ChromQuest 4.2 Quick Reference Guide

How to Use This Guide

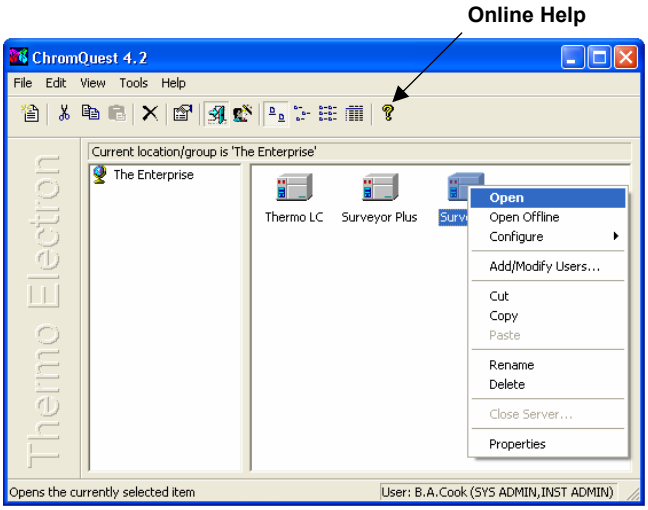
This guide contains an overview of the most common tasks that you perform in ChromQuest. For more information, see the ChromQuest Chromatography Data System User's Guide or the online Help. If you are running a Surveyor Plus system, see the Surveyor Plus Getting Started with ChromQuest manual.

Condensed instructions are included for the following key tasks:

If you are new to ChromQuest:

1. Launch ChromQuest. See the instructions in the right column of this page.
2. Open the Instrument window. See the instructions in the right column of this page.
3. Familiarize yourself with the Instrument window. See page 2.
4. Create a method that contains your instrument control parameters. Then, prepare your instrument for a run. See page 3.
5. Inject your first sample. See page 4.
6. After you acquire a preliminary run:
   - Add a custom report to your method to print a hardcopy report for each data file. See page 4.
   - Optimize the integration of your chromatogram(s). See page 4.
   - Add a Peak Table to your method for the identification and quantitation of your analytes. See page 5.
7. Create a sequence table that contains rows for your calibration standards and samples. Then, run the sequence to enter the peak responses for your analytes into the calibration table of the method and to quantitate your unknowns. See pages 5 and 6.

Main Menu Window



To Launch ChromQuest:

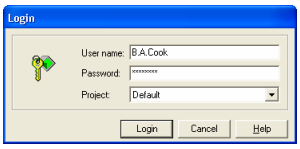
From the desktop, choose **Start > All Programs > Chromatography > ChromQuest**.

Alternatively, double-click the **ChromQuest application icon** 

ChromQuest launches and opens the Main Menu window, which is where you perform Instrument administration and System Administration functions.

To open the Instrument window:

1. From the Main Menu window, double-click the icon for your instrument  . Alternatively, right-click the icon for your instrument. Then, choose **Open** or **Open Offline** from the shortcut menu.
2. Log in. (If enabled)



See page 2

ADMINISTRATING YOUR ENTERPRISE

ChromQuest users can be given instrument administration and/or system administration privileges. Instrument administration allows you to add and configure instruments. System administration allows you to manage users and projects. To use the project management feature, you must enable logins and create at least one user. However, after you enable logins, only users with system administration privileges will be able to open the System Administration wizard and only users with instrument administration privileges will be able to add or configure instruments.

To enable System Administration:

Click the **Enterprise Login or Logout button**  to login and enable the System Administration mode.

To enable logins and project management:

1. Enable System Administration.
2. From the Main Menu menu bar, choose **Tools > Options** to display the Options dialog box.
3. Click the Enterprise tab to display the Enterprise page.
4. Select the Enable Instrument Login and Project Management checkbox.

To add users:

1. Enable System Administration.
2. From the Main Menu menu bar, choose **Tools > Options** to display the Options dialog box.
3. Click the Enterprise tab to display the Enterprise page.
4. Click **Add User** to display the User Information dialog box.
5. In the User Information dialog box, enter the appropriate information. Then, click **Save** to close the dialog box and add the user to the list of Data System Users.

To open the System Administration Wizard:

1. Enable System Administration.
2. In the Main Menu toolbar, click the **System Administration Wizard button**. 

ChromQuest opens the System Administration Wizard to the Select Administration Wizard page where you can select the User Wizard, the Instrument Wizard, or the Project Wizard.

- The User Wizard allows you to assign users access to specific instruments and projects, as well as to limit their privileges within a project.
- The Instrument Wizard allows you to limit the access of an instrument to specific users.
- The Project Wizard allows you to automate the organization of your data files, methods, sequences, and templates into project folders.

CHROM-97204 Revision A

Thermo
ELECTRON CORPORATION

FAMILIARIZING YOURSELF WITH THE INSTRUMENT WINDOW

In the Instrument window, familiarize yourself with the drop-down menus in the Menu bar, the buttons in the Command toolbar, the buttons in the Integration Events toolbar, and the shortcut menus that are accessed by right-clicking a window.

√ Tip If you cycle the power to the Surveyor AS, wait until the autosampler completes its initialization process before you open the Instrument window.

Features of the Instrument Window

Channel Selector
Lists the discrete and multi-chromatogram wavelengths that are contained in the instrument setup section of the method, as well as the scan wavelength that is currently selected, and the spectrum max plot.

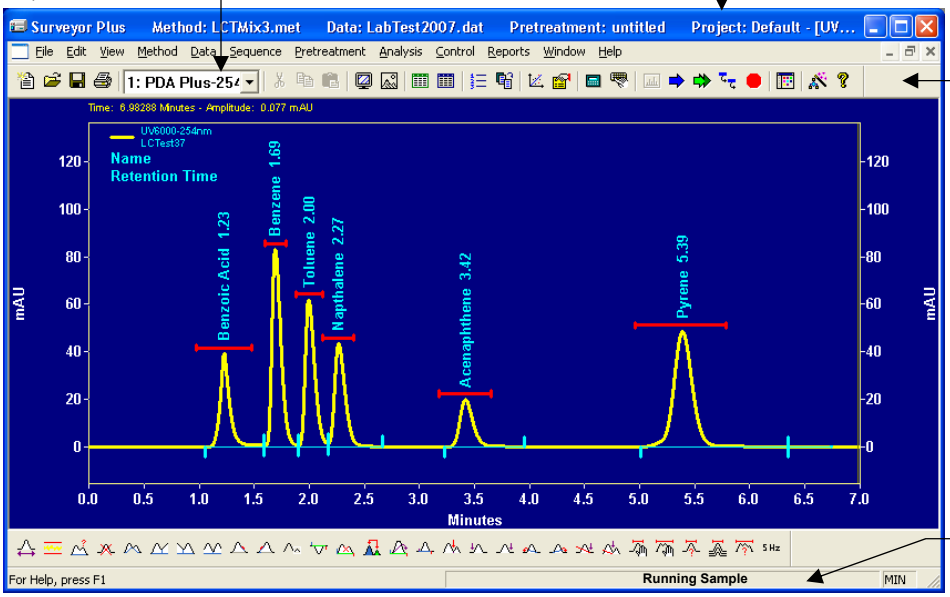
Title Bar
Lists the instrument name, the method, the data file, the pretreatment method, and the project.

Menu Bar

Command Toolbar
Contains shortcuts to the frequently used features of ChromQuest.

Drop-down Method Menu

Chromatogram Window Shortcut Menu



Integration Events Toolbar
Contains the Integration Events buttons.

Status Bar
Displays the status of the run, as well as instructions associated with the integration buttons.

Command Toolbar Buttons

Instrument Setup
Displays the Instrument Setup window in which you enter the instrument control parameters, select auxiliary traces, enter the baseline check parameters, and select a type of trigger.

Peak / Group Tables
Displays the Peak and Group tables for the detector that is currently shown in the Channel Selector list box.

Integration Events
Displays the Integration Events table for the wavelength shown in the Channel Selector list box and the method shown in the Title Bar.

Sequence Edit
Displays the Sequence table.

Sequence Process
Displays the Sequence Process dialog box.

Review Peak Calibration
Displays the Calibration window.

Edit Custom Report
Displays the custom report for the active method.

Analyze
Integrates the current data file.

Single Analysis / Calibration
Allows you to apply new sample amounts to your unknowns and enter individual calibration levels into the peak table.

Preview
Allows you to preview the baseline.

Single Run
Displays the Single Run Acquisition dialog box.

Sequence Run
Displays the Sequence Run Acquisition dialog box.

Display Run Queue
Displays the status of the sequences and single runs that have been submitted.

Stop Run
Allows you to abort the current run, the current sequence, or all items in the run queue.

Main Menu
Displays the Main Menu window in which you perform administrative tasks.

Instrument Wizard
Displays the Instrument Wizard, which guides you through the creation of methods, sequences, and sample runs.

The Method Menu

Instrument Setup Window
Allows you to do the following:

- Enter the control parameters for each of the modules in your instrument.
- Add an auxiliary trace to record the backpressure of your system during a run.
- Enter baseline check parameters if the Baseline Check option in the Configuration Options dialog box is selected.
- Select a type of trigger.

Integration Events Window
Contains the integration table(s) for your method.

Spectral Options Window
Contains the following pages: Library, Purity, Spectrum, Multi-chromatogram, and Ratio.

Peaks / Groups Window
Contains the Peak table, which is used to identify and to quantitate peaks, and the Group tables, which are used to combine peaks into groups and to calculate group totals.

Review Calibration Window
Displays the calibration table, a graphical display of the calibration points, the calibration parameters, and the regression statistics for each named peak.

Advanced Window
Contains the following pages: Export, Custom Parameters, Column / Performance, Files, and Advanced Reports.

To calculate performance parameters such as *capacity factor* and *resolution*, enter your column parameters in the Column / Performance page.

Custom Report Window
Allows you to create a report for each data file.

System Suitability Window
Allows you to enter system suitability parameters for each named peak and to perform noise and drift tests for the discrete and multi-chromatogram wavelengths in your method.

Properties Dialog Box
Contains the following pages: Description, Options, Calibration, and Audit trail.

In the Calibration page, you can do the following:

- Select the Amount / Area or the Area / Amount response factor definition.
- Select or deselect the automatic averaging of standard replicates.
- Specify the number of standard replicates in the rolling average.

CREATING A METHOD

The method contains the parameters for controlling the modules of your instrument, the parameters for identifying and quantitating your chromatographic peaks, and the parameters for determining the suitability of your system for a run. Before you can run a preliminary sample, you must create a method that contains your instrument control parameters. After you run a preliminary sample, you can graphically optimize the integration of the resulting chromatogram(s) and to you can graphically add a Peak Table for the identification and quantitation of your unknowns to the method.

To enter the Instrument Setup parameters:

To develop a new chromatographic separation, begin by entering the control parameters for your instrument:

1. From the menu bar, choose **File > Method > New**.

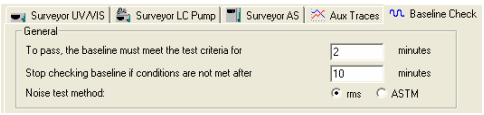
   ChromQuest opens the Instrument Setup window with the default parameters for the configured modules.

2. In the Instrument Setup window:

a. Enter the new instrument control parameters for each configured module.

b. In the Aux Traces page, select the pump pressure trace if you want to record the backpressure of your system during a run.

c. In the Baseline Check page, enter the following: the length of time for which the baseline must meet the test criteria, the maximum length of time for checking the baseline, and the test criteria.



In the example above, as soon as the baseline meets the test criteria for an interval of 2 min, the run begins. If the baseline does not meet the test criteria for 2 min within the maximum test period of 10 min, ChromQuest aborts the run or the sequence.

d. In the Trigger page, select a trigger type. Typically, the pump and detector are *externally* triggered by the autosampler.

3. Save the method by choosing **File > Method > Save AS.**

To enter the column parameters:

1. From the menu bar, choose **Method > Advanced** to display the Advanced Method Options window.
2. Then, click the **Column / Performance** tab to display the Column / Performance page.
3. Enter the following information about your column:
   - Unretained Peak Time (void volume)
   - Column Length
   - Particle Diameter
4. Select the Calculate Performance Parameters for This Channel checkbox. Then, select a Calculation Method. *This Channel* refers to the detector.
5. Save the method.

To add annotations to a trace:

After you collect a chromatogram, add annotations that will enable you to determine the performance of your chromatographic separation. These parameters typically include capacity factor, resolution, and asymmetry.

1. Right-click the Chromatogram window to access the shortcut menu.
2. Click **Annotations** to display the Trace Annotation Properties dialog box. In the Available Annotations box, double-click each annotation that you want to add to the trace (chromatogram).
3. Click **OK** to exit the dialog box.
4. Save the method.

To transfer a method:

To transfer a working method from another chromatography data system, enter the method parameters as follows:

1. From the menu bar, choose **File > Method > Method Wizard** to display the Method Wizard**.**
2. In the Method Wizard, click the **Create a Method icon**.

   ChromQuest displays the Instrument Setup window, as well as an additional toolbar at the bottom of the Instrument window.

3. Click the **Next Method Dialog button**  to move through the sections of the method. Enter the appropriate parameters in each dialog box.
4. After you have entered the contents of your method, click the **Save Method As button**  in the toolbar at the bottom of the Instrument window.

√ Tip

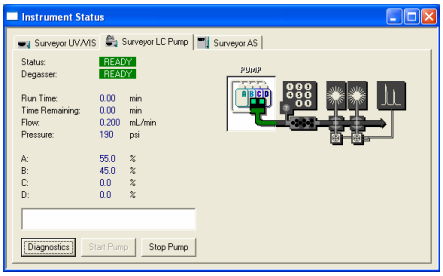
If the **Baseline Check** option in the Configuration Options dialog box is enabled, include at least one discrete channel in your scan methods.

PREPARING YOUR INSTRUMENT FOR A RUN

Before you run a sample:

- Download the method to equilibrate your column and warm-up the detector's lamps.
- Check the status of the configured modules.
- Check the volume of the solvent in your Needle Wash bottle and the volume of the solvents in the Solvent Reservoir bottles.
- Flush the syringe if it contains air or if the tubing from the Needle Wash bottle contains air.
- Preview the baseline.
- Purge the pump if the pressure is fluctuating or if the solvent lines contain air.

√ Tip 1 Bar = 14.5 psi = 0.1 MPa



To download the method:

From the menu bar, choose **Control > Download Method**.

To check the Instrument Status:

1. From the menu bar, choose **Control > Instrument Status**.
2. In the Instrument Status window, confirm that the Status readout for each of the modules of your instrument displays *Ready*, with the exception of the Status readout for the Surveyor LC Pump Plus, which displays *Pump on*, before you start a run.

To preview the baseline:

1. Click the **Preview button** 

   ChromQuest begins the baseline preview.

2. To stop previewing the baseline, click the **Stop button** 

To flush the autosampler's syringe:

1. Access the Direct Commands in ChromQuest: From the Instrument Status window, click the Surveyor AS tab to display the Surveyor AS Instrument Status page. Then, click **Diagnostics**.

   ChromQuest displays the Direct Controls page of the Diagnostics dialog box.

2. From the Direct Commands list box, select *Flush Syringe*. Enter the appropriate parameters. Then, click **Submit**.

To purge the LC pump:

1. Open the drain valve of the Surveyor LC Pump Plus by turning the drain valve knob counter-clockwise 180° to the purge position. The word DRAIN on the knob will be upside down.

2. Access the Purge group box in ChromQuest as follows: From the Instrument Status window, click the Surveyor LC Pump tab to open the Surveyor LC Pump page. Then, click **Diagnostics**.

   ChromQuest displays the Operation page, which contains the Purge group box.

3. In the Purge group box, select a solvent valve and a purge time. Then, click **Purge**.
4. After you finish flushing the solvent lines, close the drain valve by **gently** turning it clockwise as far as it will go.

Starting a Single Run

After you create a method and prepare your instrument for a run, you are ready to run a sample.

Run Information

Sample ID. The sample ID is optional.

Data File. To add an additional identifier to your data file name, click the blue arrow next to the data file text box, and then make a selection from the popup menu.

Print Method Report. To print the method custom report at the end of the run, select ☑ the Print Method Report checkbox.

Amount Values

Entries in this group box affect the quantitation of unknown run types. Quantitated peaks are divided by the Sample Amount value and the Dilution Factors values, and are multiplied by the Multiplication Factors values.

Baseline Check

To perform a noise and drift test before the autosampler injects the sample, select ☑ the Baseline Check checkbox. In addition, ensure that your method contains baseline check parameters.

Begin Run

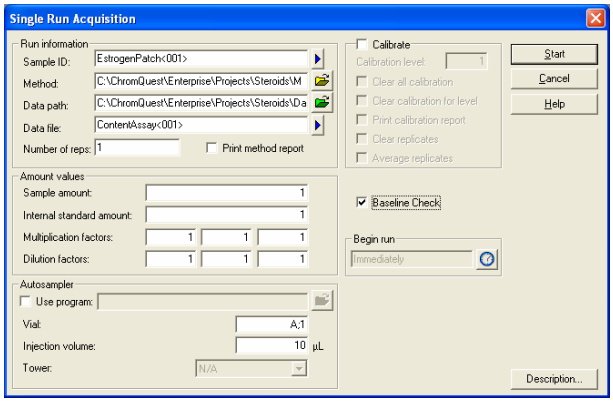
To delay the run, click the **Clock icon**  Then, select a delay time from the list.

Autosampler

Use Program. To perform a ***Pretreatment Method***, select the Use Program check box. Then, click 🗁 next to the text box to select a pretreatment method.

Vial. For the Surveyor AS, the vial locations for the standard vial types are **A;1** to **E;40**. For the AS1000 and the AS3000, the vial locations for the standard vial types are **A01** to **C40**.

Injection Volume. For the *Full Loop Injection mode*, you must match the injection volume to the configured sample loop size. For the *Partial Loop Injection mode*, inject no more than half the sample loop size. For the *No Waste injection mode*, inject at least 0.5 µL, but no more than the sample loop size less 5 µL.



To inject a single sample:

1. In the Command toolbar, click the **Single Run button**  to display the Single Run Acquisition dialog box.
2. Make the appropriate entries and selections.
3. To start the run, click **Start**.

√ Note If the requested injection volume is greater than the configured sample loop size, the run is aborted. In the *Full Loop Injection mode*, the run is aborted if the requested injection volume is not equal to the configured sample loop size.

To extend the run:

Choose **Control > Extend Run** from the menu bar.

To abort the run:

In the Command toolbar, click the **Stop button**  .

Adding a Custom Report to a Method

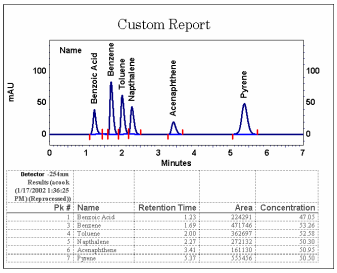
To print a report for each data file, you need to add a custom report to your method. You can add one of the four standard templates, or you can create your own custom template. After you create a custom report template, you can add it to other methods as well as the current method.

To add a Custom Report to the method:

1. Click the Edit Custom Report button  .
   If this is a new method, a blank page appears.
2. From the menu bar, choose **File > Report Template > Open** to access one of the four standard custom report templates.
   External Standard.srp
   Internal Standard.srp
   Area %.srp
   Normalization.srp
3. Save the method.

To create a new Custom Report Template:

1. In the Custom Report window, place the cursor at the desired location.
2. Right-click to display the shortcut menu.
3. Choose a menu item.
4. After you finish creating the custom report, choose **File > Report Template > Save As** from the menu bar to display the Save As dialog box.
5. Type in a name for the Custom Report Template. Then, click **Save**.
   ChromQuest adds the [.rep] extension to the file.



Pk #	Name	Retention Time	Area	Concentration
1	Benzoic Acid	1.23	224291	47.03
2	Benzene	1.69	471746	33.26
4	Toluene	2.00	362697	32.28
5	Naphthalene	2.27	272132	30.30
6	Acenaphthene	3.41	161330	30.95
7	Pyrene	5.37	553456	30.50

√ Tip

If you want the template to appear in the list that you access by choosing **Reports > View** from the menu bar, add an [.srp].

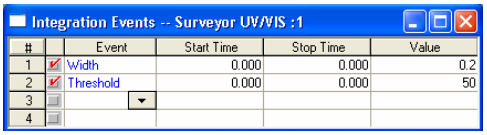
Adding Integration Events Graphically

You can optimize the integration of your chromatogram(s) by graphically adding integration events. By default, the Integration Events table for each wavelength channel contains an integration event for Width that is set to a value of 0.2 min and an integration event for Threshold that is set to a value of 50.

To graphically add integration events:

1. Use your current data file or open a stored data file.
2. From the Channel Selection list box, select a wavelength.
   Each wavelength has its own Integration table(s).
3. Click the chromatogram to activate the integration toolbar.
4. In the Integration Events toolbar, click an integration event button, and then follow the instructions shown in the status bar.
   A dialog box appears upon completion.
5. Select the Insert into Integration Events Table option button to apply the event to every data file processed with this method or select the Insert into Manual Integration Fixes Table option button to apply the event to only the current data file.
6. Click **Analyze Now** to add the event to the integration table and to apply the event to the chromatogram.
7. To review the Integration tables,
   click the **Integration Events button** 
   or the **Manual Integration Fixes button** 
   on the Command toolbar.

Note. The Integration Events tables are stored in the method file. The Manual Integration Fixes tables are stored in the data file.



#		Event	Start Time	Stop Time	Value
1	☑	Width	0.000	0.000	0.2
2	☑	Threshold	0.000	0.000	50
3					
4					

To open a stored data file:

1. Choose **File > Data > Open** from the menu bar.
   ChromQuest displays the Open Data File dialog box.
2. In the Open Data File dialog box, browse to the appropriate directory.
3. Click a data file from the list in the left pane. You can see a preview of the chromatogram(s) in the data file by clicking the **Preview button**  . You can view the file description by clicking the **Description button**  .
4. Click **Open** to open the selected data file.

ADDING A PEAK TABLE FOR IDENTIFICATION AND QUANTITATION

The peak table contains the information required to identify the peaks in the chromatogram(s), as well as the information required to build the calibration curve(s). The peak table also contains the concentration values of the check standards and the sample spikes. There is one peak table for each detector in your instrument. For multi-wavelength analyses, use the Analysis Channel column in the peak table to specify the calibration wavelength(s).

Peak / Group Tables -- PDA Plus-254nm

Named Peaks | Groups

#		Name	ID	Ret. Time	Window	Detection	Analysis Channel	Quantitate	Fit Type	Level 1	Level 2	Level 3
1	✓	Benzoic Acid	1	1.23	0.50	Ret. time	PDA Plus-254nm	Area	Linear	20	40	60
2	✓	Benzene	2	1.69	0.19	Ret. time	PDA Plus-254nm	Area	Linear	20	40	60
3	✓	Toluene	3	2.00	0.24	Ret. time	PDA Plus-254nm	Area	Linear	20	40	60
4	✓	Napthalene	4	2.27	0.29	Ret. time	PDA Plus-254nm	Area	Linear	20	40	60
5	✓	Acenaphthene	5	3.41	0.48	Ret. time	PDA Plus-254nm	Area	Linear	20	40	60
6	✓	Pyrene	6	5.37	0.83	Ret. time	PDA Plus-254nm	Area	Linear	20	40	60
7	✓											

By default, the Fit Type is Point-to-Point and the Calib Flag is Replace.

Peak Table Properties

- ☑ #
- ☑
- ☑ Name
- ☑ ID
- ☑ Ret. Time
- ☑ Window
- ☐ Ref. ID #
- ☐ ISTD. ID #
- ☐ Resolution ID #
- ☐ Units
- ☐ RT Update
- ☐ LOD
- ☐ LOQ
- ☐ Detection
- ☐ Spectrum
- ☐ Similarity
- ☑ Analysis Channel
- ☐ Quantitate
- ☑ Fit Type
- ☐ Zero
- ☑ Calib Flag
- ☐ Calib Weight
- ☐ % Calib Margin
- ☐ Scale
- ☐ Weighting Method
- ☑ 3 Levels
- ☐ STD ID #
- ☐ STD Mult.
- ☐ Manual RF
- ☐ Low Conc
- ☐ High Conc
- ☐ Check Std 1 Conc
- ☐ Check Std 1 %RD
- ☐ Check Std 2 Conc
- ☐ Check Std 2 %RD
- ☐ Check Std 3 Conc
- ☐ Check Std 3 %RD
- ☐ Check Std 4 Conc
- ☐ Check Std 4 %RD
- ☐ Check Std 5 Conc
- ☐ Check Std 5 %RD
- ☐ Spike 1 Amount
- ☐ Spike 2 Amount
- ☐ Low Spike Limit
- ☐ High Spike Limit
- ☐ Dup %RD Limit
- ☐ RF %RSD Limit

To create the Peak table:

1. Open a stored data file.
2. Click anywhere in the Chromatogram window to activate the Integration Events toolbar, and then click the **Define Peaks button**  .
3. Follow the instructions in the status bar.

   After you graphically select your peak range, ChromQuest displays the Define Peaks dialog box.
4. Make the appropriate selections in the Define Peaks dialog box.

√ Tip The Minimum Peak Area or Peak Height list box allows you to exclude peaks below the selected value from the Peak table.

5. Click **OK** to exit the dialog box.
6. Click the **Peak / Group Tables button**  to review the information in the Peak table.

To change the number of calibration levels:

1. Right-click in the Peak Tables window to display the shortcut menu.
2. Click **Properties** to display the Properties dialog box.
3. In the Properties dialog box, double-click **Levels** to display the Max # of levels text box. Type a new value into the text box. Then, press the <Enter> key.

To quantitate peaks on more than one Analysis Channel:

1. Click the peak # to highlight the entire row. Then, copy the information to a new row.
2. Click the down arrow in the Analysis Channel column. Then, select the *Analysis Channel* from the list of available wavelengths.

Note. The peak table shown above contains three concentration levels.

Before you run a set of samples…

To automatically inject a set of samples, you need to create a sequence table. To make the task easier, ChromQuest contains a Sequence Wizard. However, the Sequence Wizard does not contain all the available sequence options. You need to edit the sequence table if you want to add run types that are not available in the Sequence Wizard. After you run your sequence, you might want to modify the method, and then reprocess the data. For more information, see the following topics:

- Creating a Sequence Table Using the Sequence Wizard
- Editing a Sequence Table
- Starting a Sequence Run
- Reprocessing a Sequence

CREATING A SEQUENCE TABLE USING THE SEQUENCE WIZARD

The Sequence table contains the information that is required to automatically inject a set of samples or to reprocess a set of stored data files. ChromQuest contains a Sequence Wizard that guides you through the creation of a Sequence table.

To open the Sequence Wizard:

From the menu bar in the Instrument Window, choose **File > Sequence > Sequence Wizard.**

ChromQuest displays the Method page of the Sequence Wizard.

To create an acquisition Sequence:

1. On the Method page, select the For Acquisition option button.
2. Make the appropriate selections and entries in the Method, Unknowns, Autosampler, Calibration, and Reports pages of the Sequence Wizard.
3. After you complete your entries, click **Finish**.

   The Sequence window opens.
4. Save the Sequence table by choosing **File > Sequence > Save As** from the menu bar.

To create a sequence from existing data files:

1. On the Method page, do the following:

a. Click 🗁. Then, select a method from a ChromQuest directory.

b. Select the From Existing Data Files option button. Then, click **Next** to display the Select Files page.

2. Click 🗁 to display the Open Data Files dialog box. Then, open the ChromQuest directory that contains your data files.
3. Click the last data file that you want to reprocess, hold down the <**Shift**> key. Then, click the first data file that you want to reprocess.

   A list of the selected data files appears in the pane in the order that they will appear in the sequence table.
4. Click **Open**.
5. Click **Finish**.
6. Save the sequence.

√ Tip

In the Method page, the values entered in the Amount Values group box affect how ChromQuest reports the concentrations of the quantitated peaks in your unknowns as shown in the following equation.

$$\frac{[Unk]_C \times Multiplier\ 1 \times Multiplier\ 2 \times Multiplier\ 3}{Sample\ Amt \times Dilutor\ 1 \times Dilutor\ 2 \times Dilutor\ 3} = [Unk]_R$$

Where

$[Unk]_C$ = the concentration of the unknown determined from the calibration curve

$[Unk]_R$ = the concentration of the unknown reported by ChromQuest

Editing a Sequence Table

The Sequence Wizard allows you to create a basic Sequence table. Typical modifications to the basic sequence table include the following:

- Adding a Shutdown run type to shut down your instrument at the end of a sequence run
- Adding a Baseline Check run type to perform a baseline check at the beginning of a sequence run
- Adding an Action, such as running a shutdown if a hardware status error occurs
- Changing the Sequence Summary Template if you do not want to use the default template

Sequence: Assay.seq

Run #	Run Type	Level	Reps	Vial	Volume (µL)	Sample ID	Method	Filename	Sample Amt.	Multiplier 1	Dilutor 1	Action
1	CAL SMB CCA BLC	1	1	A;1	10	PAH001	LCTMix3.met	Cal_Assay001.dat	1	1	1	HW
2	CAL SMR	2	1	A;2	10	PAH002	LCTMix3.met	Cal_Assay002.dat	1	1	1	HW
3	CAL SMR	3	1	A;3	10	PAH003	LCTMix3.met	Cal_Assay003.dat	1	1	1	HW
4	Summary Run	0	1	A;4	10	PAH004	LCTMix3.met	Assay004.dat	20	3	5	HW
5	Summary Run	0	1	A;5	10	PAH005	LCTMix3.met	Assay005.dat	20	3	5	HW
6	Summary End	0	1	A;6	10	PAH006	LCTMix3.met	Assay006.dat	20	3	5	HW
7	Shutdown	0	1		0		Shutdown.met		1	1	1	HW

To edit the sequence:

Click the **Edit Sequence button** to open your sequence table.

You can change the run type of any row in the table. The run type options are as follows:

- Clear All Calibration
- Clear Calibration at Level
- Print Calibration Report
- Average Replicates
- Clear Replicates
- Begin Loop
- End Loop
- Shutdown
- Print Additional Reports
- Begin System Suitability
- System Suitability Standard
- End System Suitability
- Begin Summary
- Summary Run
- End Summary
- Vial Summary
- QC Check Standard
- Unspiked
- Spiked
- Spike 1 of 2
- Spike 2 of 2
- Duplicate
- Begin Calibration
- End Calibration
- Baseline Check

To minimize scrolling, you can deselect the properties that you do not need from the table. The sequence can contain the following properties:

- Run #
- Status
- Run Type
- Level
- Conc Override
- Reps
- Vial
- Volume
- Pretreatment
- Sample ID
- Method
- Filename
- Sample Amt.
- ISTD Amt.
- Multiplier 1
- Multiplier 2
- Multiplier 3
- Dilutor 1
- Dilutor 2
- Dilutor 3
- Action
- Description

To add a shutdown run type:

1. In the last row of the sequence table, double-click in the Run Type column to display the Sample Run Types dialog box.
2. Select the Shutdown run type.
3. In the Method column, click the green arrow, and then select a shutdown method.
4. Save the sequence.

To add a baseline check run type:

1. Enter the appropriate baseline check parameters in the Instrument Setup section of the method.
2. In the first row of the sequence table, double-click in the Run Type column to display the Sample Run Types dialog box.
3. Select the Baseline Check run type.
4. Save the sequence.

To add an Action:

1. If you want to perform an action for a run, click the blue arrow in the Action column to display the Action dialog box.
2. Select the tests that you want to perform.
3. For each test, select whether ChromQuest performs the action if the test passes or if the test fails. Then, select the resulting action. Some actions require additional parameters.

To change the sequence summary template:

The default template (Summary.tpl) reports the concentrations of your named peaks for the first wavelength in the Channel Selection list box.

You can access other sequence summary reports from the template directory as follows:

1. Double-click in the Run Type cell that contains the Begin Summary (SMB) run type.
2. Click the Begin Summary check box to display the contents of the Report Template text box.
3. Click to select a summary report template from the following list of templates.

   Vial Summary.tpl
   Trend.tpl
   Summary.tpl

4. Save the sequence.

√ Tip

To create your own sequence summary template:

Choose **File > Advanced Reports > New** from the Command menu bar. ChromQuest displays the Template Editor window. Click a cell in the spreadsheet. Then, click either the **Table Wizard button** or the **Function Wizard button**.

Starting a Sequence Run

To start a sequence run:

1. Click the **Sequence Run button** to open the Sequence Run dialog box.
2. Click to select a sequence file from a ChromQuest directory.
3. Select the All or the Range option button for the Run range.

   Enter a contiguous range with a dash (1-10). Enter a non-contiguous range with a comma (1-10,20-30).

   If you selected a section of the sequence before you opened the Sequence Run dialog box, notice that ChromQuest has automatically selected the ⊙ Selection option button.

4. Select a processing mode from the Processing Mode list box.

   For HPLC systems, select *Normal*. For systems that contain an HS2000 or an HS850, select *Full Download*.

5. Select a type of bracketing from the Bracketing list box.
6. To print the custom report for each data file, select ☑ the Print Method Reports checkbox. To print the sequence reports, such as the Sequence Summary report and the System Suitability report, select ☑ the Print Sequence Reports checkbox.
7. Click **Start**.

ChromQuest 4.2
Sequence Summary Report

Sequence name:	Test Mix Sequence
Analyst	B.A.Cook
PDA Plus - 254 nm	Toluene
Data Filename	ESTD
CalTestMix001.dat	1.00
CalTestMix002.dat	2.00
CalTestMix003.dat	3.00
TestMix001.dat	2.03
TestMix002.dat	2.04
TestMix003.dat	1.99
Min:	1.00
Max:	3.00
Mean:	2.01
Std Dev:	0.58
%RSD	28.75

Reprocessing a Sequence

To reprocess a sequence:

1. Click the **Process a Sequence button**.
2. Click to select a sequence file from a ChromQuest directory.
3. Select the All or the Range option button.
4. Select a processing mode from the Processing Mode list box.

   Use Stored Results shows the original results.
   Use Last Results shows the most recent results.
   Reintegrate recalculates the results.
   Review Only displays the results on the screen.

5. Select a type of bracketing from the Bracketing list box.
6. Select the Review Results check box to pause the processing after each data file. Click the green up and down arrows ⇧⇩ to move through the rows of the sequence.
7. To print the custom report for each data file, select ☑ the Print Method Reports checkbox. To print the sequence reports, select ☑ the Print Sequence Reports checkbox.
8. Click **Start**.
9. Click the **Review Peaks Calibration button** to review the calibration curve.