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 on the blue arrow next to the data file text box, and then make a selection from the popup menu. Add the .dat extension to the file name to distinguish its file type.

Print Method Report. If you want to print the method custom report at the end of the run, select ☑ the Print Method Report check box.

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 multiplied by the Multiplication Factors values.

Baseline Check

If you want to perform a noise and drift test before the autosampler injects the sample, select ☑ the Baseline Check check box. In addition, make sure that your method contains baseline check parameters.

Begin Run

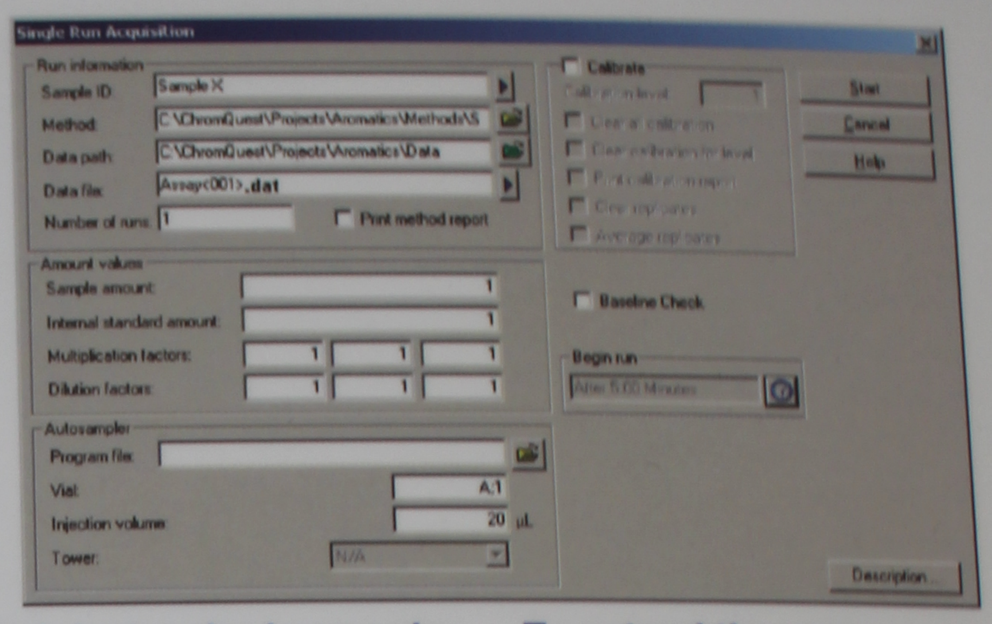
If you want to delay the run, click on the **Clock icon**, and then select a delay time from the list.

Autosampler

Program File. To select a ***Pretreatment Method***, click on next to the Program File text box. If you do not want to perform a pretreatment method, make sure that the Program File list box is empty.

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*, match the injection volume to the 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. The maximum injection volume for the no waste injection mode is 5 µL less than the sample loop size.



To inject a single sample:

1. In the Command toolbar, click on 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 on **Start**.

To extend the run:

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

To abort the run:

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

Adding a Custom Report to a Method

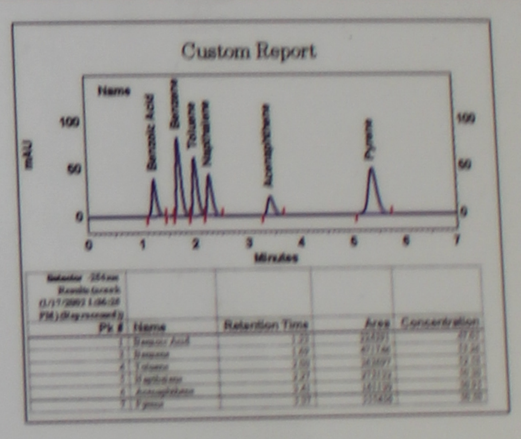
To print a report for each data file, you need to add a custom report to your method. You can add one of the four standard templates, or you can create your own custom template. After you create a custom report template, you can add it to other methods as well as the current method.

To add a Custom Report to the method:

1. Click on 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 on **Save**.
   ChromQuest adds the [.rep] extension to the file.



✓ 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] extension to the file name.

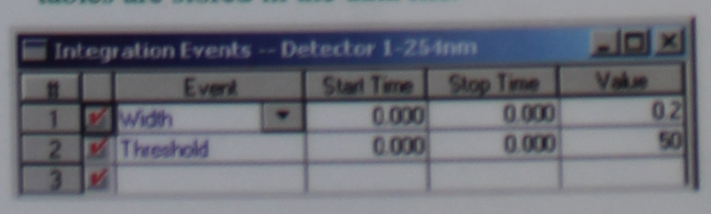
Adding Integration Events Graphically

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 on the chromatogram to activate the integration toolbar.
4. In the Integration Events toolbar, click on 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 on **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 on 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.



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, select a directory to look in.
3. Click on 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 on the **Preview button**, or you can view the file description by clicking on the **Description button**.
4. Click on **Open** to open the selected data file.