

ChromQuest 5.0 Quick Reference Guide

This guide contains an overview of the ChromQuest™ chromatography data system, with topics organized by workflow. For more information, refer to the *ChromQuest User Guide*, the manuals for the liquid or gas chromatography instruments, and the Help provided with ChromQuest. The manuals are provided as PDFs on the ChromQuest installation CD.

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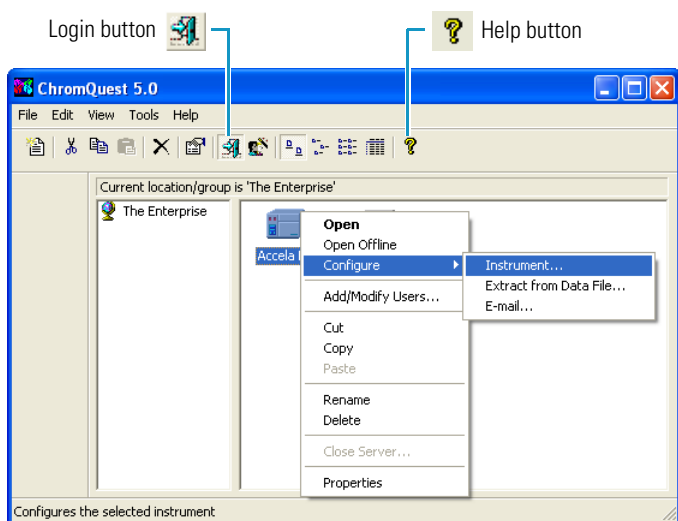
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Launching ChromQuest

❖ To launch ChromQuest or ChromQuest SI

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

For ChromQuest, the Main Menu window appears. Use this window to configure instruments and administrate ChromQuest.



For ChromQuest SI, the Instrument window appears (see page 2).

Adding and Configuring Instruments

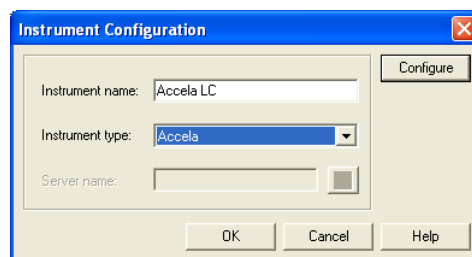
❖ To add an instrument to the Enterprise

Right-click **The Enterprise** and choose **New Instrument**.

❖ To configure an instrument


1. Do one of the following:
 - In ChromQuest, right-click the instrument icon and choose **Configure > Instrument**.
 - In ChromQuest SI, choose **Start > All Programs > Chromatography > ChromQuest SI Config**. In the ChromQuest SI Configuration dialog box, click **Instrument Configuration**.

The Instrument Configuration dialog box appears.



2. In the Instrument name box, type a name for the instrument.
3. In the Instrument type list, for a new instrument, select the instrument type.

Because selecting an instrument type erases the current instrument configuration, do not select the instrument type to modify the configuration options for an existing instrument.

4. Click **Configure**. The instrument dialog box appears.
5. In the Available modules list, double-click the icons for the instrument modules. The icons appear in the Configured modules list.
6. For PDA detectors, do the following:
 - a. In the Available modules list, double-click the **Detector** icon. The Analog icon appears in the Configured modules list.
 - b. Double-click the **Analog** icon. The Detector Configuration dialog box appears.
 - c. In the Detector model list, select **PDA** or **PDA Plus**.
 - d. Click .



Do not change the Stack number unless you are controlling more than one PDA from the same computer. The Stack number must match the rotary switch setting on the back panel of the instrument.

- e. Click **OK** to exit the PDA Plus dialog box. Click **OK** to exit the Detector Configuration dialog box.
7. To complete the configuration of each device, refer to the Help provided with ChromQuest.
 8. Click **OK** to save the configuration settings and close the instrument dialog box.

Administrating ChromQuest


You can limit access to specific tasks by assigning instrument and system administration privileges. Users with instrument administration privileges can add and configure instruments. Users with system administration privileges can manage users and projects.

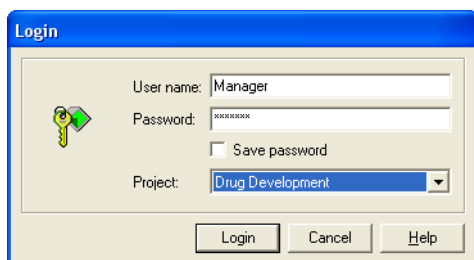
❖ To enable logins and project management

1. In the Main Menu toolbar, click  to log in and enable the System Administration mode.
2. In the menu bar, choose **Tools > Options**.
3. In the Options dialog box, click the **Enterprise** tab.
4. On the Enterprise page, select the **Enable Instrument Login and Project Management** check box.
5. Click **Add User**. The User Information dialog box appears.
6. Enter the appropriate information, and then click **Save** to add the user to the Data System Users list and close the dialog box.
7. In the toolbar, click . The System Administration wizard appears.
8. Use these wizards to create projects and assign privileges:
 - To assign users access to instruments and projects and privileges within a project, select the User Wizard.
 - To assign access to instruments, select the Instrument Wizard.
 - To create project folders for data files, methods, sequences, and templates, select the Project Wizard.

Opening the Instrument Window



❖ To open the Instrument window















1. In the Main Menu window, do one of the following:
 - Double-click the icon for your instrument .
 - Right-click the icon for your instrument and choose **Open** or **Open Offline**.
2. Log in and select a project in the Project list, if enabled. The project folder becomes the default location for data files, methods, sequence, and template files.

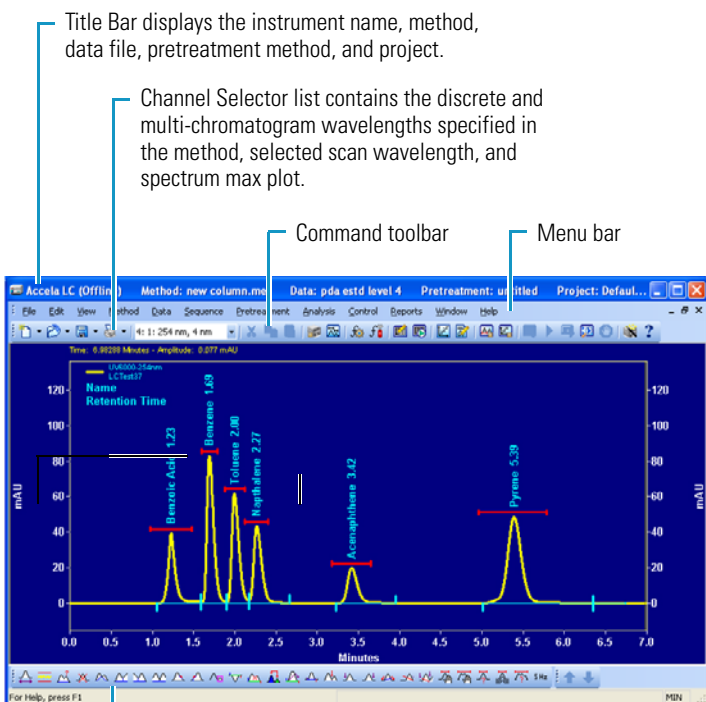


For ChromQuest SI, from the computer desktop, choose **Start > All Programs > Chromatography > ChromQuest SI**.

The Instrument window appears. Familiarize yourself with the menus, Command toolbar buttons, Integration Events toolbar buttons, and shortcut menus accessed by right-clicking the window.

Button	Tooltip	Use
	Instrument Setup	Opens the Instrument Setup window where you specify the instrument parameters, auxiliary traces, baseline check parameters, and trigger type.
	Peak/Group Tables	Opens the Peak and Group tables for the detector currently shown in the Channel Selector list.

Button	Tooltip	Use
	Integration Events	Opens the Integration Events table for the current method and the wavelength displayed in the Channel Selector list.
	Manual Integration Fixes	Opens the Integration Events table for the current data file and the wavelength displayed in the Channel Selector list.
	Sequence Edit	Opens the sequence table.
	Sequence Process	Opens the Sequence Process dialog box.
	Review Peak Calibration	Opens the Calibration window.
	Edit Custom Report	Opens the custom report for the active method.
	Analyze	Integrates the current data file.
	Single Analysis/Calibration	Applies sample amounts to the unknowns and enters calibration levels into the peak table.
	Preview	Starts a preview of the baseline.
	Single Run	Opens the Single Run Acquisition dialog box.
	Sequence Run	Opens the Sequence Run Acquisition dialog box.
	Display Run Queue	Displays the status of the submitted sequences and single runs.
	Stop Run	Stops the current run, the current sequence, or all items in the run queue.
	Instrument Wizard	Guides you through the creation of methods, sequences, and sample runs.



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

Channel Selector list contains the discrete and multi-chromatogram wavelengths specified in the method, selected scan wavelength, and spectrum max plot.

Command toolbar

Menu bar

Integration Events toolbar contains the Integration Events buttons.

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

Creating a Method





The method contains instrument control, peak identification, calibration, and system suitability parameters. To acquire data, the method must include the chromatographic conditions, such as the mobile phase composition, flow rate, analysis wavelengths, and injection type, as well as the trigger type.

❖ To develop a new chromatographic method

To add the chromatographic conditions for your application to the method, use the New Method template.

1. In the Instrument window, choose **File > Method > New**. The Instrument Setup window appears with the default parameters for the configured modules.
2. Specify the control parameters for each configured module.
3. (Optional) On the Aux Traces page, select the pump pressure trace to record the backpressure of the LC system during a run.
4. On the Trigger page, select a trigger type (typically **External**—the autosampler triggers the start of data acquisition).
5. Choose **File > Method > Save As** to save the method.

❖ To transfer an existing method created with another data system

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 . The Instrument Setup window appears with an additional toolbar () at the bottom of the window.
3. Click  to move through the sections of the method. Enter the appropriate parameters in each dialog box.
4. After you enter the contents of your method, click the **Save Method As** button  at the bottom of the window.

❖ To create a shutdown method for a Surveyor or SpectraSYSTEM LC

1. Open the Instrument Setup window.
2. On the detector page, clear the lamp check boxes and select the **Shutdown method** check box.
3. On the pump page, set the flow rate to zero and select the **Shutdown method** check box.
4. Save the method and use it at the end of a sequence to turn off the detector lamps and mobile phase flow.

Tip The Accela Pump does not support shutdown methods. To turn off the mobile phase flow at the end of a sequence run, select the **Stop after the end** in the Method Finalizing list.

Adding Column Specifications to a Method

To calculate the suitability of a chromatographic run, add information about the chromatographic column to the method.

❖ To specify the column parameters

1. From the Instrument window, open the method.
2. Choose **Method > Advanced**.
3. In the Advanced Method Options window, click the **Column / Performance** tab. The Column/Performance page appears.
4. Specify the following information about the column: unretained peak time (void volume), column length, and particle diameter.
5. Select the **Calculate Performance Parameters for This Channel** check box. Channel is the detector, not the analysis wavelength.
6. Select a Calculation Method.
7. Save the method.

Preparing the Instrument for a Run

For best results, make sure that your chromatographic system is ready before running samples.



❖ 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, before you start a run, confirm that the Status readout for each module displays **Ready**, with the exception of the Status readout for the Surveyor LC Pump Plus, which displays **Pump on**.

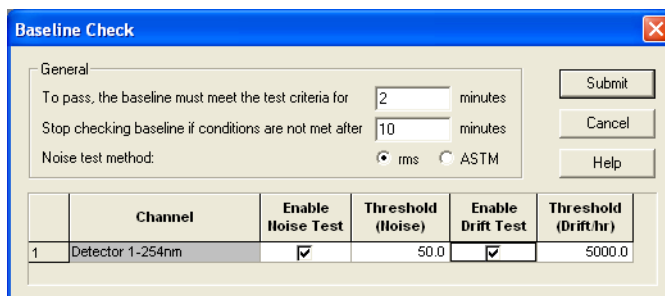
❖ To preview the baseline

1. Click the **Preview** button . The baseline preview starts.
2. To stop the baseline preview, click the **Stop** button .

❖ To perform a baseline check

1. In the Instrument window, choose **Control > Baseline Check**.
2. On the Baseline Check page, enter the following:
 - The length of time the baseline must meet the test criteria
 - The maximum length of time for checking the baseline
 - The test criteria

In the following example, as soon as the baseline meets the test criteria for an interval of 2 minutes, the run begins. If the baseline does not meet the criteria for 2 minutes within the maximum test period of 10 minutes, the run stops.






	Channel	Enable Noise Test	Threshold (Noise)	Enable Drift Test	Threshold (Drift/hr)
1	Detector 1-254nm	<input checked="" type="checkbox"/>	50.0	<input checked="" type="checkbox"/>	5000.0

Tip For scans, include at least one multi-chromatogram channel in the method.

Starting a Single Run

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

❖ To inject a single sample

1. Load the sample into the autosampler.
2. In the Command toolbar, click .
3. In the Single Run Acquisition dialog box, make the appropriate entries and selections. See the parameters table on [page 4](#).
4. To delay the start of the run, click  and select a time from the list.
5. To start the run, click **Start**.
6. To extend the run, choose **Control > Extend Run**.
7. To stop the run, click .

Run information area

Calibrate area

Amount values area

Autosampler area

Begin run area

Baseline check area

Parameter	Description
Run information area	
Sample ID	(Optional)
Method	Contains the information required to acquire and process data files.
Data path	Location where ChromQuest stores the data files.
Data file	The name of the data file. Clicking the blue arrow opens a list of unique identifiers, such as increment number.
Number of reps	Specifies the number of times the current sample is to be injected. To make one injection, use the default value of 1.
Print method report	Select this check box to print the custom report.

Amount values area
For most runs, use the default values of 1. If the method contains a calibration curve, enter multiplication factors and dilution factors to calculate the original sample concentration or amount.

$$\frac{[\text{Unk}]_C \times \text{mult factor } 1 \times \text{mult factor } 2 \times \text{mult factor } 3}{\text{sample amount} \times \text{dilution } 1 \times \text{dilution } 2 \times \text{dilution } 3} = [\text{Unk}]_R$$

$[\text{Unk}]_C$ = the concn of the unknown determined from the calibration curve
 $[\text{Unk}]_R$ = the concn of the unknown reported by ChromQuest

Autosampler area	
Use program	Clear the Use program check box unless you want the autosampler to perform a pretreatment method before it makes an injection.
Vial	The location from which the autosampler withdraws the sample. For the Surveyor or Accela Autosamplers, the allowable values are A;1 to E;40 (for vials), A;A1 to C;H12 (for 96-well plates), and A;A1 to C;P24 (for 384-well plates). For the AS3000, the allowable values are A1 to E40.
Injection volume	For partial loop and no waste injections, this is the volume that the autosampler meters into the sample loop. ChromQuest does not allow injection volumes greater than the configured sample loop size. The method specifies the injection type.

Calculate area
Use this option to inject the calibration standards one at a time.

Baseline check option
Use this option to delay an injection until the baseline stabilizes.

Begin run area
Use this feature to delay the start of the run.

Adding Annotations to a Chromatogram

Annotations include information about the chromatographic peaks such as the peak names and retention times. ChromQuest adds the peak name annotation after you create a peak table with the peak names and expected retention times.

❖ To add annotations to a trace

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

Adding a Custom Report to a Method

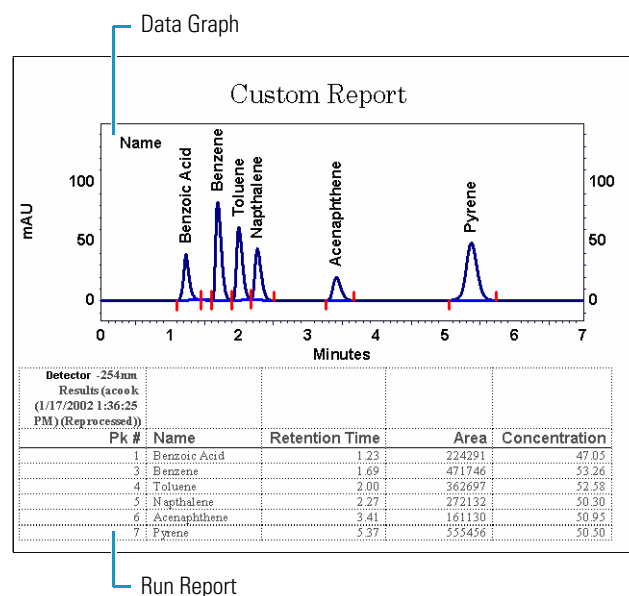
To print a report for each data file, add a custom report to the method. You can add one of the four standard templates, or you can create your own custom template.

❖ To add a custom report to the method

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

❖ To create a new custom report template

1. In the Custom Report window, place the cursor where you want the item to appear.
2. Right-click and choose an item from the shortcut menu.
3. After you finish adding items, choose **File > Report Template > Save As**. The Save As dialog box appears.
4. Type a name for the Custom Report template and click **Save**. ChromQuest adds the .srp extension to the file. To make the template appear in the Reports list, add an .srp extension.



Adding Integration Events Graphically

You can optimize the integration of your chromatograms by graphically adding integration events. By default, the Integration Events table for each wavelength channel contains the Width integration event set to a value of 0.2 minutes and the Threshold integration event set to a value of 50.

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

❖ To graphically add integration events

1. Use your current data file or open a stored data file.
2. From the Channel Selector list, select a wavelength. Each wavelength has its own Integration Events and Manual Integration Fixes tables.
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. To apply the event to every data file processed with this method, select the **Insert into Integration Events Table** option. Or to apply the event to only the current data file, select the **Insert into Manual Integration Fixes Table** option.
6. To add the event to the integration table and to apply the event to the chromatogram, click **Analyze Now**.
7. To review the Integration tables, click or .

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

❖ To open a stored data file

1. In the Instrument window, choose **File > Data > Open**. The Open Data File dialog box appears.
2. Browse to the appropriate directory.
3. Select a data file from the list in the left pane.
4. (Optional) Click to see a preview of the chromatograms in the data file. Click to view the file description.
5. Click **Open**. The Chromatogram view for the wavelength displayed in the Channel Selector list appears. When the data file contains spectral data, the Mixed View appears.

Identifying and Quantitating Analytes

The peak table contains the information required to identify the chromatographic peaks and build the calibration curves for the analytes. It also contains the concentrations of the check standards and sample spikes. There is one peak table for each detector of your instrument. For multi-wavelength analyses, use the Analysis Channel column in the peak table to specify the calibration wavelengths.

#	Name	ID	Ret. Time	Window	Detection	Analysis Channel	Quantitate	Fit Type	Level 1	Level 2	Level 3
1	Benzoic Acid		1.23	0.50 Ret. time		PDA Plus-254nm	Area	Linear	20	40	60
2	Benzonitrile		1.89	0.19 Ret. time		PDA Plus-254nm	Area	Linear	20	40	60
3	Toluene		2.00	0.24 Ret. time		PDA Plus-254nm	Area	Linear	20	40	60
4	Naphthalene		2.27	0.29 Ret. time		PDA Plus-254nm	Area	Linear	20	40	60
5	Acenaphthene		3.41	0.40 Ret. time		PDA Plus-254nm	Area	Linear	20	40	60
6	Pyrene		5.37	0.83 Ret. time		PDA Plus-254nm	Area	Linear	20	40	60
7											

❖ To create the peak table

1. Open a stored data file.
2. In the Integration Events toolbar, click .
3. Follow the instructions in the status bar. After you graphically select the peak range, the Define Peaks dialog box appears.
4. Make the appropriate selections. Use the Minimum Peak Area or Peak Height list to exclude peaks below the selected value from the Peak table.
5. Click **OK** to exit the dialog box.
6. Click to review the information in the peak table.

❖ To change the number of calibration levels

1. Right-click the Peak Tables window and choose **Properties**.
2. In the Properties dialog box, double-click **Levels** to display the Max # of levels box.
3. Type a new value in the box, and then press the ENTER key.

❖ To quantitate peaks on more than one Analysis Channel

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

Creating a Sequence

A sequence table contains the information required to automatically inject a set of samples or to reprocess a set of stored data files. The Sequence Wizard helps you create a basic sequence table.

❖ To open the Sequence Wizard

In the Instrument window, choose **File > Sequence > Sequence Wizard**.

❖ To create an acquisition sequence

1. On the Method page, select the **For Acquisition** option.
2. Make the appropriate selections and entries on the Method, Unknowns, Autosampler, Calibration, and Reports pages of the Sequence Wizard.
3. After you complete your entries, click **Finish**. The Sequence window appears with the sequence table.

Run #	Run Type	Level	Vial	Volume (µL)	Method	Filename
1	CAL SMB CCA	1	A:1	10	multilevel calibration.met	multi calibration level 1.dat
2	CAL SMR	2	A:2	10	multilevel calibration.met	multi calibration level 2.dat
3	CAL CAE SMR	3	A:3	10	multilevel calibration.met	multi calibration level 3.dat
4	Summary Run	0	A:4	10	multilevel calibration.met	multi calibration level 4.dat
5	Summary Run	0	A:5	10	multilevel calibration.met	multi calibration level 5.dat
6	Summary Run	0	A:6	10	multilevel calibration.met	multi calibration level 6.dat

4. Choose **File > Sequence > Save As** to save the sequence.

❖ To create a sequence from existing data files


1. On the Method page, do the following:
 - a. Click and select a method.
 - b. Select the **From Existing Data Files** option, and then click **Next** to display the Select Files page.
2. Click to display the **Open Data Files** dialog box, and then browse to the folder that contains the data files.
3. To create an ordered list of data files, select a data file and click **Add** for each data file that you want to reprocess. The data file appears in the Data File list at the bottom of the dialog box.
4. Click **Open**. The Select Files page appears.
5. Check the list of data files and click **Finish**.
6. Save the sequence.

Editing a Sequence Table

Use the Sequence Wizard to create a basic sequence table. Edit the sequence table to do the following:

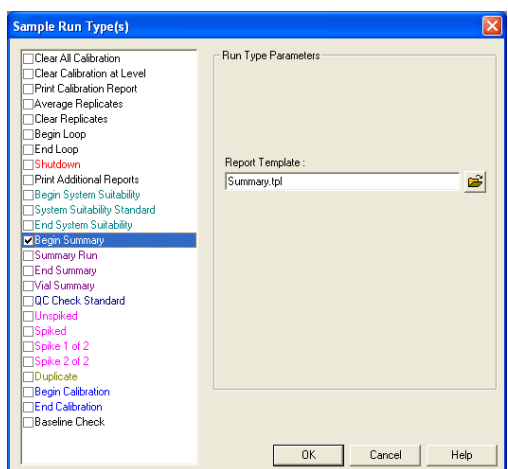
- Add a Baseline Check run type to the first row of the sequence.
- Add a Shutdown run type to the last row of the sequence.
- Add an Action, such as running a shutdown if a hardware status error occurs.
- Change the Sequence Summary template.

❖ To edit the sequence


1. Click . The sequence table appears. You can modify the sample run types for any row in the table.

❖ To modify the run type selections

1. Double-click the Run Type column in the appropriate row of the sequence. The Sample Run Types dialog box appears.



2. Select the check box for the run type of interest. You can select multiple run types for each sequence row. Make additional selections as necessary:

- To add a baseline check run type, double-click the Run Type column in the first row of the sequence table and select the **Baseline Check** check box.
- To add a shutdown run type, double-click the Run Type column in the last row of the sequence table and select the **Shutdown** check box. In the Method column, select a shutdown method.
- To change the sequence summary template, double-click the Run Type cell that contains the Begin Summary (SMB) run type. Select the **Begin Summary** check box to display the contents of the Report Template box. Click  to browse for and select a summary report template.

3. Save the sequence.

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

Sequence Summary Report



Sequence name: multilevel 3.seq
Analyst: System

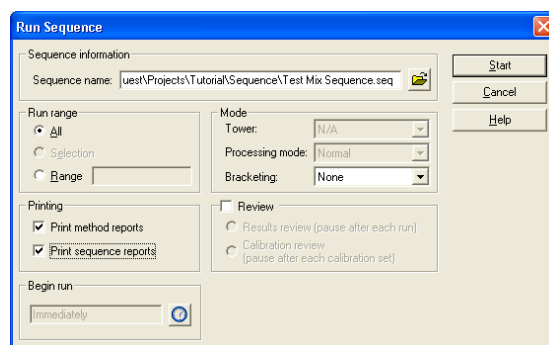
Channel A	Peak1	Peak2	Peak3	Peak4
Data Filename	ESTD	ESTD	ESTD	ESTD
multi calibration level 1. dat	10.00	5.00	15.00	10.00
multi calibration level 2. dat	20.00	6.00	20.00	20.00
multi calibration level 3. dat	30.00	7.00	25.00	30.00
multi calibration level 4. dat	39.76	0.00	0.00	0.00
multi calibration level 5. dat	50.00	9.00	35.00	50.00
multi calibration level 6. dat	51.95	9.18	36.22	51.56

For information on creating a custom summary report template, refer to the ChromQuest Help.

Starting a Sequence Run






❖ To start a sequence run

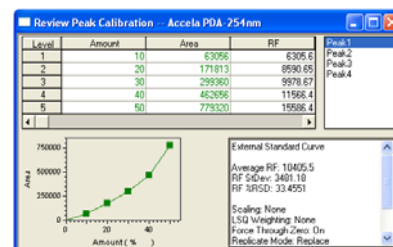
1. Click  to open the Sequence Run dialog box.
2. Click  to browse for and select a sequence file.
3. Select the **All** or the **Range** option for the Run range. Enter a contiguous range with a dash, as in 1-10. Enter a non-contiguous range with a comma, as in 1-10,20-30.
4. Select a processing mode from the Processing Mode list.
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.
6. To print the custom report for each data file, select the **Print Method Reports** check box. To print the sequence reports, such as the Sequence Summary report and the System Suitability report, select the **Print Sequence Reports** check box.
7. Click **Start**.



Reprocessing a Sequence

❖ To reprocess a sequence

1. Click . The Sequence Process dialog box appears.
2. Click  to browse for and select a sequence file.
3. Select the **All** or the **Range** option.
4. Select a processing mode from the Processing Mode list:
 - Use Stored Results shows the original results.
 - Use Last Results shows the most recent results.
 - Reintegrate recalculates the results.
 - Review Only displays the results in the Instrument window.
5. Select a type of bracketing from the Bracketing list.
6. Select the **Review Results** check box to pause the processing after each data file. Click the blue up and down arrows   to move through the sequence rows.
7. To print the custom report for each data file, select the **Print Method Reports** check box. To print the sequence reports, select the **Print Sequence Reports** check box.
8. Click **Start**.
9. To review the calibration curve, click .



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