has been subtracted. To actually subtract the baseline, you must select *Subtract Blank Baseline* in the Integration Parameters window in the Data Handling Method Section. If you subtract a blank baseline that has been manually edited, it will be documented in the report.

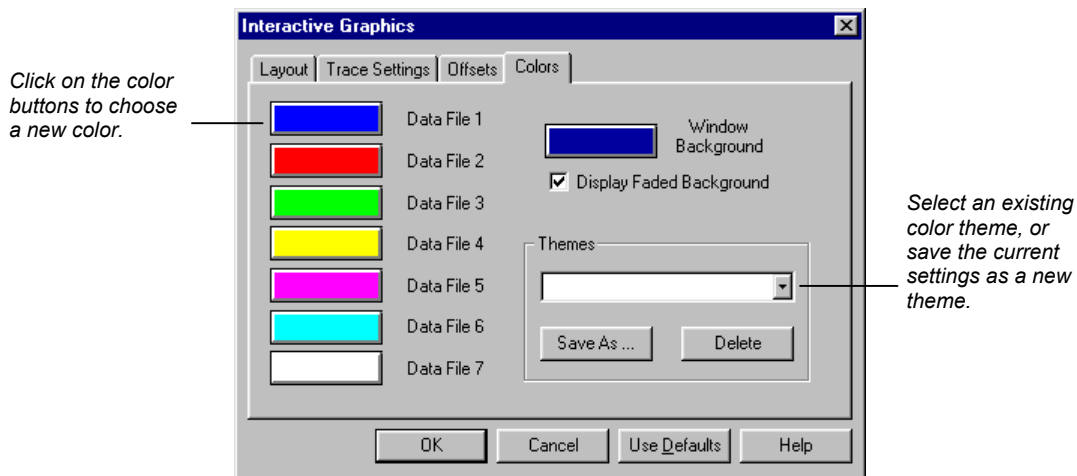
Offsets

Time and amplitude offsets affect the “3D” appearance of multiple chromatograms when displayed in overlay mode. When offsets are performed by percentage, the distance between traces appears fixed regardless of the scaling. When offsets are performed by a value, the distance between traces changes as the scaling changes.



Colors

You may specify the colors for each of the seven possible chromatogram traces that can be displayed simultaneously in Interactive Graphics. You may also specify the background color of the Chromatogram Display Window, and whether the background is a solid color or is a faded gradient. You may save your color settings as a theme, which can be restored later.



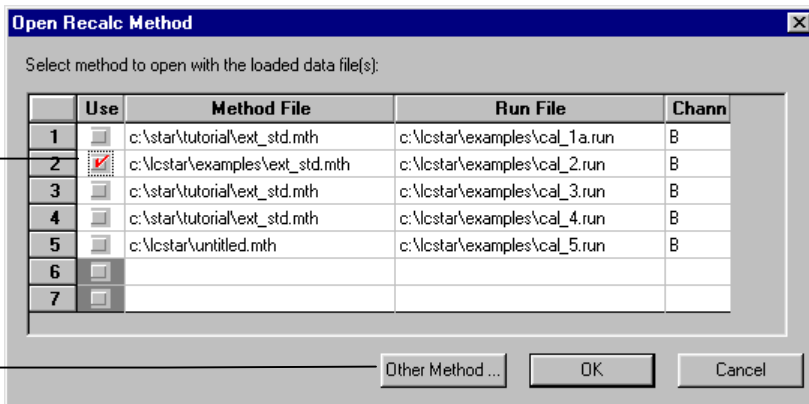
Selecting a Method

When a chromatogram is initially opened in Interactive Graphics, the Method used to perform the most recent calculation of the chromatogram is automatically opened. If this method cannot be found, a new untitled Method will be opened.

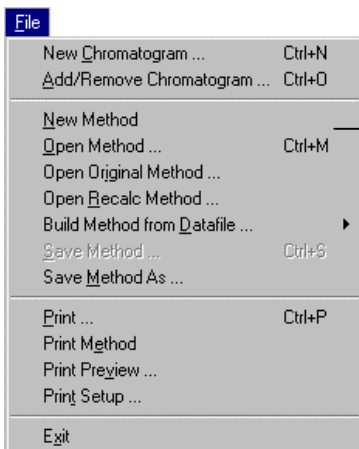
If multiple chromatograms are opened at once and more than one Method was used on the set, you are prompted to select the Method to open, or you can browse for another Method.

Select the method you wish to use with the chromatograms you opened.

If you wish to use another method, you may browse for it here.

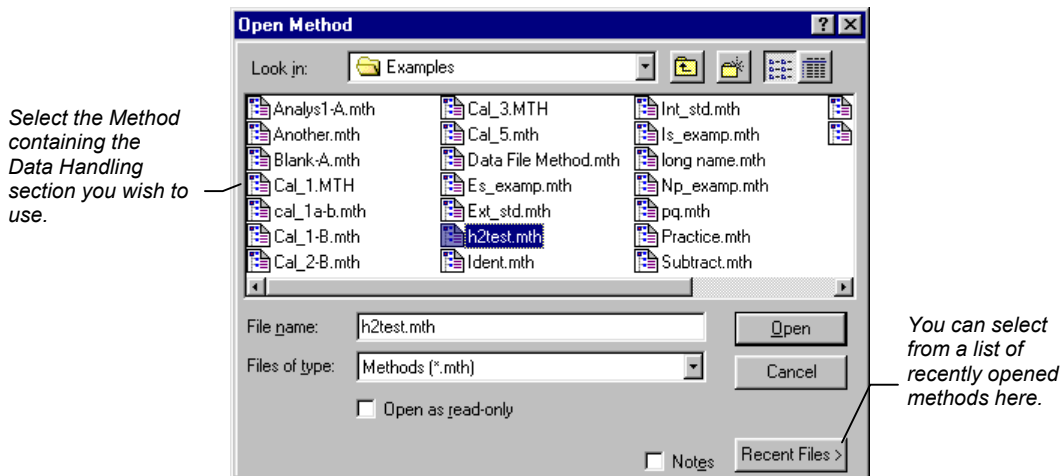


If you wish to use Data Handling parameters from a Method file already stored on disk but not automatically opened when you selected the chromatogram, you can choose one from the File menu.

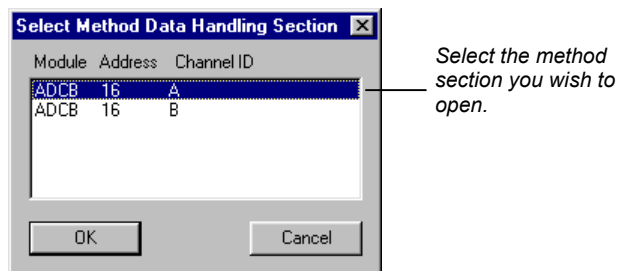


Select the Open Method command.

The Open Method dialog box is displayed.



If the Method you select contains more than one Data Handling section, you will be prompted for the section to use.



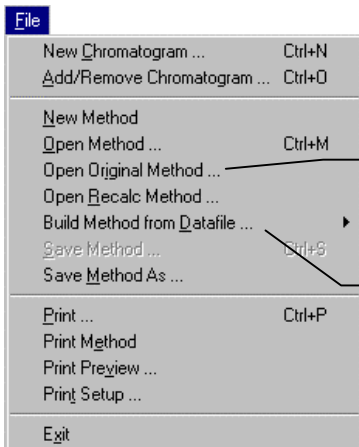
If you wish to open the Method originally used with any chromatogram that is currently opened in Interactive Graphics, you may do so by selecting Original Method... from the File menu.

Building a Method from the Data File

When a calculation is performed on a Data File using parameters in the Data Handling section of a Method, that Method section is copied into the Data File. You may build a new Method from the Data Handling parameters stored in a Data File. Modifications to the new Method do not affect the Method file that was used originally when

the Data File was acquired from the detector. You may use the Method created from one chromatogram channel to recalculate results for another Data File.

Build a new Method from an open chromatogram by using the File menu.



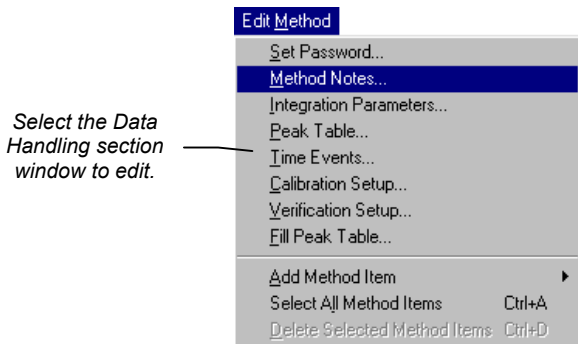
This item allows you to select from the methods used when the chromatograms were originally generated.

Select Build Method from Data File. If multiple chromatograms are open, a cascading menu allows you to select the Data File to use.

When you select *Build Method from Data File*, you are prompted for the name of the temporary Method file to be created. This new Method then becomes the active Method.

Changing the Data Handling Parameters

The Edit Method menu provides access to the Data Handling Method section windows for the open Method.



Select the Data Handling section window to edit.

Edit the Notes associated with the Method. Method notes are printed with the method, and can be viewed when selecting the method.

The following Method editing windows can be opened from the Edit Method menu. Refer to the section [Data Handling Fundamentals on page 69](#) for more information about Data Handling Method parameters.

Integration Parameters

Integration parameters affect peak detection, peak size calculation and results calculation. Refer to the on-line help in Interactive Graphics for details on all Integration Parameters fields.

Integration Parameters

Peak Detection

Subtract Blank Baseline

Initial S/N Ratio: 10

Initial Peakwidth: 2 sec

Initial Tangent Height %: 10

Peak Measurement

Measurement Type

Peak Area

Peak Height

Sg. Rt. Height

Initial Peak: []

Reject Value: 500

Monitor Noise

Before every run

Once at start of method

Fixed value: 1 μ Volts

Peak Result Calculation

Report Unidentified Peaks

Report Missing Peaks

Normalize Results

Save Cancel

Peak Table

The Peak Table is used to identify peaks so that results may be calculated. Refer to the on-line help in Interactive Graphics for details on all Peak Table fields. Right-click in a column header for formatting option. Refer to [page 23](#) for the procedure for filling a Peak Table.

	Retention Time	Peak Name	Ref	Std	RRT	Standard Peak Name	Group	Level 1 Amount
1	5.674	2-Octanone	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>		0	12
2	6.969	1-Octanol	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>		0	12
3	7.507	n-Decane	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>		0	12
4	8.474	2,6-dimetphe	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>		0	20
5	8.997	n-Dodecane	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>		0	12
6	9.324	2,4-dimetani	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>		0	12
7	10.856	n-Tridecane	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>		0	12

Buttons: Add, Insert, Delete, Fill Down, Sort

Buttons: Define Peak Windows..., Print, Save, Cancel

Specify peak identification windows.

Select a column then click here to replicate the first entry on all subsequent rows.

Sort peaks by retention time.

When you click on the Define Peak Windows button, the Peak Identification Window dialog box is displayed.

Peak windows are defined by an absolute time plus a percentage of the retention time. These values are added to and subtracted from the retention time to determine the peak window.

Define Peak Windows	
Define Reference Peak Windows	
Width (minutes):	0.10
Retention Time %:	2.0
Define Other Peak Windows	
Width (minutes):	0.10
Retention Time %:	2.0
Unretained Peak Time	
Time (minutes):	0.00
Save Cancel	

Reference peaks are marked in the Peak Table with a check in the Ref column.

This is used with relative retention time peaks (RRT) to compute relative retention times for all peaks in the Peak Table.

Time Events

Time events affect peak detection and baseline placement. Refer to the on-line help in Interactive Graphics for details on all Time Events fields. See [page 24](#) for details on graphically editing time events.

	Time	Event	Value / End Time	Description
1	0.0100	II	3.9000	(End time:0.0-1440.00 min)
2	6.6209	VB	9.7144	(End time:0.0-1440.00 min)
3				
4				
5				
6				
7				

This field describes acceptable values for the Value / End Time cell.

Calibration Setup

Calibration Setup parameters determine the type of calibration to be performed, as well as calibration acceptance criteria. Refer to the on-line help in Interactive Graphics for details on all Calibration Setup fields. For more information on calibration, refer to the [Calibration section on page 45](#).

Parameters in this window only apply when a calibrated calculation type is selected.

The number of levels determines the number of amount columns shown in the Peak Table.

Displays calibration curves.

The screenshot shows the 'Calibration Setup' dialog box with the following sections and controls:

- Calibration Type:** Radio buttons for % (No Calibration), Internal Standard, External Standard, and Normalized %.
- Number of Calibration Levels:** A numeric spinner set to 4.
- Multi-Level Parameters:**
 - Curve Defaults:** Origin: ; Fit: .
 - View Curves...** button.
 - Weighted Regression:** Apply this weighting scheme to each peak: .
- Replicate Treatment:**
 - Keep Replicates Separate
 - Average Calibration Replicates
 - Averaging Weight:** Apply this weight to new replicates (%): .
 - Replicate Tolerance:**
 - Always add new replicates
 - Never add new replicates
 - Add replicates within this tolerance (%): .
 - Out of Tolerance Action...** button.
- Calibration Range Tolerance:**
 - Peaks outside the range + tolerance generate calibration range errors.
 - Range Tolerance (%): .
 - Out of Tolerance Action...** button.
- Edit/Lock Calibration Data...** button.
- Save** and **Cancel** buttons at the bottom.

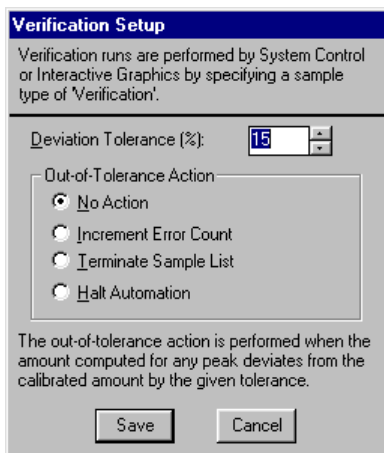
Specify action taken when a calibration point is not within the given tolerance.

Specify action taken when an analysis run is outside the calibrated range.

Edit calibration coefficients. Locked coefficients are not updated by calibration runs.

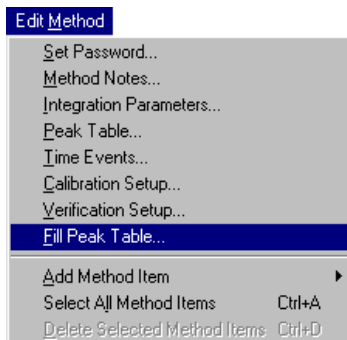
Verification Setup

Verification Setup options affect the behavior of verification runs. Refer to the on-line help in Interactive Graphics for details on all Verification Setup fields. For more information on verification, refer to the section *Calibration Verification on page 54*.



Filling the Peak Table

The fastest way to build a Peak Table is to create one from the detected peaks in the active chromatogram. To do so, pull down the Edit Method menu.



Select the Fill Peak Table command.

The Fill Peak Table window is displayed at the top of the screen, above the Chromatogram Display Window.

Fill Peak Table

	Retention Time	Peak Name	Ref	Std	RRT	Standard Peak Name	Group	Level 1 Amount
1	5.673	2-Octanone	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>		0	12
2	6.970	1-Octanol	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>		0	12
3	7.507	n-Decane	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>		0	20
4	8.473	2,6-dimetphe	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>		0	12
5	8.997	n-Dodecane	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>		0	12

Fill table from selection

Save Cancel

Add
Insert
Delete
Sort

When you check this, peaks detected in any region that you select in the Chromatogram Display Window are automatically added to the peak table.

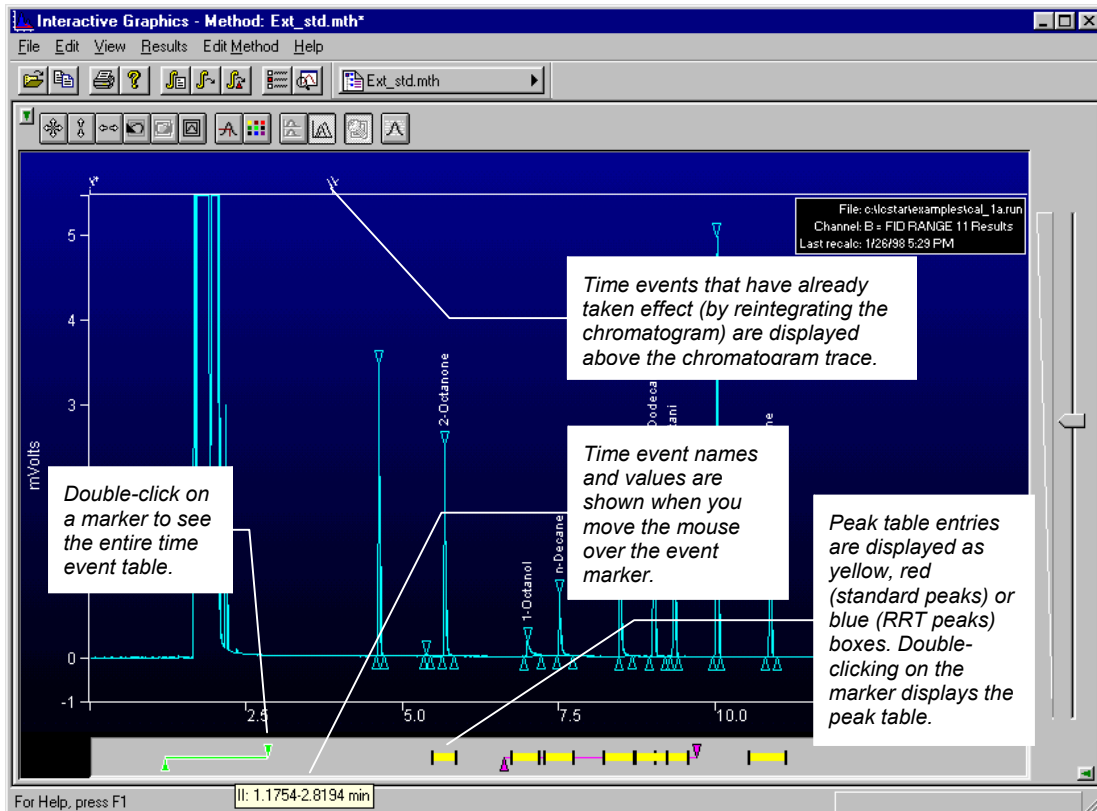
The Fill Peak Table window is nearly identical to the Peak Table window, except that you may click on any peak displayed in the Chromatogram Display Window to add an entry into the table. A default name and peak parameters are entered with the retention time of the selected peak. Click on the peaks of interest in the display, zooming and scrolling if necessary to bring the peaks into view. After all peaks have been added, click on the Save button.

Interactive Editing of Timed Events

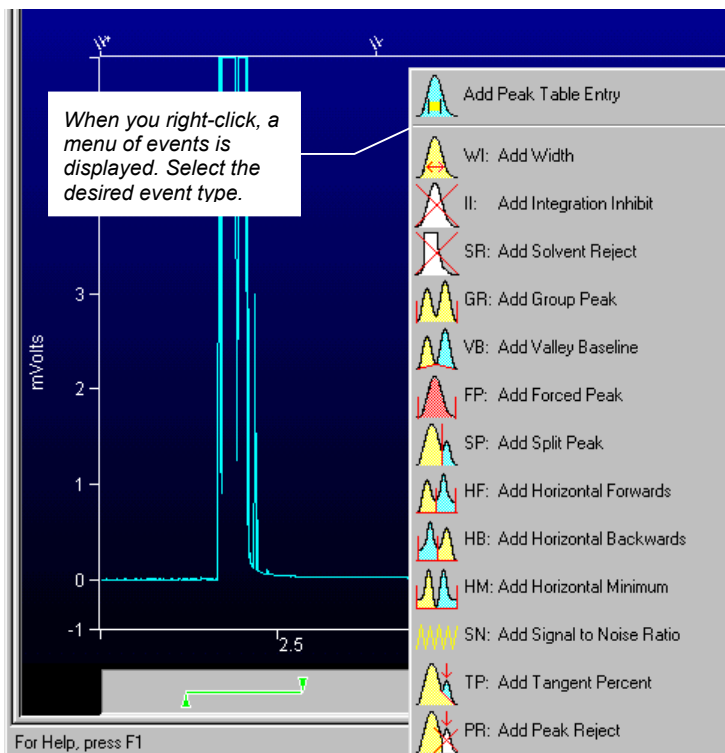
Certain integration parameters can be set to affect only portions of the chromatogram. This is useful to account for changes in the chromatographic signal during the course of the run, or to better integrate partially fused peaks or peaks that occur on a drifting baseline.

These timed integration events can be edited from the Time Events window displayed from the Edit Method menu, or they can be graphically placed on the chromatogram display. Peak table entries can also be graphically placed on the chromatogram using the same technique. Time events that are added to the chromatogram take effect when you perform a reintegration.

The Visual Method Editing Window is displayed below the chromatogram.

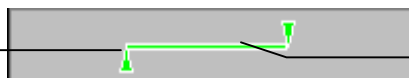


To add a new time event, right-click in the Interactive Time Events window at the time where you wish the event to occur.



The event is added at the point where you right-clicked.

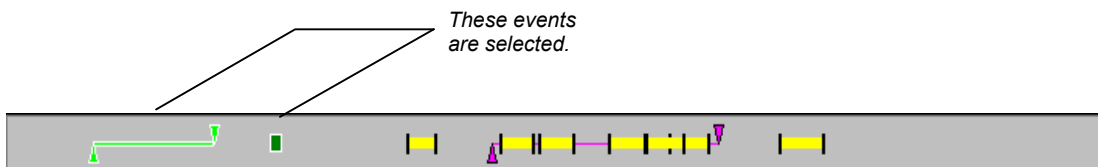
Drag a time range endpoint to change the range.



Drag the center of a time range to move the entire range.

When you change the width of a peak table entry (the yellow, red or blue boxes), all peak table entries are adjusted to reflect the new window size. Refer to *Peak Table* on page 20 for more information on peak identification windows.

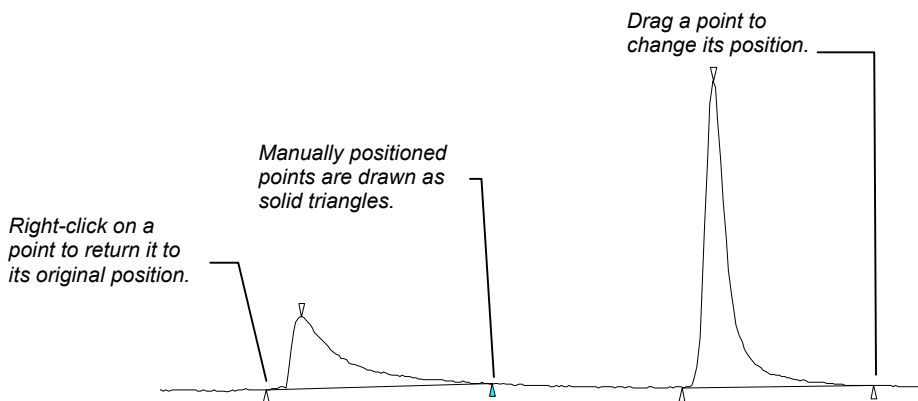
You may select multiple events by holding the Shift key down while clicking on them, or by dragging over all the events with the mouse.



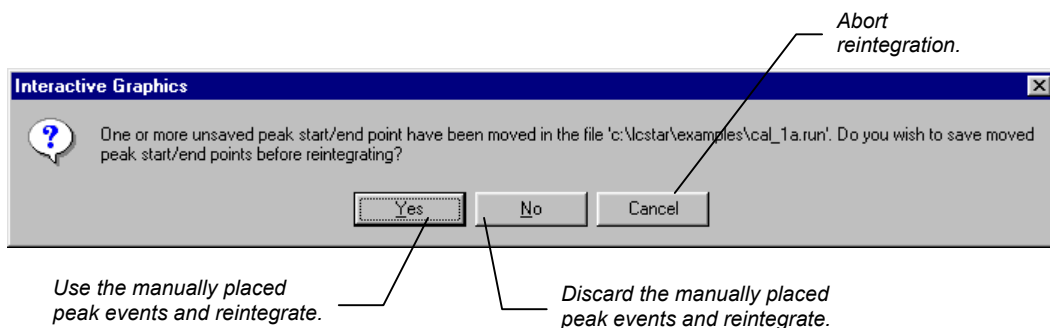
Use the control key to toggle the selection state and the delete key to delete selected events. Right-click on the event to see a menu of options.

Moving Peak Start and End Points

Peak start and end points are indicated on the chromatogram as lines or triangles (depending on the options selected in the Preferences dialog box). You may change the position of these points by dragging them with the mouse.



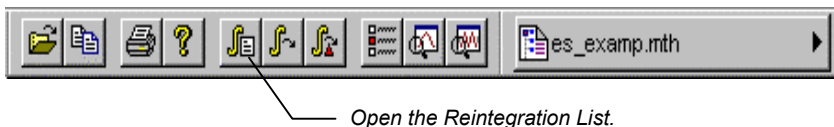
When you perform reintegration on a chromatogram with manually positioned peak events, you are asked whether you wish to include the changes when calculating results.



If you use the manually positioned peak events, peaks whose areas are affected by the event will be flagged with a "U" (user-modified) in the results report.

Calculating Results

Results can be calculated for all opened chromatogram channels using the Data Handling parameters in the active Method. Open the Reintegration list by clicking on the button in the Main toolbar, or by selecting it from the Results menu.



The Reintegration List is displayed.

Set the run type (analysis, calibration, verification, baseline).

If you are calculating results using an Internal Standard, edit the amount for standard peaks here.

Run DH	Data File	Sample Name	Sample Type	Cal. Level	Internal Standard	Unidentified Peak Factor	Multiplier
<input checked="" type="checkbox"/>	c:\lstar\examples\cal_1a.run	12.0 NP	Analysis		Amount(s)	0	1
<input type="checkbox"/>					Amount(s)		
<input type="checkbox"/>					Amount(s)		
<input type="checkbox"/>					Amount(s)		
<input type="checkbox"/>					Amount(s)		
<input type="checkbox"/>					Amount(s)		
<input type="checkbox"/>					Amount(s)		

Indicates channels on which to run Data Handling. An unchecked row indicates that no new results will be calculated for the corresponding chromatogram.

Save changes and calculate results.

Save changes but do not run Data Handling

Calculate Results

Save Changes

Cancel

Calibration Coefficients

Incorporate New Calibrations into Data Set

Clear Coefficients at Start of List

If a calibration run is specified, either add calibration points to existing data, or replace existing data with new calibration points.

After reintegration, the chromatogram display will be redrawn with any changes to peak events and colored markers indicating where timed integration events took place.

You may also quickly reintegrate all open chromatograms using the parameters in the Reintegration List by using the Reintegrate Now command, selected from the Main toolbar or the Results menu.



Run Data Handling using parameters stored in the Reintegration List.

Reintegrate peaks after clearing any manually positioned peak events.

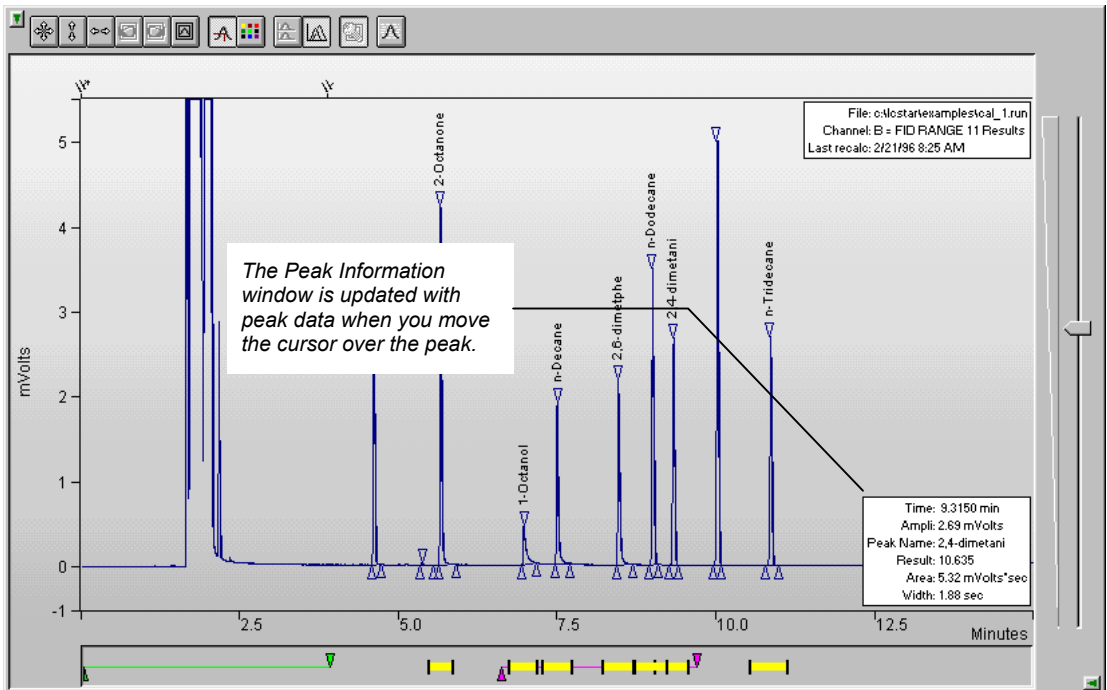
Viewing Results

You may view results for each peak by enabling the Cursor/Peak Information display from the Chromatogram Display Toolbar.



Click on this button to enable the display of peak information.

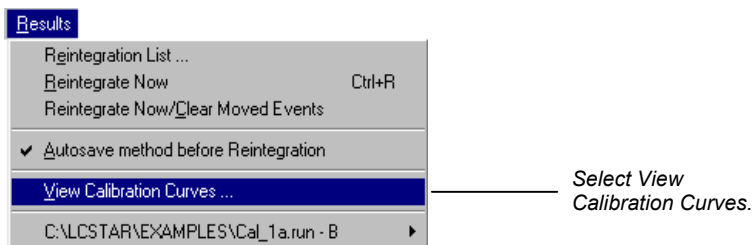
The Cursor/Peak Information display can also be enabled from the Trace Settings tab in the Preferences dialog box.



Other results viewing functions are available by right-clicking on the chromatogram trace. When you do, a popup menu lists all report options available. This list will vary depending upon the post-run applications that you have installed. The same list is also available from the Results menu, listed under the Data File name.

Viewing Calibration Curves

If you are performing calibrated calculations (external standard, internal standard or normalized percent), you may view the calibration curves associated with the active Method. Pull down the Results menu.



The Calibration Curve window is displayed if calibration data exists in the active Method. If you have not yet performed any calibration runs with the active Method, or if you have cleared calibration coefficients without adding any new calibration data, a message box will tell you that no calibration data exists in the Method.

You may overlay curves with different fit parameters to determine the best type of fit to use for your data.

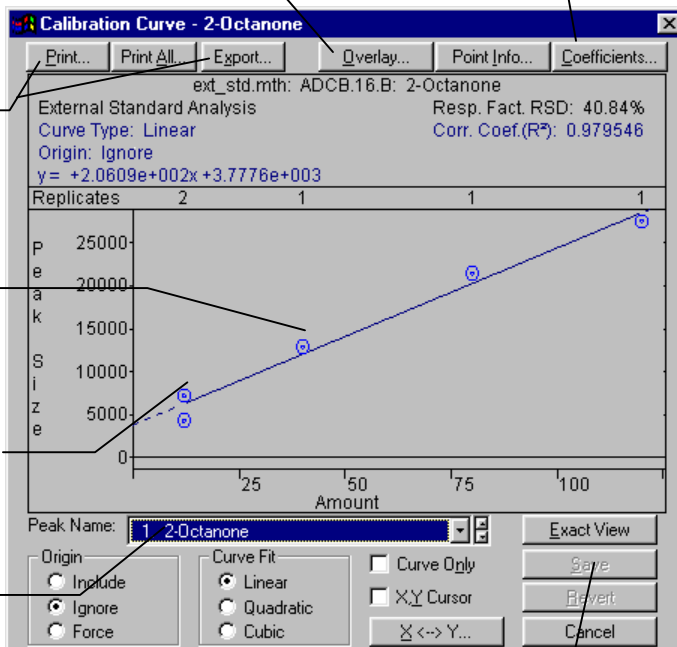
You may manually enter calibration coefficients.

You may print or export the selected curve or curves for all peaks in the peak table.

Right-click on a calibration point to exclude it from the curve fit calculation.

Double-click on a calibration point to see more information.

Select the peak whose curve you wish to view.

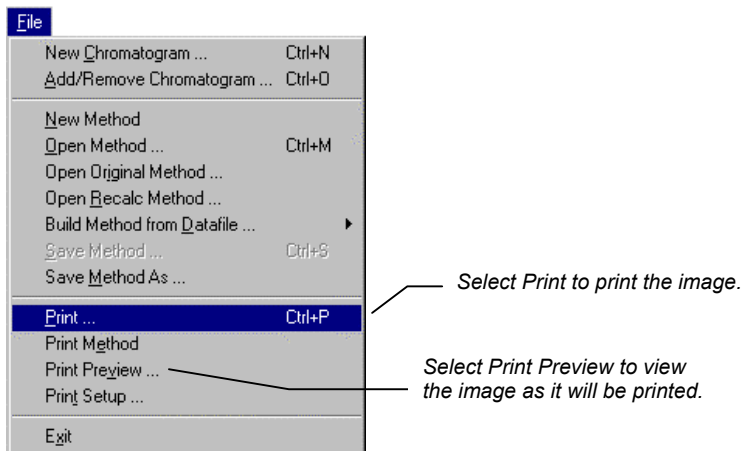


Changes made here only affect the stored calibration data and are documented in the results report and calibration block report.

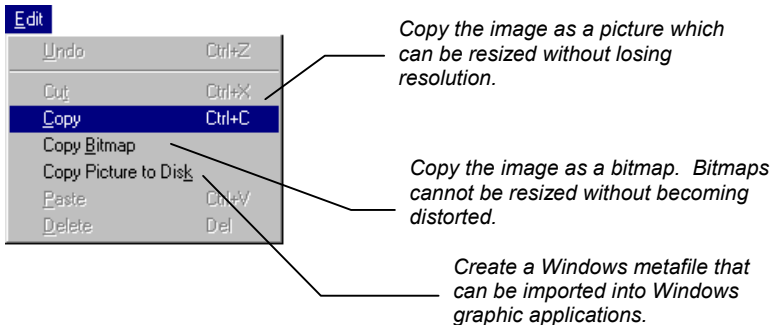
Refer to the on-line help in Interactive Graphics for a complete description of all fields in the Calibration Curve window.

Printing and Copying the Chromatogram Display

You may wish to print the image displayed in Interactive Graphics, or paste it into another document. To print the image displayed in the Chromatogram Display Window, pull down the File menu.



To copy the image to the clipboard for use in other Windows applications, pull down the Edit menu and click on the Copy item.



Images that are generated using *Print*, *Copy* or *Copy Picture to Disk* always have a white background with no attenuation control, toolbar scroll bars or borders. Color is preserved when printing to a color printer, otherwise colors are changed to black. Images generated using *Copy Bitmap* are exactly as they appear on screen.

Exit Interactive Graphics

When you exit Interactive Graphics or when you remove a .RUN file from Interactive Graphics by removing it from the chromatogram display, you will be prompted to save changes to the file. If you want the latest set of calculated results and method parameters to be saved in the RUN file, then select Yes and the new results and method parameters will be added to the file.

Batch Recalculations

Performing Recalculations in System Control

You can recalculate a group of Data Files from System Control. You do so by creating a RecalcList containing the names of the Data Files you wish to recalculate. A RecalcList can be created by selecting *New RecalcList* from the File menu, or by clicking on the *Create a new Automation File* button in the System Control toolbar.



Select New RecalcList.

If you are using a RecalcList that has already been created, use the *Open RecalcList* menu item or the *Open an Automation File* button on the toolbar to select it.

The RecalcList window is displayed.

Enter names of Data Files to recalculate.

Right-click on column headers for formatting options.

	Data File	Sample Name	Sample Type	Cal. level	Inj.	Recalc Notes	AutoLink	Amount Std (IS, N% only)
1			New Calib Block					
2	c:\star\examples\parais1.r	Calib. Level #1	Calibration	1	1	none	none	0.55
3	c:\star\examples\parais2.r	Calib. Level #2	Calibration	2	1	none	none	0.55
4	c:\star\examples\parais3.r	Calib. Level #3	Calibration	3	1	none	none	0.55
5	c:\star\examples\parais4.r	Sample #1	Analysis		1	none	none	0.55
6	c:\star\examples\parais5.r	Sample #2	Analysis		1	none	none	0.55
7	c:\star\examples\parais6.r	Sample #3	Analysis		1	none	none	0.55
8			New Calib Block					
9	c:\star\examples\parais7.r	Calib. Level #1	Calibration	1	1	none	none	0.55
10	c:\star\examples\parais8.r	Calib. Level #2	Calibration	2	1	none	none	0.55

Begin the recalculation.

Data Handling parameters are identical to those in the SampleList.

Browse to find Data Files on disk.

Refer to the on-line Help in System Control/Automation for a complete description of all RecalcList fields.

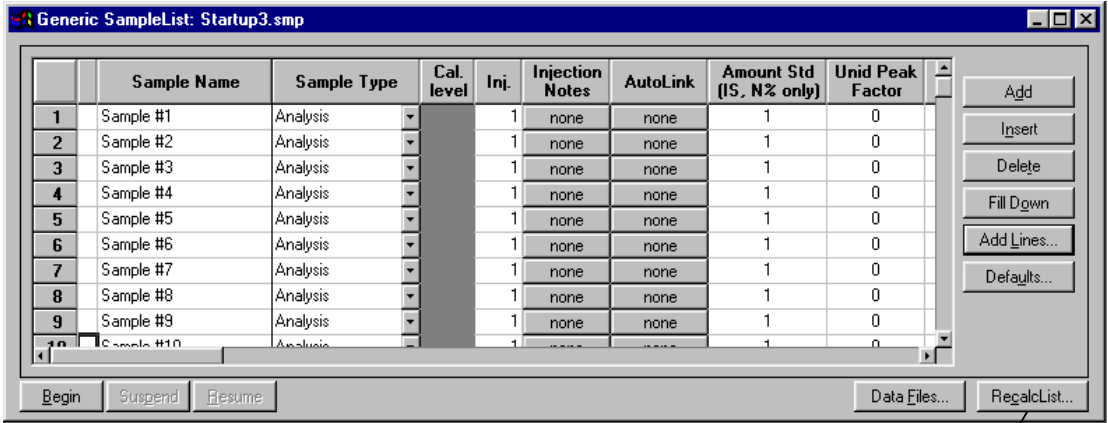
When you press the Begin button, you are prompted for your name, the instrument, and for the Method to use.

Select the Method to use for the recalculations.

Recalculate results or print reports (no recalculation performed).

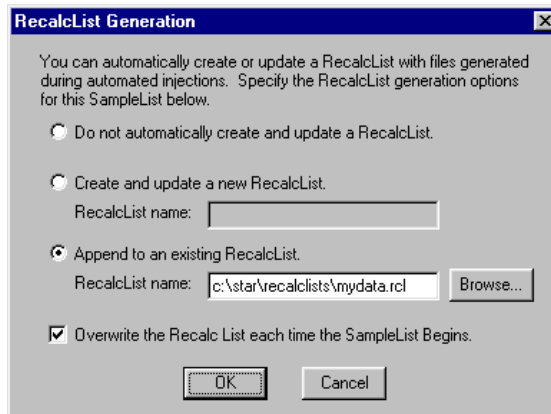
Generating a RecalcList after Injections

When you use a SampleList to perform injections in System Control, a RecalcList can be automatically generated containing the names of all the Data Files produced from the run.



Click on the RecalcList button for RecalcList generation options.

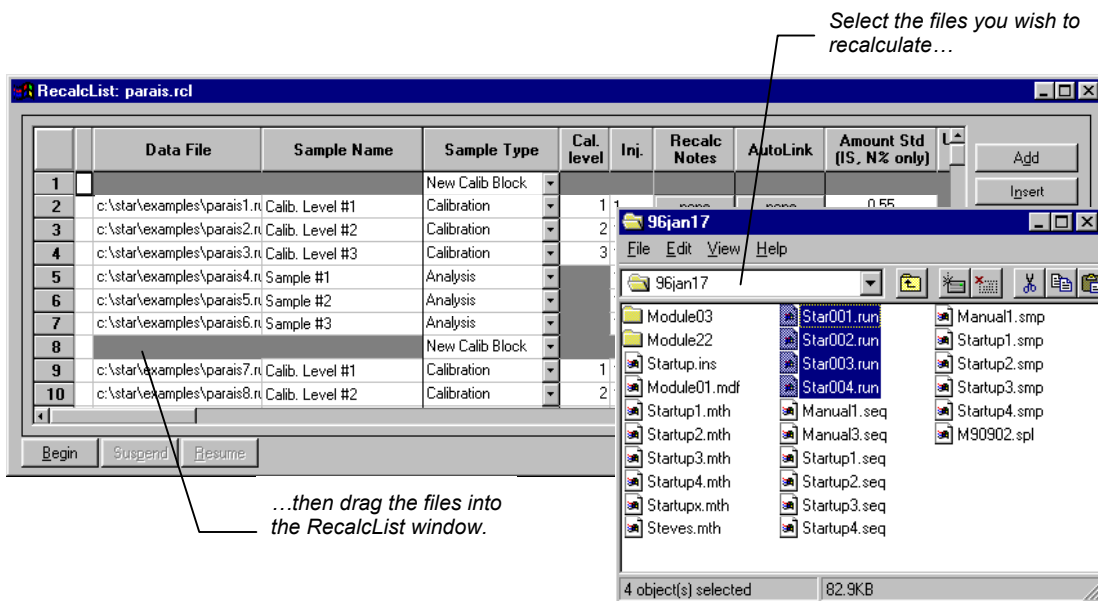
The RecalcList Generation dialog box is displayed.



If you choose to create a new RecalcList every time the SampleList is executed, a number will automatically be appended to the RecalcList file name, if necessary, to avoid overwriting an existing file. If you specify “Overwrite the Recalc List each time the SampleList begins”, then name specified with the Create or Append options is always used as entered without appending a number. If you choose to append entries to an existing RecalcList, you may have both the SampleList and RecalcList open simultaneously in System Control during automation and see the RecalcList get updated with new entries.

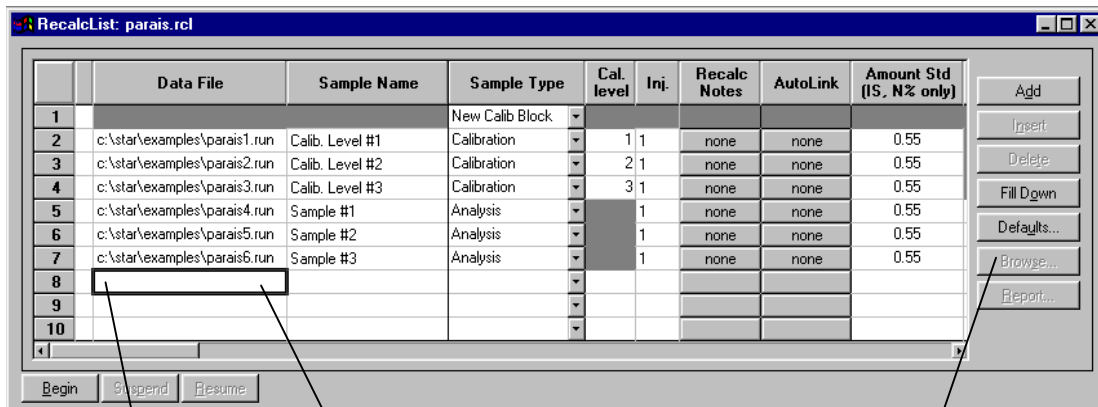
Generating a RecalcList from Saved Data Files

You may create a RecalcList containing Data Files stored on disk. Open or create a new RecalcList from the File menu or toolbar in System Control. Then, use the Windows Explorer to list the Data Files that you wish to recalculate.



The RecalcList window is filled with the Data Files. Default entries are added to each row of the RecalcList corresponding to the values used in the original processing of the Data File.

You may also add Data Files to a RecalcList one at a time.



As you make changes to the RecalcList in System Control, the changes are saved at the time that you make them. If you are editing a RecalcList and wish to save it under a different name, use the Automation File Editor.

Specifying Per-Sample Data Handling Parameters

Most Data Handling parameters are specified in the Method used during the recalculation. Some parameters may vary on a per-sample basis, and are therefore specified in the RecalcList. The following Data Handling parameters can be specified on a per-sample basis:

- Unidentified Peak Factor
- Multiplier
- Divisor
- Amount for Internal Standard Peak(s)

These parameters are represented by cells in the spreadsheet.

If you have multiple internal standard peaks, or wish to specify different per-sample Data Handling parameters for each channel of a detector in an instrument, you do so by clicking on the Multi-Channel/Multi-Standard button in the spreadsheet row for each sample. The following dialog box is displayed.

Select the specific detector channel here.

Columns for each standard amount can be entered.

Data Handling Channels For Method Startup3.mth, Sample 'Sample #1'

#	Detector Channel	Calculation Type	Unid Peak Factor	Multiplier	Divisor	Standard Peak 1	Amount Standard 1
1	ADCB.01 Channel A	Internal Std	0	1	1	Peak 1.000	1
2	ADCB.01 Channel B	Internal Std	0	1	1		
3							
4							

Edit the Calibration Setup for the active Method.

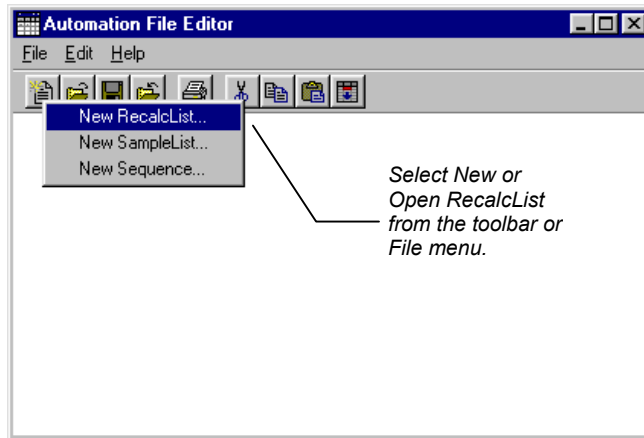
Edit the Peak Table for the active Method.

Editing RecalcLists from the Automation File Editor

You can edit existing RecalcLists or create new ones using the Automation File Editor instead of System Control/Automation. This is useful if System Control is already using a RecalcList, or if you wish to save the RecalcList under a new name.

Click on the Edit Automation Files button.

The Automation File Editor window is displayed.



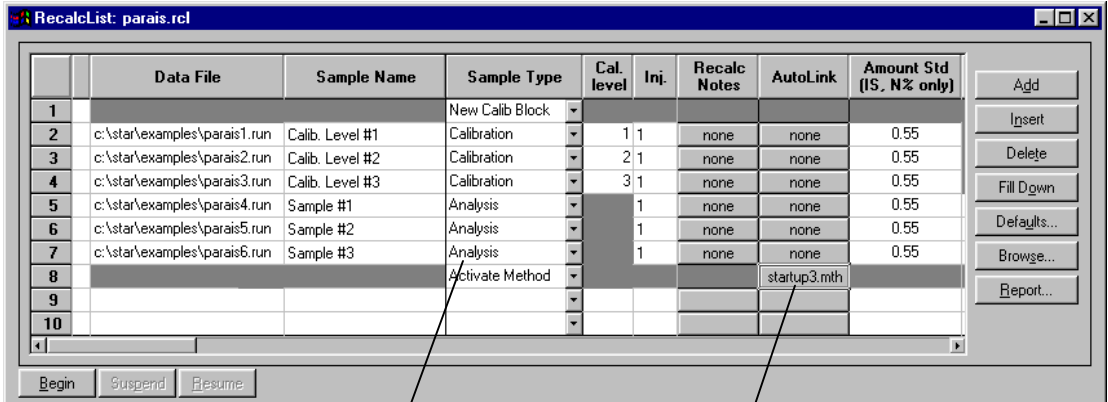
Editing the RecalcList from the Automation File Editor is the same as editing from System Control, except changes to the RecalcList are not saved until you explicitly select Save or Save As. If you attempt to edit a RecalcList using the Automation File Editor while the same file is in use by System Control, you will be denied access.

Using More than One Method for Recalculations

The Star Workstation allows you to perform batch recalculations using more than one Method. There are two ways in which this can be accomplished. The first is by changing the active Method from within the RecalcList. The second is by using a Sequence.

Changing the Method in the RecalcList

You may change the Method used during recalculations by activating a Method in a RecalcList row. Activation of Methods in the RecalcList is performed the same way as in the SampleList.

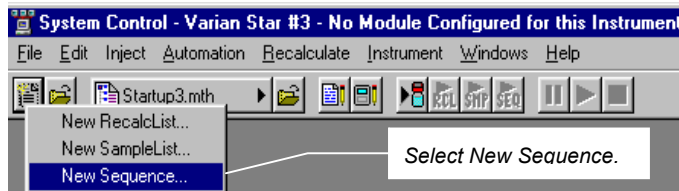


Select Activate Method as the Sample Type.

Select the Method in the AutoLink cell.

Using a Sequence

A Sequence allows you to specify multiple Methods and RecalcLists to be processed during automation. In addition, you may perform automated injections followed by automated recalculations in the Sequence. A Sequence can be created by selecting *New Sequence* from the File menu, or by clicking on the *Create a new Automation File* button in the System Control toolbar.



If you are using a Sequence that has already been created, use the *Open Sequence* menu item or the *Open an Automation File* button on the toolbar to select it.

The Sequence window is displayed.

You may specify injections followed by recalculations.

Enter the Method and RecalcList to use. You may enter any number of

	Action	Method	Sample/RecalcList
1	Inject	c:\star\2887_a-a.mth	c:\star\startup3.smp
2	Recalc	c:\star\analysis.mth	c:\star\myrecalcs.rcl
3	Print	c:\star\examples\another.mth	c:\star\myrecalcs.rcl
4	Pump(s) Off		
5	Lamp(s) Off		
6	Print Message Log		
7			
8			

Press Begin to start the Sequence.

Specify Recalc as the Sequence action.

Browse for a Method or RecalcList file in the active cell.

Calibration

Types of Calibration



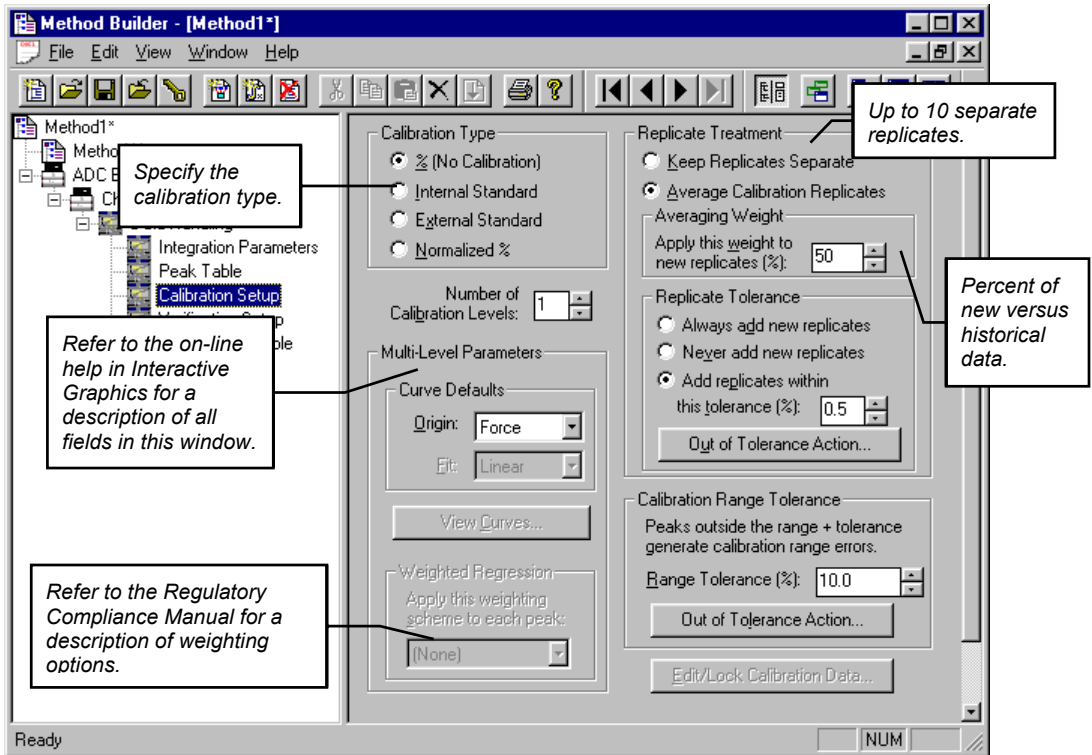
There are three types of calibration available with the Star Workstation: External Standard, Internal Standard, and Normalized Percent. Refer to the section, *Data Handling Fundamentals on page 69*, for a brief description of each calibration type. Refer to the Regulatory Compliance Manual for a complete description of the algorithms used by each type to calculate results.

Preparing the Method for Calibration

In order to generate quantitative results for the compounds in your samples, you must identify the peaks of interest and specify your calibration parameters. This is done by using the Peak Table and Calibration Setup window in the Data Handling section of the Method. The Data Handling Method section can be edited from the Interactive Graphics or the Method Builder applications. The Method Builder application can be invoked anywhere a Method name appears in a Quick Link button. Refer to the sections *Interactive Graphics and Data Handling on page 3* and *Building Methods* in the Data Acquisition Operation Manual for details on the procedure for creating and editing Data Handling Method sections.

Calibration Setup

The Calibration Setup window contains parameters that affect the type of calibration calculations that will be performed by your Star Workstation.



Peak Table

The Peak Table contains amounts for each level (the number of which is specified in the Calibration Setup), and the internal standard peak designations.

Specify internal standard peaks. *Enter amounts for each level.*

The screenshot shows the 'Method Builder' window for a file named 'E_s_examp.mth'. The interface includes a menu bar (File, Edit, View, Window, Help), a toolbar, and a tree view on the left showing the method structure. The main area contains a table with the following data:

	Retention Time	Peak Name	Ref	Std	RRT	Standard Peak Name	Group	Level 1 Amount
1	5.674	2-Octanone				1-Octanol	0	12
2	6.969	1-Octanol		<input checked="" type="checkbox"/>		1-Octanol	0	12
3	7.507	n-Decane				1-Octanol	0	12
4	8.474	2,6-dimetphe				1-Octanol	0	20
5	8.997	n-Dodecane				1-Octanol	0	12
6	9.324	2,4-dimetani				1-Octanol	0	12
7	10.856	n-Tridecane				1-Octanol	0	12
8								
9								
10								

Buttons on the right side of the table include: Add, Insert, Delete, Fill Down, and Sort. At the bottom of the table area are buttons for 'Define Peak Windows...' and 'Print'. The status bar at the bottom left shows 'Ready' and the bottom right shows 'NUM'.

Refer to the appropriate standard peak.

Automated Calibration

You calibrate your Method by injecting calibration samples using System Control. Calibration samples are specified in the SampleList.

To clear previously stored calibration data, enter a New Calib Block line.

The screenshot shows a software window titled "Generic SampleList: 8200 attached to SWLab 3800.smp". The main area is a table with the following columns: Sample Name, Sample Type, Cal. level, Inj., Injection Notes, Amount Std (IS, N% only), and Unid Peak Factor. The table contains several rows, including calibration standards and unknown samples. Callouts point to specific cells in the table:

- A callout points to the "Sample Type" column for the first three rows, stating: "Select the Calibration sample type."
- A callout points to the "Cal. level" column for the first three rows, stating: "Enter the calibration level for this injection."
- A callout points to the "Amount Std" column for the first three rows, stating: "Specify internal standard amounts."
- A callout points to the "Inj." column for the first three rows, stating: "Enter the number of replicates for each level."

At the bottom of the window, there are buttons for "Begin", "Suspend", "Resume", "Data Files...", and "RecalcList...". On the right side, there are buttons for "Add", "Insert", "Delete", "Fill Down", "Add Lines...", and "Defaults...".

Sample Name	Sample Type	Cal. level	Inj.	Injection Notes	Amount Std (IS, N% only)	Unid Peak Factor
1	New Calib Block					
	Calibration	1	3	Standard	10	
	Calibration	2	3	Standard	20	
	Calibration	3	3	Standard	30	
5	Unknown #1		1	Unknown	10	0
6	Unknown #2		1	Unknown	10	0
	Analysis		1	Unknown	10	0
	Analysis		1	Unknown	10	0
	Analysis		1	Unknown	10	0

You can also calibrate your Method using previously collected Data Files, recalculating them as calibration samples. Add the Data Files to the RecalcList.

	Data File	Sample Name	Sample Type	Cal. level	Inj.	Recalc Notes	AutoLink	Amount Std (IS, N% only)
1			New Calib Block					
2	c:\star\examples\parais1.r	Calib. Level #1	Calibration	1	1	none	none	0.55
3	c:\star\examples\parais2.r	Calib. Level #2	Calibration	2	1	none	none	0.55
4	c:\star\examples\parais3.r	Calib. Level #3	Calibration	3	1	none	none	0.55
5	c:\star\examples\parais4.r	Sample #1	Analysis		1	none	none	0.55
6	c:\star\examples\parais5.r	Sample #2	Analysis		1	none	none	0.55
7	c:\star\examples\parais6.r	Sample #3	Analysis		1	none	none	0.55
8			New Calib Block					
9	c:\star\examples\parais7.r	Calib. Level #1	Calibration	1	1	none	none	0.55
10	c:\star\examples\parais8.r	Calib. Level #2	Calibration	2	1	none	none	0.55

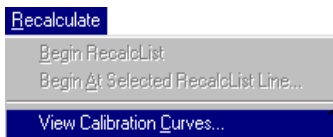
Enter the Data Files to be used as calibration samples.

Select the Calibration sample type.

Enter the calibration level for this Data File.

Inspecting Calibration Curves

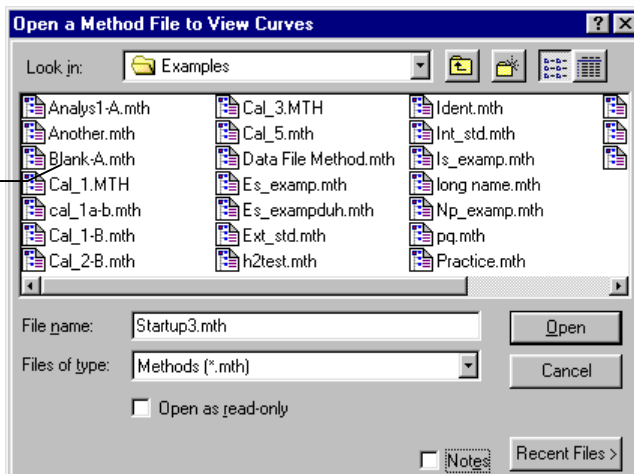
Calibration Curves can be viewed and edited from System Control. Pull down the Recalculate menu.



Select View Calibration Curves.

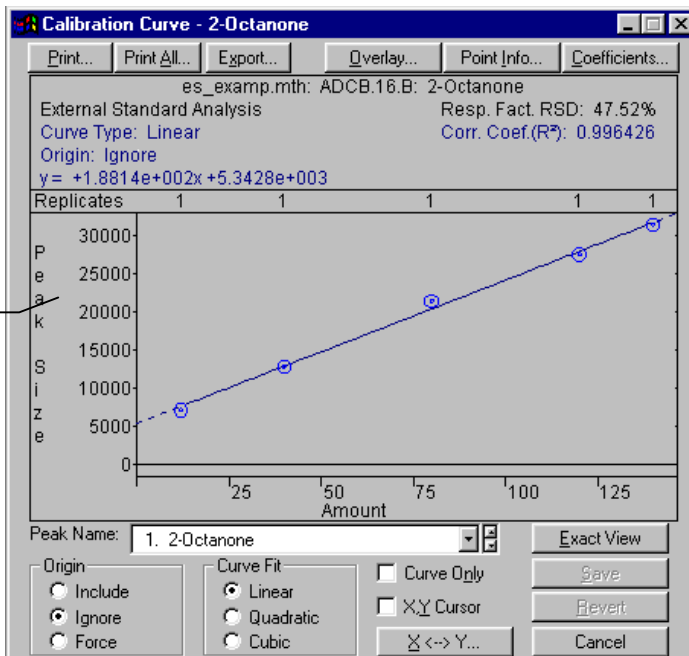
You are prompted for the Method containing the calibration curves to view. The active Method for the instrument is selected by default.

Select the Method.

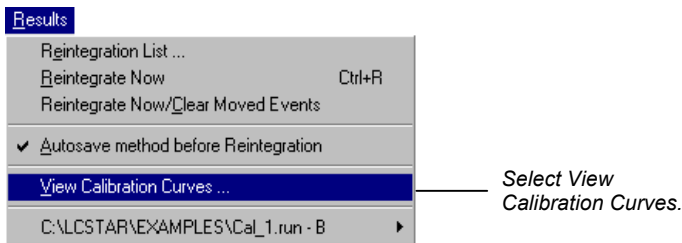


If curves exist for more than one channel, you are prompted for the channel. The Calibration Curve window is displayed for the selected channel's curves.

Refer to [page 31](#) for a description of this window.

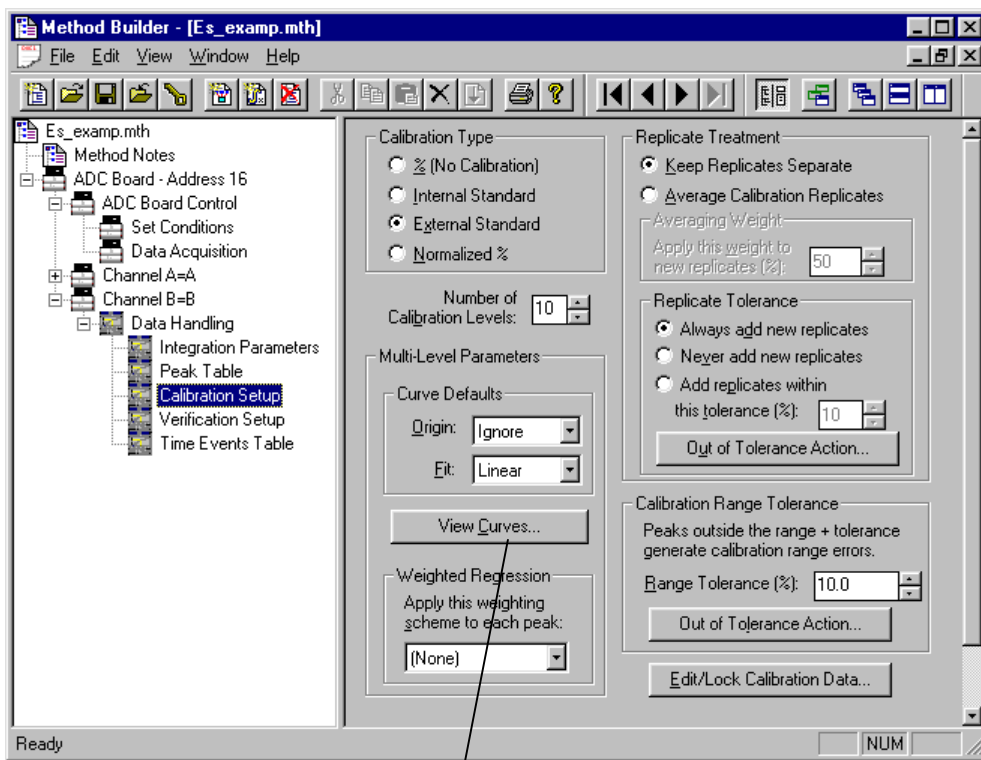


You may also view Calibration Curves for the active Method in Interactive Graphics. Pull down the Results menu.



The Calibration Curve window is displayed.

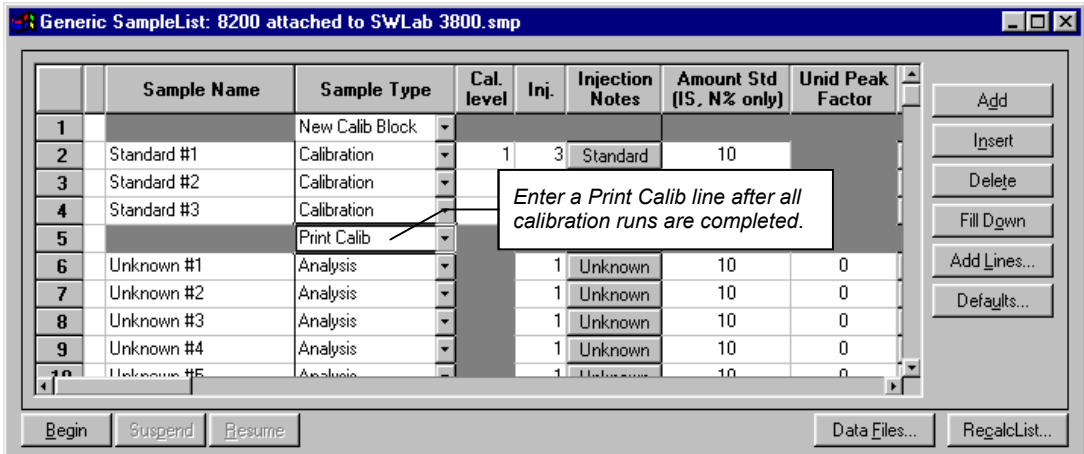
You may also view Calibration Curves from the Calibration Setup window in the Data Handling section of the Method.



Select View Curves.

Generating Calibration Block Reports

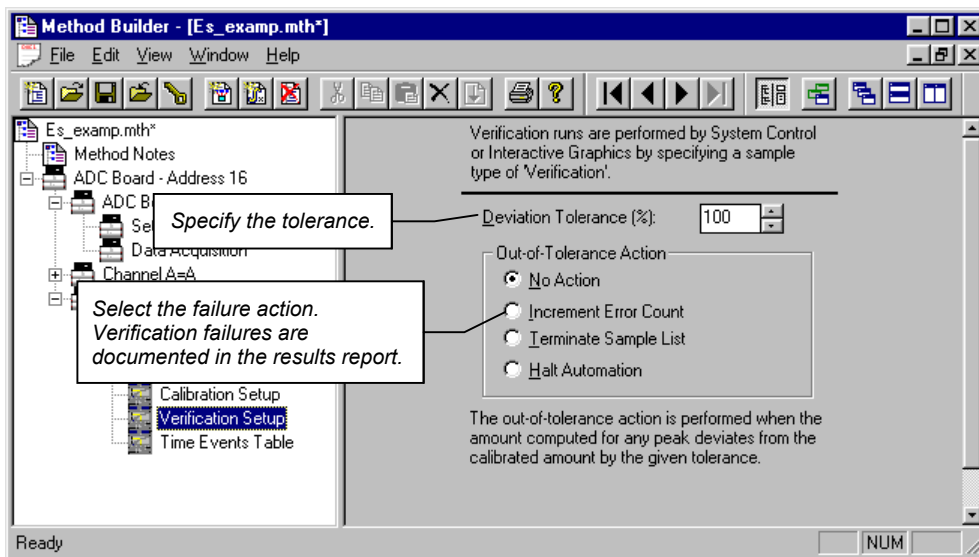
As you create calibration information in System Control, you may wish to generate a Calibration Block Report documenting the calibration curves and replicate statistics for each peak. Open the SampleList (shown) or RecalcList window.



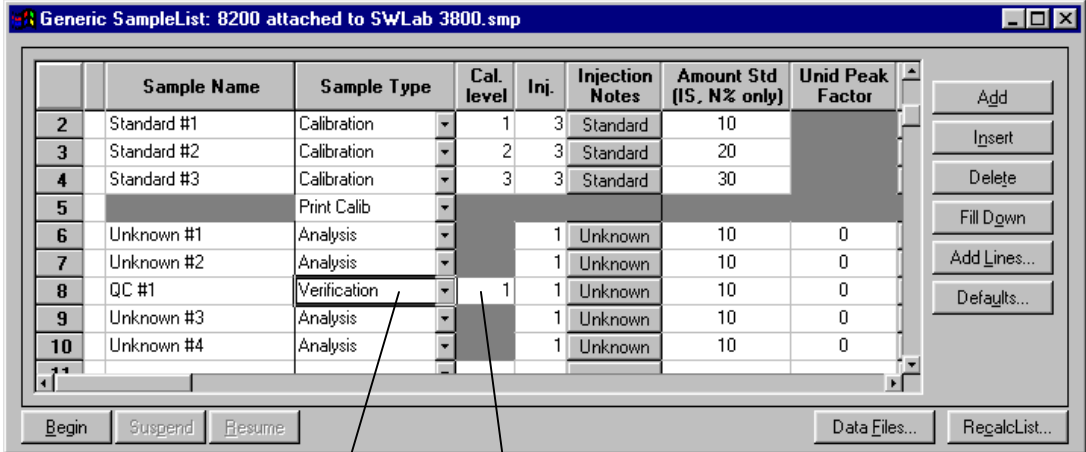
A Calibration Block Report is printed when the SampleList or RecalcList line is encountered during automation. The format of the Calibration Block Report is determined by parameters set in the Calibration Block Report Format window in the Report section of the Method. Refer to the section [Generating Reports on page 57](#) for details on the Report Method section.

Calibration Verification

You may wish to periodically check the validity of your calibration data as you perform analytical injections. You do so by injecting a verification sample with known amounts for each compound and comparing them to amounts calculated from the calibration curves. If the amounts deviate more than a given tolerance, a verification failure occurs and a number of failure actions can take place. Verification failure options are specified in the Verification Setup window in the Data Handling Method section.



Verification samples are entered into the SampleList (shown) or RecalList.



Select the Verification sample type.

Specify the calibration level corresponding to the known amounts in the sample.

Refer to the on-line help in Report for details on the format of the results report for Verification runs.

Generating Reports

This section contains information on generating Standard Reports. For information about using other reporting applications such as the Star Custom Report Writer, refer to the manuals specific to those applications.

The Standard Report Method Section



Report formatting parameters are specified in the Report section of the Method. The Report Method section is a post-run application section and applies to a specific detector channel. You create a Report Method section for each channel of each detector for which you wish to generate a report. Refer to the Data Acquisition Operation Manual for details on the procedure for creating and editing Method sections.

The Report Method section contains four editing windows. Each one is described below.

Print Options

Print options allow you to specify the report title, whether the report includes the chromatogram, results or both, along with other parameters that affect report generation.

Method Builder - [Es_examp.mth*]

File Edit View Window Help

Es_examp.mth*
Method Notes
ADC Board - Address 16
ADC Board Control
Set Conditions
Data Acquisition
Channel A=A
Data Handling
Standard Reports
Print Options
Results Format
Chromatogram Format
Calibration Block Report
Star Custom Report Writer
Channel B=B
Data Handling

Print Copies: 1

Single Run Reports

Title: _____

Print Chromatogram

Print Results

Suppress Printout on Injections

Convert Results to ASCII

Calibration Block Reports

These parameters affect the Calibration Block Report printed from a Sample/RecalcList in System Control using the "Print Calib" action.

Print Report

Convert Report to ASCII

Only prints when performing recalculations or print actions from System Control. Use this to avoid automated injection delays due to printer problems. Refer to page 35 for details on batch recalculations.

Creates an ASCII file containing the results report. The file is named based on the Data File name and channel label, with the extension ".txt".

Ready NUM

ASCII file conversion creates text files that are required by certain Advanced Applications used with the Star Workstation.

Results Format

Results format specifies the layout and contents of the results report. Refer to the on-line help in Report for details on the results report fields and format.

The screenshot shows the 'Method Builder' window with the following settings and callouts:

- Results Table:**
 - Amount Units:** [Empty text box] *Uses the group number set in the Peak Table.*
 - Number of Decimal Digits:** 4
 - Show Peak Group Totals
- Run Documentation:**
 - Run Log (Method/Module Documentation)
 - Error Log (Instrument Errors)
 - Calibration Report (Curve Coefficients)
 - Revision Log (Changes to Results)
 - Notes (Sample Notes)

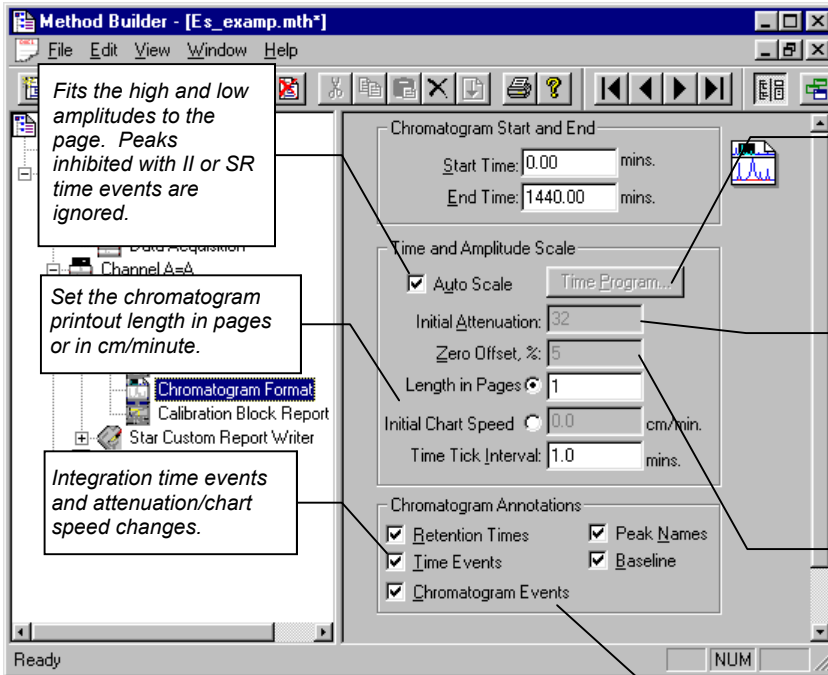
Callout boxes on the left side of the interface provide further details:

- Top Callout:** Contains the Method used during the injection, along with the Module Information specified in System Control.
- Middle Callout:** Calibration coefficients and replicate statistics for each peak.
- Bottom Callout:** Date, time and Method name logged for each recalculation of the Data File.

A callout box at the bottom right explains the 'Notes' option: Notes entered for the Sample in the SampleList and RecalList in System Control, or the Reintegration List in Interactive Graphics.

Chromatogram Format

Chromatogram Format specifies the length of the chromatogram, the scaling of the plot, and the plot annotations.



Fits the high and low amplitudes to the page. Peaks inhibited with II or SR time events are ignored.

Set the chromatogram printout length in pages or in cm/minute.

Integration time events and attenuation/chart speed changes.

When not using Auto Scale, you can time program attenuation and chart speed settings.

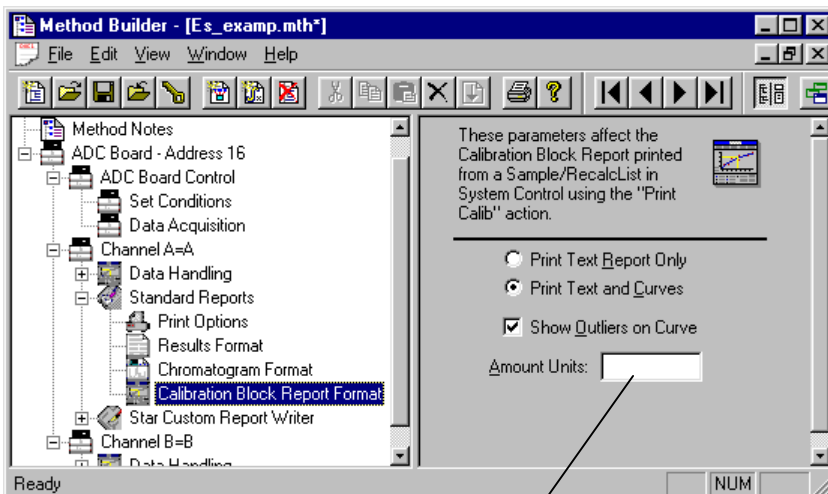
When not using Auto Scale, sets the magnification of the amplitude axis. 4096 displays the maximum detector range, 1 displays the highest magnification.

When not using Auto Scale, sets the offset of the baseline as a percentage of the full page.

Peak start, end and apex.

Calibration Block Report Format

These options affect the Calibration Block Report generated when a Print Calib entry is added to a SampleList or RecalcList in System Control.



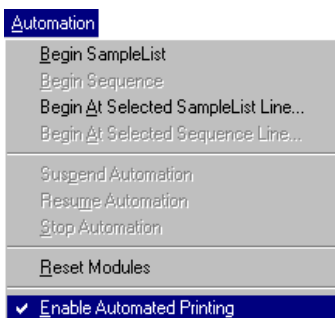
*Amount units label
the X axis of the
curve.*

Refer to the on-line help in Report for details on all fields in the Report Method section.

Automated Report Generation

Once you have added Report sections to your Method, automated reports can be generated from System Control after each injection, after recalculations, or by the use of the Print action in the Sequence window (see page 42).

You may choose to disable automated Report printing during the course of an automated sequence of injections or recalculations. You can do this by disabling automated printing from the Automation menu in the Instrument window.

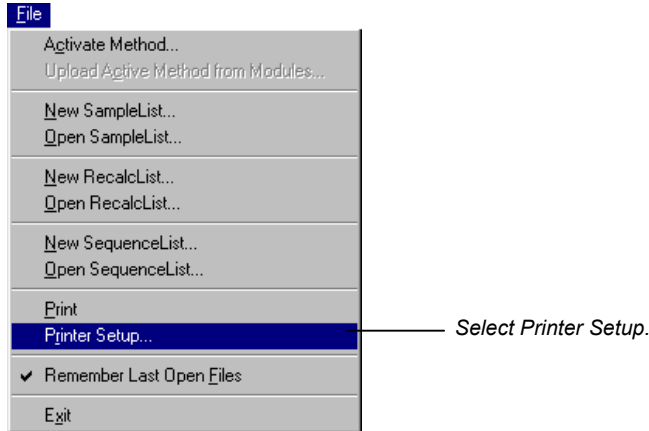


When this item is not checked, report printing is disabled. ASCII file generation is still performed if specified in the Report Method section.

Disabling automated printing is analogous to disconnecting the printer—automation continues but no reports are printed. This is useful if you are about to run out of printer paper but do not wish to suspend automation.

Automated Printing to Multiple Printers

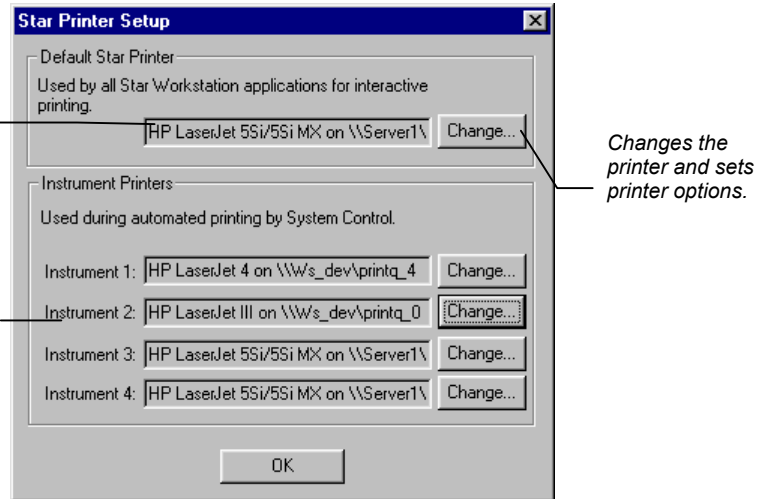
If you are running automation on more than one instrument, you may wish to designate a separate printer for each instrument to avoid interleaving of reports. Pull down the File menu in System Control (or any Star Workstation application).



The Star Printer Setup dialog box is displayed.

This printer is used when you print documents from any Star Workstation application interactively.

These printers are used during automated report generation from System Control.

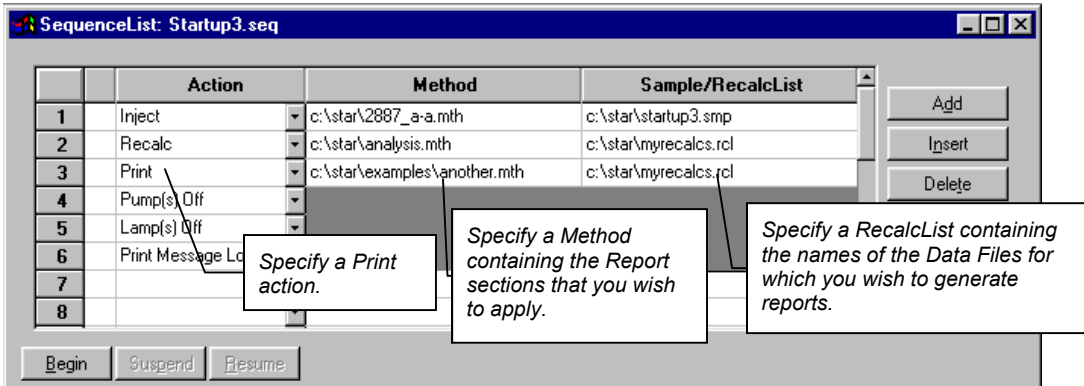


Batch Report Printing without Recalculating

When you perform batch recalculations in System Control, reports are automatically generated using the Report parameters in the active Method. You may wish to print reports for a batch of Data Files without recalculating them.

Batch Printing in System Control

Create or open a Sequence from the File menu or toolbar.



Refer to the section [Generating a RecalcList after Injections on page 37](#) for details on creating, editing and saving RecalcLists. Refer to the section [Using a Sequence on page 42](#) for more information on the Sequence window.

Batch Printing with Batch Report

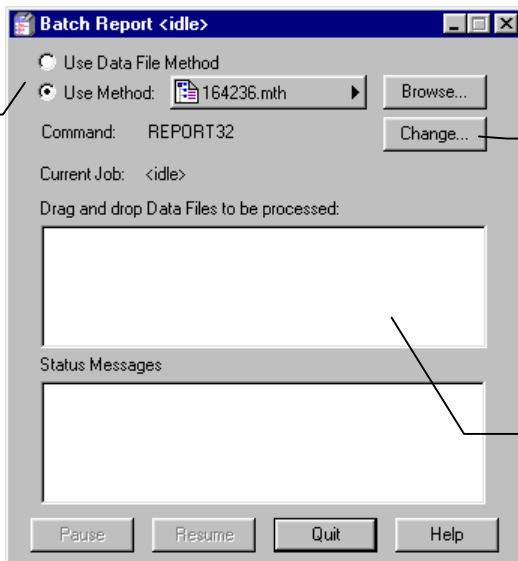
You may print reports for a set of Data Files without using System Control.



Click on the Batch Reporting icon in the Star Toolbar.

The Batch Report window is displayed.

Reports are printed using the formatting options stored in the Method last used to process the Data Files, or from the specified Method.



You may specify the post-run application to invoke. Use REPORT32 for standard reports.

Use the Windows Explorer to drag and drop Data Files into the Batch Report window.

As each report is generated, the Status Messages window is updated.

Viewing a Report for a Single Run

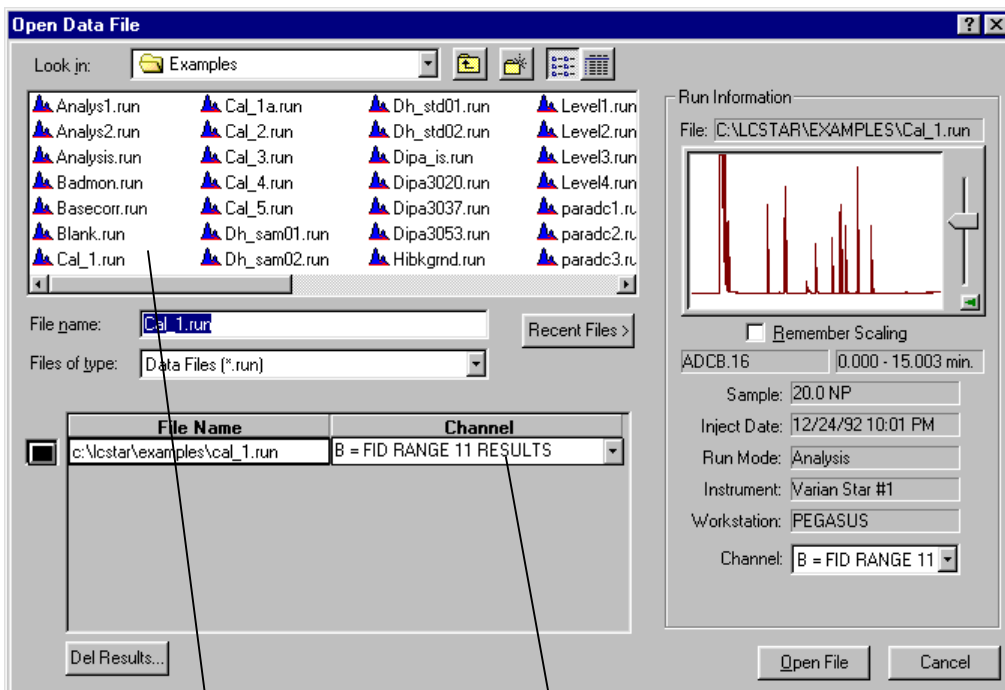
Note: Other reporting applications such as the Star Custom Report Writer can be used to view reports for Data Files. Details about these applications are documented in the manuals specific to the application.

Report viewing and printing options are available from any Data File Quick Link button, or by right-clicking on a chromatogram trace in Interactive Graphics. You may also select a Data File and view its chromatogram and results report by invoking the Standard Report application from the Star Toolbar.



Click on the Standard Reports icon in the Star Toolbar.

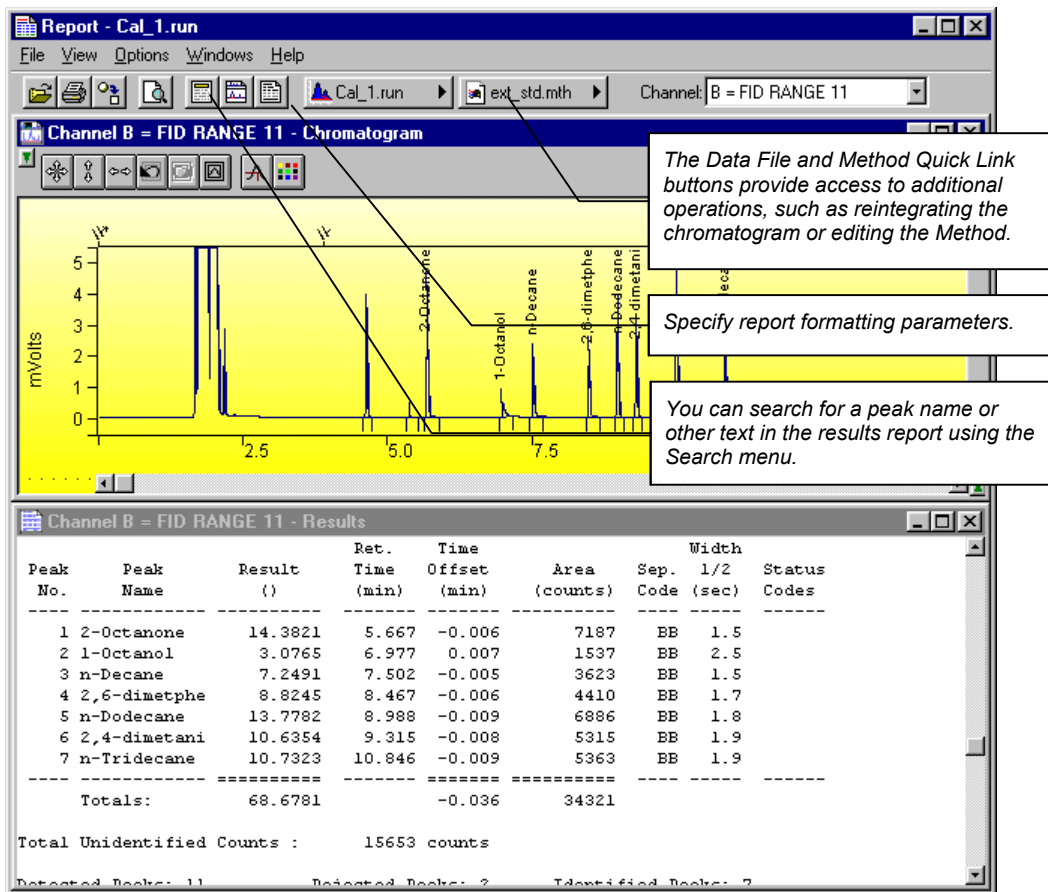
The Open Data File dialog box is displayed.



Select the Data File.

Select the channel in the Data File whose report you wish to view.

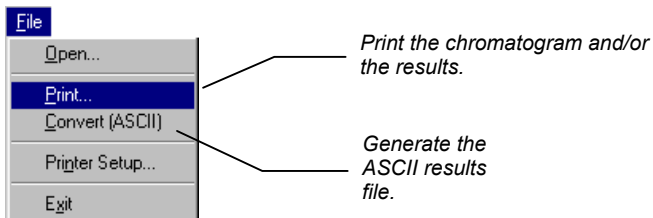
The chromatogram and results report are displayed.



The chromatogram is shown with the magnification, offset and time range specified in the Report Method section most recently used on this Data File channel. The results report is shown as it will appear when printed. When you zoom in on the chromatogram display, the chromatogram options in the Report Method section are updated.

Click on the Report Title, Chromatogram Options, or Results Options buttons in the toolbar, or select the corresponding items from the Options menu, to change the report format.

From the Report application you may print the report, generate an ASCII representation of the results report. Pull down the file menu.



You can also access these functions from the Report toolbar.

Data Handling Fundamentals

Introduction

Even after optimizing your chromatographic conditions to provide the best separation possible, you may still have unresolved peaks or other situations requiring special post-run Data Handling operations. For instance, you may want to exclude solvent peaks from the total area when doing area percent calculations. You may want to ensure that a very small peak in one part of the chromatogram is detected, and not rejected as a noise peak. Another common use for special post-run Data Handling is to fine tune your quantitation method. This section will provide an overview of both how the Star Workstation software performs the peak processing and how you can use the software to most efficiently meet your Data Handling needs.



Refer to the [Calibration section on page 45](#) for more information on calibration and verification procedures. Refer to the Regulatory Compliance Manual for a complete description of Data Handling algorithms and calculations. Refer to the on-line help in Interactive Graphics for descriptions of all of the fields in the Data Handling section of the Method.

Performing a Pilot Run

You may wish to use a pilot run to adjust the Data Handling parameters to their proper settings. You can use Interactive Graphics to edit the Data Handling section of your Method, and save this along with the Instrument Control sections for automatic data analysis on your production runs.

Data Handling Methods can be developed using an iterative approach. You change Method parameters, then reintegrate, and then determine if the results of your changes are appropriate. If not, you repeat these steps until you have the desired results. The Interactive Graphics application in the Star Workstation is designed to facilitate this iterative process. You can view your pilot run and create a Peak Table by clicking on peaks of interest with the mouse. You can add timed integration events graphically using the Interactive Time Events window. You can even generate and review calibration curves used to calculate results. Refer to the section *Interactive Graphics and Data Handling on page 3* for more information on these procedures.

Peak Detection

The Star Workstation software reduces the raw data collected from the chromatograph into a results report in four steps:

- Peak detection
- Peak integration (and final baseline determination)
- Peak identification (if a Peak Table is present)
- Results calculations

Peak detection is the process in which the peak start, apex, and end points are determined. This is also the step where fused peaks are identified as a mother/tangent peak pair, or as two valley separated main peaks.

The programmable time events that affect the peak detection process are Peak Width, Signal to Noise Ratio, Inhibit Integrate, Tangent Percentage, and Forced Peak. These are discussed in more detail later in this section.

Once the peaks are detected, the area for the peaks is determined in the peak integration step. The first part of this step is to process any Split Peak events. This event causes a previously detected peak to be treated as two separate peaks. Tied to both peak detection and peak integration is baseline placement. The four time events which affect baseline placement do not affect peak detection. These events are Valley Baseline, Horizontal Forward, Horizontal Backward, and Horizontal Minimum.

After areas for all peaks have been calculated, the optional step of peak identification is done. Before peaks are identified, they may be excluded from consideration by the Solvent Reject event or the Peak Reject event. Also, several peaks may be treated as one peak by the Group Peak event. Peak identification is the process by which peaks detected in the first step, and integrated in the second, are matched by retention time with a list of peaks you have previously entered in the Peak Table. As described below in more detail, Interactive Graphics provides a fast and efficient means of building the Peak Table using your pilot run.

The final step is to perform one or more of a large variety of possible calculations producing the final results. This produces results in a state suitable for printing or exporting by the Report application.

Peak Width Determination

In general, peaks are wider in liquid chromatography than they are in gas chromatography. To account for potential wide differences in peak width from run to run, you can set an initial peak width parameter. The lower the peak width value, the more accurate the placement of peak events. However, if set too low, a wide low peak may not be detected.

Peaks tend to widen with the retention time. The Data Handling software can account for this by automatically programming peak width events at appropriate times. This way, early eluting narrow peaks can use a low and more accurate peak width setting, while later eluting wide peaks will be properly detected with a higher peak width setting. To do automatic peak width programming, the peak detection software monitors peak widths as peaks are detected. If it determines that peaks are getting too wide relative to the current peak width setting, it programs a new, wider peak width. Although it is rarely necessary, the software is also able to automatically program narrower peak width settings.

Instead of letting the software automatically program peak width settings as needed, you can manually program your own peak width setting. The act of manually programming a peak width event disables automatic peak width programming. In the vast majority of cases, automatic peak width determination is all that is needed.

Adjusting the Signal To Noise Ratio

The Signal to Noise Ratio (S/N ratio) also affects the peak detection process. When you lower the S/N ratio, more small noise peaks are detected. Conversely, increasing the S/N ratio causes fewer small peaks to be detected. In the extreme case, a high S/N ratio may cause some larger peaks of interest to remain undetected, particularly if you have manually programmed peak width value that is too low. Another effect of a high S/N ratio value is that peak start and end events tend to be closer to the peak apex, especially when there is a lot of tailing, or a sloping baseline. This can result in valley separated peaks incorrectly considered baseline resolved.

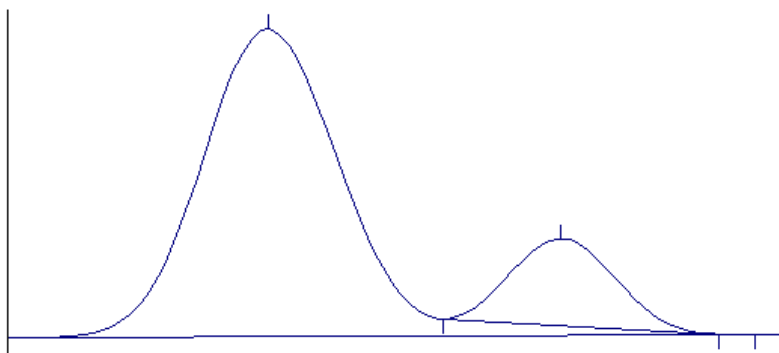
The optimal setting for this value depends on your analyses. You want to set this value low enough so that all the peaks in which you are interested are detected, but high enough so that extraneous noise “peaks” are not detected. If you want small peaks to be detected in one part of the chromatogram, but not in another, you can program different S/N ratio values at different times in the chromatogram.

Rejecting Solvent Peaks

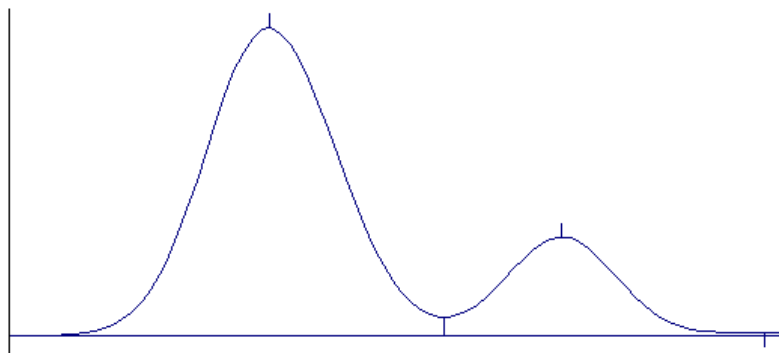
In many types of chromatographic analyses, you will have a large, essentially unretained solvent peak elute at the beginning of your run. This represents the solvent in which your sample is contained, and is not pertinent to your results. You have two options for removing the peak from your results—using the Inhibit Integrate or the Solvent Reject event. Generally you will use Inhibit Integrate unless an analyte of interest is a shoulder peak or is tangent to the solvent peak. Remember that Inhibit Integrate occurs at the first step of peak processing, during the peak detection phase. Its effect is to remove the section of the chromatogram specified by the event from consideration while peak detection is in progress. With the Inhibit Integrate event, regardless of the specific location where the event ended, the next detected peak always starts a new baseline. This is why a Solvent Reject event is used if your analyte of interest is a shoulder peak or is tangent to the solvent peak. This allows the peak detection algorithms to correctly determine the baseline points for the shoulder or tangent peak, while still removing the solvent peak from your final results calculations.

Skimming Fused Peaks

Fused peaks are peaks that elute next to each other and are not baseline resolved. The peak detection software treats fused peaks as either valley separated peaks, tangent peaks, or as fused tangent peaks. The Tangent Percentage value affects which peaks are considered valley separated peaks and which are tangent peaks. The Tangent Percentage value represents the percentage of the peak height of the second peak to the first fused peak. If the peak height of the second peak is a lower percentage than the Tangent Percentage value relative to the first peak, then the peak is considered a tangent, otherwise it is considered a main peak. The rule of thumb is that the higher the programmed Tangent Percentage value, the more peaks are considered tangents. Note that a tangent peak can only be detected following a main peak. Tangent skimming cannot be done on leading tangents.



Tangent Skimmed Peak



Valley Separated Peaks

Fused tangent peaks are a special case of tangent peaks. Once it is determined that more than one peak is tangent to a main peak, the tangents themselves could be valley separated.

Splitting Fused Peaks

Occasionally, the Data Handling software will not detect a shoulder peak, especially if there is no clear valley between the fused peaks. It will treat all of the area as one peak, even if you expect two peaks to be present. In this case, you would use the Split Peak event. This splits one peak into two valley separated peaks.

Forcing Peaks

Forcing peaks is a way of defining your own baselines. You might use this if, after adjusting the S/N ratio and peak width, a peak you are interested in is still not detected. Alternatively, you can use the Forced Peak event as a way of grouping multiple peaks so that they are reported as one peak (see also the Group Peak event).

The Forced Peak event causes peak events to be placed at the start and end times of the event and a baseline is drawn between the two. The apex is taken to be the highest data point in the time range for the event. This event supersedes all other peak detection events, so the Peak Width, Signal to Noise Ratio, Inhibit Integrate, and Tangent Percentage settings have no effect on the forced peak placement.

Identifying Peaks

Peaks are identified with the use of the Peak Table in the Data Handling section of the Method. The main purpose of the Peak Table is to list the names of your compounds and their expected retention times. Since retention times may vary slightly from run to run, you can specify a window of time during which the Workstation will try to identify a particular peak. The peak window is the actual span of time on the chromatogram that the software searches for the peak, centered around the retention time you entered for that peak. If the peak falls within that time window, it will be identified, otherwise it will not be identified. You may choose to report unidentified peaks, but these peaks cannot be accurately quantified (refer to the on-line help

in Interactive Graphics for a description of the unidentified peak factor).

If your peaks tend to drift, you can automatically modify their peak windows by marking a peak as a reference peak. Non-reference peaks will have their peak windows adjusted by the same percentage that the reference peaks have deviated from their expected retention times, accounting for the direction of change.

Interactive Graphics provides an easy way to build a Peak Table using your pilot run. You select the Edit Method→Fill Peak Table menu item, and one by one click on the peaks in your pilot run which you want to identify in your production runs. As you click on a peak, a new entry is added to the Peak Table with the retention time and a default name. You can also fill the Peak Table with all the peaks in a selected time range by checking the *Fill Table from Selection* checkbox in the Fill Peak Table window. When you have added all the peaks of interest, you can change the default names to real compound names.

Building a Calibration Curve

In order to determine absolute amounts of an analyte, you need to compare the peak area from a run in which the amount is unknown to a run in which you have injected a known amount of the compound. A sample that contains known amounts of the compounds to be analyzed (analytes) is called a calibration standard. When you inject a calibration standard, you designate the run as a Calibration Run. You enter amounts (for each analyte in the calibration standard) into the Peak Table. Note that this is the same table used for identifying your analytes.

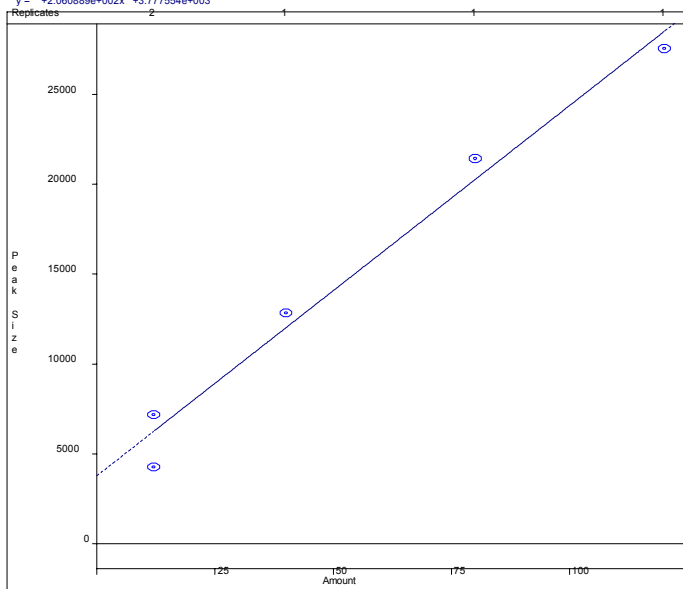
Sometimes you will want to do several calibration runs, and in each successive calibration run you inject different calibration standards with different amounts of each analyte. This is called multipoint or multilevel calibration. The Star Workstation allows you to calibrate with up to ten levels. Each level represents the amount of each analyte injected for each of the different calibration standards. Multilevel calibration can be more accurate than single level calibration, because you calibrate over large range of analyte amounts. For more accuracy, you may want to repeat injections at a

given level. This is a way of averaging out variations from injection to injection.

Regardless of the number of calibration runs you perform, the result of the calibration runs is a calibration curve. The calibration curve for an analyte is generated by plotting the peak size on the y axis and the injected amount of the analyte on the x axis for each calibration run you have performed, and then calculating the best line through the points. There are options to do a linear, quadratic or cubic fit through the points.

Calibration Curve Report
File: c:\startutorial\ext_std.mth
Detector: ADC Board, Address: 16, Channel ID: B

External Standard Analysis
Curve Type: Linear
Origin: ignore
y = +2.060889e+002x + 3.777554e+003
2-Octanone
Resp. Fact. RSD: 40.84%
Corr. Coef.(R²): 0.979546



Sample Calibration Curve Using Linear Fit

When you inject a sample with unknown amounts of your analytes, you designate the run as an Analysis Run. After identifying a peak as discussed above, the peak is quantified using the calibration curve. The peak area, which is determined after the second step of peak processing, is used as the y value in the calibration curve equation. This lets you calculate the x value which is the analyte amount.

External Standard Calibration

The External Standard calibration type is the most common method of calibrating an analysis. To calculate results with this technique, you must first perform a calibration run with a standard mixture. The calibration curve manager automatically generates a curve by plotting the known amounts of standards, as entered in the Peak Table, against the corresponding peak sizes, as calculated by the software. When you inject a sample in an analysis run, the Star Workstation calculates the amount of the analyte from the coefficients for the curve and the size of the sample peak.

Internal Standard Calibration

When you use the Internal Standard calibration type, you calibrate with regular calibration standards but you also add a known amount of another analyte, the internal standard, to each calibration standard and sample. When you make an injection, any variation in the injection volume will be reflected by a detectable variation in the amount of the internal standard. Fluctuations may also be caused by the process used to prepare the samples. In this case, adding the internal standards before sample preparation corrects for recoveries. Your Peak Table may contain as many as eight internal standard peaks. Each non-standard peak refers to the internal standard peak to use for calculations. Having multiple internal standards allows you to match each peak to a standard with similar chemical properties, which should have a similar recovery.

In generating the curve for an Internal Standard Calibration, you plot ratios: the peak size divided by the standard peak size on the y axis and amount of standard divided by the amount of internal standard on the x axis. Even if your injection volume varies slightly, the ratio of the sample to the internal standard will remain constant.

Normalized Percent Calibration

The Normalize Percent calibration type gives a percentage amount of each analyte relative to the total amount of all analytes in the sample, adjusted for varying detector response to the different analytes. It is analogous to a regular percentage calculation, except that the percentages are based on peak sizes that have been corrected for the relative detector response for each peak. It is also analogous to the Internal Standard calibration type in that the amounts are determined using a calibration curve based on ratios of sample to internal standard. An alternative method of generating ratios of amounts is to use either Internal Standard or External Standard calibration types and choose *Normalize Results* in the Integration Parameters window in the Data Handling section of the Method.

Choosing a Calibration Type

Your choice of which calibration type to use depends on your regulatory requirements and sample workup techniques. If you can very accurately measure your standard amounts, using an external standard calibration type is the easiest. The Internal Standard calibration type accurately accounts for variances in injection volume. You would also choose Internal Standard calibration if you have varying loss during sample preparation. In this case, you would add a known amount of your Internal Standard compound before sample preparation, and sample loss during preparation will be accounted for.

Advanced Applications

System Suitability Application

Creating System Suitability Reports

The System Suitability Application performs simple computations on data files acquired by the Star Chromatography Software. The program can operate under automation as an AutoLink application, or interactively.

When operating under automation, a report is automatically generated, and the automation sequence can automatically be aborted if user-defined tests fail.

When operating interactively, the program can process individual files or operate on a batch of files via drag-and-drop from an application such as the Windows Explorer. The System Suitability program is available from the Star Interactive Graphics application, and from the data file Quick Link button on the Star Toolbar.

The following calculations and tests can be performed by the System Suitability application:

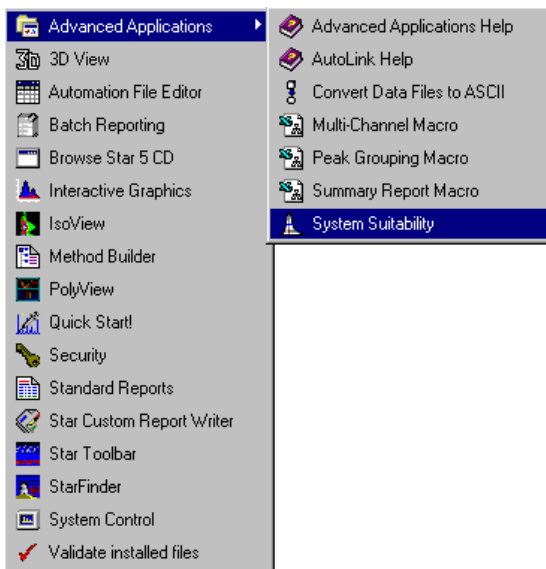
- Peak Resolution
- Peak Tailing
- Capacity Factor
- Theoretical Plate Calculation
- Noise Calculation & Hi/Low Tests.
- Drift Calculation & Hi/Low Tests.
- Baseline Shift Calculation & Hi/Low Tests.
- Hi/Low Tests on up to 10 peaks for raw peak size or calculated results.

Interactively Using the System Suitability Application

There are several different methods for interactively using the System Suitability application to create the report for Star Workstation data file. System Suitability can be started from the Star Advanced Application menu, from the data file Quick Link button, or from the Star Interactive Graphics application.

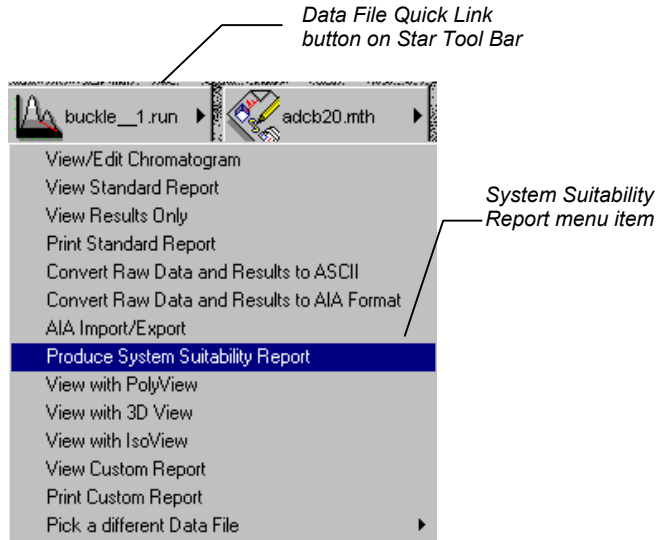
Running System Suitability from the Advanced Applications Menu

System Suitability is an item on the *Star Workstation Advanced Application* menu as show in the figure below:



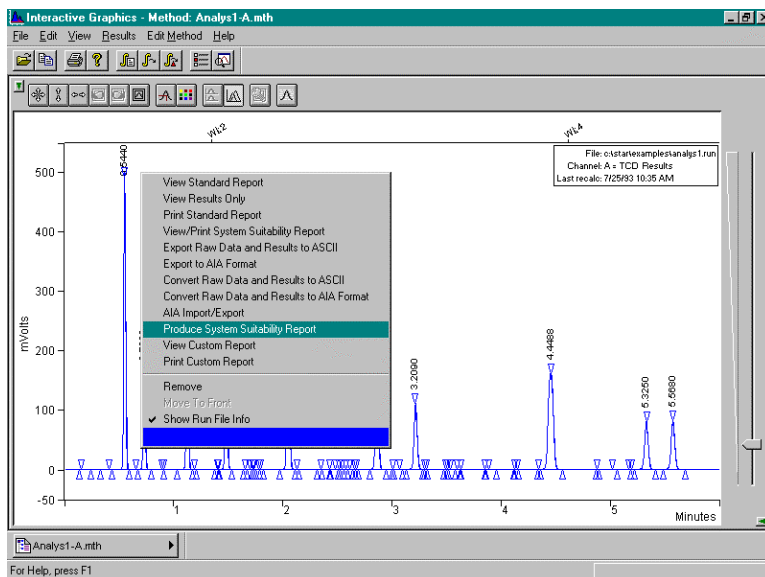
Running System Suitability from the Star Toolbar

To launch System Suitability from the Star Toolbar, click on the data file Quick Link button and then select the Produce System Suitability Report item from the pop-up menu. The System Suitability Report for the current Quick Link data file will be created.



Creating a System Suitability Report from Interactive Graphics

To launch System Suitability from the Star Interactive Graphics application, click the right mouse button anywhere in the chromatogram display area and then on the Convert Raw Data and Results to ASCII item from the pop-up menu. The System Suitability Report for the current data file will be created.

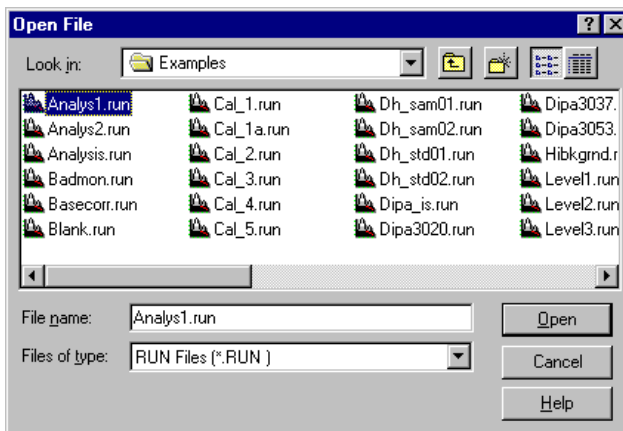


Selecting a System Suitability Method

When you run the System Suitability application, you will be prompted to open a method. The method is a text file that contains the parameters for the report. The default method file name is SSMETH.TXT, although, if desired, additional method files can be built. The various options available in a System Suitability method file are discussed in the section labeled *System Suitability Method File Parameters*.

Selecting a Data File for the System Suitability Report

When you run System Suitability from the *Star Workstation Advanced Application* menu, after you select a method file, a dialog where you can select the data file to be processed will be displayed.



System Suitability Drag-And-Drop Operation

The System Suitability application also supports drag-and-drop operation with the Windows Explorer. To use this mode of operation, open the Windows Explorer, select one or more Star data files, and then drag them into the System Suitability window before releasing the left mouse button.

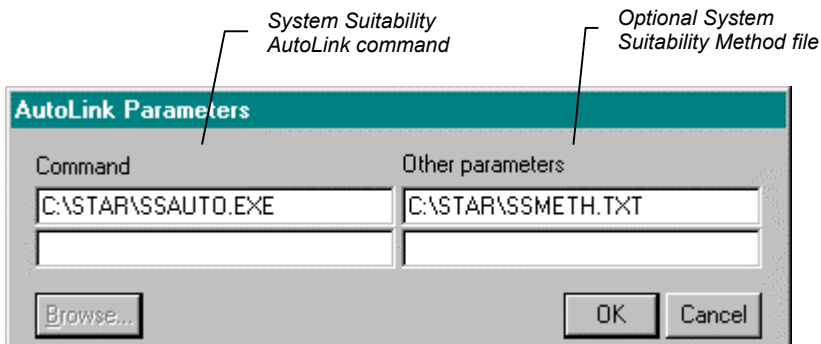
Automated Use of System Suitability

Creation of System Suitability Reports can be automated using the *AutoLink* mode of operation. In this mode of operation, the System Suitability application is automatically launched from a Star SampleList or RecalcList to process the current data file. To run System Suitability for a line in the Star SampleList or RecalcList, scroll horizontally to the column titled *AutoLink* and click on its button to display the press the button to display the *AutoLink Parameters* dialog. Enter the following items:

Command: `C:\STAR\SSAUTO.EXE`

Other Parameters: `C:\STAR\SSMETH.TXT`

When the SampleList or RecalcList is executed, the System Suitability report for the current data file will be created using the parameters in the method file specified by the *Other Parameters* field, or the default method SSMETH.TXT, if the *Other Parameters* field is blank. The report will also be printed if printing is enabled, as determined by the *Enabled Automated Printing* menu item in System Control.



System Suitability Method File Parameters

System Suitability method files contain the settings for the report parameters and options. A method file is a text file that contains a series of lines with the setting for each option. Each option line has the form *Key = Value*. *Key* is a fixed string that is recognized by System Suitability. *Value* is the setting for the option. Any text editor program that save standard ASCII text files (for example Notepad or Wordpad) can be used to edit System Suitability method files.

The first line in a System Suitability method file must be [SYSSUIT]; this identifies the file as a System Suitability method file. Following this line, the parameters shown in the following table can be used.

Parameter	Description
MethodType	Must be SYSSUIT
ReportTitle=Sys...	Title you want displayed on the report.
ColName	Column type / brand

Parameter	Description
ParticleSize	Particle size in microns (unless modified by SizeLabel, described below)
SizeLabel	Use this field to specify something else than Particle Size, such as "Film Thickness (um)"
Length	Column length, followed by optional unit (m or cm only). If no unit is provided, or if the unit is not recognized, the default unit is centimeters.
Diameter4	Column diameter, in millimeters (unless modified by DiameterLabel, described below)
DiameterLabel	Use this field to specify something else than Diameter (mm), such as "Diameter (microns)" or "Channel Thickness (um)".
ColID#	Column ID number
TailHeight	Percent of peak height at which peak tailing is calculated. Default = 5.
VoidPeakTime	The void volume of the chromatographic system expressed in minutes. This time is determined by the retention time of an unretained compound and for most systems is evident as a solvent peak. This field must be filled in to calculate capacity factor (k').
ResPeak1	Name of 1st peak for resolution test
ResPeak2	Name of 2nd peak for resolution test
ResHi	Resolution limit, High
ResLo	Resolution limit, Low
ResAbort	1 = Abort sequence if resolution test fails, 0=Don'tabort
TailPeak	Name of peak for Tailing check
TailHi	Tailing limit, high
TailLo	Tailing Limit, low
TailAbort	1 = Abort sequence if tailing test fails,. 0=Don't
ResultPeaks	Number of peaks for Result Checks (0-10).

Parameter	Description
ResultPeakN	Name of Nth peak for Result Check
ResultHiN	High Limit for Calculated Result for Nth peak.
ResultLoN	Low limit for Calculated Result for Nth peak.
RawResultHiN	High Limit for Raw peak size (counts) for Nth peak.
RawResultLoN	Low limit for Raw peak size (counts) for Nth peak.
ResultAbortN	1 = Abort sequence if Peak N fails a test, 0=Don'tabort.
NoiseStart	Start Time for Noise calculation, in minutes.
NoiseEnd	End Time for Noise calculation, in minutes.
NoiseFactor	Factor applied to RMS noise to estimate Peak-to Peak noise.
NoiseHi	High Limit for noise value, in microUnits.
NoiseLo1	Low limit for noise value, in microUnits.
NoiseAbort	1 = Abort sequence if Noise test fails, 0=Don't
DriftStart	Start Time for Drift calculation, in minutes.
DriftEnd	End Time for Drift calculation, in minutes.
DriftHi	High Limit for Drift value, in milliUnits/hour.
DriftLo	Low limit for Drift value, in milliUnits/hour.
DriftAbort	1 = Abort sequence if Drift test fails, 0=Don't abort
BaseStart1	Start Time for first Baseline segment, in minutes.
BaseEnd1	End Time for first Baseline segment, in minutes.
BaseStart2	Start Time for second Baseline segment, in minutes.
BaseEnd2	End Time for second Baseline segment, in minutes.
BaseHi	High Limit for Baseline Shift value, in milliUnits.

Parameter	Description
BaseLo1	Low limit for Baseline Shift value, in milliUnits.
BaseAbort	1 = Abort sequence if Baseline Shift test fails, 0=Don't abort
Extension	File Extension for saved reports
StoragePath	Specifies a full path for the storage of the report files. If no parameter is provided, the file is stored in the same location as the Star data file.
WidthInMinutes	Report Peak Width in minutes (1=yes, 0=no (default))
ShowUnidentified	Report Unidentified Peaks (0=no, 1=yes (default))
ShowNotes	1 = Show Original Notes only (default). 2 = Show Original AND additional notes. 0 = No Notes
ShowVersion	1 = Show Program's Internal Version Number. 0 = Don't show
PointSize	Specifies the size in points of the Courier font requested by the program. A larger point size results in a bigger font. This provides some flexibility in dealing with unsupported printer drivers.
FirstChannel LastChannel	These parameters define a range of channels to be processed. A report will be created for each channel containing results. By default, the range includes all channels in the data file. This feature is useful to process a given channel with a given set of parameters. In the special case where different channels result from using different columns, multiple AutoLink commands can be set up selecting the proper set of parameters for each channel. This field must have a numerical value. For an ADCB file, Channel A is 1 and Channel B is 2. Do NOT use A or B as a value.

System Suitability Peak Calculations

The following are the calculations used in the System Suitability application:

T1: Retention time of the peak of interest.

T2: Retention time of the next peak.

W1: Width at half height for peak at *T1*.

W2: Width at half height for peak at *T2*.

L: Length of the column in centimeters

T0: Void volume (Time of unretained peak).

TL: Retention time of leading edge at X% height.

TT: Retention time of trailing edge at X% height.

Calculation	Formula
Theoretical plates (N):	$N = 5.5452 (T1/W1)^2$
Theoretical plates/meter (PM):	$PM = N(100/L)$
Capacity factor (k'):	$k' = (T1/T0)-1$
Resolution (R):	$R = 2(T2-T1)/(1.699(W1+W2))$
Peak tailing (T):	$T = (TT-TL)/(2(T1-TL))$

Noise Calculation and Tests

The noise is calculated by doing a linear least squares fit on the specified baseline segment, then by computing the Root Mean Square value of the deviations of the data points from this line. A user-specified factor (NoiseFactor, default value 5) is applied to the noise measured so that it can be converted to estimated peak-to-peak noise. The noise calculation is performed if valid start and end times are provided. Tests of the noise value against high or low limits are conducted if limits are specified in the method.

Drift Calculation and Tests

The drift is the slope of the line resulting from a linear least squares fit on the specified baseline segment. The drift calculation is performed if valid start and end times are provided. Tests of the drift value against high or low limits are conducted if limits are specified in the method.

Baseline Shift Calculation and Tests

The Baseline Shift calculation measures the difference in amplitude between two baseline regions. GC users can use it to measure and check column bleed, while LC users can measure the amplitude of a baseline gradient, and - for example - detect contaminated solvents.

The shift is calculated as the difference between the average of the signal calculated for the two regions specified (Average of second region - Average of first region). The value is calculated and reported if valid start and end times are provided for both regions. Tests of the drift value against high or low limits are conducted if limits are specified in the method.

Summary Report Macro

Creating Star Summary Reports

The Summary Report Application is an Microsoft® Excel macro that summarizes the data from a series of individual chromatographic runs and prepares Quality Control charts that indicate trends in the data. Processing is based on the data files listed in a Workstation RecalcList. The Summary Report Application extracts information (either results, retention times, peak areas, or peak heights) from each individual report file, transfers it to a table called the Summary Report and creates Quality Control charts of selected groups of the data.

Names of peaks summarized

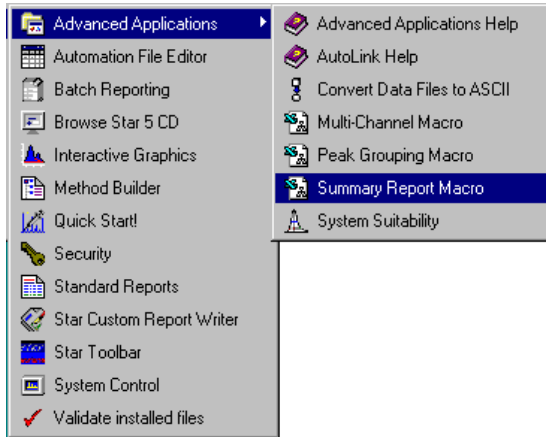
List of data files included in Summary Report

1	2	3	4	6	7	8	
1	SUMMARY REPORT CONTROL WORKSHEET - Retention Time Summary						
2							
3							
4	Sample	Data	Inj.	Peak Names			
5	Name	File	Mode	#	Internal Std	C1 Paraben	Un Paraben 1
6	Calib. Level #1	ies\parais1.RPA	C	1	0.2037	0.783	1.004
7	Calib. Level #2	ies\parais2.RPA	C	1	0.2017	0.776	1
8	Calib. Level #3	ies\parais3.RPA	C	1	0.206	0.7707	1.003
9	Sample #1	ies\parais4.RPA	A	1	0.2007	0.776	
10	Sample #2	ies\parais5.RPA	A	1	0.2037	0.769	
11	Sample #3	ies\parais6.RPA	A	1	0.2007		
12	Calib. Level #1	ies\parais7.RPA	C	1	0.2047	0.7817	1.007
13	Calib. Level #2	ies\parais8.RPA	C	1	0.1977	0.7737	0.9977
14	Calib. Level #3	ies\parais9.RPA	C	1	0.2037	0.762	1.0037
15				Average	0.2025	0.7740	1.0026
16				Std. Deviation	0.0025	0.0068	0.0033
17				Rel. Std. Deviation (%)	1.2537	0.8847	0.3261
18							

Statistics for summarized data

Starting the Summary Report Macro

The Summary Report macro can be started from the *Advanced Applications* menu item found on the *Star Workstation* menu as shown below:

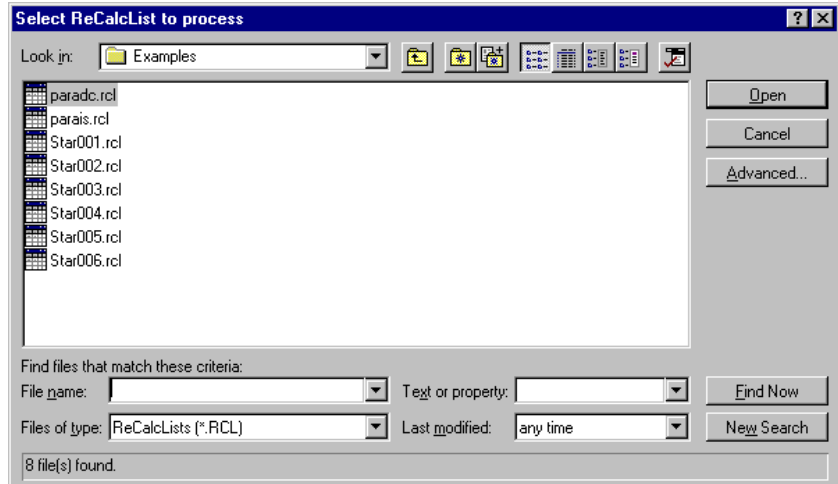


Once the Summary Report macro has been loaded, an item labeled *Star* will be added to Excel's main menu. *Summary Reports* is an item on the *Star* menu.



Creating Summary Reports

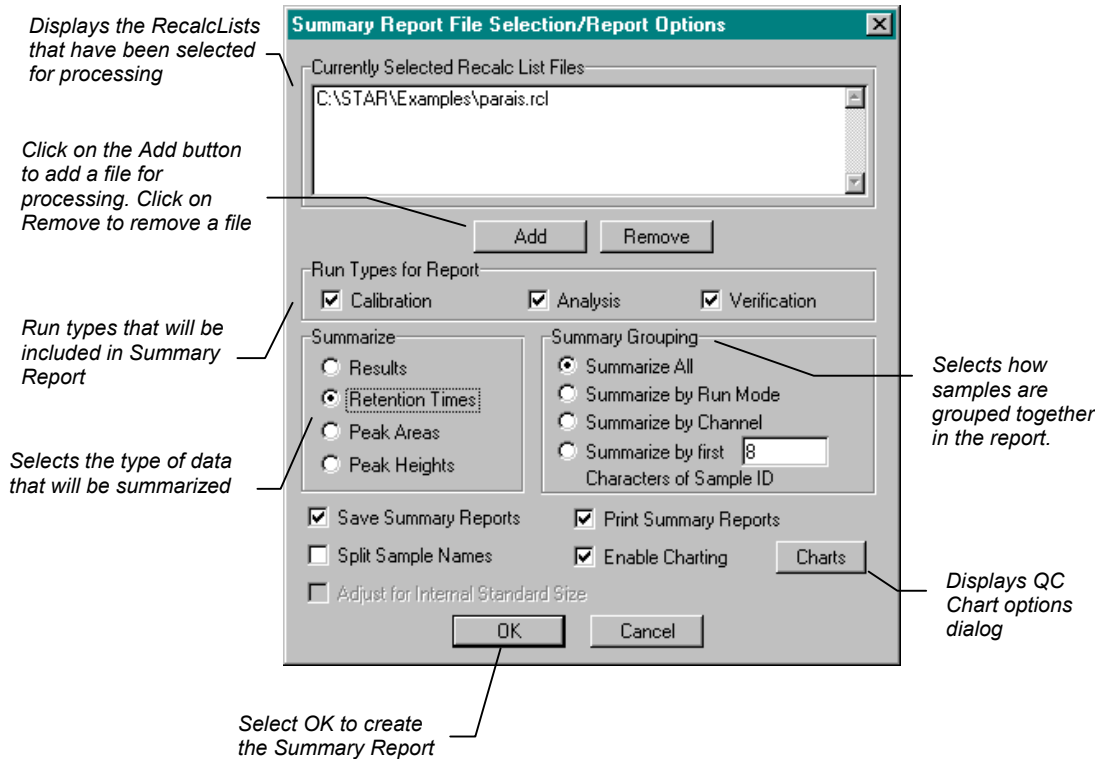
To create a Summary Report for the data files listed in one or more Star RecalcLists, select the Process Recalc List item from the Star Summary Report menu. A file selection dialog box will be displayed. This dialog is used to select the Star RecalcList files that the Summary Report will be created from.



After you select the RecalcList file to be processed and have clicked on the Open button, the Summary Report File Selection/Report Options dialog will be displayed.

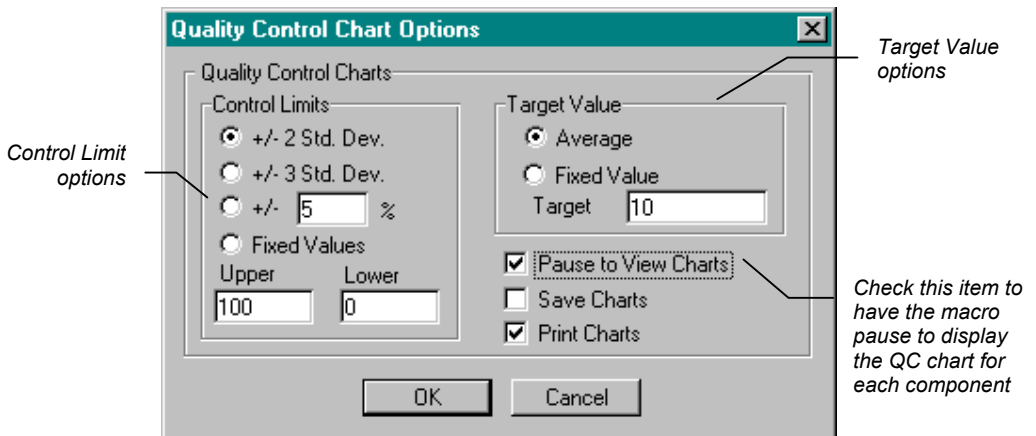
Summary Report Options

The Summary Report File Selection/Report Options dialog displays the various options available in the macro.



Quality Control Chart Options

The Summary Report File Selection/Report Options dialog contains a checkbox item labeled *Enable Charting*. Checking this item enables the creation of Quality Control charts for each named peak found in the data files that are processed. When the *Enable Charting* item is checked, the Charts button will be enabled. Clicking on the *Charts* button will display a dialog where the various options for the QC Charts can be set.



Sample Grouping Options

The Summary Report File Selection/Report Options dialog option buttons for selecting how the summarized data will be grouped together. The grouping options are:

- *Summarize All* - All data is grouped together
- *Summarize by Run Mode* - All data files having the same run mode (Calibration, Analysis, or Verification) are grouped together.
- *Summarize by Channel* - All data from the same detector channel is grouped together.
- *Summarize by first n Characters of Sample ID*. Data is grouped together based up on the first *n* characters of the Star Sample ID field.

Individual statistics (average, standard deviation, and relative standard deviation) will be reported for the data in each group.

Split Sample Name Option

This option is for users who are using the Summary Report macro in conjunction with a Varian 3600 gas chromatograph that has Twin-Tower autosamplers. When this option is enabled and the Summary Report macro detects a comma (,) in the Sample Name field, the contents of the Sample Name field to the left of the comma will be assigned to the data associated with channel A of the data file and the contents of the Sample Name field to the right of the comma will be assigned to the data associated with channel B of the data file. This effectively allows the data for a single line of a RecalcList to be treated as two separate samples.

Adjust for Internal Standard Size Option

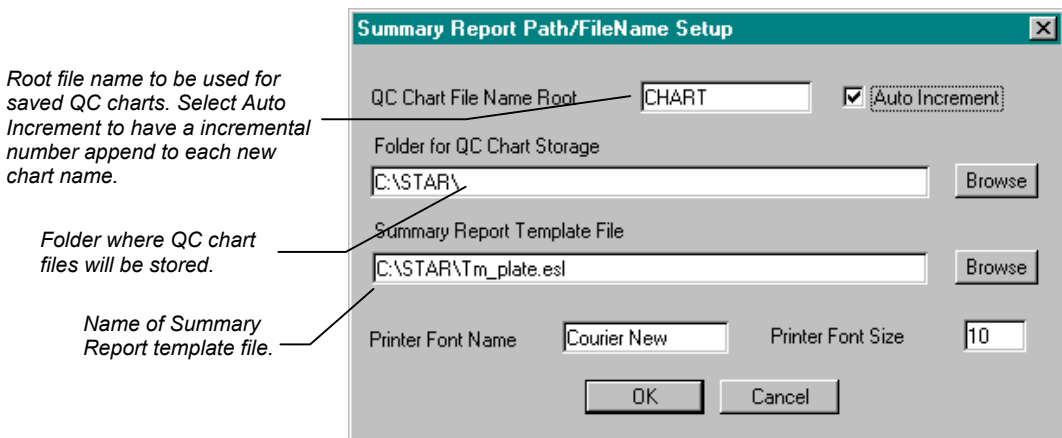
For Internal Standard calculations, this options allows the size of summarized peak areas or heights to be adjusted based upon the amount of Internal Standard that has been added to the sample. The following formula is used calculate the reported peak area or height:

$$\frac{(\text{AnalytePeak Area or Height})(\text{Amt.Std})}{(\text{ISPeakArea or Height})}$$

If this option is not selected, then raw area or height values will be reported.

Configuring File and Path Options

The Path/File Name Setup Dialog Box can be accessed by selecting the *Configure Paths* item from the Star Summary Report menu in Excel. This dialog box is used to select, and then save, some options for the macro. Among these options are the names and location for charts, the name of the Summary Report template file, and the name and size of the font used when the macro sends output to a printer. Once you set the options in the dialog box, they are saved to disk and remain in effect until you choose to change them. The Path/File Name dialog box is shown.



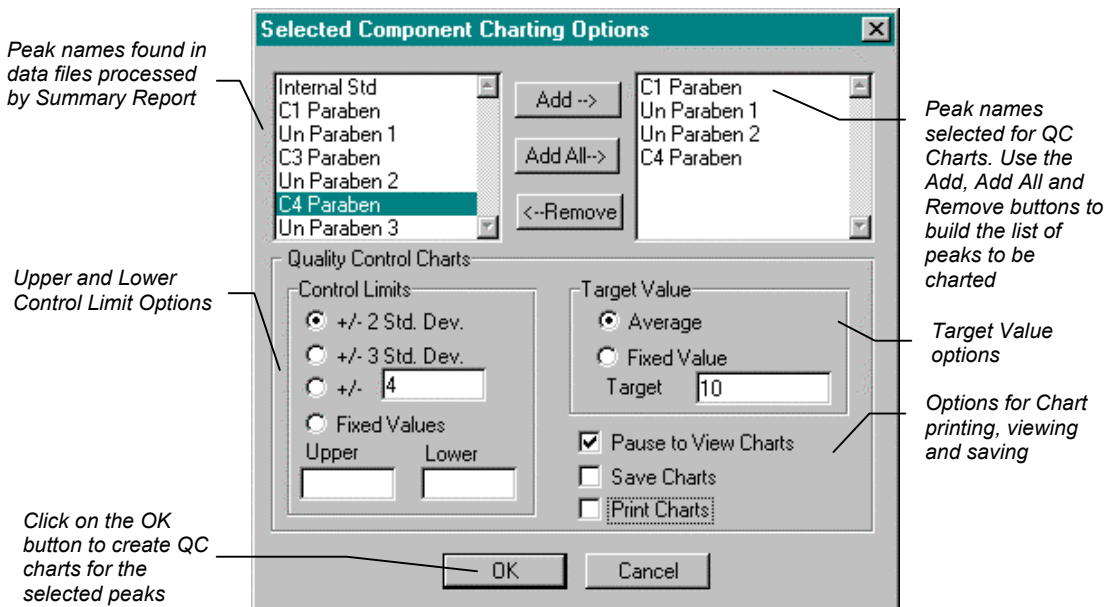
The Summary Report Template file field contains the name of the spreadsheet file that the macro will use to built the Summary Report from. Normally, the default template file, TM_PLATE.ESL can be used for processing as the macro will read the sample information from the SampleLog file and the analyte names from the data files listed in the RecalcList. However, if desired, other template files can be used by the Summary Report macro. For example, a template with the analyte names for the samples already filled in could be used.

Once you have entered your selections into the Configuration dialog box click on the *OK* button to save the changes as part of the Summary Report macro. The entries that you make will remain in effect until you change them. If you decide not to save the entries you have made in the dialog box, click on the *Cancel* button.

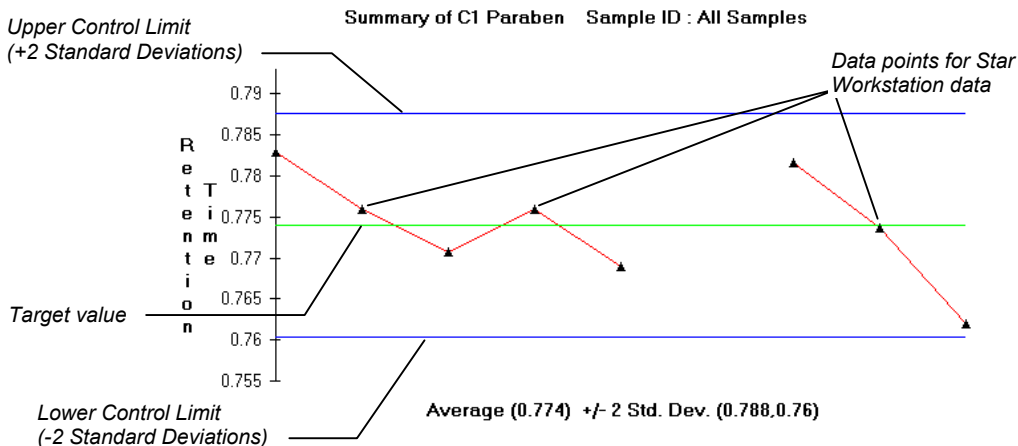
Quality Control Charts

The Summary Report macro can create Quality Control, or QC, charts for the each peak found in the data files that are processed. An individual QC chart can be created for each peak in each Summary Report group. A QC chart plots each individual data point, plus a target value (the average, or a user-definable value), and the upper and lower control limits (± 2 , ± 3 Standard Deviations, or a user-defined value).

The Summary Report macro File Selection/Report Options dialog contains an option for selecting creation of QC charts; when this option is enabled, the macro will automatically create a QC chart for each peak found in the data files that are processed. A second method of creating QC charts is to use the *QC Charting* item on the Star Summary Report menu in Excel. Using this menu item after a Summary Report has been created allows you to create QC charts for selected peak names. The peak name selection is done using the dialog box shown below



After you select the peak name, choose the charting options, and click on the OK buttons, the QC charts for the selected peaks will be created. The figure below shows an example QC chart created by the Summary Report macro.

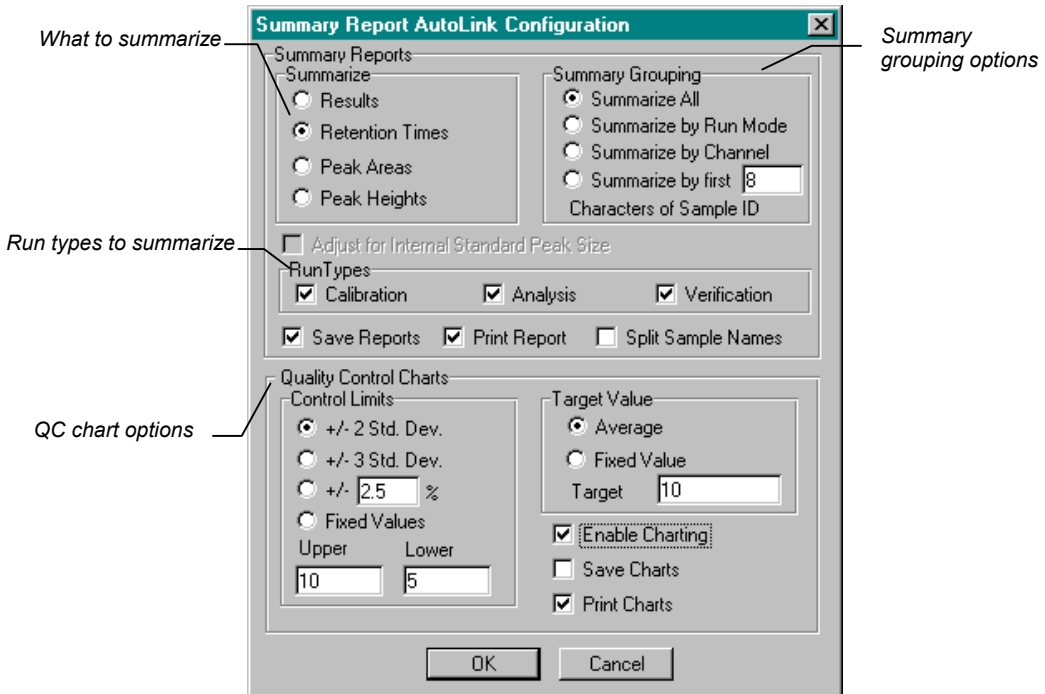


Running the Summary Report Macro Using AutoLink

When used with Star Chromatography Software, the Summary Report macro can be run from System Control as an AutoLink application. This allows Summary Reports to be automatically created from the data files listed in a RecalcList. When the Summary Report macro is run as an AutoLink application, Excel will be loaded and the macro will generate the summary report and QC charts. When the macro completes, Excel will exit and control will be returned to the Workstation software.

Summary Report Macro - Default AutoLink Configuration

The default AutoLink parameters for the Summary Report macro are set up in the dialog box shown in the figure below. This dialog box can be accessed by selecting the Configure AutoLink item from the Star Summary Report menu in Excel.



Summary Report AutoLink Command Line

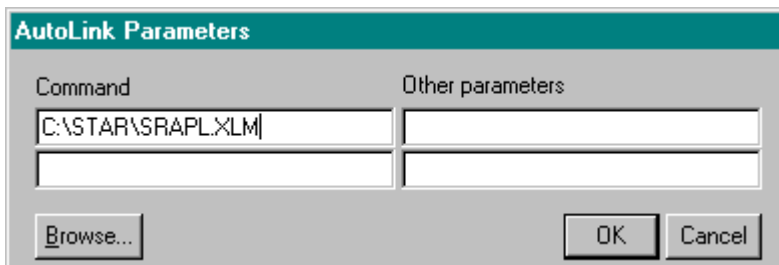
For running the Summary Report Macro as an AutoLink application, the macro SRAPL.XLM is used. This macro is responsible for the DDE communication between Excel and System Control and for starting up the main Summary Report macro, SUMRPT.XLM.

Since the Summary Report Macro processes RecalcList files, when run as an AutoLink application it should be called after the completion of the last injection of the SampleList or last recalculation of a RecalcList. This is done by adding an additional sample to the end of the SampleList or RecalcList and setting its Sample Type to *AutoLink*. Clicking on the *AutoLink* button for this sample will bring

up a dialog box where the application file name and application parameters are entered. For Summary Report, the complete path for SRAPL.XLM is entered into the *Command* field. For example, if the Summary Report macro is installed in the directory C:\STAR\SUM_RPT, the AutoLink command line entry would be

C:\STAR\SRAPL.XLM

The figure below shows an example of how to set up the SampleList AutoLink dialog box for use with the Summary Report macro.



Using the AutoLink Other Parameters Field

The *Other Parameters* field of the AutoLink dialog box can be used to pass the name of an initialization file containing parameters for the Summary Report macro to override the values set in the AutoLink Defaults dialog box. The file must be an ASCII text file which contains the text [AUTOLINK] on a line by itself. Following the [AUTOLINK] section heading, will be the parameter names used for each option. Following each parameter name will be an equal sign and the value to be assigned to the option.

The table below describes the parameter names which can be entered in the [AUTOLINK] section of an initialization file passed in the AutoLink *Other Parameters* field:

Parameter	Description
Datatype	Data type to Summarize. 1 = Results, 2 = Retention Time, 3 = Peak Areas, 4 = Peak Heights
RunTypes	Run Types to include. 1 = Calibration, 2 = Analysis, 4 = Verification. Run types are additive, i.e. 3 = Calibration and Analysis, 7 = include all types.

Parameter	Description
Template	Name of Summary Report template file
ISAdjust	Adjust peak areas and heights for Internal Standard peak size. 0 = Don't Adjust, 1 = Adjust.
Charting	Quality Control Chart flag. 0 = Don't create charts, 1 = Create charts.
QCLimits	Quality Control Chart Limit type. 1 = ± 2 Std. Dev., 2 = ± 3 Std. Dev., 3 = \pm Fixed Average, 4 = \pm Fixed Upper/Lower
QCAverage	Quality Control Chart fixed average value
QCFixedUpper	Quality Control Chart fixed upper limit.
QCFixedLower	Quality Control Chart fixed lower limit.
TargetType	Quality Control Chart target type. 1 = Average, 2 = Fixed Value.
PrintCharts	Quality Control Print Charts flag. 0 = Don't print charts, 1 = print charts.
SaveCharts	Quality Control Save Charts flag. 0 = Don't save charts, 1 = save charts.
PrintSum	Print Summary Report flag. 0 = Don't print Summary Report, 1 = Print Summary Report.
SaveSum	Save Summary Report flag. 0 = Don't save Summary Report, 1 = Save Summary Report.
SummaryType	Summary Report summarization. 1 = Summarize all, 2 = Summarize by run mode, 3 = Summarize by detector channel, 4 = Summarize by first <i>n</i> characters of Sample Name.
SummaryNameLength	Sample Name length for Summarize by Sample Name.
SplitNames	Split sample names flag. 0 = Don't split name, 1 = split names.

AutoLink Timeout Setting

By default, the Workstation System Control application will wait 120 seconds for an AutoLink application to complete. If the application has not completed within this amount of time, System Control assumes that the application has terminated abnormally and generates an RAI Timeout error.

In some cases, the default timeout period of 120 seconds may not be long enough to allow the Summary Report application to complete. If necessary, use the following procedure to modify the AutoLink timeout period:

1. Use the Windows Notepad editor to open the file STAR32.INI located in the directory where Windows is installed.
2. Find the *RAITimeOutSeconds* entry and change the timeout value to the number of seconds you want System Control to wait for an AutoLink application to complete. For example, if you want to set the timeout to 4 minutes, the entry should read:

```
RAITimeOutSeconds=240
```

3. Save the edited STAR32.INI file.
4. Restart System Control so that the change will take effect.

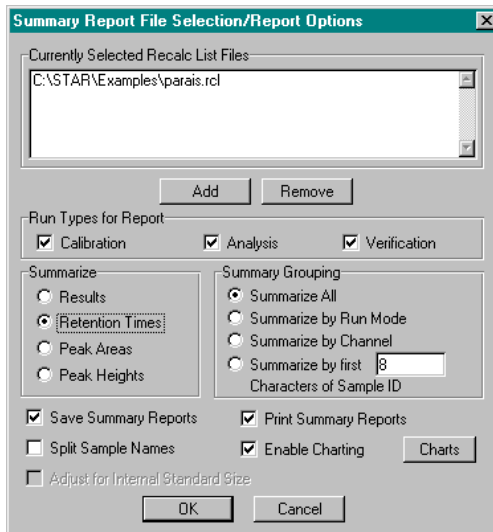
Tutorial - Creating Summary Reports

In this exercise, you will use the tutorial files stored in the directory C:\STAR\EXAMPLES to prepare a Summary Report. The report will summarize and plot the retention times for all of the files in the original RecalcList.

Note: If the Star software is not installed in the folder C:\Star, you will need to use the System Control application to edit the tutorial RecalcList in order to substitute the proper folder name for C:\STAR\EXAMPLES in the path for the tutorial data files.

1. Start the Summary Report Application by clicking on Windows *Start*→*Programs*→*Varian Star Workstation*→*Advanced Applications*→*Summary Report Macro*. Microsoft Excel will be loaded and an item labeled *Star* will be added to Excel's menus.

- To select the Star Workstation RecalcList file that will be processed, select *Summary Report Process RecalcList* from the Star menu in Excel. Use the dialog box to select the RecalcList file that will be processed; *C:\STAR\EXAMPLES\PARAIS.RCL* for this tutorial. Click on the *OK* button to display the report options dialog. Set up the dialog box as shown in the figure below and click on the *OK* button to create the Summary Report.



- As the macro executes, it will extract the retention time information from each Star data file and prepare a Summary Report and the QC Charts. As the chart for each analyte is created, the macro will pause and display the chart; when you are ready to view the chart for the next analyte, click on the *Continue* button. When the macro completes, the completed Summary Report will appear.
- At this time, you can summarize additional RecalcLists by selecting *Summary Report Process RecalcList* or quit macro processing (by closing Excel).

Tutorial - Creating Summary Reports Using AutoLink

The following tutorial uses the System Control application and the tutorial files in the C:\STAR\EXAMPLES folder to run the Summary Report macro in an AutoLink application. Before going through the tutorial listed below, it is recommended that you use the procedure outlined in section the section labeled *AutoLink Timeout Setting* to increase the AutoLink timeout to 240 seconds.

1. Start the Summary Report Application by clicking on Windows *Start*→*Programs*→*Varian Star Workstation*→*Advanced Applications*→*Summary Report Macro*. Microsoft Excel will be loaded and an item labeled *Star* will be added to Excel's menus.
2. From the Excel menu, select *Star Summary Report Configure AutoLink* and verify that the AutoLink defaults are set as shown in the figure below. Click on the *Save* button after making any necessary changes and then use the Excel *File Exit* option to close Excel.

The image shows a dialog box titled "Summary Report AutoLink Configuration". It contains several sections for configuring the summary report:

- Summary Reports**
 - Summarize**: Radio buttons for Results, Retention Times, Peak Areas (selected), and Peak Heights.
 - Summary Grouping**: Radio buttons for Summarize All (selected), Summarize by Run Mode, Summarize by Channel, and Summarize by first 8 Characters of Sample ID.
 - Adjust for Internal Standard Peak Size
- RunTypes**: Checkboxes for Calibration (checked), Analysis (checked), and Verification (checked).
- Save Reports, Print Report, Split Sample Names
- Quality Control Charts**
 - Control Limits**: Radio buttons for +/- 2 Std. Dev. (selected), +/- 3 Std. Dev., +/- 2.5 % (with a text box containing 2.5), and Fixed Values. Below are text boxes for Upper (10) and Lower (5).
 - Target Value**: Radio buttons for Average (selected) and Fixed Value. Below is a text box for Target (10).
 - Enable Charting, Save Charts, Print Charts

At the bottom are buttons for OK and Cancel.

3. Start the System Control Application and use the *Instrument* menu to access one of the instruments available on the Workstation.
4. Use *FileOpen RecalcList* to open and activate the Summary Report tutorial RecalcList file named PARAIS.RCL located in the C:\STAR\EXAMPLES folder.
5. Use *File Method Activate* to activate the Summary Report tutorial method file named PARAIS.MTH located in the C:\STAR\EXAMPLES folder.
6. Use the *Windows* menu to access the active RecalcList window (PARAIS.RCL).
7. Add a new sample to the end of the list and set the Sample Type for the new sample to *AutoLink*. Click on the *AutoLink* button for this sample and enter the following into the *Command* field of the dialog box:

C : \STAR\SRAPL.XLM

8. The *Other Parameters* field should be left blank. Click on the OK button after making the entry to the *Command* field. Note that you can also use the *Browse* button to locate the macro file to be run.
9. Start the RecalcList reintegration using the *Recalculate Begin RecalcList* menu item. The nine samples listed in the RecalcList will be reintegrated. After the last sample is reintegrated, the Summary Report macro will be activated as the AutoLink application. When the data has been summarized, the macro will print control charts and the Summary Report for the data. When the macro completes, Excel will close itself and control will be returned to System Control.

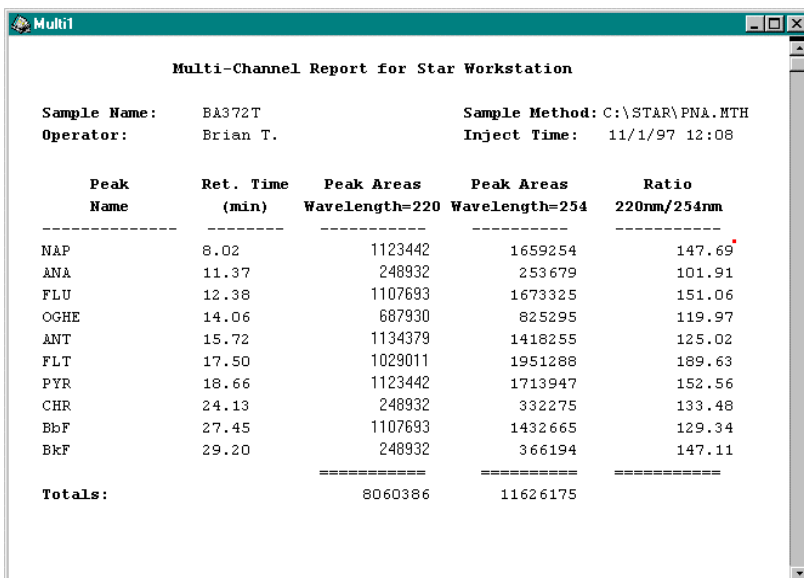
Multi-Channel Report Macro

Creating Multi-Channel Reports

The Multi-Channel Report macro for the Varian Star Chromatography workstation is an Excel macro that can generate reports combining data from any number of detector data channels contained in a Star data file.

The macro also allows custom reports to be generated through the use of Microsoft Excel spreadsheet template files.

The figure below shows an example report created by the Multi-Channel Report Macro.

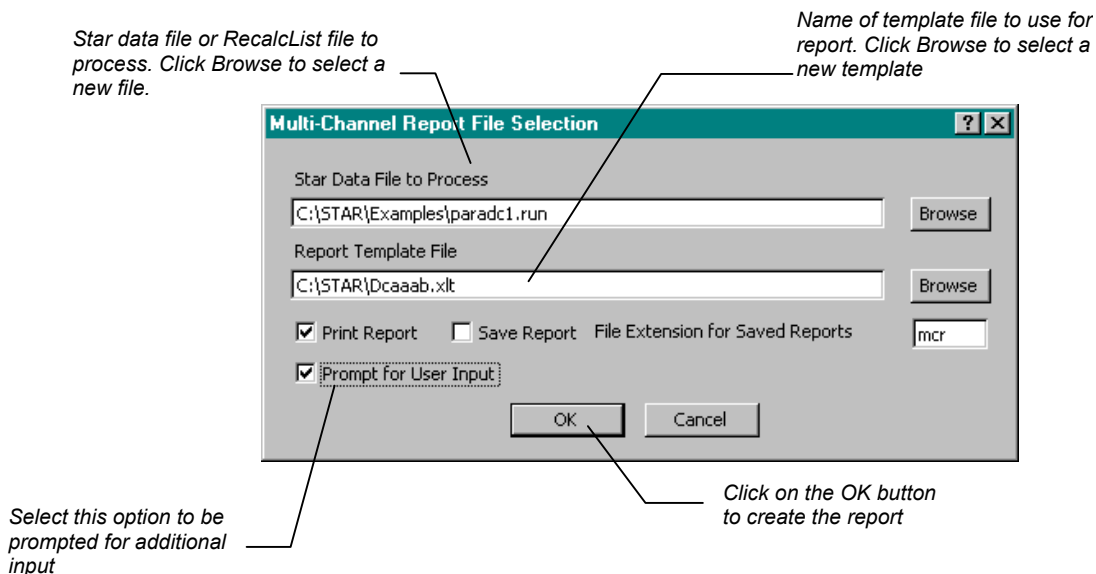


The screenshot shows a window titled "Multi1" containing a report titled "Multi-Channel Report for Star Workstation". The report includes sample and operator information, sample method and inject time, and a table of peak data. The table has five columns: Peak Name, Ret. Time (min), Peak Areas Wavelength=220, Peak Areas Wavelength=254, and Ratio 220nm/254nm. A totals row is at the bottom.

Peak Name	Ret. Time (min)	Peak Areas Wavelength=220	Peak Areas Wavelength=254	Ratio 220nm/254nm
NAP	8.02	1123442	1659254	147.69
ANA	11.37	248932	253679	101.91
FLU	12.38	1107693	1673325	151.06
OGHE	14.06	687930	825295	119.97
ANT	15.72	1134379	1418255	125.02
FLT	17.50	1029011	1951288	189.63
PYR	18.66	1123442	1713947	152.56
CHR	24.13	248932	332275	133.48
BbF	27.45	1107693	1432665	129.34
BkF	29.20	248932	366194	147.11
Totals:		8060386	11626175	

Multi-Channel Report Macro - Interactive Use

To run the Multi-Channel Report macro interactively, select *Multi-Channel Macro* from the Star Advanced Application menu. After Excel has loaded, select *Create Report(s)* from the Star Multi-Channel Report menu in Excel. The File Selection dialog will be displayed. This dialog is shown below:

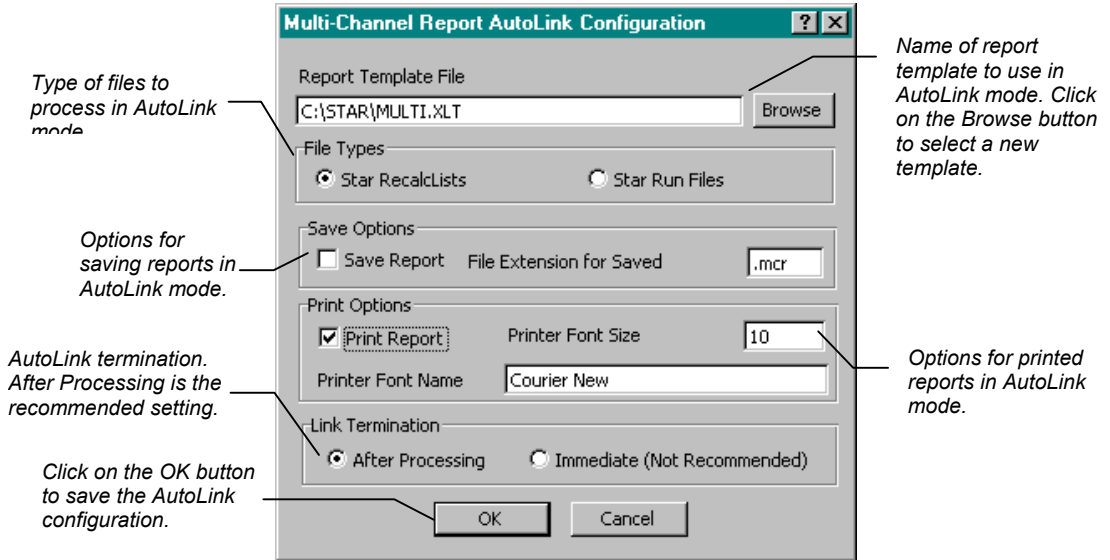


Running the Multi-Channel Macro as an AutoLink Application

When used with Star Chromatography Software, the Multi-Channel Report macro can be run from System Control as an AutoLink application. This allows reports to be automatically created either for a single data file or for all data files in a RecalcList. When the macro is run as an AutoLink application, Excel will be loaded and the macro will generate its report(s). When the macro completes, Excel will exit and control will be returned to the Workstation software.

Multi-Channel Macro - Default AutoLink Configuration

The default AutoLink parameters for the Multi-Channel Report macro are set up in the dialog box shown in the figure below. This dialog box can be accessed by selecting the Configure AutoLink item from the Star Multi-Channel Report menu in Excel.



Note that the AutoLink parameters set in this dialog box are used by the macro unless you override them by using the *Other Parameters* field of the AutoLink dialog.

Multi-Channel Macro AutoLink Command Line

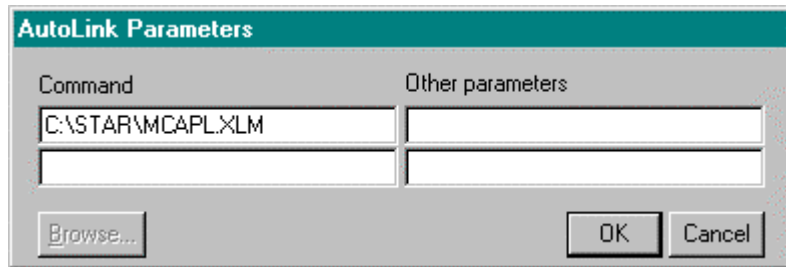
For running the Multi-Channel Report macro as an AutoLink application, the macro MCAPL.XLM is used. This macro is responsible for the DDE communication between Excel and System Control and for starting up the main macro, MULTCHAN.XLM.

The Multi-Channel Macro can be activated either after the completion of a single sample or the completion of all the samples in a SampleList or RecalcList. To have the macro run following the completion of a single sample, use the AutoLink dialog box for the sample in the SampleList or RecalcList. To run the macro after all samples in a SampleList or RecalcList have been processed, add an

additional sample to the end of the list and set its Sample Type to *AutoLink*. In either case, the complete path to MCAPL.XLM is entered into the 'Command' field in the AutoLink dialog box. For example, if the Multi-Channel macro is installed in C:\STAR, the AutoLink command line entry should be:

C : \STAR\MCAPL.XLM

The figure below shows an example of how to set up the AutoLink dialog box for use with the Multi-Channel Report macro.



Using the AutoLink Other Parameters Field

The *Other Parameters* field of the AutoLink dialog box can be used to pass the name of an initialization file containing parameters for the Multi-Channel Report macro to override the values set in the AutoLink Defaults dialog box. The file must be an ASCII text file which contains the text [AUTOLINK] on a line by itself. Following the [AUTOLINK] section heading, will be the parameter names used for each option. Following each parameter name will be an equal sign and the value to be assigned to the option.

The table below describes the parameter names which can be entered in the [AUTOLINK] section of an initialization file passed in the AutoLink *Other Parameters* field:

Parameter	Description
Print	Print Report Flag. 0 = Don't print reports, 1 = Print reports.
Save	Save Report Flag. 0 = Don't save reports, 1 = Save reports.

Parameter	Description
Template	Name of Multi-Channel report template file.
UserPrompt	User Prompt Flag. 0 = Don't prompt for additional input. 1 = Prompt for additional input.
FileType	Type of file to process. 1 = Run file, 2 = RecalcList file.
ReportExt	File extension to use for saved reports.

AutoLink Timeout Setting

By default, the Workstation System Control application will wait 120 seconds for an AutoLink application to complete. If the application has not completed within this amount of time, System Control assumes that the application has abnormally terminated and generates an 'RAI Timeout' error. If necessary, this timeout period can be changed by using the following procedure:

1. Use the Windows Notepad application to open the file 'STAR32.INI' located in the directory where Windows is installed.
2. Find the 'RAITimeOutSeconds' entry and change the timeout value to the number of seconds you want System Control to wait for an AutoLink application to complete. For example, if you want to set the timeout to 4 minutes, the entry should read:

RAITimeOutSeconds=240

3. Save the edited 'STAR32.INI' file.
4. Restart System Control so that the change will take effect.

Multi-Channel Report Templates

The Multi-Channel Report macro allows you to use custom report templates that define the layout of the reports that are generated by the macro. When you create a custom Multi-Channel Report template, you decide what information will appear on the report. The report template that is used by the macro to create a report is defined in the File Selection dialog box. The figure below shows an example Multi-Channel Report template file.

Dcexmp1						
	1	2	3	4	5	6
1						
2			Moose Bay Gas Company			
3			Gas Analysis Laboratory			
4						
5	Initial Sample Time:	<i>inject_timea</i>				
6	Initial Vessel PSI:	<i>user_value1</i>				
7						
8	Final Sample Time:	<i>inject_timeb</i>				
9	Final Vessel PSI:	<i>user_value2</i>				
10						
11			Initial Sample		Final Sample	
12	Peak Name	Time	Result	Area	Result	Area
13						
14	<i>peak_names</i>	<i>peak_times</i>	<i>peak_resultsa</i>	<i>peak_areasa</i>	<i>peak_resultsb</i>	<i>peak_areasb</i>
15			=====	=====	=====	=====
16	Totals:		0	0	0	0
17						
18	Names					
19						
20						
21						

The report templates used by the Multi-Channel Report macro are Excel Template (.XLT) files. When an .XLT worksheet is opened, Excel loads a copy, rather than the original; this allows the file to be modified and saved without the original copy being destroyed. You use standard Excel functions to create the templates that will be used by the Multi-Channel Report macro.

The Multi-Channel Report macro recognizes certain key words in a report template. These key words correspond to information, such as peak names and results, that appear in Star Workstation results reports. When the macro is building its final report, it searches the template for these key words. When a key word is found, the

corresponding information from the current result report is inserted into the Multi-Channel report template. Your templates can also include Excel formulas which use the data from the workstation reports to perform custom calculations.

The following three sections describe setting up custom report templates for use with the Multi-Channel Report macro.

Multi-Channel Template Keywords

The keywords recognized by the Multi-Channel Report correspond to information that can be retrieved from a Workstation result file being processed by the macro. When the macro recognizes a keyword, it will replace the keyword with the corresponding information from the Workstation report file. The keywords recognized by the Multi-Channel macro are listed in the table below. When a keyword is placed in a cell in the template, the font of the cell must be in italics; this can be done easily by using the italic button which appears on the Excel toolbar.

Note that the last character of most of the keywords in the keyword table is an *x*; when you insert the key word in a report template cell, you must replace the *x* with a channel designator to identify which data channel the information should be retrieved from. The channel designator can be an *a* (ADC channel A), a *b* (ADC channel B), *fr* (3800 front detector), *mi* (3800 middle detector), *re* (3800 rear detector), or 2 numeric characters in the range 01 to 38 (9050 or 9065 channel number). For example, the keyword *sample_namex* appears in the table. If you wish to retrieve the Sample Name from channel 03 of a 9065 detector, enter *sample_name03* into the report template. Note that for channel numbers less than 10, that a leading 0 character must be included in the channel designator at the end of the keyword (01, 02, etc.).

Key Word	Action
<i>addressx</i>	Include contents of Bus Address field from Workstation report
<i>amt_std x</i>	Include contents of Amount Standard field from Workstation report
<i>channelx</i>	Include contents of Channel field from Workstation report
<i>detectorx</i>	Include contents of Detector Type field from Workstation report
<i>divisorx</i>	Include contents of Divisor field from Workstation report

Key Word	Action
<i>inject_timex</i>	Include contents of Injection Date field from Workstation report
<i>inst_namex</i>	Include contents of Instrument from Workstation report
<i>methodx</i>	Include contents of Method File field from Workstation report.
<i>multiplierx</i>	Include contents of Multiplier field from Workstation report
<i>noisex</i>	Include contents of Noise field from Workstation report
<i>notesx</i>	Include contents of Notes field from Workstation report
<i>offsetx</i>	Include contents of Baseline Offset field from Workstation report
<i>offset_totx</i>	Include contents of Time Offset field from Totals line of Workstation report
<i>operatorx</i>	Include contents of Operator field from Workstation report
<u>peakname@areax</u>	Include area count for 'peakname' (replace 'peakname' with actual name)
<u>peakname@ndrsltx</u>	Include result for 'peakname' (replace 'peakname' with actual name). If there is no result for this peak, 'n.d.' will be put into the report.
<u>peakname@rsltx</u>	Include result for 'peakname' (replace 'peakname' with actual name)
<u>peakname@rtx</u>	Include retention time for 'peakname' (replace 'peakname' with actual name)
<u>peakname@rtoffx</u>	Include retention time offset for 'peakname' (replace 'peakname' with actual name)
<u>peakname@sepcodex</u>	Include baseline separation code for 'peakname' (replace 'peakname' with actual name)
<i>peak_areasx</i>	Include contents of Peak Areas (or Heights) column from Workstation report
<i>peaks_detectedx</i>	Include contents of Detected Peaks field from Workstation report
<i>peaks_identifiedx</i>	Include contents of Identified Peaks field from Workstation report
<i>peak_measx</i>	Include contents of Peak Measurement field from Workstation report
<i>peak_numbersx</i>	Include contents of Peak Numbers column from Workstation report
<i>peak_names</i>	Include Peak Names found in all channels referenced in the report current
<i>peak_offsetsx</i>	Include contents of Peak Retention Time Offsets column from report
<i>peak_resultsx</i>	Include contents of Peak Results column from Workstation report
<i>peaks_rejectedx</i>	Include contents of Rejected Peaks field from Workstation report

Key Word	Action
<i>peak_sep_codesx</i>	Include contents of Peak Separation Codes column from Workstation report
<i>peak_timesx</i>	Include contents of Peak Retention Times column from Workstation report
<i>peak_totsex</i>	Include contents of Area/Height field from Totals line of Workstation report
<i>peak_widthsx</i>	Include contents of Peak Widths column from Workstation report
<i>report_headerx</i>	Include header lines from Workstation report
<i>report_summaryx</i>	Include summary lines from Workstation report
<i>result_totsex</i>	Include contents of Result field from report Totals line of Workstation report
<i>runfilex</i>	Include contents of Method File field from Workstation report
<i>run_modex</i>	Include contents of Run Mode field from Workstation report
<i>run_timex</i>	Include contents of Run Time field from Workstation report
<i>sample_namex</i>	Include contents of Sample Name field from Workstation report
<i>sample_ratex</i>	Include contents of Sample Rate field from Workstation report
<i>titlex</i>	Include contents of Title field from Workstation report
<i>tot_unidentx</i>	Include contents of Total Unidentified Counts field from Workstation report
<i>user_valuen</i>	Include User Value n entered by user (n = 1 to 6)
<i>workstationx</i>	Include contents of Workstation field from Workstation report

The key word *peak_names* does not have to have an channel designator appended to it. Using this keyword will cause the macro to retrieve the analyte names which appear in any of the workstation reports being processed (analyte names which appear in multiple data channels reports are not duplicated). When the macro recognizes this keyword it will insert the number of cells needed to accommodate all the analyte names. These new cells will be inserted at the location where the *peak_names* key word appears in the template.

The key words *peak_numbersx*, *peak_names*, *peak_resultsx*, *peak_timesx*, *peak_offsetsex*, *peak_areasx*, *peak_sep_codesx*, and *peak_widthsx* will insert a number of new cells vertically at the location they are placed in the template. Be sure to take this into account if you use these key words in any templates that you create.

To have one of the values from a workstation report included in a calculation on the report template, put the appropriate keyword (such as *user_value1*, or *amt_stda*) in a cell on the template, and then use the Excel *Formula Name* command to give this cell a named reference. This name can then be referenced by a formula on the template, even if its original location changes when new cells are inserted.

The Multi-Channel Report Configuration dialog box contains a *Prompt for User Values* check box, which, if enabled, will cause the macro to display a dialog box where the user can enter up to 6 values each time the macro generates a report. The user values also have keywords so that they can be included in a report template. These key words are *user_value1* through *user_value6*. Including the *user_value* keywords on a report template is useful if you need to incorporate additional data into the reports created by the macro.

Multi-Channel Report Template Formulas

The Multi-Channel Report templates which you build can include Excel formulas which perform calculations using the values taken from the workstation reports being processed. Any of the worksheet functions available in Excel (such as the SUM or AVERAGE functions) can be used on the Multi-Channel Report templates that you create. For information on the functions available in Excel, refer to the Excel On-Line Help.

The following paragraphs describe some guidelines for using formulas on Multi-Channel Report templates that you build.

If you want to have a report include the result, retention time, retention time offset, area counts or baseline separation code for a particular peak use one of the *peakname@*, keywords (*peakname@rsltx*, *peakname@rtx*, etc.) When you use one of these keywords, substitute the actual name of the peak of interest for '*peakname*' in the keyword. For example, if you would like to have the area counts for the peak named Benzene from channel B included in the report, the keyname you should use is *Benzene@areab*. Refer to keyword table for the text of the keywords you can use with individual peaks.

If you want your report templates to be able to perform calculations based on the results of the analytes in the workstation reports, build a row on the template that contains the keyword *peak_names* (using this keyword will cause the macro to insert a vertical column of cells which contain the analytes common to both the channel A and channel B report files) plus the keyword which correspond to the items you want to include in the calculation (*peak_resultsa*, *peaks_resultsb*, *peak_areasa*, *peak_areasb*, etc.). Next, in the same row of the worksheet, pick the cell where you want the calculation to occur and use the *Formula Notes* command to enter *dual_calc* into the cell's Note. Then you must enter a valid Excel formula that performs the desired calculation into the cell. Since your calculation will probably involve a value from the same row of the worksheet, the formula should use the Excel *OFFSET()* command to reference the correct value.

For example, if you want to have the formula in the cell multiply the analyte results by 10, and the analyte results are located two columns to the left, the formula which you would enter would look this:

```
=OFFSET(RC,0,-2)*10
```

To Excel, this says take the value that is offset from the current location by 0 rows and -2 columns (2 columns to the left), multiply that value by 10, and put the result in the current cell.

Note that a calculation formula involving analyte results, such as the one described above, only has to be put into one location on the report template in order for it to occur for all analytes present in the workstation reports. The Multi-Channel Report macro will duplicate the formula so that the calculation will occur for each analyte in the report.

A report template can also contain formulas which, based on an analyte name, will look up a value in a table, for example, a BTU value. The Excel function *VLOOKUP()* can be used to perform this table lookup. For example, suppose that you want to multiply the result for an analyte by its standard BTU or Specific Gravity value. The BTU and Specific Gravity values can be looked up from a table, which might look like this:

Analyte	BTU	S.G.
Butane	3251.9	2.0068
Ethane	1769.6	1.0382
Methane	1010	0.5539
Propane	2516.1	1.5226

You could enter this table on the report template and give it a name, such as *Parms*, by highlighting the cells which make up the table and then using the Excel *Define Name* command. Note that in the table above, the first row would not be included as part of the defined *Parms* table because these cells just identify the columns and are not part of the data that you want to be able to look up. Also notice that the analyte names listed in column 1 of the table are in alphabetical order; this is required by the *VLOOKUP()* function (the Excel *Data Sort* command can be used to sort the entries in a table).

To have Excel look up a value from this table, the *VLOOKUP()* command can be used. For example, to look up the BTU value for Butane, the Excel function would look like this

```
=VLOOKUP("Butane",Parms,2)
```

The 2 in the above function tells Excel to get the value from the 2nd column of the table named *Parms*. To look up the Specific Gravity value for Butane, the function would be

```
=VLOOKUP("Butane",Parms,3)
```

In a Multi-Channel Report template you will probably want to use the *VLOOKUP* function in conjunction with the *OFFSET* function so that you can look up a value based on the analyte name which appears in the same row of the report. For example, suppose the analyte names will appear in column 1 of the report, analyte results will appear in column 2, and in column 3 you want to multiply the analytes result by its BTU value from the *Parms* table. The Excel formula which would do this is:

```
=VLOOKUP(OFFSET(RC,0,-2),Parms,2)*OFFSET(RC,0,-1)
```

The above formula will look up the BTU value based on the analyte name in the current row, and multiply the BTU value by the result in the current row. The cell containing the above formula would also

have to have dual_calc entered into its Note (*Formula Note*). This entry in the cell's Note is required so the Multi-Channel report macro knows that the formula must be duplicated for all of the analytes which appear in the workstation result reports.

For further information on the use of the Excel OFFSET() and VLOOKUP functions, please refer to the On-Line Help in Excel.

Note: If you build a Multi-Channel report template that contains a lookup table, make certain that the contents of the table have been sorted by the names which appear in the first column of the table; if the lookup table is not sorted correctly, the Excel VLOOKUP() function will not return the correct values. Also, if the lookup table contains analyte names, they must exactly match the names which appear in the workstation report files to be processed by the macro.

Creating New Multi-Channel Report Templates

Perform the following steps, to create a new report template for use with the Multi-Channel Report macro.

1. Use the Excel *File New* menu command to open a new worksheet.
2. Customize the report template using the keywords described in the section labeled *Multi-Channel Template Keywords*.
3. You can put fixed text that you want to appear in the report anywhere on the template, such as in a cell that is to the left of a cell that contains a keyword. The fixed text that you enter can be in any available font or point size and you can adjust the row heights and column widths as much as necessary.
4. After you have entered all of the fixed text, keywords, and formula onto the template, you must define the area of the report that will be printed. To do this, use the mouse and select all the cells that make up the area you want to be printed out. Next, use the *File Page Setup* menu item and access the *Page* tab and make sure that the *Print Area* range is set to the range of cells that you have selected. After you have done this, click on the *OK* button.

5. Next, select a cell in column 1 that is below the print area you defined in the previous step. Type the text 'Names' into this cell and then use the *Insert Note* menu to put a *Text Note* of 'Compnames' into this cell. The Multi-Channel report macro uses this cell location for the temporary storage of the peak names found in the various report files that it processes.
6. Finally, select the Excel *File Save As* menu command. In the dialog box that appears, click on the button labeled *Options*; this will bring up another dialog box that has a drop down list box labeled *File Format*. Set the file format to *Template* and then click on the *OK* button. Next, enter a new file name for the report template; this file name should have a file extension of .XLT. After you have entered the new file name, click on the *OK* button to save the new report template to disk.
7. To set up the Multi-Channel Report macro to use the report template you have created, press *Ctrl+F* to bring up the Configuration dialog box, In this dialog box, enter the file name of the template you created into the *Multi-Channel Report Template File Name* field. If you want to use the template when the macro is run as an AutoLink application, enter the template file name into the AutoLink Defaults dialog box.

Example Multi-Channel Report Templates

The directory containing the Multi-Channel Report macro has several report template files that you can use as examples for building your own custom templates. The template files you can find in this directory are shown below.

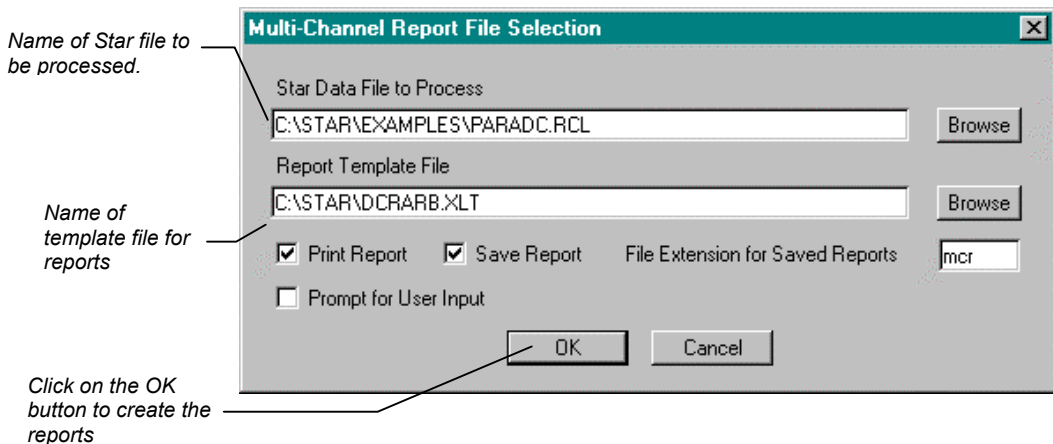
Template File	Description
DCAAAB.XLT	Creates a report that divides the area counts from channel A peaks by the area counts from the channel B peaks
DCABAA.XLT	Creates a report that divides the area counts from channel B peaks by the area counts from the channel A peaks

Template File	Description
DCRARB.XLT	Creates a report that divides the results for A peaks by the results for the channel B peaks
DCRBRA.XLT	Creates a report that divides the results for B peaks by the results for the channel A peaks
MULTI.XLT	Creates a report that divides the area counts from 9065 detector channel 07 by the area counts from 9065 detector channel 12.

Tutorial - Creating Multi-Channel Reports

In this Tutorial, you will use the files stored in the directory C:\STAR\EXAMPLES to generate Multi-Channel reports. If your Star Workstation software is not installed in the default folder of C:\STAR, before performing this tutorial you will need to start the System Control application and edit the RecalcList PARADC.RCL so that the data files file names reference the actual location on disk.

1. Start the macro by selecting the Multi-Channel Macro item from the Star Advanced Application menu. After the macro has loaded, you will have a Star menu item near the right-hand side of the Excel menu bar. From the Star Multi-Channel Report menu select *Create Report(s)*. The dialog shown below will be displayed.



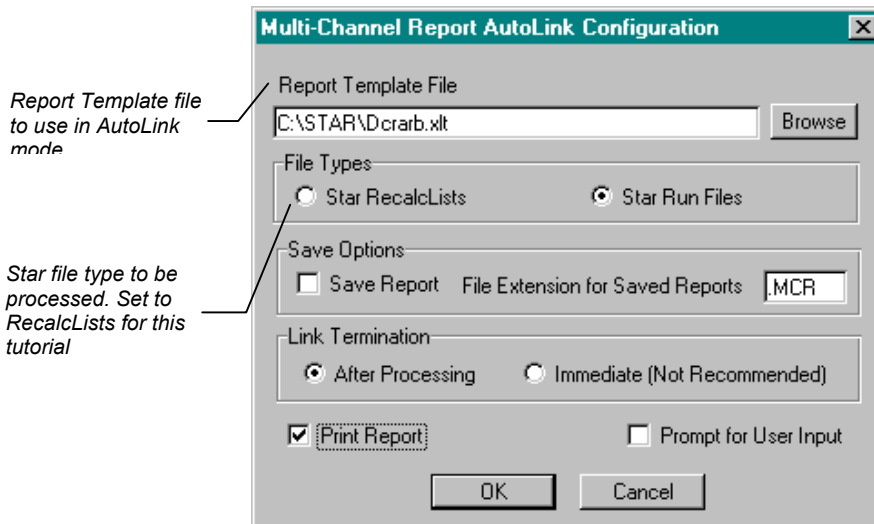
2. The File Selection dialog box should be set up as shown above. The RecalcList name should be

C:\STAR\EXAMPLES\PARADC.RCL and the Report Template File name should be C:\STAR\DCRARB.XLT (this template divides the channel A results by the channel B results). You should also select the *Print Report* and *Save Report* options. After you have set up the dialog box as shown, click on the *OK* button to create the reports for the three data files in the RecalcList. When the macro completes, the Multi-Channel report for the last data file in the RecalcList will be displayed on the screen.

Tutorial - Creating Multi-Channel Reports Using AutoLink

In the following tutorial you can use the System Control application and the macro tutorial files installed in C:\STAR\EXAMPLES to run the Multi-Channel Report macro as an AutoLink application. Before going through this tutorial, it is recommended that you use the procedure outlined in the section labeled *AutoLink Timeout Setting* to increase the AutoLink timeout to 240 seconds.

1. Start the macro by selecting the Multi-Channel Macro item from the Star Advanced Application menu. After the macro has loaded, you will have a Star menu item near the right-hand side of the Excel menu bar. From the Star Multi-Channel Report menu select *Configure AutoLink* The dialog shown below will be displayed.



2. The AutoLink Configuration dialog box should be set up as shown above. The Report Template File name should be C:\STAR\DCRARB.XLT (this template divides the channel A results by the channel B results). You should also select the *Print Report* and *Save Report* options. After you have set up the dialog box as shown, click on the *OK* button to save the settings and then use the *File Exit* menu item to close Excel.
3. Start the System Control application and use the *Instrument* menu to access one of the instruments available on the Workstation.
4. Use *File Open RecalcList* to open the RecalcList named C:\STAR\EXAMPLES\PARADC.RCL.
5. Use *File Activate Method* to activate the method file named C:\STAR\EXAMPLES\PARADC.MTH.
6. Use the *Windows RecalcList* menu to access the active RecalcList window
7. Add a new sample to the end of the list and set the Sample Type for the new sample to *AutoLink*. Click on the *AutoLink* button for this sample and enter the following into the *Command* field of the dialog box:

C : \STAR\MCAPL . XLM

8. The *Other Parameters* field should be left blank. Click on the *OK* button after making the entries.
9. Start the recalculation using the *Recalculate Begin RecalcList* menu item. The three samples listed in the *RecalcList* will be reintegrated. After the last sample is reintegrated, the Multi-Channel macro will be activated as the *AutoLink* application and the macro will create and print the Multi-Channel reports for each of the three runs. When the macro completes, control will be returned to System Control and Excel will close itself.

Peak Grouping Macro

Creating Reports with the Peak Grouping Macro

The basic Star Chromatography Software allows each peak in a method peak table to be assigned to a peak group number. The report created by using the method will contain a section displaying the total for each peak group.

The Peak Grouping macro provided similar capabilities to the basic Star software, except that a descriptive name, such as 'Olefins Totals' or 'Aromatics Total', can be assigned to each group number. The Peak Grouping macro also prints two additional data fields, Sample Description 1, and Sample Description 2 near the top of the report it creates.

The macro groups peaks together based upon group numbers. Peaks are assigned to a group number and the macro calculates and reports the summarized results for each of the group numbers. The macro contains an editor function that is used to assign peaks to a group number.

The peak grouping macro can run either interactively, or automatically, by using the Star Workstation *AutoLink* feature.

Creating Group Files

Before running the Peak Grouping macro to create a report, you must create a group file spreadsheet that contains the information related to which peaks will be grouped together. This is done by using the group file editor. You use the group file editor to enter the

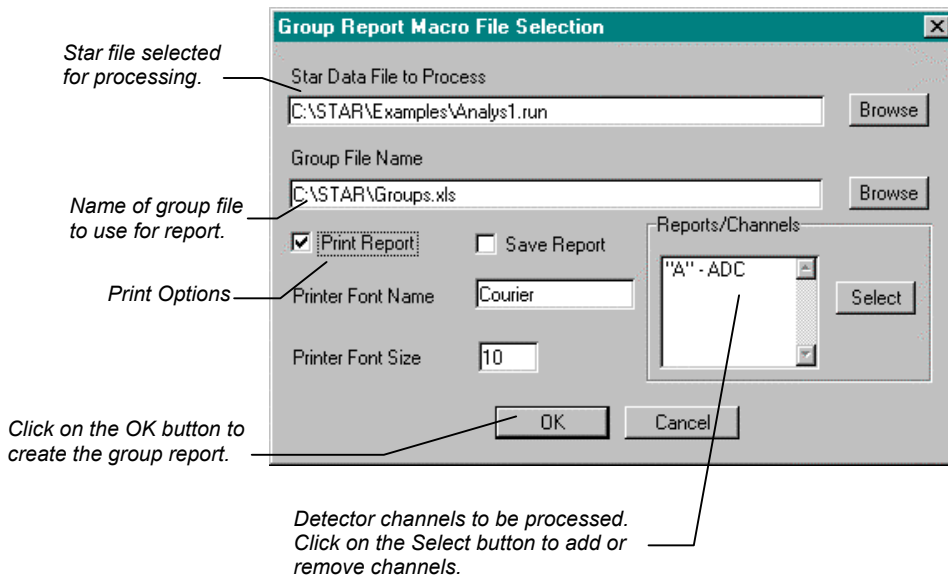
peak names and assign each peak to a group number. The group file editor is also used to enter a descriptive name for each of the group numbers.

Use the following steps to create or edit a group file for use with the Peak Grouping macro:

1. Access the group file editor either by selecting the Configure Groups item from the Star Peak Grouping menu in Excel.
2. For each peak that you enter into the *Peak Name* column enter an appropriate group number for the peak in the *Group Number* column. If you want to create a group that calculates the total for all unidentified peaks, leave the cell in the *Peak Name* field blank.
3. Each group number that you will be using also needs to have a descriptive name given to it. This name, rather than the group number, is used in the report that the macro creates. Enter each group number into the *Group Number* column and then enter a name for each of the groups into the *Group Name* column.
4. After you have entered all the information into the group file, either click on the *Save* button to save to the current file name or click on the *Save As* button to save to a new file name. If you decide you do not wish to save any of the information you have entered, click on the *Exit* button and then choose No when you are asked if you wish to save changes.
5. The group files that you create are used by the macro to create its reports. When the macro is run interactively, the group file to be used is entered into the *File Selection* dialog box. When the macro is run automatically using AutoLink, the macro uses the group file that has been entered into the *AutoLink Defaults* dialog box, or alternatively, the group file name that is passed in the AutoLink *Other Parameters* field.

Peak Grouping Macro - Interactive Use

To run the Peak Grouping macro interactively, select *Peak Grouping Macro* from the Star Advanced Application menu. After Excel has loaded select, *Process Files* from the Star Peak Grouping menu in Excel. The File Selection dialog will be displayed. This dialog is show below:

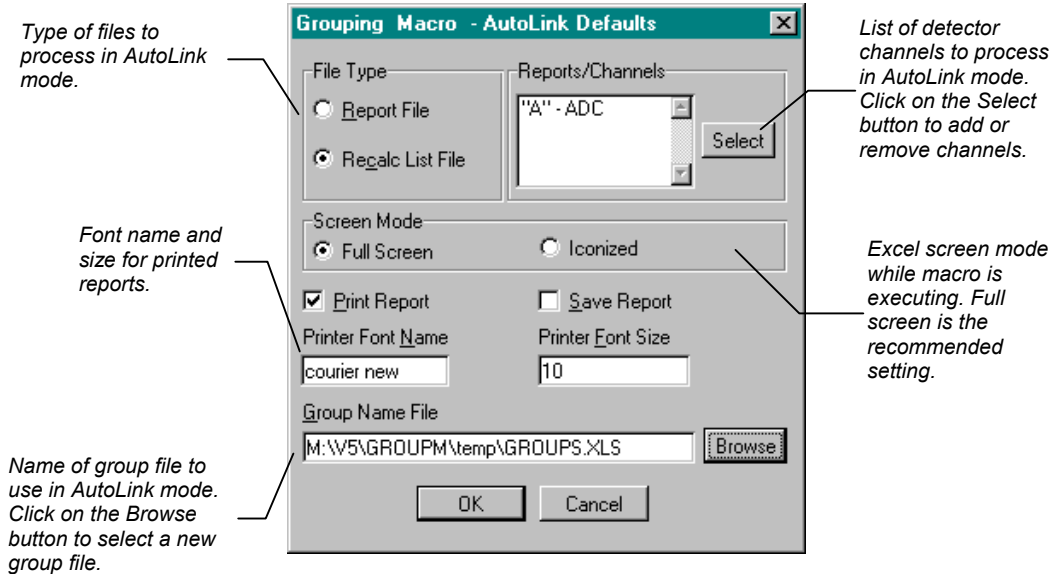


Running the Peak Grouping Macro as an AutoLink Application

When used with Star Chromatography Software, the Grouping macro can be run from System Control as an AutoLink application. This allows Group reports to be automatically created either for a single sample or for all the samples in a SampleList. When the Grouping macro is run as an AutoLink application, Excel will be loaded and the macro will generate the group report(s). When the macro completes, Excel will exit and control will be returned to the Workstation software.

Peak Grouping Macro - Default AutoLink Configuration

The default AutoLink parameters for the Peak Grouping Macro are set up in the dialog box shown in the figure below. This dialog box can be accessed by selecting the Configure AutoLink item from the Star Peak Grouping menu in Excel.



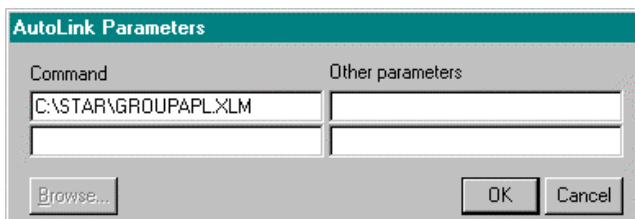
Grouping Macro AutoLink Command Line

For running the Grouping macro as an AutoLink application, the macro GROUPAPL.XLM is used. This macro is responsible for the DDE communication between Excel and System Control and for starting up the main Grouping macro, GRPBYNUM.XLM.

The Grouping Macro can be activated either after the completion of a single sample or the completion of all the samples in a SampleList or RecalcList. To have the macro run following the completion of a single sample, use the AutoLink dialog box for the sample in the SampleList or RecalcList. To run the macro after all samples in a SampleList or RecalcList have been processed, add an additional sample to the end of the list and set its Sample Type to *AutoLink*. In either case, the complete path to GROUPAPL.XLM is entered into the *Command* field in the AutoLink dialog box. For example, if the Grouping macro is installed in C:\STAR, the AutoLink command line entry should be:

C:\STAR\GROUPAPL.XLM

The following figure shows an example of how to set up the AutoLink dialog box for use with the Grouping macro.



Using the AutoLink Other Parameters Field

The *Other Parameters* field of the AutoLink dialog box can be used to pass the name of an initialization file containing parameters for the Peak Grouping Report macro to override the values set in the AutoLink Defaults dialog box. The file must be an ASCII text file which contains the text [AUTOLINK] on a line by itself. Following the [AUTOLINK] section heading, will be the parameter names used for each option. Following each parameter name will be an equal sign and the value to be assigned to the option.

The table below describes the parameter names which can be entered in the [AUTOLINK] section of an initialization file passed in the AutoLink *Other Parameters* field:

Parameter	Description
Print	Print Report Flag. 0 = Don't print reports, 1 = Print reports.
Save	Save Report Flag. 0 = Don't save reports, 1 = Save reports.
GroupFile	Name of peak grouping file.
FileType	Type of file to process. 1 = Run file, 2 = RecalcList file.
FontName	User Prompt Flag. 0 = Don't prompt for additional input. 1 = Prompt for additional input.
FontSize	Type of file to process. 1 = Run file, 2 = RecalcList file.
ChannelCount	Number of detector channels to be processed.
Channel <i>n</i>	Name of detector channel <i>n</i> , where <i>n</i> is a value of 1 to ChannelCount setting.

Grouping Macro AutoLink Log File

Each time the Grouping macro is run as an AutoLink application, it records its activity in a log file named GRAPLLOG.XLS. This log file can be found in the directory where the Group macro is installed (normally C:\STAR). To examine the log, use Excel to open the file as a spreadsheet. If errors occur in the macro while running as an AutoLink application, the log file will record the location of the error within the macro sheet. The log file may be deleted if it grows too large; a new AutoLink log file will be automatically created by the macro.

AutoLink Timeout Setting

By default, the Workstation System Control application will wait 120 seconds for an AutoLink application to complete. If the application has not completed within this amount of time, System Control assumes that the application has abnormally terminated and generates an 'RAI Timeout' error. If necessary, this timeout period can be changed by using the following procedure:

1. Use the Windows Notepad application to open the file 'STAR32.INI' located in the directory where Windows is installed.

2. Find the 'RAITimeOutSeconds' entry and change the timeout value to the number of seconds you want System Control to wait for an AutoLink application to complete. For example, if you want to set the timeout to 4 minutes, the entry should read:

```
RAITimeOutSeconds=240
```

3. Save the edited 'STAR32.INI' file.
4. Restart System Control so that the change will take effect.

GOTO Application

Star Workstation GOTO Application

GOTO is an AutoLink application to jump within a Sample List or Recalc List. It can be used to create loops.

Using the GOTO Application

To use the GOTO application in a Star Workstation SampleList or RecalcList, click on the *AutoLink* button for the appropriate line (normally the last line in the SampleList or RecalcList); the *Command* and *Other Parameters* fields for the GOTO application are as follows:

```
Command: C:\STAR\GOTO.EXE <line-number>  
Other Parameters: Inject , or Recalc , or Print
```

This sets the next Sample List or Recalc List line to be executed to the line number passed on the command line. If *Other Parameters* are specified, this action will only take place if the current automation action matches the action in the *Other Parameters* field.

Note: The line numbers in a Sample List file will not apply to the Recalc List file. Therefore, if you plan to use the Recalc List, you should always specify *Inject* in the *Other Parameters* field; this will prevent the GOTO command from executing when the RecalcList is recalculated.

The GOTO application may display any of the following messages in the Message Log:

Error Messages

<line-number> is not a valid line number

<other-parameter> is not a valid sequence action

Info Messages

Next SampleList line set to <line-number>

Next Recalc List line set to <line-number>

Goto: Sequence action mismatch; no action taken

The GOTO application can be combined with the WAIT application to create systems that perform injections on a specific time table.

WAIT Application

Star Workstation WAIT Application

WAIT is an AutoLink application that waits for a specified time before terminating; it can therefore be used to perform injections on a specific time table.

WAIT.EXE is installed in the directory where the Star Workstation resides.

Use of the WAIT Application

To invoke WAIT, insert a line into the SampleList immediately before the desired sample. Set the Sample Type for the inserted line to AutoLink. The AutoLink parameters should be set as follows:

```
Command:      WAIT hours:minutes:seconds
Other Parameters: <none>
```

Hours - 0-23

Minutes - 0-59

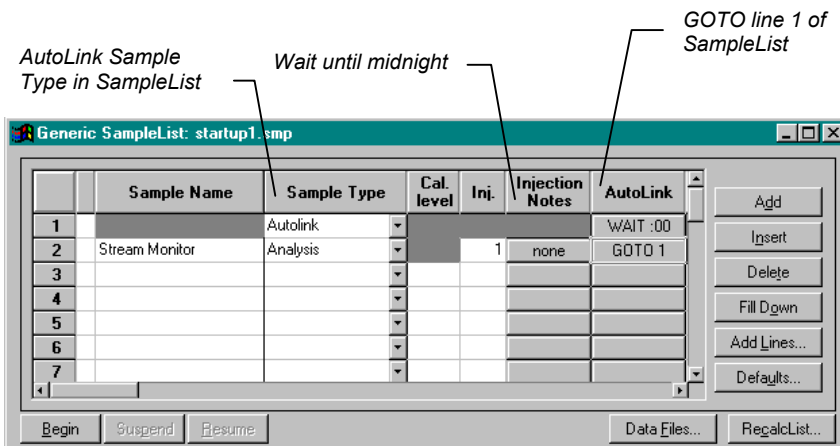
Seconds - 0-59

For example, WAIT 15:03:56 will wait for 3:03:56 PM, unless this time is already passed, in which case there will be no wait.

Fields in the time specification can be omitted. In this case, trailing fields are defaulted to zero, while leading fields are interpreted as the next matching hour or minute. The following table illustrates examples of use of the WAIT application.

AutoLink Command	Explanation
WAIT 13:	Wait until 13:00:00
WAIT 13:10	Wait until 13:10:00.
WAIT :13	Wait until the next occurrence of 13 minutes after the hour. At 12:15, this command would wait for 13:13. At 12:10, this command would wait for 12:13.
WAIT :13:00	(same as above).
WAIT ::13	Wait until the next occurrence of 13 seconds after the minute.

The following sample list shows how WAIT and GOTO can be used to create an infinite loop that performs an injection every hour on the hour to monitor a process stream:



More complex functions may require several WAIT commands. For example, to inject every 2 hours, the above example should be modified as follows:

AutoLink Command	Explanation
WAIT :01	Wait until 1 minute past next hour.
WAIT :00	Wait until next hour
none	Inject Sample
GOTO 1	Goto first line of SampleList

To specify in the evening that an analysis is to start early in the morning, the following AutoLink commands should be inserted at the beginning of the SampleList:

AutoLink Command	Explanation
WAIT 23:59	Wait until midnight
WAIT 5:00	Wait until 5:00 a.m.
none	Inject Sample

Capsule Application

CAPSULE.EXE is a Windows program that you can use to run external applications using the AutoLink feature of the Star Workstation's System Control application. The programs that CAPSULE.EXE can run do not have to have any Windows DDE capabilities; CAPSULE.EXE can start up a program and take care of the required DDE interface with System Control. CAPSULE.EXE allows the automated activation of Windows, and even DOS-based, programs that were not written specifically to use the AutoLink feature of the Star Chromatography Workstation.

Operation

To use CAPSULE.EXE to run another program from System Control, use the AutoLink dialog box for the sample in the Workstation Sample List or Recalc List. The Command field in this dialog box will always be CAPSULE.EXE.

The 'Other Parameters' field in the AutoLink dialog box of the Workstation SampleLog or Sample List is used to tell CAPSULE.EXE what program it needs to execute as well the parameters for the program to be run. The syntax for the 'Other Parameters' field is:

```
application, filetype
```

where:

application - Required; Filename of application that you want to run. The application can be a Windows .EXE or a DOS .BAT file.

filetype - Optional; Type of Workstation file name to be passed to the application. Items are:

- 0 - None
- 1 - Current Workstation data file, minus .RUN extension (DEFAULT)
- 2 - Current Workstation Recalc List file, minus .RCL extension
- 3 - Current Workstation Sequence file, minus .SEQ extension
- 4 - Current Workstation Method file, minus .MTH extension

- 5 - Current Workstation SampleList file, minus .SMP extension
- 11 - Current Workstation data file, including .RUN extension
- 12 - Current Workstation Recalc List file, including .RCL extension
- 13 - Current Workstation Sequence file, including .SEQ extension
- 14 - Current Workstation Method file, including .MTH extension
- 15 - Current Workstation SampleList file, including .SMP extension

For example, if you want CAPSULE.EXE to run a program named C:\STAR\SUMRPT.EXE, pass it the name of the current Recalc List file minus the .RCL extension (e.g. C:\STAR\MYSAMP), the 'Other Parameters' field would be:

```
C : \STAR\SUMRPT . EXE , 2
```

Notes on automating DOS Applications or Batch files:

If you are automating a DOS mode program, you should create a .BAT file that executes this program and passes it any necessary command line parameters. If needed. If desired, you can directly set the *Properties* for each program. If you need different sets of Properties for different operating conditions, create multiple shortcuts to this program and set different properties for each shortcut.

Star AutoLink

The Varian Star Workstation includes the AutoLink feature. This feature allows external programs to exchange information with the Star System Control application (CHEMIS32.EXE). Programs that use AutoLink can request the names of the files currently active for an instrument, such as the name of the current data file or the name of the currently active method. Programs can also send information to System Control in order to store text into the instrument Message Log or to perform automation actions such as activating a method or suspending further injections.

The AutoLink feature is implemented using a messaging protocol based on Microsoft's Dynamic Data Exchange (DDE). The DDE topics and items, along with the rules for invocation and termination, used to implement AutoLink is called the Remote Application Interface.

The AutoLink interface is used by standard Star Workstation applications, such as the Report application (REPORT32.EXE) and the Excel Summary Report macro (SUMRPT.XLM). Through the use of AutoLink, it is possible to enhance the Star Workstation software with applications that perform specialized functions such as custom reports or automated result transfer to external LIMS systems.

Modes of AutoLink Operation

Star AutoLink has two different modes of operation: post-run and asynchronous. The difference in these two modes of operation is related to when and how the AutoLink conversation is established by the application.

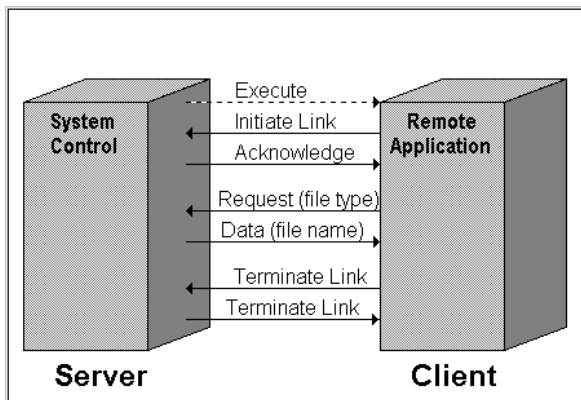
Post-Run AutoLink Mode

In the post-run mode of operation, a program name is entered into the AutoLink command field of a line in a Star SampleList or RecalcList. The AutoLink program is automatically started by System Control when data handling/processing for the line has been completed. Upon starting, the AutoLink program establishes the DDE conversation with System Control and requests or sends the required data using the supported AutoLink topics. Once the program has performed its processing (creating a report, transferring data, etc.), it closes the DDE conversation and terminates itself. Following termination of the DDE conversation, System Control will continue with the next line in the SampleList or RecalcList.

In the post-run mode of operation it is important that the application can:

1. Automatically initiate the DDE conversation with System Control.
2. Use the AutoLink topic strings to request the information that it needs to perform its processing.
3. Close the DDE conversation and terminate itself when it has completed its processing.

Below is a diagram showing the relationship between System Control and a remote application in the post-run mode of operation.



Asynchronous AutoLink Mode

In the asynchronous mode of operation, an AutoLink conversation can be started with System Control at any time. However, in this mode of operation, the DDE topic string must include information about which instrument number data is being requested from or sent to. This is done by appending a colon (':') and the instrument number onto the end of the topic string. For example, 'LAST_RUN' is a valid post-run AutoLink topic; if you want to use this topic in an asynchronous mode conversation to request the last data file for Instrument #2, the actual topic string would be 'LAST_RUN:2'.

The available DDE topics for AutoLink conversations are discussed in the next section.

DDE Application, Topic, and Items Supported by AutoLink

DDE topics and items are text strings used to establish transactions and exchange information between applications running under Windows. See the Microsoft Windows SDK or your development language's documentation for a further discussion of DDE.

AutoLink defines specific DDE topics and items that are used in the exchange of data between System Control and the AutoLink application. Below are the topics and items specified by AutoLink.

Application Name

CHEMIS32

To establish an AutoLink conversation with Star System Control, use an application name (also referred to as a server or service name) of CHEMIS32.

Topic

AUTOLINK

This topic establishes a conversation between System Control (CHEMIS32.EXE) and the AutoLink application. Information items may be sent to System Control by the AutoLink application or requested from System Control. The information items are specified with the appropriate item string. The SEND_FILENAME topic has been obsoleted, and should be replaced by AUTOLINK.

Items

LAST_RUN

This item requests the name of the last Run file processed by System Control (from either an Inject or Recalc automation action). The return value of this item is a string representing the file name of the last Run file processed (created or recalculated) by the system.

CUR_MTH

This item requests the name of the active Method in System Control when the remote application was invoked. The return value of this item is a string representing the active Method file name.

CUR_SMP

This item requests the name of the active Sample List in System Control when the remote application was invoked. The return value of this item is a string representing the active Sample List file name.

CUR_RCL

This item requests the name of the active RecalcList in System Control when the remote application was invoked. The return value of this item is a string representing the active RecalcList file name.

CUR_SEQ

This item requests the name of the active Sequence in System Control when the remote application was invoked. The return value of this item is a string representing the active Sequence file name.

OTHER_PARMS

This item requests additional parameters entered by the user in System Control. These parameters are freeform text and must be parsed by the application. The return value of this item is a string representing the user-entered parameters.

REMOTE_RESULT

This item sends a response string to System Control. This response is displayed in the Sequence Log and, depending upon the response code, appropriate action is taken. The response string is in the form:

response_code uniqueID descriptive_text

The **response_code** is one of the following strings: INFO, WARNING, FATAL. INFO responses are simply displayed by System Control in the Message Log with no other action taken. WARNING responses cause System Control to increment the Error Counter. Two identical FATAL responses in a row abort the current SampleList or RecalcList. The **uniqueID** is an ASCII representation of an integer between 10000 and 32767. This number is used by System Control to determine if two identical fatal errors have occurred in a row, so the number should be unique to a particular response. The **descriptive_text** is displayed in the Message Log window and should provide information about the response to the user. This is a "poke" item type.

GET_AUTOSAMPLER_TYPE

This item requests the type of autosampler that is currently active in the instrument that invoked the AutoLink application. The return value of this item is a string representing the autosampler type. Possible autosampler type strings are 8200, 8200S, 8134, 9100, 9300, AI200 or Generic. If the string returned from this item is 'Generic', then there is no autosampler being controlled on the instrument, and the generic Sample List is being used.

GET_INSTRUMENT_ID

This item requests the numerical ID representing the instrument that invoked the AutoLink application. This ID is the same as the numerical ID displayed in the Configuration Screen in System Control (e.g. Instrument 1: Varian Star). The return value of this item is a string representing the instrument number (ranging from 1 to the maximum number of instruments allowed in System Control).

GET_INSTRUMENT_NAME

This item requests the name that the user has associated with the instrument that invoked the AutoLink application. The return value of this item is a string representing the instrument name.

GET_OPERATOR_NAME

This item requests the name of the operator that the user has associated with the instrument that invoked the AutoLink application. The return value of this item is a string representing the operator name.

GET_CURRENT_SEQUENCE_ACTION

This item requests the automation action. The return value of this item is a string representing the current action. Valid actions are 'Inject', 'Recalc' and 'Print'.

GET_PRINT_SWITCH

This item requests the setting of the 'Enable Automated Printing' switch for an instrument. A string of 'on' will be returned if this switch is enabled and a string of 'off' will be returned if this switch is disabled. Applications may wish to suppress printing when this topic returns 'off'.

STATUS_PRINTING

This item informs System Control that the remote application is printing a report. The state indicator in the System Control title bar will show "Printing" when this item is received, and System Control will monitor the print spooler to insure that the print jobs are complete before continuing with the next automation action. No additional information is passed with this item. This is a poke item type.

STATUS_COMPUTING

This item informs System Control that the remote application is performing a calculation. The state indicator in the System Control title bar will show "Computing" when this item is received. No additional information is passed with this item. This is a poke item type.

REPORTS_GENERATED

This item causes System Control to increment the "Reports Generated" counter displayed in the Instrument Status window and reported in the Sequence Log. The number of reports generated by the remote application is passed as a string by this item. This is a poke item type.

CALCULATIONS_PERFORMED

This item causes System Control to increment the "Recalculations" counter displayed in the Instrument Status window and reported in the Message Log. The number of calculations performed by the remote application is passed as a string by this item. This is a poke item type.

SET_NEXT_SAMPLELIST_LINE

This item sets the next line in the current Sample List that will be executed by System Control. The line number is passed as a string representing the next line (line numbers start at 1) to be executed. The current action specified in the active Sequence List must be "Inject". If the current action is not "Inject", the active Sample List will still be modified, but the injection status will be reset when the Sample List is next executed. The injection status of all lines before the specified line number are marked as complete. If the line specified is less than or equal to zero, the item has no effect. If the line specified is greater than the last line in the Sample List, then all lines will be marked as complete. If the line number specified is less than the current line, then the injection status of the lines starting at the specified line and continuing through the current line will be reset to zero (i.e. no injections complete). The resulting Recalc List entry will reflect the actual sequence of injections. This is a poke item type.

SET_NEXT_SAMPLELOG_LINE

This item sets the next line in the current Recalc List that will be executed by System Control. The line number is passed as a string representing the next line (line numbers start at 1) to be executed. If the current action is not "Recalc", the active Recalc List will still be modified, but the completion status will be reset when the Recalc List is next executed.

The completion status of all lines before the specified line number are marked as complete. If the line specified is less than or equal to zero, the item has no effect. If the line specified is greater than the last line in the Recalc List, then all lines will be marked as complete. If the line number specified is less than the current line, then the completion status of the lines starting at the specified line and continuing through the current line will be reset to incomplete (i.e. no recalc/print performed). This is a poke item type.

ABORT_CURRENT_SEQUENCE_LINE

This item causes System Control to abort the current Sample List or Recalc List and continue with the next line in the active Sequence. A string is passed with this item and is displayed in the Sequence Log window. This is a poke item type.

ABORT_CURRENT_SEQUENCE

This item causes System Control to abort the current line in the Sample List or Recalc List, and prevent any further line from being executed in the active Sequence. A string is passed with this item and is displayed in the Sequence Log window. This is a poke item type.

ARE_ALL_MODULES_READY

This item requests whether or not all modules assigned to an instrument are ready. A string of '1' will be returned if all assigned modules are ready and a string of '0' will be returned if one or more assigned modules are not ready.

GET_PROMPT_AT_AUTOMATION_SWITCH

This item requests whether or not the instrument will display the 'Instrument Parameters' dialog box when a Sample List or RecalcList is started. A string of '1' will be returned if this dialog box will be displayed and a string of '0' will be returned if the dialog box will not be displayed.

IS_INSTRUMENT_COMPLETE

This item requests whether or not all modules configured for the instrument have completed logging on. A string of '1' will be returned if all modules have completed their log on and '0' will be returned if one or more modules still have not logged on.

GET_STATE

This item requests the current state of a instrument. The possible strings returned from the use of this AutoLink item are: 'offline', 'hungbus', 'online', 'notready', 'equilibrating', 'allmodulesready', and 'hasrunningmodule'.

GET_MODULE_NAMES

This item requests the names and bus address of the modules assigned to an instrument. The returned string will contain a comma-delimited list of modules and address, with each modules and buss address separated by a period. For example, if an instrument has an ADCB board at address 16 and a 3400 GC at address 17, the returned string would be 'ADBC.16,3400.17'.

GET_SAMPLE_INJECTION_COUNT

This item requests the number of injections performed for the current line of the SampleList. A string containing the number of injections will be returned.

GET_INJECTION_COUNT

This item requests the total number of injections performed by the current SampleList. A string containing the number of injections will be returned.

SET_ACTIVE_METHOD

This item activates a specified method for an instrument. The string passed with this item should contain the complete file specification of the method to be activated. This is a poke item type.

SUSPEND_AUTOMATION

This item causes System Control to suspend automation. The current line of the Active SampleList or RecalcList will be completed, but no further lines will be executed until automation is resumed. The string passed with this item will be stored in the instrument Message Log. This is a poke item type.

RESUME_AUTOMATION

This item causes System Control to resume automation following a suspend action. The string passed with this item will be stored in the instrument Message Log. This is a poke item type.

START_PUMPS

This item causes System Control to start any Star LC pumps configured for an instrument. The string passed with this item will be stored in the instrument Message Log. This is a poke item type.

STOP_PUMPS

This item causes System Control to stop any Star LC pumps configured for an instrument. The string passed with this item will be stored in the instrument Message Log. This is a poke item type.

Note: When used with an asynchronous mode AutoLink conversation, you must append a colon (':') and the instrument number onto the end of all of the above AutoLink topic strings. For post-run AutoLink conversations, it is not necessary to specify an instrument number.

Developing AutoLink Applications

Refer to On-Line Help file AUTOLINK.HLP, which provides sample code for Visual Basic and C programs and allows you to copy sample code into your application.

File Access Routines

The following functions can be used to read records from a Star RecalcList file. Their calling syntax is described in the On-Line Help File AUTOLINK.HLP.

OpenSampleLog
GetSampleLogRecordCount
SampleLogGetRecordType
SampleLogGetRunFilePath
SampleLogGetSampleName
SampleLogGetSampleLevel
SampleLogGetSampleType
SampleLogGetSampleAmountStandard
SampleLogGetSampleInjection
SampleLogGetSampleUnidentifiedPeakFactor
SampleLogGetSampleMultiplier
SampleLogGetSampleDivisor
SampleLogGetSampleNotes
SampleLogGetSampleAutoLinkCommand
SampleLogGetSampleAutoLinkParameters
SampleLogGetSampleAutoLinkInvocation
SampleLogGetRecordAutoLinkCommand
SampleLogGetRecordAutoLinkParameters
SampleLogGetRecordAutoLinkInvocation
SampleLogGetControlRecord
SampleLogRecordDone
CloseSampleLog