

Agilent G2070BA GC ChemStation

Familiarization Guide



Notices

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In This Guide

This guide contains a step-by-step exercise to help you become familiar with your Agilent G2070BA GC ChemStation software used with the Agilent 7890A GC. Revisions covered by this manual includes B.04.03.

To successfully complete this exercise, you need the following:

Agilent G2070BA GC ChemStation software

• Agilent 7890A GC with:

GC Inlet: Split/Splitless Inlet with EPC

(default inlet configuration)

Column: HP-5 30 m × 320 μ m × 0.25 μ m

Sample: P/N 5188- 5372

Detector: FID

ALS Agilent 7693 or 7683 automatic liquid

sampler (Optional)

Before operating your instrument, be sure to read all safety and regulatory information included with the instrument.

1 Startup the System

This chapter includes a startup checklist for instrument readiness.

2 Create a Method for Qualitative Analysis

This chapter describes how to the method is created by uploading the GC method parameters from the GC and saving. It also describes how to create an acquisition method that will be used to identify the compounds in an Agilent standard sample.

3 Run a Single Sample

This chapter describes how a sample is prepared for data acquisition. The ALS is loaded with the sample, the solvent wash vial, and a solvent waste vial. Finally, the sample is run and the logbook, showing the actions taken during the run, is reviewed.

4 Qualitative Data Analysis

This chapter explains how to set up data analysis options, modify integration results, perform manual interactive integration of peaks, print area percent reports, and edit the data analysis part of the method.

5 Create and Run a Sequence

This chapter describes how to create a sequence and acquire data for the calibration samples which are used in the next chapter to update the calibration curve.

6 Create a Calibration Method

This chapter describes how to setup a calibration table with compounds and calibrators to identify unknown samples. This new calibration table is then used with a reprocessing sequence to report on the quantity of compounds found in these samples.

7 Easy Sequence

This chapter describes how to use a template based sequence creation system to create a recalibration sequence that fits into a daily workflow requiring re-calibrations before processing samples.

8 Create a Maintenance Method

This chapter describes how to create and store a method to use for instrument shutdown and maintenance tasks. Using this type of method helps prevent damage to the instrument electronics and columns, and avoid injuries such as burns or shocks.

Where to Find Information

Hardware

In addition to this document, Agilent provides several learning products that document how to install, operate, maintain, and troubleshoot Agilent instruments. This information can be found on the Agilent Technologies GC and GC/MS Hardware User Information and Utilities DVDs that ship with your instrument.



Included on these DVDs is an extensive collection of localized online help, videos, and books for current Agilent gas chromatographs, mass selective detectors, ion traps, and GC samplers including:

- · Getting Familiar documentation
- Safety and Regulatory guides
- Site Preparation checklists
- Installation information
- · Operating guides
- Maintenance information
- · Troubleshooting details

Software

For more information on the G2070BA GC ChemStation in addition to this book, refer to the on-line help.

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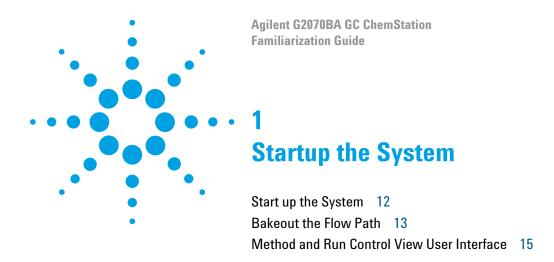
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In this chapter, a startup checklist is reviewed for instrument readiness. The GC's analysis flow path is baked out. The Agilent ChemStation is started and a brief description of the user interface is given.

Start up the System

This procedure starts with the GC turned off and all hardware previously configured. Items requiring a possible change in configuration to suit a particular method are addressed here. These include the column, gas types used in pneumatic controllers, inlet liners and O-ring, and septums.

- 1 Review the Agilent 7890A Gas Chromatograph Safety manual (P/N G3430-90013) and Agilent 7890A Gas Chromatograph Operating manual (P/N G3430-90010) for important safety information and start up details before powering on your instrument.
- **2** Gather the following:
 - Evaluation column, HP- 5 30 m x 0.32 mm x 0.25 μ m (19091J- 413)
 - FID performance evaluation (checkout) sample (PN 5188- 5372)
 - Chromatographic- grade iso-octane
 - 4- mL solvent and waste bottles or equivalent for autoinjector
 - 2- mL sample vials or equivalent for sample
- **3** Verify the following:
 - Capillary column jet installed. If not, select and install a capillary column jet.
 - Capillary column adapter installed (adaptable FID only).
 If not, install it.
 - Chromatographic- grade gases plumbed and configured: helium as carrier gas, nitrogen, hydrogen, and air.
 - Empty waste vials loaded in sample turret.
 - 4-mL solvent vial with diffusion cap filled with iso-octane and inserted in Solvent A injector position.
- 4 Verify that the split/splitless (S/SL) inlet septum, liner, and O-ring are clean, properly installed, and in good condition. See the procedure in the 7890A Maintenance manual (G3430-90010).
- 5 Install a conditioned (HP-5 30 m x 320 μ m x 0.25 μ m) column in the GC. Attach the column inlet to the S/SL inlet and its outlet to the FID. See the procedure in the 7890A Maintenance manual (G3430-90010).
- 6 Verify that the He carrier gas line valve is open and the carrier gas is attached to the GC inlet flow module.

- 7 Verify that the H2, makeup gas, and air gas line valves are open and these lines are attached to the GC FID module.
- **8** Verify that the GC is connected to a grounded power source.
- **9** Power on the 7890A GC.
- 10 To specify the column configuration, from the GC keypad press [Config][Col 1] (or [Config][Col 2]).

The column dimensions are located on a metal tag located on the column basket.

- a Scroll to the **Length** line, type the column length, in meters, followed by [**Enter**].
- **b** Scroll to **Diameter**, type the column inside diameter in microns, followed by [**Enter**].
- **c** Scroll to **Film thickness**, type the film thickness in microns, followed by [**Enter**]. The column is now defined.
- d Scroll to Inlet. Press [Mode/Type] to select a gas pressure control device for this end of the column. Select the front or back inlet location with the split/splitless inlet and press [Enter].
- e Scroll to **Outlet**. Press [**Mode/Type**] to select a gas pressure control device for this end of the column. Select the front or back detector location with the FID and press [**Enter**].
- f Scroll to Thermal zone. Press [Mode/Type] to see the available choices. Select the GC Oven and press [Enter].
- 11 To specify carrier gas flow to the column, from the GC keypad, press [Col 1] (or [Col 2]).
 - a Scroll to Mode. Press [Mode/Type], select Constant Flow and press [Enter].
 - b Scroll to Velocity and enter 30 to set the column velocity to $30~\rm cm/s$. The Pressure and Flow values are calculated and displayed by the GC.

Bakeout the Flow Path

- 1 Purge the column with carrier flow for at least 20 minutes before heating the column. The HP-5 column in our example has a maximum temperature of 325 °C. Do not exceed the maximum temperature noted on your column.
- **2** To set up the inlet temperature and flow:
 - a From the GC keypad, press [Front Inlet] (or [Back Inlet] if the Split/Splitless is located there) and with Temperature selected press [On/Yes] and enter 300 °C or 25 °C above

- the normal operating temperature, to turn on the inlet heater and set its temperature.
- b Press [Up Arrow] to select Mode and press [Mode/Type] to select Split mode and press [Enter].
- c Press [Down Arrow] to select Pressure and press [On/Yes] to open the carrier gas control valve.
- d Press [Down Arrow] twice to select Split flow, enter
 200 mL/min and press [Enter]. Split ratio will be calculated for you.
- 3 To set the column temperature from the GC keypad, press [Oven] and with Temperature selected press [On/Yes] and enter 225 °C, or 25 °C above the GC method final oven temperature. This turns on the oven heater and set its temperature. Do not exceed the column manufacturer's maximum temperature limit.
- **4** To set up the FID:
 - a From the GC keypad, press [Front Det] (or [Back Det] if the FID is located there) and with Temperature selected press [On/Yes] and enter 325 for the detector Temperature to turn on the detector heater and set its temperature to 325 °C.
 - b Press [Down Arrow] to select H2 Flow and press [On/Yes] and enter 30 mL/min.
 - c Press [Down Arrow] to select Air Flow and press [On/Yes] and enter 400 mL/min.
 - d Press [Down Arrow] to select Makeup and press [On/Yes] and enter 25 mL/min.
 - e Press [Down Arrow] to select Flame and press [On/Yes] to ignite the flame.
 - f To check the FID baseline output, press [Down Arrow] to view the Output. It should be between 5 pA and 20 pA and relatively stable. (If using a gas generator or ultra pure gas, the signal may stabilize below 5 pA.) If the output is outside this range or unstable, resolve this problem before continuing.
 - **q** If the output is too low:
 - Check that the electrometer is on.
 - Check that the flame is lit.
- **5** Bakeout the flow path for a minimum of 30 minutes.

Method and Run Control View User Interface

- 1 Power on the PC and log into Windows.
- 2 From the Windows start icon, click **All Programs**, click **Agilent ChemStation**, then click the on-line ChemStation program for your instrument.

The ChemStation user interface is displayed. Click the **Method and Run Control** button located in the left pane at the bottom, to display the ChemStation **Method and Run Control** view, if that view is not displayed.

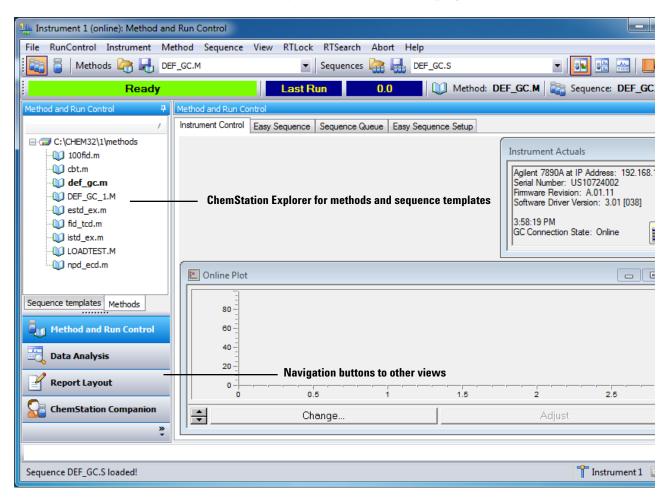


Figure 1 Method and Run Control view user interface

The **ChemStation Explorer** allows for easy access to specific files (e.g. methods and sequences in **Method and Run Control** view) and fast access to other ChemStation views.

1 Startup the System

The ChemStation user interface is displayed as views that group software functionality according to typical analytical tasks. The following three standard views are present in all software configurations:

- the Method and Run Control view for controlling and acquiring data from the instrument
- the **Data Analysis** view for reviewing and reevaluating data that has been acquired
- the Report Layout view for designing specific report layouts

The **Data Analysis** view extends the standard toolbar to specific data analysis modes including integration, calibration, reporting, annotation, and signal comparison. These separate data analysis modes are supported with a mode-specific toolset.

The **Report Layout** view allows you to graphically define the layout of a specific report style. It also uses a set of toolbars specific to this task.

The **ChemStation Explorer** is used to navigate through sequences, methods, and data files. Use the **Navigation Buttons** to switch the ChemStation Views.

Configure Method and Run Control Views

The Instrument Control tab in the Method and Run Control view displays several view components that assist in monitoring the instrument. You select these components from the View menu. Figure 2 shows where to select these view components listed on the menu as Online Signals, Instrument Actuals, Sampling Diagram, GC Instrument Diagram, ChemStation Status, and Logbook.

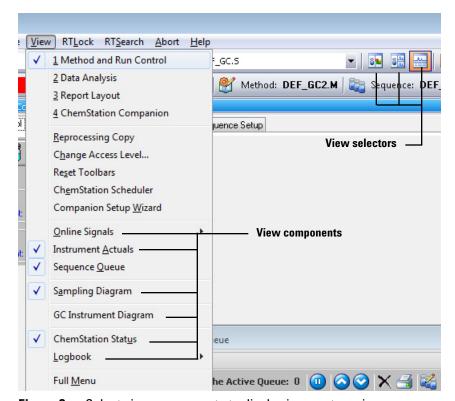
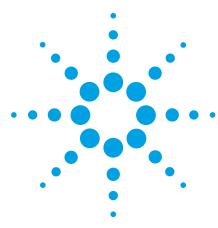


Figure 2 Select view components to display in a custom view

The view selectors shown in Figure 2 allow you to store 3 different groupings of these view components. First click on a view selector icon to display the group of UI components on the **Instrument Control** tab selected for that icon. Next you can select additional (unchecked) view components from the **View** menu or select an existing view component (checked) to remove it from the **Instrument Control** tab. Likewise you can configure the other two view selector icon to display different component groupings.

1 Startup the System





Create a Method for Qualitative Analysis

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This chapter describes how to create an acquisition method that will be used to identify all compounds in an Agilent standard sample.

Introduction

The acquisition method presented in this chapter will be used to find the known compounds in the Agilent sample PN 5188-5372. The sample compounds are contained in a iso-octane solvent as shown in Table 1. Three 0.5 mL ampules are included.

 Table 1
 Sample compound list

Compound	Concentration in iso-octane	
n-Tridecane	2.36 mg/L	
n-Tetradecane	2.36 mg/L	
n-Penta-decane	23.6 mg/L	
n-Hexadecane	23.6 mg/L	

The data acquisition parameters used in this method are taken from the FID performance section in the Chromatographic Checkout chapter of the *Agilent 7890A Gas Chromatograph Advanced User Guide* (G3430-90015). If your inlet and detector are different than the Split/Splitless - FID setup used in our example, find your detector and inlet in the Chromatographic Checkout chapter of this manual and use the parameters found there for good separation of these sample compounds.

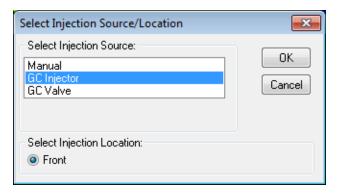
Edit the Entire Method

With on-line session connected to the 7890A, upload the current method from the GC and Save with a new Method Name such as default.m or first connect.m.

- 1 Click the **Method** menu then click **Edit Entire Method**..., to create the method. The **Edit Method** dialog box opens.
- 2 Mark the Method Information and Instrument/Acquisition checkboxes only. Clear the Data Analysis and Run Time Checklist checkbox.

The **Data Analysis** part of the method will be updated after the run.

- 3 Select **OK** to close the **Edit Method** dialog box. If **Method Information** was selected, the **Method Information** dialog box opens.
- 4 In the **Method Comments** field, enter a description of this method.
- 5 Select **OK** to close the **Method Information** dialog box and display the **Select Injection Source/Location** dialog box.



- **6** From the **Select Injection Source** dropdown list, select your source. Only configured injector sources are listed.
 - If you are injecting from the GC using the Automatic Liquid Sampler (ALS), select GC Injector.
 - If you are manually injecting select **Manual**.
 - If using a valve select **GC valve**. The GC used for this example does not have valves installed.
- 7 In the **Select Injection Location** area, select an injection location of **Front**, **Back**, or **Dual**.
- 8 Select **OK** to close the **Select Injection Source/Location** dialog box and display the **Setup Method** window.

Check the GC configuration

- 1 Select the **Configuration** button, ______ to specify pressure units, configure a column, and specify gas types for pressure and flow controllers associated with detectors, inlets, and auxiliary devices.
- With the Miscellaneous tab selected, select the Pressure Units type. Under Valve Configuration set up valves if installed or set all Valve Types to Not Installed. Review the online help for an explanation of Slow fan and Thermal Aux Type.

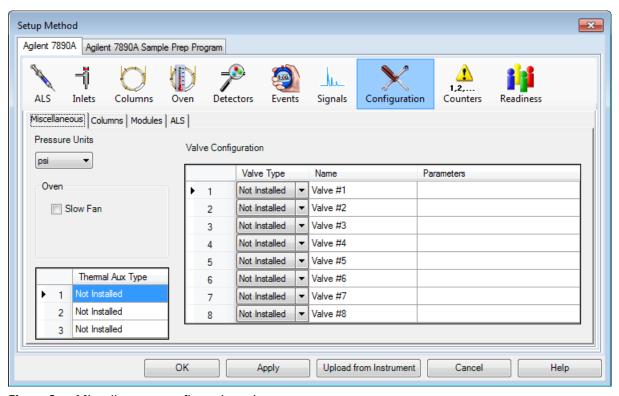


Figure 3 Miscellaneous configuration tab

Table 2 lists a description of the **Setup Method** window buttons.

 Table 2
 Setup method window buttons

Button	Action		
Apply	Downloads any settings that have been changed to the GC.		
ОК	Downloads any settings that have been changed to the GC and closes the Setup Method window.		
Upload from Instrument	If setpoints are changed via the keyboard, they can be uploaded to the ChemStation.		
Cancel	Discards any settings that have been changed and closes the Setup Method window.		
Help	Displays help topics for the current parameter.		

3 Select the Columns tab to display the column configuration parameters. The HP-5 checkout column is listed in the Column position 1.

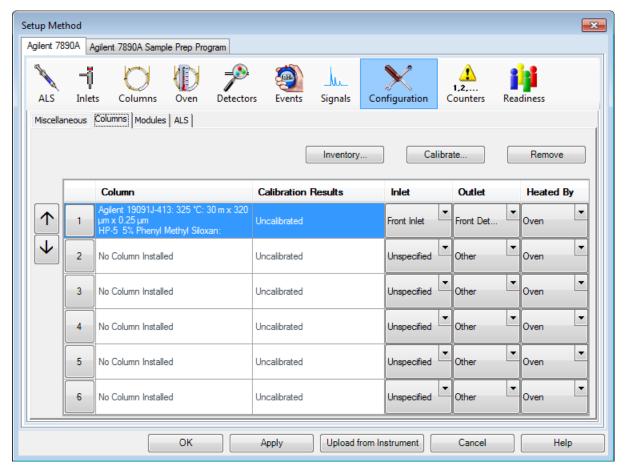


Figure 4 Columns configuration tab

- 4 If the HP-5 is not listed under **Column**, or another column will be used, click the **Inventory** button and add it to inventory before listing it here. See "Add a column to ChemStation local inventory" on page 36.
- 5 Use the up and down arrow keys to move the HP-5 column into one of the six column positions. The column is generally installed in the 1 position.
- **6** For the **Inlet** pressure for this column, select the location of the Split/Splitless inlet from the dropdown.
- 7 For the column **Outlet** pressure select the FID location.
- 8 For the column **Heated By** select **Oven** from the dropdown.
- 9 Click the **Apply** button and select the **Modules** tab.

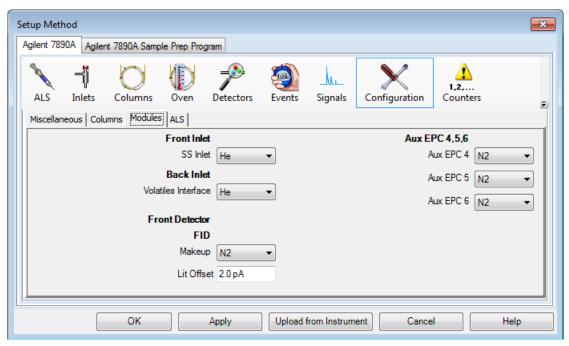


Figure 5 Modules configuration tab

- 10 Select He or H_2 as the carrier gas from the dropdown for the inlet connected to column 1.
- 11 Select He or N_2 as the Makeup gas from the dropdown for the Front Detector.
- 12 Click the Apply button and select the ALS tab.

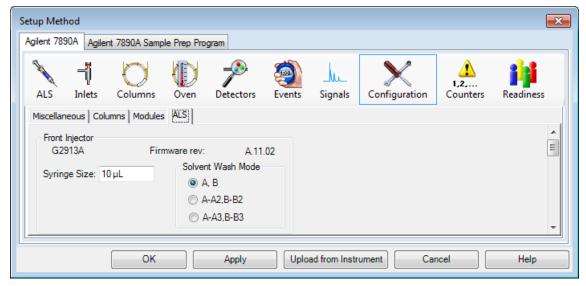


Figure 6 ALS configuration tab

13 Enter a Syringe Size of $10 \mu L$.

14 Select a Solvent Wash Mode of A, B.

The other **Solvent Wash Mode** options, **A-A2**, **B-B2** and **A-A3**, **B-B3**, are used with sequences.

15 Click the **Apply** button to download any edits to the GC.

Set the GC readiness state

The 7890 GC readiness state is reached when all GC parameters specified here are within their method specified setpoints. This Readiness requirement can also be set from the 7890A GC keypad.



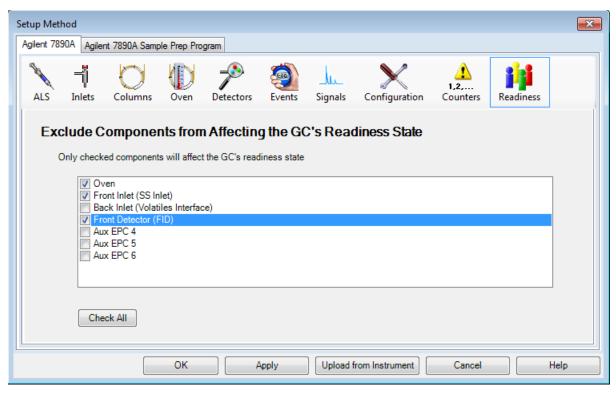


Figure 7 Readiness state component selection

- 2 Select the **Oven**, **Front Inlet** and **Front Detector** (both attached to column 1). These selections require the GC to wait until all setpoints related to the oven, inlet, and detector are held at a steady value before allowing a run to begin.
- 3 Click **Apply** to download these selections to the GC.

Set the GC oven parameters



1 Select the **Oven** button, displayed.

The **Oven** parameters are

For this example, the FID Checkout Oven program is used.

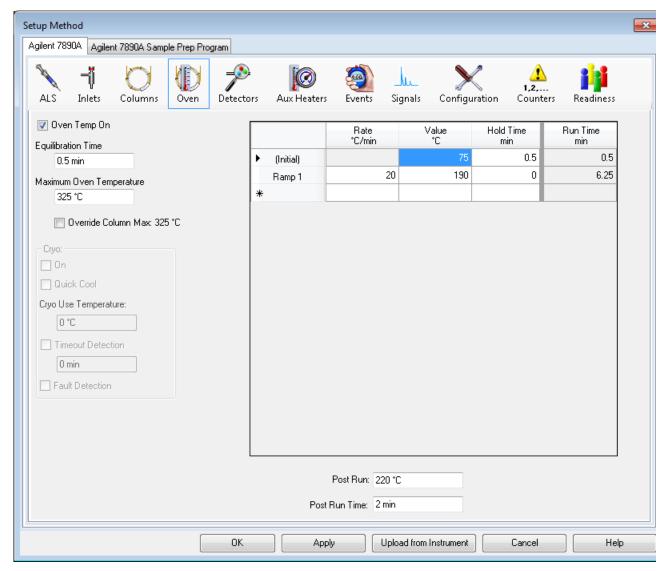


Figure 8 GC oven parameters

- 2 Mark the Oven Temp On checkbox.
- 3 In the **Equilibration Time** field, enter 0.5 min to shorten the default time of 3 min.
- 4 In the **Maximum Oven Temperature** field, enter 325 °C. This is the maximum temperature for the HP-5 column.
- 5 Clear the Override Column Max. 325 °C checkbox.

6 In the **Oven Ramp** table, enter the settings shown in Table 3.

Table 3 Oven ramp settings

Oven Ramp	Rate	Value	Hold Time
	°C/min	°C	min
(Initial)		75	0.5
Ramp 1	20	190	0

- 7 In the **Post Run** field, enter 220 °C.
- 8 In the **Post Run Time** field, enter 2 min to hold the 220 °C oven temperature for 2 minutes after the run is finished.
- **9** Select **Apply** to download these settings to the GC.

Set the GC column parameters



- Select the **Columns** button, . The **Column** parameters are displayed
- 2 Check the Column information in the **Selection** list.
 - Column: 19091J-413 (HP-5 30 m x 320 μ m x 0.25 μ m)
 - In: front or back (split/splitless inlet position)
 - Out: FID
- 3 Mark the Control Mode checkbox.
- 4 Select **Flow** in the Control Mode area.
- 5 In the Flow Setpoint field, enter 6.5 mL/min. The Pressure, Average Velocity, and Holdup Time Setpoints are calculated and displayed in the corresponding fields.
- **6** Select **Apply** to download these settings to the GC.

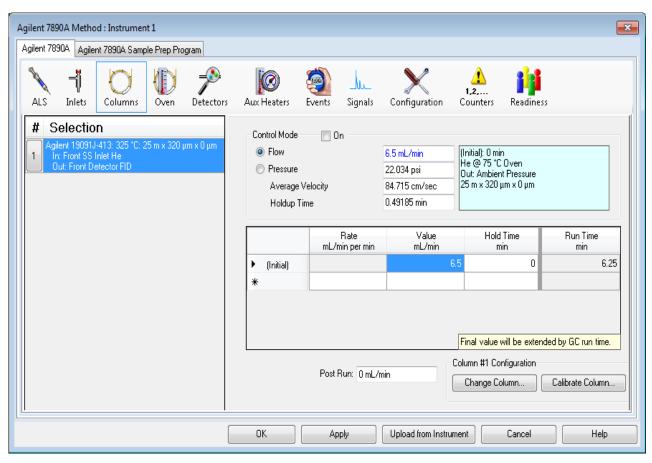


Figure 9 GC columns parameters

Set the GC inlet parameters

1 Select the **Inlets** button, . The **Inlet** parameters are displayed.

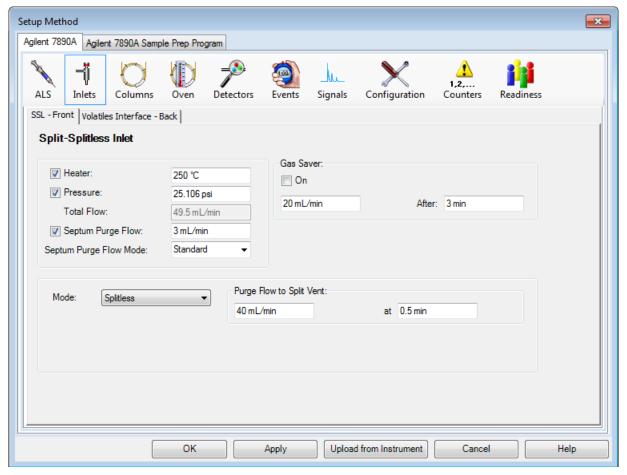


Figure 10 GC inlet parameters

- 2 Select the **front** or **back** tab, depending on your hardware configuration.
- 3 Mark the **Heater** checkbox and enter **250** °C in the corresponding **Setpoint** field.
- 4 Mark the **Pressure** checkbox. The **psi** in the corresponding **Setpoint** field is automatically set when the column flow rate is set.
- 5 Mark the **Septum Purge Flow** checkbox and enter **3 mL/min** in the corresponding **Setpoint** field.
- 6 From the **Septum Purge Flow Mode** drop down list, select **Standard**.

Gas Saver reduces the carrier gas flow rate from the split vent after a sample is within the column. The program maintains column head pressure and flow rate while purge and split vent flow rates are decreased. See online help for details. In general, start Gas Saver after inlet purge time for splitless injection or 2 minutes after a split injection. Reduced flow rates continue until the next run. To use Gas Saver, select it and enter:

- The reduced split vent flow rate you want (in mL/min)
- The time, in minutes, when flow rate is to decrease after a run has started

Keep Gas Saver 15 mL/min above the maximum column flow rate during the run.

- 7 In the **Mode** area select **Splitless**.
- 8 In the Purge Flow to Split vent area:
 - a In the field, enter 40 mL/min.
 - **b** In the **at** field, enter 0.5.
- 9 Select Apply.

Set the GC injector parameters

If you are not using the autosampler, skip this section.



- 1 Select the **ALS** button,
- 2 Select the **Front Injector**, **Back Injector**, or **Dual** tab, depending on your hardware configuration.
- 3 In the **Injection** area:
 - a Verify that the 10 μL Syringe Size matches your hardware configuration.
 - **b** In the **Injection Volume** field, enter 1.
- 4 In the Washes and Pumps area:
 - a For Solvent A Washes, enter 5 in the Postlnj field.
 - **b** For **Sample Washes**, enter 3 in the **Prelnj** field.
 - c For Sample Pumps, enter 5 in the Prelnj field.
- 5 Select the **Advanced** button, . Additional options are displayed in the window.
- 6 In the Plunger Speed area, select Fast.
- 7 Select Apply.

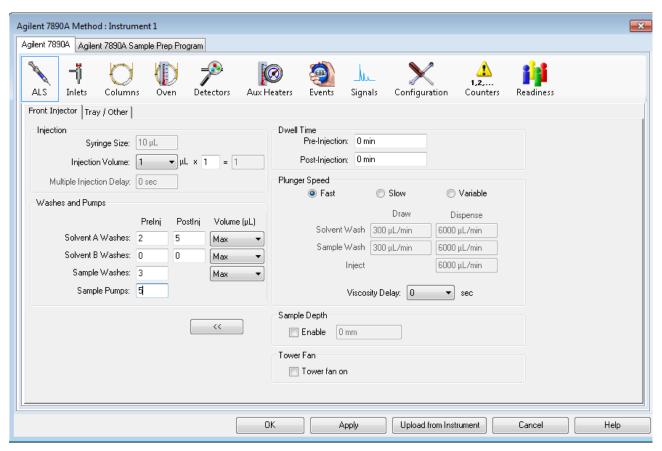


Figure 11 ALS parameters

Set the GC detector



- 1 Select the **Detectors** button,
- 2 Select the **Heater** checkbox and enter **300** for the heater setpoint.
- 3 Select the **H2 Flow** checkbox and enter **30** mL/min for the **H2 Flow** setpoint.
- 4 Select the Air Flow checkbox and enter 400 mL/min for the Air Flow setpoint.
- 5 Select the **Makeup Flow** checkbox and enter **25** mL/min for the **Makeup Flow** setpoint.
- 6 Select the **Flame** checkbox to ignite the flame. When igniting the flame, the detector will attempt ignition several times.
- 7 Select Apply.



Figure 12 Detector parameters

Set the GC signals parameters



- I Select the **Signals** button, Signals .
- 2 From the Signal Source dropdown list, select Front (or Back) Signal (FID) for the signal source.

When using multiple detectors you may assign specific signals to both the Front Signals and the Back Signals. See the online help for configuration instructions.

- 3 For the Data Rate / Min peak Width select 20 Hz/.01 min from the dropdown menu.
- 4 In the **Signal Source** dropdown list, select **None** for the other signal sources.

2 Create a Method for Qualitative Analysis

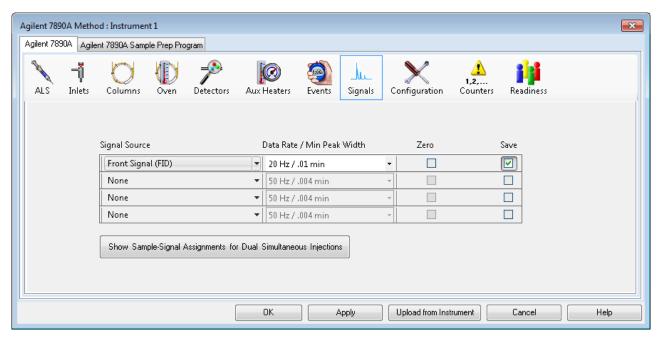


Figure 13 GC signals parameters

Select **OK** to download the selected parameters to the GC and close the **Setup Method** window.

Save the method

- 1 From the **Method** menu select **Save Method As** to display the **Save Method As** dialog.
- 2 Enter checkout.M in the **Method File** field.
- 3 Click **OK** to save the current ChemStation method as **checkout.m** method.

If the Method Audit Trail is enabled you are prompted to enter an Audit Trail comment. Enter a comment and click **OK** to close the dialog.

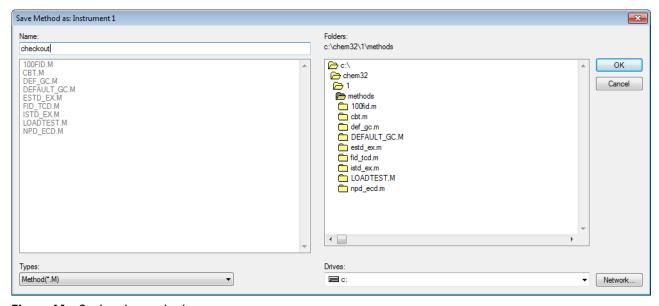


Figure 14 Saving the method

General Information for Editing the GC Parameters

Open the GC edit parameters window

- 1 From the **Instrument** menu select **Edit Agilent 7890 Parameters** to display the **Setup Method** window. See Figure 8 on page 27.
- 2 When a parameter button at the top of the screen is selected, the button is highlighted in blue and the settings for that parameter are displayed in the right panel. The GC instrument status is shown in the left panel.

Add a column to ChemStation local inventory

1 Select the **Configuration** icon to display the columns configured for the instrument.

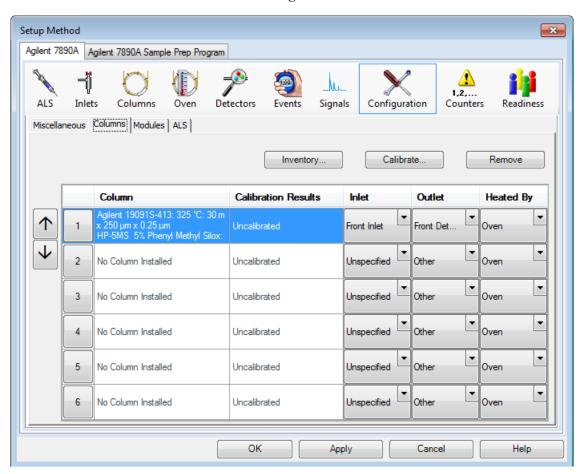


Figure 15 Columns configured for the instrument

2 Click **Inventory** to display the **Install Column 1** dialog box containing a list of columns in local inventory.

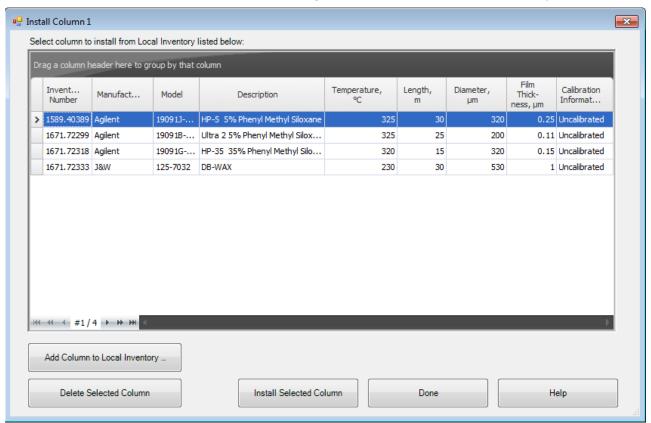
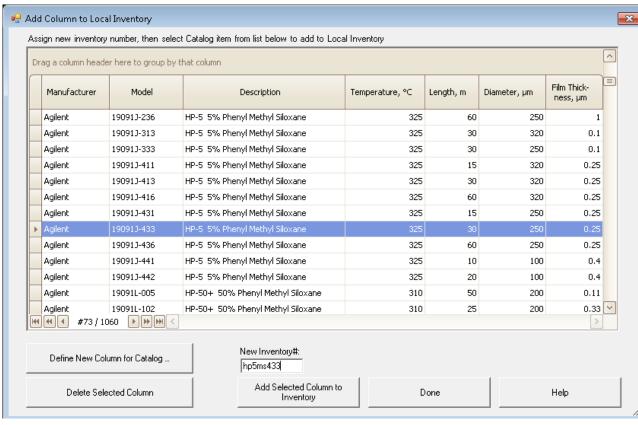


Figure 16 The local inventory of columns



3 Click Add Column to Local Inventory to display the Add Column to Local Inventory dialog box.

Figure 17 The catalog of columns

- 4 Scroll down the list of columns to model number 19091J-433 and enter the column serial number hp5ms433 as the New Inventory# or select the default. The column serial number is found on the column tag.
- 5 Click Add Selected Column to Inventory to display the Install Column 1 dialog box with the selected column now added to the local inventory list.



Figure 18 Local inventory with the added column

Columns added to local inventory can be quickly added and configured for the instrument. See "Select and configure a column" on page 39.

Select and configure a column

This example selects a column previously added to local column inventory and configures it as column number 1. See "Add a column to ChemStation local inventory" on page 36.

1 Select the **Configuration** icon and click on the **Column** description for column 1 to select it. The column number selected here will be replaced with the column we are adding.

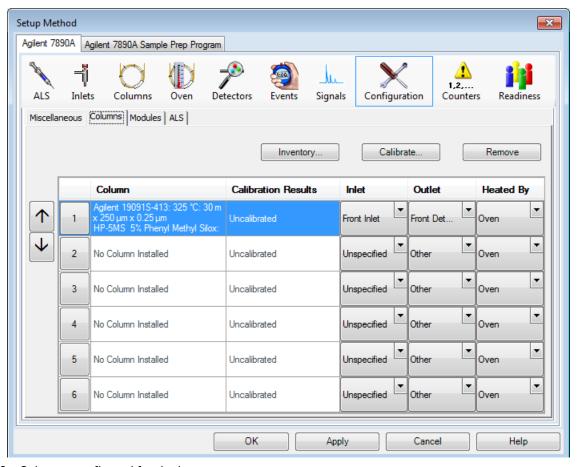


Figure 19 Columns configured for the instrument

2 Click **Inventory** to display the **Install Column 1** dialog box containing a list of columns in local inventory.

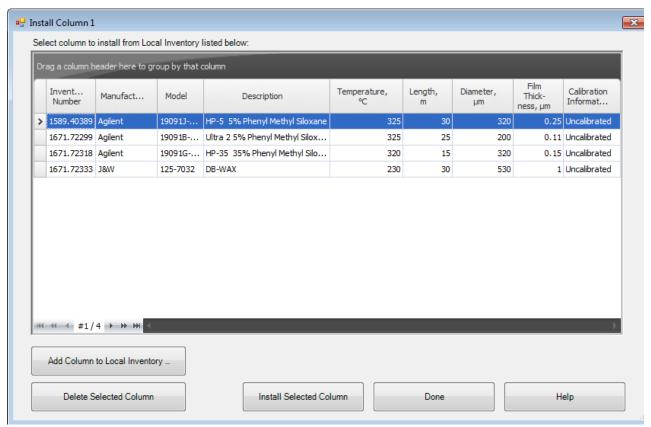


Figure 20 The local inventory of columns

3 Select a column from the local inventory list and click **Install Selected Column** to display the **Configuration** panel for **Setup Method** with the selected column replacing the previously configured column 1 for the instrument.

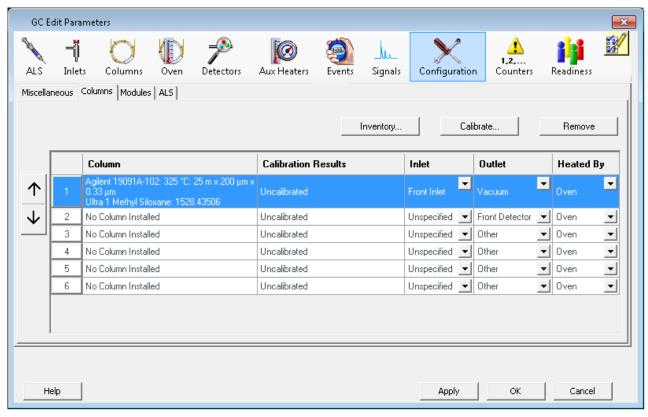


Figure 21 Columns configured for the instrument

- 4 Under the **Inlet** heading dropdown, select the item the column inlet is attached to.
- 5 Under the **Outlet** heading dropdown, select the item the column outlet is attached to.
- 6 Under the **Heated By** heading dropdown, select the method for controlling the column temperature.

Change a column directly from the Setup Method Columns dialog

- 1 From the **Setup Method** dialog with the **Columns** icon selected (Figure 9 on page 29), click **Change Column** to display the **Edit Properties of Installed GC Column** dialog.
- 2 You can specify a column by setting the parameters in the dialog and clicking **OK** or optionally you can replace the column selected for the current method with one specified in inventory.
- To select a column from inventory, click **Replace with Inventory** to display the **Install Column 1** dialog (Figure 20 on page 40).

4 Select a column from the local inventory list and click **Install Selected Column** to display the **Setup Method** for **Columns** dialog with the selected column replacing the previously configured column 1 for the instrument.

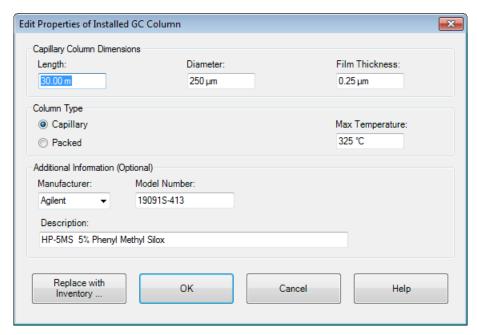


Figure 22 Edit properties of installed GC column

Upload parameters from the 7890A GC

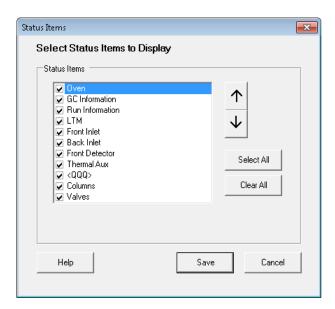
From the **GC Edit Parameter** dialog, right mouse click in the right panel and select **Upload Method from GC**.

Also, from the main menu you can select Instrument > Upload Method from Agilent 7890A.

Customize the status panel view

1 In the status panel, select the **Setup Actuals** button, the **Status Items** dialog box opens.





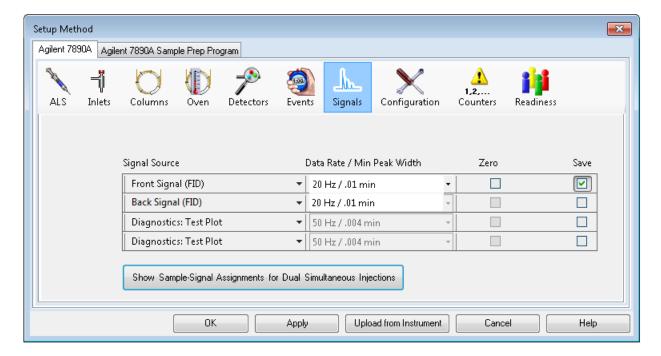
- 2 Mark the checkboxes of the items in the **Status Item** list that you want to have displayed in the status panel.
- 3 To move an item up or down in the displayed list, select the item and then the up or down arrow buttons until it is in the desired position.
- 4 Select **Save** to save the settings and return to the **GC Edit Parameters** window.

Assigning Signals with Dual Simultaneous Injections

Dual Simultaneous Injections require a front and back inlet to make the simultaneous injections. They also require a Front and Back detector for analysis of these analytical streams. These analytical streams can be further spit to enter two or more detectors. A procedure is required for assigning each of these signals to the front or back signal location.

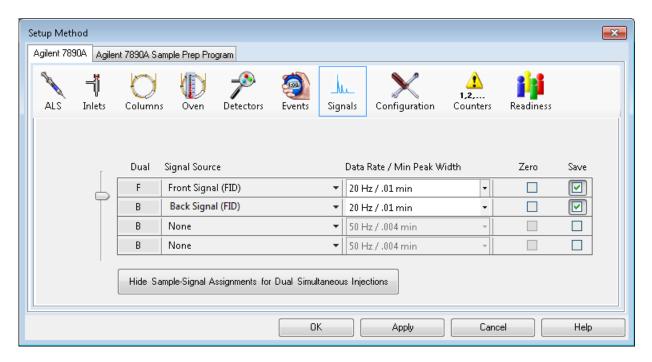
Signal Assignments for Dual Simultaneous Injections

1 From the **Setup Method** dialog, click on the **Signals** icon.



- 2 For the first item in the table, select a **Signal Source** associated with the front inlet from the dropdown menu.
- **3** For the next item in the table, select a **Signal Source** associated with the back inlet from the dropdown menu.
- 4 For each detector **Signal Source** entered in the table, enter a **Data Rate/Min Peak Width**.
- 5 Select **Zero** for each signal you wish to zero at the start of the run.
- **6** Save the data for each signal by selecting the **Save** checkbox.
- 7 If you disable the **Save** feature, data from the signal can be plotted on the online plot, but will not be stored for analysis.

8 Click Show Signal Assignments for Dual Simultaneous Injections to display a Dual column and slider selector on the left side of the table.



- 9 Move the slider to display F in the Dual column of all Signal Sources associated with the front inlet. The other Signal Sources are associated with the back inlet.
- 10 Click **Apply** to download these setting to the GC.
- 11 Save the method.

2 Create a Method for Qualitative Analysis





Run a Single Sample

Prepare the Sample 48
Load the Method 48
Complete the Run Time Checklist 49
Run the Method 50
View the Current Logbook File 51
View the Log of the Run 52

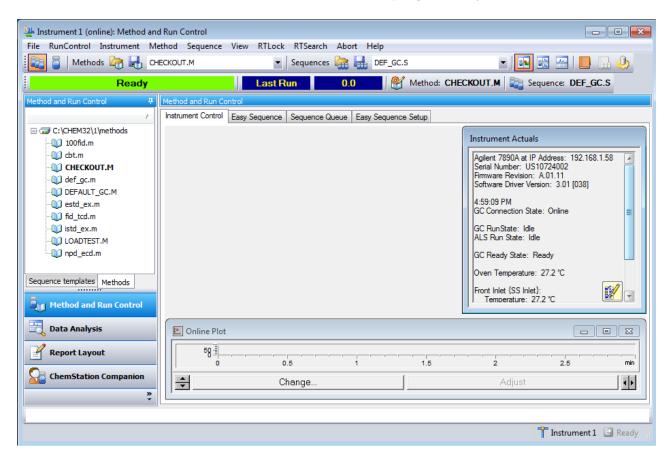
In this chapter, a sample is prepared and run for data acquisition.

Prepare the Sample

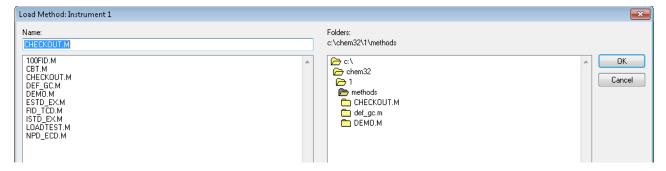
- 1 Fill a sample vial with the contents of the 0.5 mL ampule, Agilent sample p/n 5188-5372, and cap the vial.
 - If you are not using an ALS skip the remaining steps.
- 2 Place the sample vial into position 1 of the GC sample tray.
- **3** For solvent wash mode **A**, **B**:
 - Fill a solvent wash vial with iso-Octane and place it in injector turret location **A**.
 - Place a waste vial in injector turret location **W**.

Load the Method

1 To start the GC ChemStation, from the Windows start icon, click **All Programs**, click **Agilent ChemStation**, then click the online ChemStation program for your instrument.



2 Select the Load Method button, Methods to open the Load Method window. Navigate to and select checkout.M.



3 Select **OK** to load the method and close the dialog box.

Complete the Run Time Checklist

On the **Run Time Checklist** dialog, you will mark the check box for each section of a method that you want to be run.

- 1 In the Method and Run Control view in the Method menu click Run Time Checklist to display the Run time Checklist dialog.
- 2 In the Check Method Selections to Run area, for this example:
 - a Mark the Data Acquisition check box.
 - **b** Mark the **Standard Data Analysis** check box.
 - c Clear the other check boxes.
- 3 You can optionally mark the Save Method with Data check box.
- 4 Select **OK** to set the sections of the method to run and close the dialog box.

Run the Method

1 Open the **RunControl** menu and choose **Sample Info**.

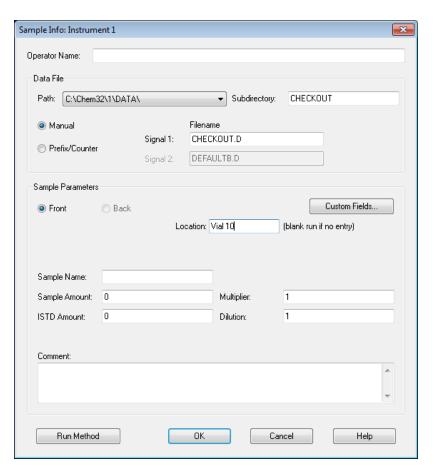


Figure 23 Start a single sample run

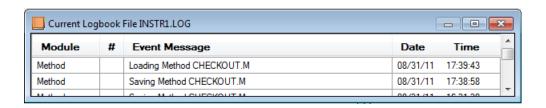
- 2 In the **Operator Name** field, enter your name.
- 3 In the Data File area:
 - a For the Path accept the default shown.
 - **b** Enter CHECKOUT as a subdirectory name.
 - c Select Manual and enter checkout.D in the Signal 1 field.

- 4 In the Sample Parameters area:
 - a Select Front or Back to specify the location of the ALS.
 - **b** In the **Sample Name** field, enter a name for your sample (optional).
 - c In the **Location** field, enter the tray location where the vial is located. Here we entered 10 and the system changes our entry to Vial 10. Vial position numbers are labeled on the trays. If you are making a blank run do not locate a vial at the specified position.
 - The 7693 sample tray has 150 labeled vial positions
 - The 7683 sample tray has 100 labeled vial positions
 - **d** If not using a tray the vial locations are, 101 for front and 201 for back.
 - **e** The **Sample Amount** field and the **ISTD Amount** fields are not required for Qualitative calculations.
 - f For the Dilution and Multiplier fields keep the default value of 1
 - **g** In the **Comment** field, enter a comment (optional).
- 5 Click **Run Method** to close the dialog box and start the run. The ready state indicator changes to Run. The data acquired during this run is used later starting in "Setup Data Analysis Options" on page 54.

View the Current Logbook File

The Current Logbook File lets you review event messages from the instrument.

1 In the Method and Run Control view select the Show/Hide current online Logbook button to display the Current Logbook File dialog for the instrument.

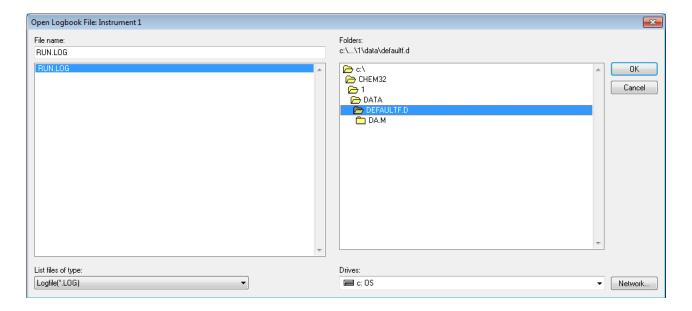


- 2 To print the log select View>Logbook>Print Logbook.
- 3 To save the log in another location select **View>Logbook>Save** As.

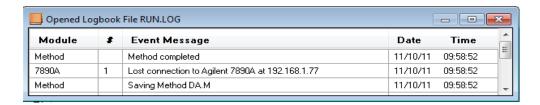
View the Log of the Run

The system keeps a logbook named RUN.LOG that records all instrument error and status messages prior to and during data acquisition. This logbook is stored with each data file.

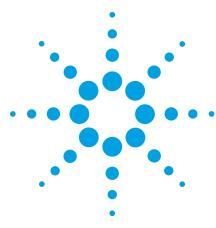
1 In the Method and Run Control view select View>Logbook>Open Logbook to display the Open Log Book dialog.



- 2 Use the right pane to browse to the data directory that contains the run log that you wish to view.
- 3 Select RUN.LOG from the left pane and click **OK** to display the **Open Log Book File** dialog for the selected data file.







Qualitative Data Analysis

Setup Data Analysis Options 54
Edit Integration Events 57
Manually Integrate Peaks 61
Modify the Method to Print a Report 63

Qualitative data analysis identifies the compounds in your sample by:

- Integrating the peaks in your acquisition data. Integration is a tool for finding the peaks in a chromatogram and determining their size and retention time.
- Identifying the compound by the peak's retention time
- Allowing interactive manual integration of peaks
- Reporting the identity of the compound(s) found for each peak

This chapter reviews each of these processes.

Setup Data Analysis Options

1 From the Windows **Start** button select **All Programs>Agilent ChemStation** and click the name of your Offline Instrument.

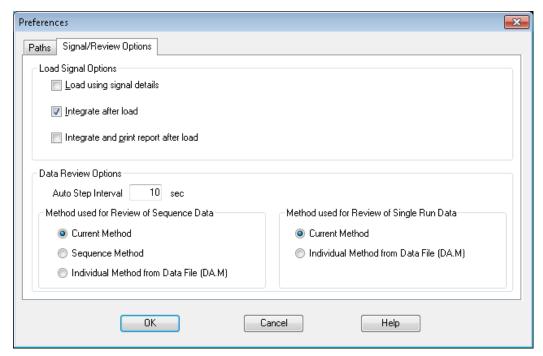
The ChemStation is displayed in offline mode.

2 Click the **Data Analysis** button in the ChemStation Explorer window to view the **Data Analysis** window.

The Integration tab Integration is selected by default.

3 Click the View Preferences icon to display the Preferences dialog.

When we load a data file we can set an option to automatically integrate the file after it is loaded.



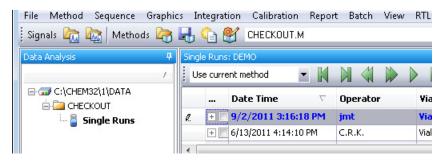
- 4 Under the Signal/Review Options tab, in the Load Signal Options Area, select Integrate after load.
- 5 In the Data Review Options area, for the Method used for Single Run Data select Current Method. This is the master method.
- 6 Click **OK** to close the dialog.

- 7 Select Graphics>Signal Options, to display the Signal Options dialog to set the Autoscale feature.
- 8 In the **Ranges** area select **Autoscale** and click **OK** to close the dialog.

The algorithm for autoscale does not work by selecting peaks. It splits the data points into "buckets", then looks at the max and min in each bucket, throws out the largest, and uses the second largest to base the scaling on. This is not necessarily the second largest peak (it depends on the size of the data point "buckets").

9 Double click the **ChemStation Explorer** tree **CHECKOUT** subdirectory to load all single run data files into the **Navigation Table**.

Data files are organized into Single runs and Sequences.

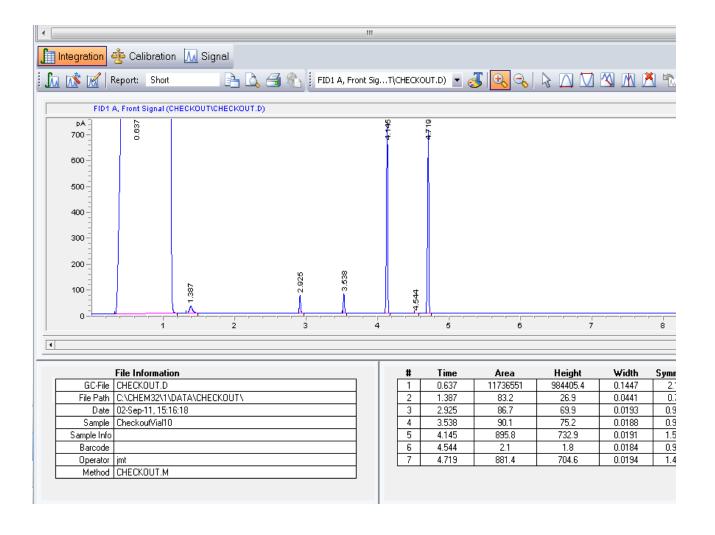


- 10 Navigate to the **CHECKOUT.D**. data file in the **Navigation Table**. This is the acquisition data file created from our sample run.
- 11 Double-click the **CHECKOUT.D**. data file line in the table. The data file is loaded and its chromatogram is displayed according to its method settings.

The data file is automatically integrated and the chromatogram is automatically scaled to fit the in the window.

If the chromatogram displays only a single large peak, you may not have set the **Autoscale** feature, as described in Step 7

4 Qualitative Data Analysis



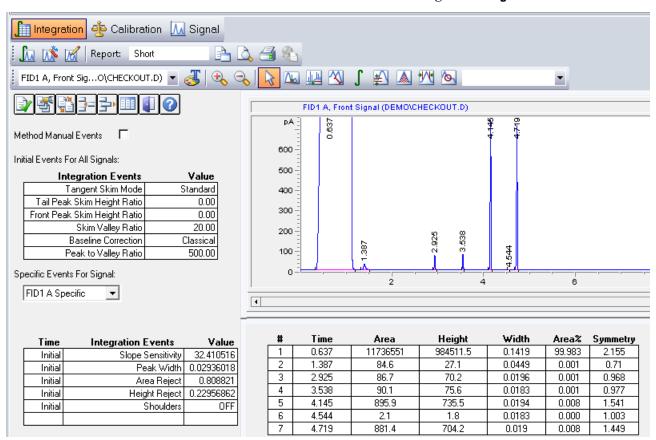
Edit Integration Events

Display integration events

When the data analysis part of your method is run, the chromatogram is integrated. Most chromatograms can be successfully integrated using the ChemStation default auto integration parameters. However, you may edit these auto integration event values and add additional integration events for your specific method.

- 1 Click the **Auto Integrate** icon to calculate suitable initial integration event parameters for the loaded signal.
- 2 Select the Edit/Set Integration Events Table icon M.

The **Integration Event Table** displays next to the chromatogram. Here, the lower integration events table displays the initial time values we created using **Auto Integrate**.



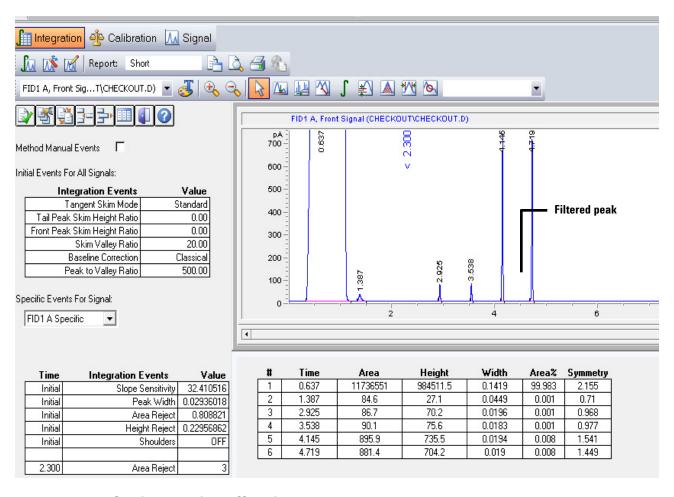
4 Qualitative Data Analysis

Set area reject

To demonstrate how Integration Events are used to filter peaks, we will remove the peak located at time **4.554** using the **Area Reject** event and then remove the peaks located at times **0.637** and **1.387** by turning the integrator off before it reaches these peaks and then turning the integrator back on after these peaks are processed.

To remove a peak using the **Area Reject** event:

- 1 Select **FID1 A Specific** from the **Specific Events for Signal** drop down menu. In this example this is the front detector signal shown in the chromatogram. These events apply to this signal only.
- 2 Click on the **Area Reject** icon _____, mouse over the chromatogram, and observe the vertical line that moves with the cursor.
- 3 Move the vertical line to the **2.3** minute time and click the left-mouse button. The **Area Reject** event is added to the Integration Events table at this time and given a **Value** of **0**.
- 4 Set the **Area Reject Value** to **3.0** in the Integration Events table and click to complete this edit. This peak at **4.554** minutes is filtered out and removed from the table.

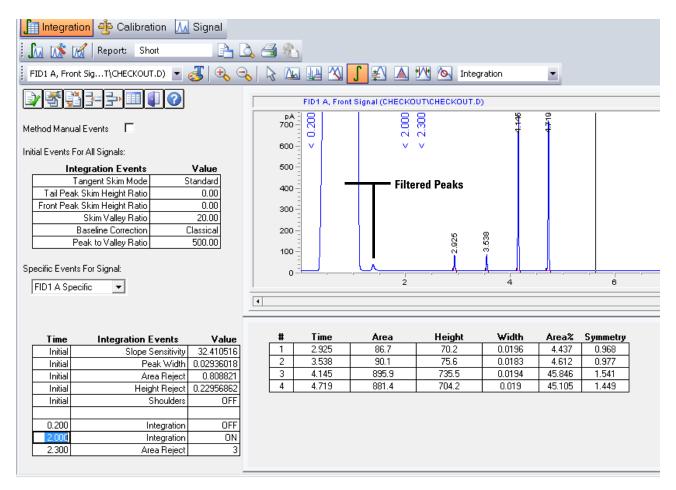


Set integration off and on

To remove peaks using the Integration Off/On event:

- 1 Click on the **Integration** icon \int , mouse over the chromatogram, and observe the vertical line that moves with the cursor.
- 2 Move the vertical line to the 0.2 minute mark and click the left-mouse button. The **Integration OFF** event is added to the Integration Events table at this time.
- **3** Move the vertical line to the 2.0 minute mark and click the left-mouse button. The **Integration ON** event is added to the Integration Events table at this time.
- 4 Click on 1 to complete this edit.

4 Qualitative Data Analysis



The peaks located between times **0.637** and **1.387** are now filtered out and removed from the table.

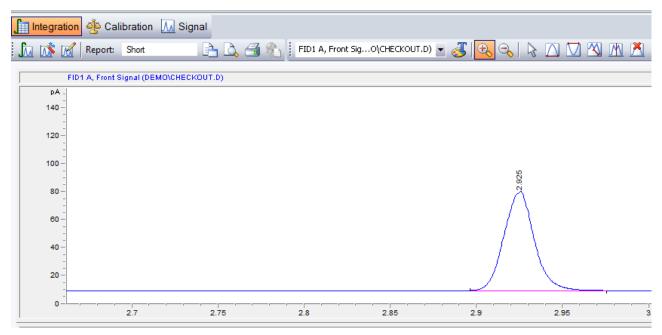
Note the times displayed vertically at < 0.200, < 2.000, and < 2.300 in the graph above. These times are also shown in the lower left **Integration Events** Table. These are the times we entered for the integrator to stop and start and the time that area reject starts.

The Peak table in the lower right that originally contained 7 peaks now contains only 4 peaks.

Manually Integrate Peaks

Manual peak integration allows interactive modification of peak integration for a data file. A set of graphic tools allows modification of the chromatogram directly. These changes can be saved with the data file (available since ChemStation revision B.04.01) or saved with the method. This section examines manual integration saved with data files.

- 1 Load a signal data file by selecting File > Load Signal from the menu to display the Load Signal dialog.
 - You can also load the file from the navigation table, which is read only.
- 2 In the right pane select the CHECKOUT folder where the data file is located then, from the left panel, select the CHECKOUT.D data file to be integrated and click OK.
- 3 Click the **Integrate** icon to integrate the signal with the specified method's integration events.
- Select the **Zoom In** icon then, click and drag the left mouse button to zoom in on the peak of interest at 2.92 minutes in the chromatogram.



Select the Manual integration: Remove integrated Peak(s) from the Integration Results icon , then click the peak at 2.92 minutes to delete its peak. The peak table located below the chromatogram no longer contains this peak.

4 Qualitative Data Analysis

- 6 Select the Manual integration: Draw Peak baseline(s) and integrate icon , then click and drag the right mouse button to draw an integration baseline on the peak. When you release the button, the peak will be integrated and added to the peak table located below the chromatogram.
- 7 Other tools available include:
 - The **Undo** icon to undo the last manual event edit
 - The **Zoom out** icon
 - The Draw Negative Peak Baseline icon 🚺
 - The Tangent Skim One Peak icon
 - The Split Manually Integrated Peaks icon
- 8 Click the **Save** icon to save the current manual integration events to this data file. This is the recommended method for saving a manual integration.

When a manual integration events file is saved with the data file, the **Manual Events** column of the **Navigation Table** is marked with the symbol.

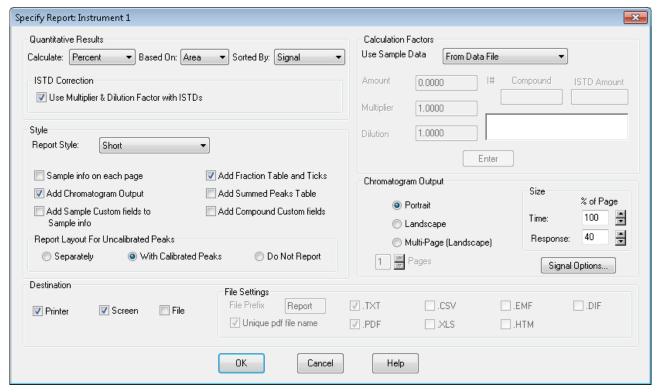
9 The **Delete** icon is used to delete all manual events from the data file. The manual integration file remains with the data file until this delete action is saved. Click the **Save** icon to permanently delete the current manual events file from this data file.

Modify the Method to Print a Report

1 Click the Specify Report Calculation and Print Style icon display the Specify Report dialog.

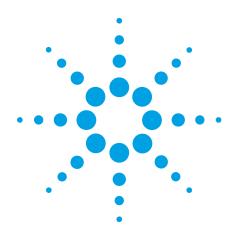


You can also select this dialog from the menu by selecting **Report > Specify Report**.



- 2 To create an area percent report, in the Quantitative Results area, select Percent for Calculate, Area for Based On and Signal for Sort By.
- 3 For destination select **Printer** and **Screen**.
- 4 Click the Identify Peaks, calculate and preview results icon to view the Report. To Print the Report, from the main menu select Print > Report.
- Click the Identify Peaks, calculate Results and Print Reports iconto send a copy of the report to the printer.
- 6 Click the **Save Method** icon to save the report specification to the method or select **Method** > **Save Method**As to create a method with a new name.

4 Qualitative Data Analysis



Create and Run a Sequence

Sequence Data File Storage 66
Prepare the Samples 68
Set the Sequence Parameters 69
Create and Run a Sequence 70
Partial Sequence 73
Sequence Reprocessing 76

A sequence is a list of samples to be analyzed and a designated method to be used for each analysis. Once defined, the sequence may run unattended, automatically processing the samples defined in the sequence.

When an ALS is installed, the entire analysis, from injection of the sample through reporting of results, can be automated to save you time.

The data files generated when running the sequence in this chapter will be used to create a calibration curve in the next chapter.

Sequence Data File Storage

Before creating a sequence, check the unique folder creation setting is on. See "Set the sequence preference" below.

When this Data Storage preference (Unique Folder Creation ON) is selected, sequences are reprocessed from the Data Analysis view. It will not be possible to reprocess any sequence using this data storage selection from Method & Run Control\Sequence\Sequence Parameters.

All data files, copy of the sequence table template (Sequence.S), all methods used in the sequence table, the batch (.B) file, and the sequence log are stored together in one folder under the Data Directory (C:\Chem32\1\Data). Generally, this folder is called the sequence folder or sequence container. Each data file also contains two methods, ACQ.M and DA.M.

For more detailed information on this subject please see the *Agilent ChemStation Getting Started with New ChemStation Workflow* manual (G2170-90044).

Table 4	Method type.	location, and	use with Unio	ue Folder Creatio	n ON preference set
---------	--------------	---------------	---------------	-------------------	---------------------

Method	Location of Method	Acquisition	Reprocess	Data Review
Master Method	C:\Chem32\1\Methods	Yes	No	Yes
Sequence Method	C:\Chem32\1\Data\ Subdirectory\Sequence_container\	No	Yes	Yes
DA.M	C:\Chem32\1\Data\ Subdirectory\Sequence_container\Data.d	No	No	Yes
ACQ.M	C:\Chem32\1\Data\ Subdirectory\Sequence_container\Data.d	No	No	No

Set the sequence preference

- 1 Start a ChemStation online session.
- 2 From the main menu select View > Preferences to display the Preferences dialog.

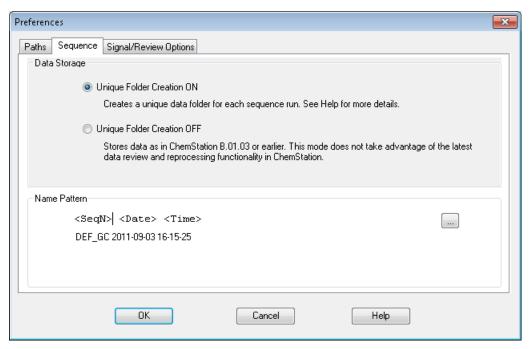


Figure 24 Setting the sequence preference

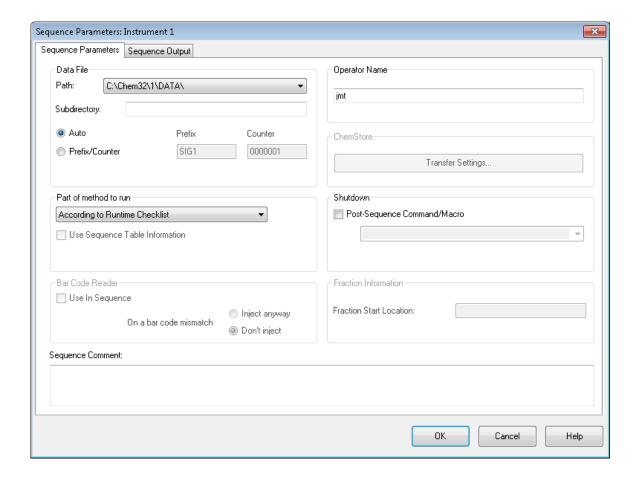
- 3 Under the **Data Storage** area select **Unique Folder Creation ON**. This option specifies that each time a sequence is run, the system creates a unique directory where it stores all files related to the completed sequence run including its methods, logs, batch files, and data files.
- 4 In the **Name Pattern** area, optionally change the default name pattern for the sequence container (storage directory). This default name pattern is made using the sequence name with a time stamp appended to assure its uniqueness. See the online help for other naming options.
- **5** Click **OK** to close the dialog.

Prepare the Samples

- Fill a sample vial with the contents of the 0.5 mL ampule, Agilent sample p/n 5188-5372 and cap the vial. Mark this vial as the 23.6 mg/ μ L calibration standard.
- 2 Fill a sample vial with the contents of the 0.5 mL ampule, Agilent sample p/n 5188-5372. Add an equal amount iso-Octane to the vial for a 1:2 serial dilution and mix the vial contents.
- 3 Remove 0.5 mL from this vial, place it in a new vial, and cap the original vial. Mark this capped vial as the 11.8 mg/ μ L calibration standard.
- 4 Take the uncapped vial from the previous step and add 0.5 mL of iso-Octane to the vial for a 1:2 serial dilution and cap the vial. Mark this vial as the 5.9 mg/ μ L calibration standard.
- 5 Make an unknown concentration sample in a vial by diluting a 23.6ug/mL solution. Cap and mark this vial unknown sample.
- 6 If you are not using an ALS skip the remaining steps.
- 7 If you are using an ALS:
 - a Place the sample calibration vials into positions **20** through **22** of the GC sample tray. Place the lowest concentration level in position **20**, and the other two in order of increasing concentration.
 - **b** Place the unknown sample vial in position **23**.
 - **c** Fill a solvent wash vial with iso-Octane and place it in injector turret location **A** for solvent wash mode **A**, **B**.
 - **d** Place a waste vial in turret location **W** specified for solvent wash mode **A**, **B**.

Set the Sequence Parameters

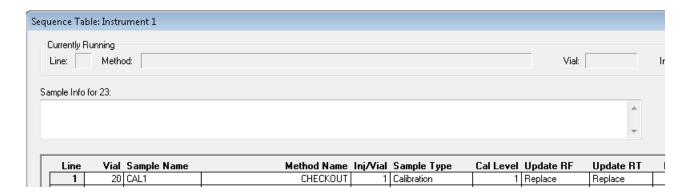
- 1 With the ChemStation running in online mode, click the Method and Run Control button to display the Method and Run Control view with the Instrument Control tab selected.
- 2 Load the CHECKOUT.M method.
- 3 From the **Sequence** menu, select **New Sequence Template** to clear any entries from the current sequence table.
- 4 From the Sequence menu, select Sequence Parameters to display the Sequence Parameters dialog.



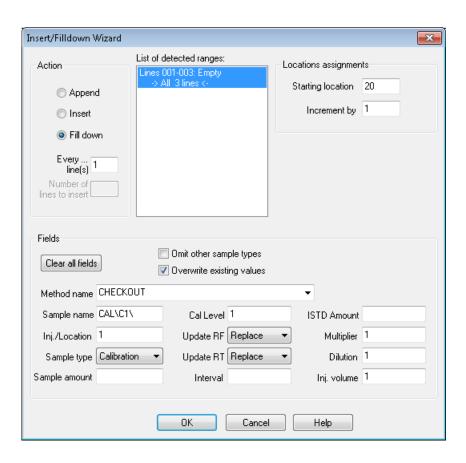
- With the Sequence Parameters tab selected, select a Data File Path from the drop down. If the required path is not shown, access the Preferences dialog to add it.
- 6 In the Part of method to run area, select According to Runtime Checklist.
- 7 Enter your name in the **Operator Name** field.
- 8 Click **OK** to close the dialog.

Create and Run a Sequence

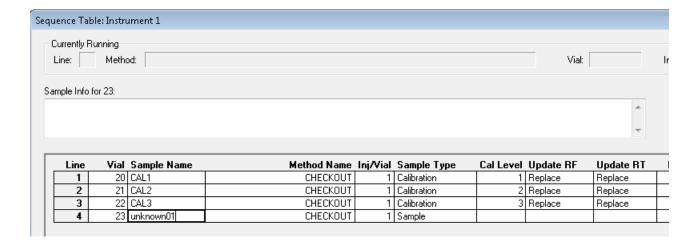
1 From the **Sequence** menu, select **Sequence Table** to display an empty **Sequence Table** dialog.



- 2 Click the **Append Line** button twice to add two lines to the table.
- 3 Click the Insert/Filldown Wizard button to display the Filldown Wizard dialog.
- 4 In the Action area select Fill down and In the List of detected ranges, select both lines.
- In the Location assignments area, set the Starting location to 20 and the Increment by value to 1. This specifies that the first vial is located in position 20 and the other vials are in locations 21 and 22 in the ALS tray.
- 6 In the Fields area, click the Clear All Fields button and do not select Omit other sample types.
- 7 Select the CHECKOUT method from the Method name drop down list and select Calibration from the Sample type drop down list.
- 8 In the **Sample name** field enter CAL\C1\. The \C1\ parameter creates samples names CAL1, CAL2, and CAL3. For other applicable configurations click the **Help** button.

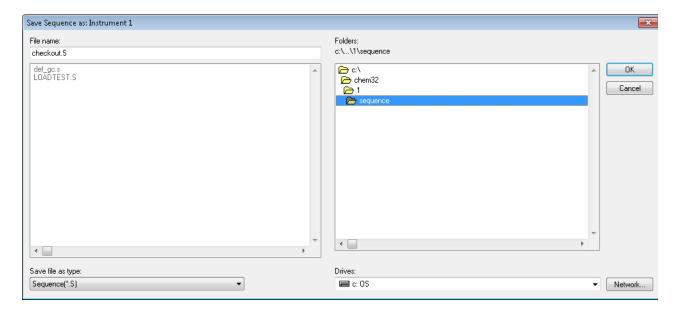


- 9 Click **OK** to close the dialog and fill in the required columns in the **Sequence Table**.
- 10 In the **Sequence Table Cal Level** column, for samples 2 and 3, change the entries to **2** and **3**.
- 11 Click the **Append Line** button to append a line to the table.
- 12 Enter a Vial number of 23 and a Sample Name of unknown01.

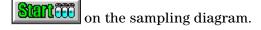


- 13 Click **OK** to close the dialog.
- 14 From the main menu select **Sequence > Save Sequence As** to open the **Save Sequence as** dialog and enter CHECKOUT as the sequence name. For the location use the chem32/instrumentNumber/sequence directory. This is the directory where the sequence templates are stored.

This sequence becomes the current default sequence.



15 From the main menu select **Sequence > Run Sequence** to run the **CHECKOUT.s** sequence or click the Start Sequence button





The sequence acquires data files for all three calibration samples and our unknown sample.

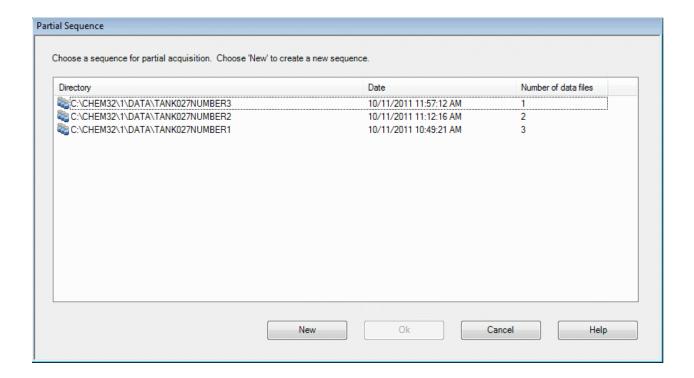
In the next chapter we will create a calibration table using data acquired with this sequence.

Partial Sequence

Partial Sequence can be used to acquire data into a new sequence container or to add runs to an existing sequence container. It can also be used to preview the run order of the sequence or to select specific runs for data acquisition or data reprocessing.

- 1 From the **Method and Run Control** display, select the **Sequence** menu in the tool bar.
- 2 Select Partial Sequence.

A list of sequence containers are shown with the last run sequence listed first.



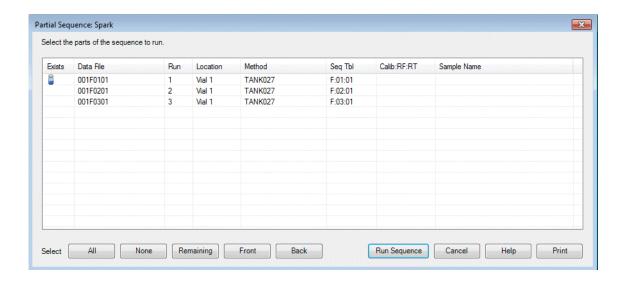
Acquire data into an existing container

- 1 To acquire data into an existing sequence container, first select the sequence container from the list and click **0k**.
 - While the selected sequences are being parsed, a timeline shows the progress. You can click to abort the process.

5 Create and Run a Sequence

All runs are displayed in order. If the runs exceed the viewable area, use the vertical scroll to view more of the listings.

2 Select the run/s desired for data acquisition/ analysis/ reprocessing.



In the sequence shown in the dialog box, only one sample was run. The completed run is shown by a vial icon in the **Exists** column.

It is possible to select all samples, only the remaining samples, or just the front or back samples.

3 Select **All** if you want to re-run all 3 samples.

OR

Select the **Remaining** button if you want to run the other samples and run 2 and 3 will be highlighted.

4 Select **Run Sequence**. The sequence container will now include 3 completed runs.

Acquire data into new sequence container

1 To place this data into a new container, select **All** and each line is highlighted.



2 Select the **Run Sequence** button. A new sequence container is created with the 3 data files.

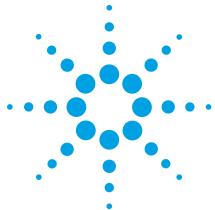
The new container is automatically named.

Sequence Reprocessing

Reprocessing is accessed from the Data Analysis view. It uses copies of method and sequence files in the sequence container; however not all parameters can be changed. Only the relevant Sequence Parameter fields for reprocessing are accessible.

During reprocessing, all changes in the DA.M are overwritten. All new methods are written into the Sample Container.





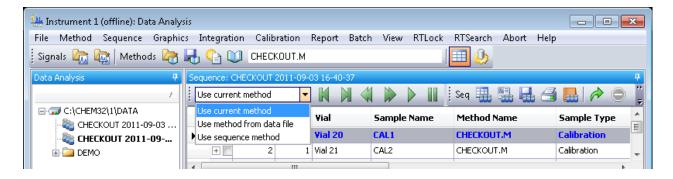
Create a Calibration Method

Create a Calibration Table 78
Reprocess the Sequence 83

This chapter describes how to add compounds to the calibration table stored in your method. After a compound is identified, quantitative data analysis determines the amount of the compound in your sample by comparing the response from a known measured amount of the compound, stored in the calibration table, to the response from an unknown amount of compound.

Create a Calibration Table

Start an offline session of the ChemStation and select **Data Analysis** view from the **ChemStation Explorer**.

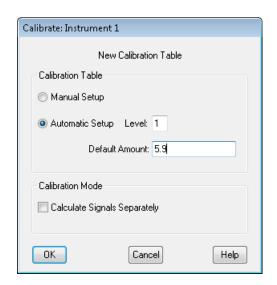


- 2 In **ChemStation Explorer**, double click the sequence you just acquired to load its 4 data files into the navigation table. The unique sequence name, which includes a time stamp, is displayed to the right of a three blue sample vial icon. This sequence name is displayed in bold when its sample data is displayed in the navigation table.
- 3 Select **Use sequence method** from the drop down menu.
- 4 In the navigation table, double click the 1st calibrant data row to load and display its chromatogram.

NOTE

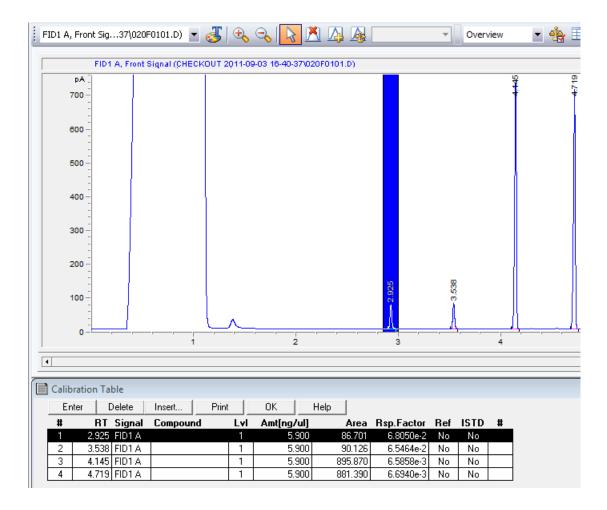
The navigation table is read only.

5 From the Calibration menu select New Calibration Table to display the Calibrate dialog.



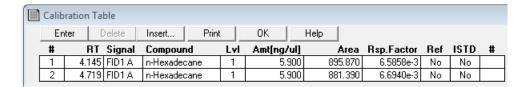
6 With Automatic Setup Level selected for level 1, set the Default Amount to 5.9 ng/ μ L and click OK to display the Calibration Table below the chromatogram of the 1st calibrant with 4 integrated peaks entered.

This view is in **Data Analysis** with the **Calibration** tab selected. The units label shown in the **Amt** column can be changed in the **Calibration Settings** dialog accessed by selecting **Calibration** > **Calibration Settings** from the main menu.



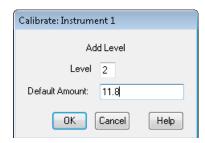
- 7 To quickly locate a **Calibration Table** entry for a peak in the chromatogram, use the select peak tool and click on the chromatogram peak to highlight its row in the **Calibration Table**.
- 8 Click the delete peak tool 2 and the cursor changes to a peak symbol with an "X" over it. Click this cursor on the peaks in the chromatogram at 2.9 minutes and 3.5 minutes to delete them from the Calibration Table.
 - The **Calibration Table** now only contains the peaks at **4.1** and **4.7** minutes.
- **9** For the peak at **4.1** minutes enter n-Penta-decane as the **Compound** name.

10 For the peak at **4.7** minutes enter n-Hexadecane as the **Compound** name.



Add levels to a calibration table

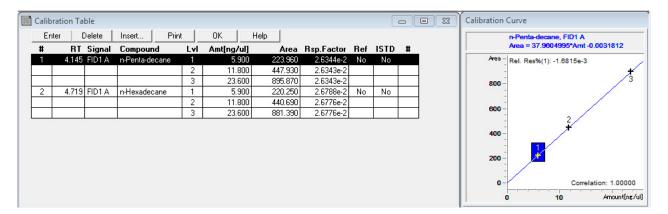
- 1 In the navigation table, double click the 2nd calibrant data row to load and display its chromatogram.
- 2 From the Calibration menu select Add Level to display the Calibrate dialog.



- 3 With Level set to 2, set the Default Amount to 11.8 ng/ μ L and click OK to display a level 2 added to the Calibration Table for both compounds.
- 4 In the navigation table, double click the 3rd calibrant data row to load and display its chromatogram.
- From the **Calibration** menu select **Add Level** to display the **Calibrate** dialog.

6 Create a Calibration Method

6 With Level set to 3, set the Default Amount to 23.6 ng/ μ L and click **OK** to display a level 3 added to the Calibration Table for both compounds.



7 Save this calibration table to the sequence method by selecting Method > Update Sequence Method from the main menu.

Reprocess the Sequence



1 Run sequence reprocessing by clicking the

icon.

The report is printed and now contains the concentration of the unknown sample. If you are satisfied this sequence method, you can update this method to the master method for next analysis.

To update this method to the master method, select MethodUpdate Master Method from the main menu.

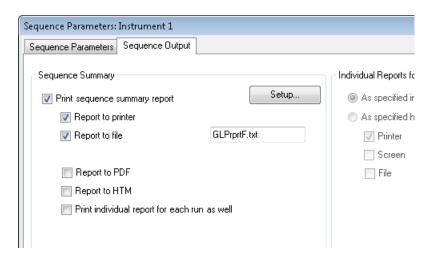
Sequence summary report

The tools shown in the navigation table will allow you to make changes to this file without going to the **Method and Run Control** view.

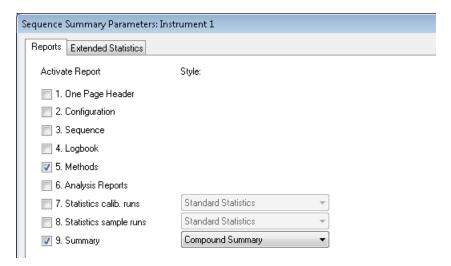
1 With the sequence loaded, open the **Sequence Parameters** dialog by clicking on the icon shown below.



2 Select the **Sequence Output** tab and deselect the **Print individual** reports for each run checkbox.



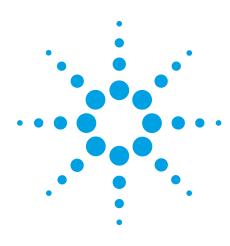
3 Select the **Setup** button to display the **Sequence Summary Parameters** dialog with the **Reports** tab selected.



- 4 Items 5 and 9 are selected. Select item 9. Summary, with Compound Summary selected from the dropdown. Click OK to close the dialog.
- 5 To reprocess the sequence, select the Start sequence reprocessing tool displayed below.



- 6 The sequence will reprocess. You will notice that the status bar turns blue to indicate the sequence is reprocessing. The method and a Compound Summary should print at the end of the sequence.
- **7** Examine the method. You should see the record of your action in the Change History.
- 8 Save the sequence to accept changes if desired.



Easy Sequence

Create an Easy Sequence Template 86
Create an Easy Sequence from a Sequence Template 93
View the Sequence Queue 96
Edit a Sequence in the Sequence Queue 101

The ChemStation **Easy Sequence** feature allows you to create a template (called an Easy Sequence Template) that contains information you routinely use in sequences.

This template (the **.est** file) includes sample attributes that do not typically change from sequence-to-sequence, such as the number of samples in a sequence, sample naming conventions, data storage locations, calibrants, response factors, and so on.

After this template is created, it is used over and over again, as the starting point for creating new sequence files. The sequence files created from an Easy Sequence Template are called Easy Sequence files (.es files).

This chapter describes:

- How to create an Easy Sequence Template (.est file)
- How to create an Easy Sequence from that template (.es file)
- How to add the Easy Sequence to the sequence queue.

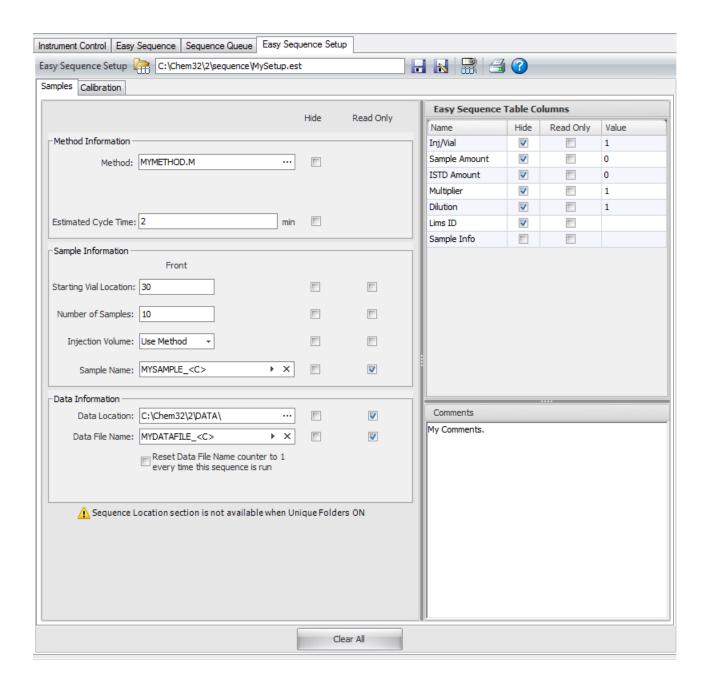
Create an Easy Sequence Template

When you create an Easy Sequence Template (.est file) you will enter sample and calibration attributes that will not typically change from one sequence to another. Both processes, entering sample information and entering calibration information, are described in this Chapter.

Sample information

To enter sample details for the template:

- 1 Select the **Easy Sequence Setup** tab from the Method and Run Control window.
- If not already highlighted, select the **Samples** tab. This screen shows the sample attributes you may specify as the starting point for your sequences. The information you enter here will be pre-filled when this template is used as the starting point for an Easy Sequence.



To begin, identify the method you would like used for your sequences.



- 3 In the **Method Information** area, click the ellipsis in the **Method** field, then browse to and select the method you want. For this example, we are using **MYMETHOD.M**.
- 4 Enter an **Estimated Cycle Time** for each run. This is for information purposes only. It is used by the ChemStation to provide an estimated completion time for queued sequences. For this example, use two minutes.

Estimated cycle time

Estimated cycle time is the GC cycle time, which is oven + Data Analysis + cool down. GC ready to GC ready.

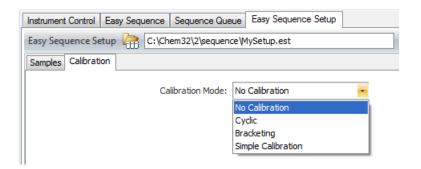
Estimated cycle time only shows when the sequence is running in the queue and is not required, just a user estimate. Nothing depends on its accuracy.

Calibration information

Once you have saved the sample information for the Easy Sequence Template, as described in the previous section, you may add calibration details.

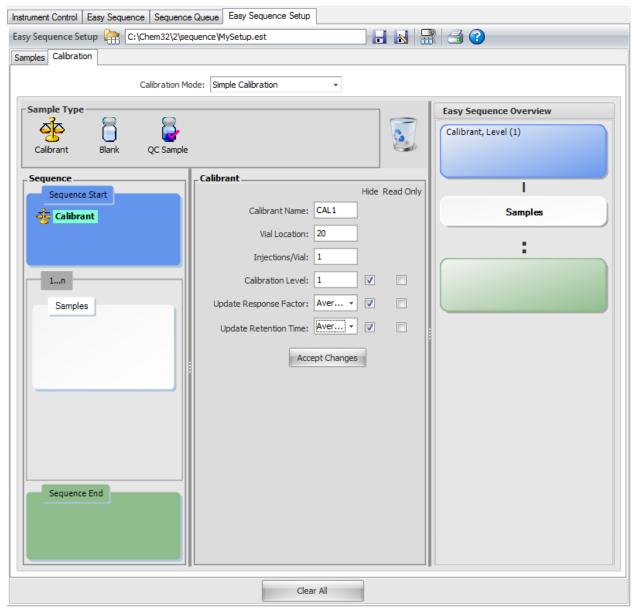
1 Before moving to the **Calibration** tab, be sure to save your changes to the **Samples** section. If you do not, those details will be lost when you click the **Calibration** tab.

After saving the **Samples** section, click the **Calibration** tab.



2 For this example, select **Simple Calibration**, from the **Calibration Mode** drop-down menu.

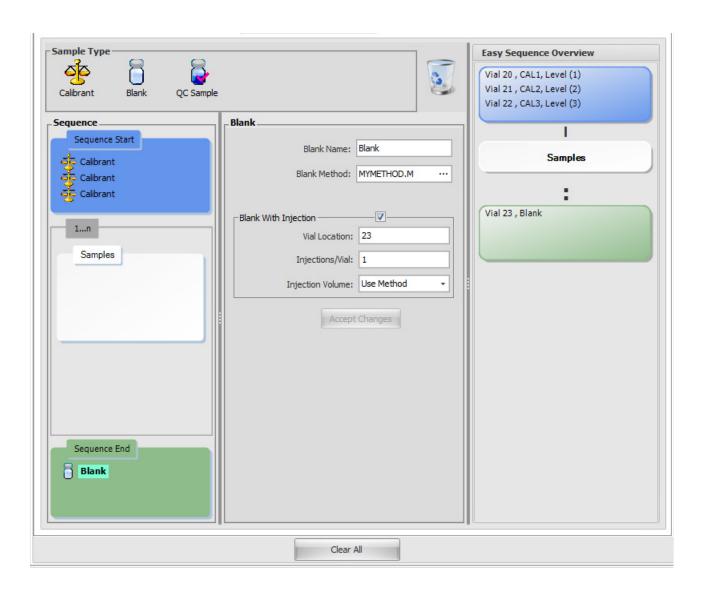
7 Easy Sequence



- For each calibrant you want included in the sequence template you will:
 - a Drag the Calibrant icon from the Sample Type area to the Sequence Start area, in the left column.
 - b Enter the calibrant details (Vial Location, Injections/Vial, Calibrant Level, Response Factor, and Retention Type), in the center column.
 - Click Accept Changes to update the template. Notice the updated details in the right column under Easy Sequence Overview.

For this example enter 3 calibrants:

Calibrant Name:	CAL1	CAL2	CAL3
Vial Location:	20	21	22
Injections/Vial:	1	1	1
Calibration Level:	1	2	3
Update Response Factor:	Average	Average	Average
Update Retention Time:	Average	Average	Average



- 4 Next, for this example, add a Blank to end the sequence. Similar to how you entered calibrants:
 - a Drag the icon for a Blank sample from the Sample Type area to the Sequence End area.
 - **b** In the center column, specify a **Blank Name**.
 - **c** Click the ellipsis and select a method to be used to run the sample, and click **OK**.
 - d To use a solvent blank, select the Blank with injection, enter a Vial Location, and specify the Injection Volume.
 - e Click Accept Changes to update the template.
- 5 Review the Easy Sequence Overview panel (in the right column) to verify the calibration information is as you
 - expect, and click the Save icon \blacksquare to save the changes to the template.

That completes the process of creating a sequence template.

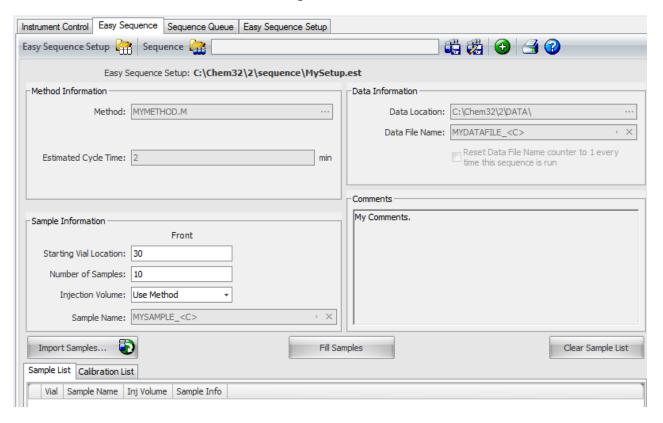
The next section describes how you may now use this template to easily create a sequence.

Create an Easy Sequence from a Sequence Template

Now that you have created an Easy Sequence Template (.est file), you can use it to create an Easy Sequence (.es file).

To create an Easy Sequence from an Easy Sequence Template:

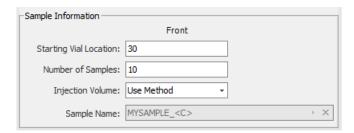
- 1 From the Method and Run Control panel, access the **Easy**Sequence tab.
- 2 Click the Open Easy Sequence Setup icon to load the template.
- **3** Browse to the template you wish to use and click **OK** to load the template.



4 This is your starting point for your new sequence. Notice the default information is the information you entered in your Easy Sequence Template (the .est file).

Notice the greyed out fields: Method, Estimated Cycle Time, Sample Name, Data Location, Data File Name. These are the fields that were set to **Read Only** when this template was created.

7 Easy Sequence



5 Modify these default values, to create the sequence you need.

For this example, make the **Sample Information** match the example shown above.

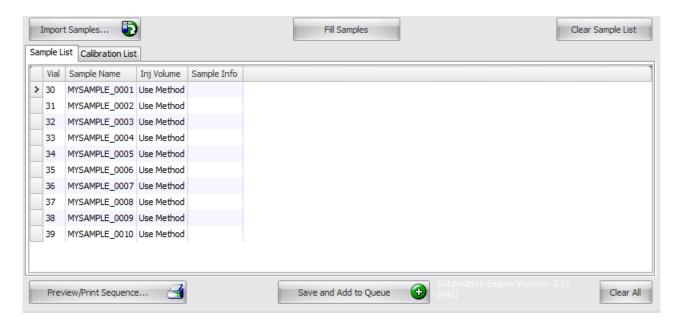
a Starting Vial Location: 30

b Number of Samples: 10

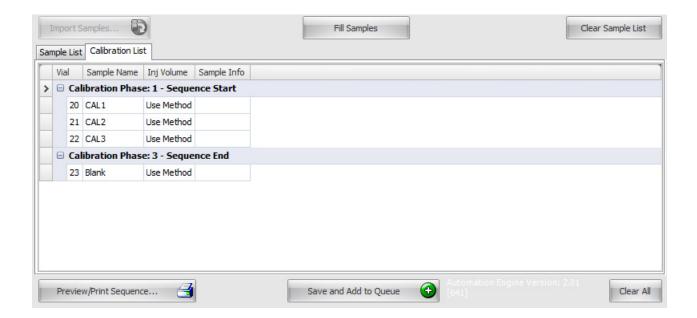
c Injection Volume: Use Method:

6 Click the **Fill Samples** button to populate the samples list.

This will add the number of samples defined in the **Number of Samples** field the **Samples List**.



7 Because we are running calibration samples in this example, click the Calibration List tab, to view the calibration samples. That completes the entries needed to create the sequence.



- 8 To review a report for this sequence, click the **Preview/Print** Sequence button.
- **9** Use the scroll bar to see the bottom portion of the report.
- 10 Click **Print Sequence...** to print a copy if you desire.
- 11 Click the **Close** button to return to the Sample table.
- 12 To save and run this sequence, click the Save and Add to Queue button.
- 13 Enter a filename for this sequence, and click Save.

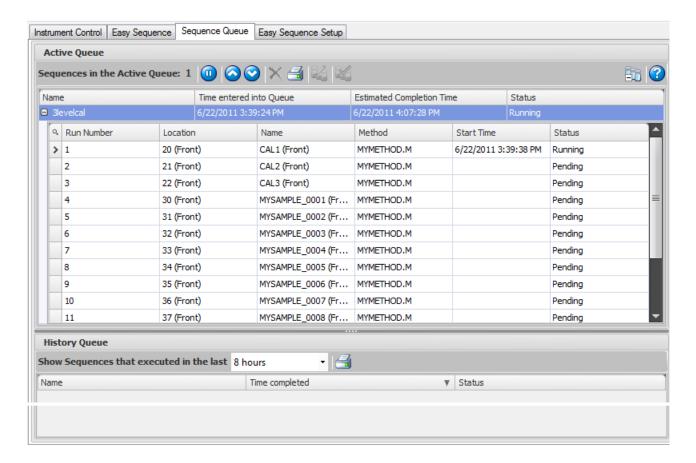
That concludes the process. The Easy Sequence is now saved and has been added to the Sequence Queue.

Review the next section of this document for details on the Sequence Queue.

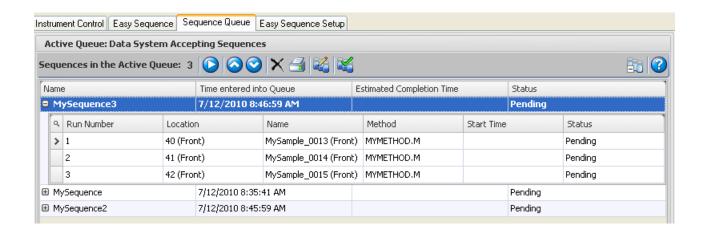
View the Sequence Queue

When you save an Easy Sequence, as described in the preceding section, it is automatically saved to the Sequence Queue.

1 To view the active sequence queue and the queue history, click the **Sequence Queue** tab.



- 2 Look at the top of the queue to see sequences that are currently running and scheduled to run (pending).
- 3 Look at the bottom of the screen (the History Queue section), to see the completed sequences.
 - You may click the **History** icon in the upper right corner of the screen, to toggle the **History Queue** on or off.
- 4 Click the plus or minus sign next to the sequence name, to expand or collapse details for each sequence in either the current queue or the history queue.



5 To move a sequence to a different time slot, highlight the sequence and click the **Move** icon .

The above graphic shows MySequence3 was moved ahead of MySequence.

Sequence queue considerations

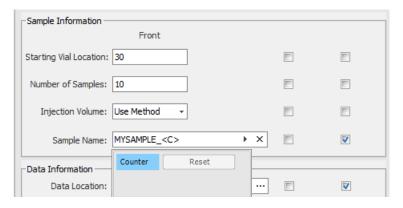
The Easy Sequence acquisition begins as soon as the data system is ready, unless Paused from the Queue.

- Once an Easy Sequence is started, it cannot be changed from the Easy Sequence UI. It becomes a ChemStation sequence (.s) and can be opened and edited in the Sequence Table.
- If any changes are made to the running sequence in the Sequence Table and the sequence is not saved, the queue will be paused at the sequence conclusion. Saving the sequence will be necessary before the next sequence in the queue will begin.
- Only pending Easy Sequences in the queue can be edited.
- If an error occurs at any point in the execution of a sequence, the ChemStation sequence will abort and the Easy Sequence will be sent to the History Queue with an error status. You must reload the Easy Sequence (.es), modify as needed, and resend to the queue.

Priority sample

- Pause the Queue if using Easy Sequence.
- Pause Sequence from RunControl menu.

- Use RunMethod (F5) to specify sample, method, and injection information.
- After running all priority samples, Resume Sequence.

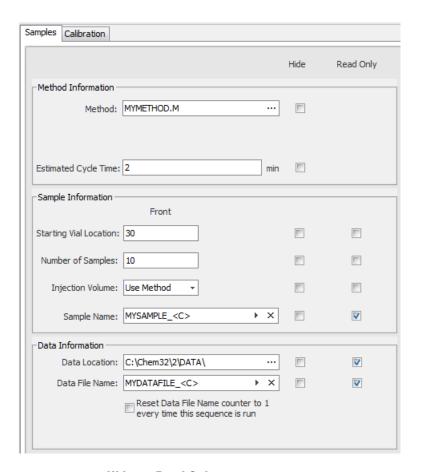


- 6 Next, fill in the global **Sample Information**. Include the:
 - **Starting Vial Location** of the first sample vial (30 for this example.)
 - **Number of Samples** (10 for this example.)
 - Injection Volume (For this example, leave this set to Use Method.)
- 7 In the Sample Name field, enter the name you wish to use for the samples in your sequences, and the way you want each sample name to increment. For this example, enter MySample_ for the Sample Name, then click the right arrow at the right end of the field to display the sample naming options, and select Counter.

Counter adds a sequential number to the end of the sample name for each sample created. In this example, MySample_1 will be the first, MySample_2 for the next, and so on.



- In the **Data Information** area, enter the desired **Data Location** for storing the data files, the **Data File Name**, and naming convention. For this example, use the default location, **MyDataFile**_ for the **Data File Name**, and add a **Counter** on the end of this name, similar to the Sample Name.
- **9** For this example, check the **Reset Data File Name** counter. This will reset the Data File Name counter to 1 every time the sequence is run.

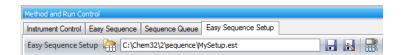


10 Select the **Hide** or **Read Only** check boxes to specify the parameters that you would like to be available when this template is used to create a sequence.

For this example, set the **Sample Name**, **Data Location**, and **Data File Name** to **Read Only**, and leave all other fields unchecked. Later, when this template is used to create a sequence, parameters defined as:

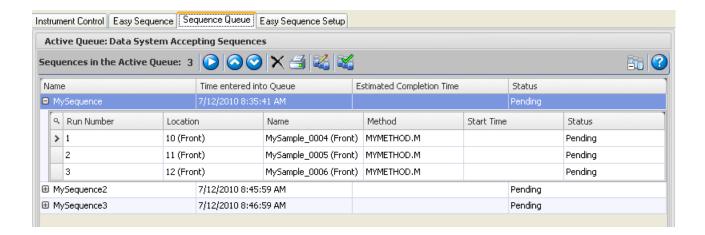
- **Show** (where nothing is checked) will be editable
- Read Only will be shown, but will not be editable

- Notice, **Method Information** parameters are always **Read Only**.
- 11 Use the **Comments** field to specify any additional sequence information or external links that you would like to pass on to anyone using this template to create a sequence. To enter a comment, click inside the comment box and type the appropriate information.
- Sequence Setup As icon to display the Save Easy Sequence Setup As dialog, then enter a name for this template, MySetup for this example, and click Save to save the template.
- 13 Notice this new template name, **MySetup.est**, is now displayed in the **Easy Sequence Setup** title bar. Now you may enter the calibration details, as described in the next section, to complete the template.



Edit a Sequence in the Sequence Queue

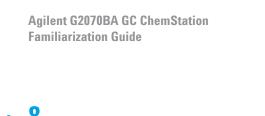
1 Select the sequence you want to edit in the active queue. (Only Easy Sequences, those created with an Easy Sequence Template, can be opened with the Easy Sequence editor.)



- 2 Click the **Edit Sequence** icon, to open the editor. If the sequence you selected was scheduled to run next in the sequence queue, the sequence queue automatically pauses.
- **3** Edit the information as necessary, (change the vial position for example), then click the **Fill Sample** button to update the sequence table.
- 4 Click **OK** to save the changes and return to the sequence table
- 5 Click the **Resume Queue** icon to resume the sequence.

Note that this changes the instance of the sequence in the sequence queue **only**. The original easy sequence (the **.es** file) and the easy sequence template (the **.est** file) do not change.

7 Easy Sequence



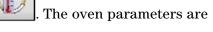
Create a GC Maintenance Method 104
Use the Maintenance Method 105
Shut Down the GC 106

Create a Maintenance Method

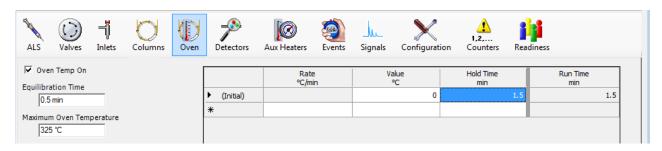
This chapter describes how to create and store a method to use for instrument shutdown and maintenance tasks. Using this type of method helps prevent damage to the instrument electronics and columns, and avoid injuries such as burns or shocks.

Create a GC Maintenance Method

- 1 Select View > Method and Run Control.
- 2 Click the Instrument menu then click Edit Agilent 7890A Parameters to edit the currently loaded method. The Edit Method dialog box opens.
- 3 Select the **Oven** button, displayed.



- 4 In the **Value** field, enter 35°C.
- 5 Mark the Oven Temp On checkbox.



6 Select the **Inlets** button, displayed.



. The inlet parameters are

- 7 Select the **front** or **back** tab, depending on your hardware configuration.
- 8 Mark the **Heater** check box, and enter 35°C in the corresponding field.
- **9** Mark the **Pressure** check box. Column flow must be maintained to prevent damage to the column when hot.



10 Select the **Detectors** button, parameters are displayed.

. The detector

- 11 Select the **front** or **back** tab, depending on your hardware configuration.
- **12** Mark the **Heater** check box, and enter 35°C in the corresponding field.
- **13** Mark the makeup gas on, and clear other gas and flame check box.



- 14 Select the **AUX** button,
- 15 Clear the On check box for any Aux x Heater and select OK.



- 16 Select Method>Save Method As. The Save Method As dialog box opens.
- 17 In the Method File field, enter maintenance.
- 18 Select OK.

Use the Maintenance Method

To use the maintenance method, load the method, access the **Setup Method** window, and right mouse click in the right panel. Select **Download Method to GC** from the context menu. A confirmation message is displayed.



Select $\mathbf{0K}$ to close the message and return to the \mathbf{Setup} \mathbf{Method} window.

When the GC enters the Ready state, perform the maintenance.

WARNING

Hot surfaces on the GC can possibility cause a skin burn injury. Before maintenance, make sure the oven, inlets, detectors and heated parts are cooled down, or wear heat-resistant gloves.

At the next power on, the GC and ChemStation will start up with its heated components maintained at a safe temperature.

Shut Down the GC

- In Method and Run Control, view, load the GC maintenance method.
- 2 Access the **Setup Method** window.
- 3 Right mouse click in the right panel and select Download Method to GC from the context menu. A confirmation message is displayed.



- 4 Select **OK** to close the message and return to the **Setup Method** window.
- 5 Close the **Setup Method** window.
- **6** When the GC enters the Ready state, exit the ChemStation.
- 7 Turn off the power to the GC.
- **8** Turn off the carrier gas and gases to the detectors.
- **9** Power off the PC and all peripheral equipment.



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