

Agilent MassHunter Data Acquisition Software for 5975/5977 Series GC/MSD

Familiarization Guide



Agilent Technologies

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In This Guide...

This manual will serve as a familiarization or quick reference guide for first-time users of MassHunter Data Acquisition.

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

1 Introduction

Chapter 1 provides an overview of how to start up and tune your system.

2 Create a Scan Method

In Chapter 2 you will learn how to edit, save, and run a data acquisition Scan method.

3 Create a SIM Quantitation Method

In Chapter 3 you will learn how to create a SIM method.

4 **Running Samples**

Chapter 4 describes how to run a single sample and how to run a sequence.

5 General Information

Chapter 5 includes miscellaneous information on commonly used features in MassHunter.

Where to Find More Information

Accompanying your hardware and software is a comprehensive collection of **manuals**, **videos**, **user applications**, and **method development tools**. These are located on the:

- Agilent GC and GC/MS Manuals and Tools DVD set
- Agilent GC/MS Software Information and Manuals memory stick

	To Install Your Hardware Library
	Insert Disk 1 into your DVD drive and follow the prompts.
	This can be installed by anyone who has authority to copy information onto the receiving computer.
(To Install Your Software Library
	To Install Your Software Library Insert the memory stick into a USB port and follow the prompts.

See the **Agilent 5977 Series MSD System Quick Start** document (**G3870-90103**) for more details on how to install this information on your computer.

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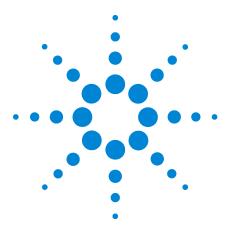
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Introduction

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Included in this Chapter is a general list of steps to follow when you start up your hardware. Also included is a brief introduction to tuning and an explanation of how to run an autotune on the instrument.



Start up the Hardware

Below is a general list of steps to follow when you start up your hardware.

- 1 Review the Agilent Gas Chromatograph and MSD Operating Guides for important safety information and start up details before powering on your instruments.
- 2 Verify that the inlet septum, liner, and O-ring are clean, properly installed, and in good condition.
- **3** Install a conditioned column that is appropriate for your method in the GC. Attach the column inlet to the inlet and its outlet to the MSD transfer line. See the Agilent MSD Operation Manual for details.
- **4** Verify the ion source is installed.
- 5 Verify the carrier gas required by your method is attached to your inlet.
- **6** Power on the Agilent GC.
- 7 From the GC keypad, turn off the oven, Aux 2 heated zone (GC/MSD transfer line), and inlet heater. If equipped, turn off any GC detectors.
- 8 Before you turn on or attempt to operate the MSD verify the following:
 - The vent valve must be closed (the knob turned all the way clockwise).
 - All other vacuum seals and fittings must be in place and fastened correctly.
 - The front side plate screw should not be tightened.
 - The MSD is connected to a grounded power source.
 - The GC/MSD interface extends into the GC oven.
 - A conditioned capillary column is installed in the GC inlet and in the GC/MSD interface.
 - The GC is on, but the heated zones for the GC/MSD interface, the GC inlet, and the oven are off.
 - Carrier gas of at least 99.9995% purity is plumbed to the GC with the recommended traps.
 - The foreline pump exhaust is properly vented.
- **9** Open the MSD analyzer top cover.
- **10** Close the MSD vent valve.

- 11 Press the Power button on the front of the MSD to power it on. The foreline pump will make a gurgling noise.Press lightly on the metal box mounted on the MSD side board until the air noise stops to ensure a correct seal.
- **12** Close the MSD analyzer top cover.
- **13** One the MSD local control panel:
 - a Press Menu repeatedly until Maintenance appears.
 - **b** Press **Item** repeatedly until **Pumpdown** appears.
 - c Press Yes/Select to start the pumpdown.

The pumpdown is completed automatically and does not require operator actions.

After the turbo pump starts and the ion gauge valve reaches 100 mTorr, allow the MSD to operate for a minimum of 2 hours before acquiring sample data.

Tune your MS

Tuning is the process that adjusts the MS for good performance over the entire mass range. Using a known compound as a calibrator, the tune parameters are set to achieve sensitivity, resolution, and mass assignments for the known calibration ions.

Tuning is performed using either the autotune or manual tune features.

The autotune program described in this section adjusts the MS for good performance over the entire mass range and is recommended for most applications.

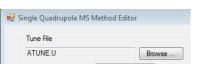
Manual tune allows you to adjust an MS tune parameter while viewing the results easily in profile scans and spectra.

Manual tuning is used:

- To achieve maximum sensitivity by sacrificing some resolution
- To tune specifically for the very low end of the mass range (< 150 amu)
- To tune with a compound other than the standard calibrator

Run Autotune

- **1** From the PC desktop, select the Instrument Control shortcut icon to open MassHunter Data Acquisition.
- 2 Select Method/Load Method then navigate to and select the method you want to use for data acquisition (e.g., default.m in the MassHunter/GCMS/1/methods directory), and click OK.
- **3** To check which Tune file is currently associated with your method, in the Instrument Control view, click the **Instrument MS Parameters** icon to display the Quadrupole Method Editor dialog.
- 4 In the Tune File group, verify the tune file shown is the one you wish to use for this method. (Atune.U is a good choice.) Click **Browse** and select a new one if necessary.



5 Click the **MS Tune** icon to display the Select Tune Type dialog.



💀 Select Tune Type	
Tune MSD	
QuickTune	
Manual Tune	
OK Cancel	Help



- **6** Select **Tune MSD** to perform a complete autotune, or select **Quick Tune** to adjust peak width, mass assignment, and abundance, without changing ion ratios. Alternatively, select **Manual Tune** to display the Manual Tune dialog and graphs for doing manual edits to the Tune file.
- 7 Click **OK** to close this dialog and start the tune.
- 8 Wait for the tune to complete and to generate the report.
- 9 To evaluate the tune results, select Evaluate Tune from the Checkout menu. To view history of tune results, in the Instrument Control view select Checkout > View Previous Tunes....

See the online Help provided with your MassHunter Data Acquisition software for additional information about tuning.

1 Introduction



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Create a Scan Method

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A good way to create a new method is to begin with an existing one, edit the settings, and save it as a new method, using the **Edit Entire Method** option.

This chapter describes how to use the **Edit Entire Method** option to open the default method and modify its Method Information and Instrument/Acquisition settings to represent a scan method, then save it as a new method name.



Edit the Entire Method Option - Overview

For this example, we will modify the Method Information and Instrument/Acquisition settings of the default method to represent a scan method. During this process you will be presented with 7 primary dialogs. Each is described on the following pages.

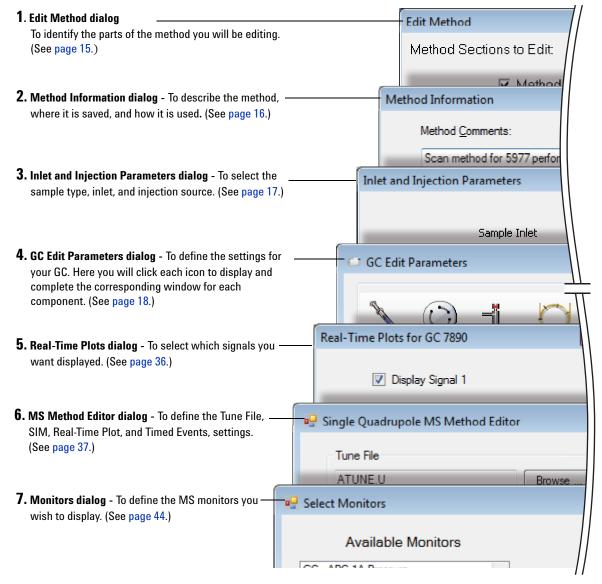


Figure 2 Edit the entire method option - overview

1) Edit Method Dialog

The first dialog you will see when you select the **Edit Entire Method** option is the Edit Method dialog.

Here you will identify the parts of the method you want to address as you create your method.

To begin the process:

- 1 Click the Load Method icon , or select Method/Load Method.
- 2 Navigate to and select the method you want to start with (e.g., default.m in the MassHunter/GCMS/1/methods directory), and click OK.
- **3** Select **Method/Edit Entire Method**...The dit Method dialog opens.
- 4 Check each section you want included in this method.
 - **Method Information** To provide a description of the method, specify whether or not to save a copy of the method with the collected data, and define what parts of the method sections to run.
 - **Instrument/Acquisition** To have the Edit Entire Method process display all the dialogs required to edit the acquisition parameters for both the GC and MS parts of the currently loaded method.
 - **Data Analysis -** To display the Data Analysis portions of the method. Data Analysis settings are beyond the scope of this guide, so we are not including data analysis in our example.
- 5 Click **OK** to close the Edit Method dialog and continue. The Method Information dialog opens.

Edit Method	×							
Method Sections to Edit:								
Method Information								
Instrument / Acquisition								
🗖 Data Analysis								
OK Cancel Help								

Figure 3 Edit Method dialog

2) Method Information Dialog

In the Method Information dialog you will provide a description of the method, decide whether or not to save a copy of the method with the collected data, and define what parts of the method sections to run. For example:

- 1 In the **Method Comments** field, enter a description of this method.
- 2 Mark the **Save Copy of Method With Data** checkbox. This causes MassHunter to save a copy of the method along with the sample data collected.
- 3 In the **Method Sections to Run** group box, mark the **Data Acquisition** checkbox only. This specifies that the Data Acquisition will run when this method is used, but the data analysis and post-run macros will not be run.
- 4 Click **OK** to close the Method Information dialog. Because we are running the Edit Entire Method option, and we did check the Instrument/Acquisition option in the previous step, the Inlet and Injection Parameters dialog displays next.

Method Information	×
Method <u>C</u> omments:	
Scan method for 5977 performance sample	
Save Copy of Method With Data	
Method Sections to Run	
Pre-Run Macros/Commands	_
Instrument Control: Browse	
Data Analysis: Browse	
☑ Data <u>A</u> cquisition	
Data Anal <u>v</u> sis	
Post-Run Macros/Commands	
Instrument Control: Browse	
Data Analysis: Browse	
OK Cancel <u>H</u> elp	

Figure 4 Method Information dialog

3) Inlet and Injection Parameters Dialog

In the Inlet and Injection Parameters dialog you will specify the Sample inlet and Injection Source and the inlet and MS locations.

- 1 From the Sample Inlet dropdown list, select GC.
- 2 From the **Injection Source** dropdown list, select your source.
 - If you are injecting from the GC using the Automatic Liquid Sampler (**ALS**), select **GC ALS**.
 - If you are manually injecting or using another injection source, select **Manual**.
- 3 Mark the **Use MS** checkbox to allow MassHunter to turn on the MS analyzer and save the MS sample data acquired during the run. Uncheck this box only if you do no want to collect Mass Spec data. For example, you would uncheck this box if you are running a GC (non-MS) detector and you were acquiring data for the GC detector only.
- 4 In the **Inlet Location** box, select the location where your inlet is attached to the MS through the column.
- **5** In the **MS Connected to** box, select the location where your inlet is attached to the MS through the column.
- 6 Click **OK** to close the Inlet and injection Parameters dialog. Because we are running the Edit Entire Method option, the **GC Edit Parameters** window displays next.

Inlet and Injection	Parameters			×
	Sample Inlet	GC	•	
	Injection Source	GC ALS	•	
		🔽 Use MS		
- Inlet Location	Front	C Rear	C Dual	
MS Connected to	• Front Inle	et	🔿 Rear Inlet	
ОК		Cancel	Help	

Figure 5 Inlet and Injection Parameters dialog

4) GC Edit Parameters Dialog

The **GC Edit Parameters** window contains several icons. Each icon contains one or more panels where you will define the GC instrument settings. We will go through each one here.

To begin, we will address the Configuration panel because some of the settings made here will affect settings in other panels.

GC Configuration panel

On the **Configuration** panel, there are four 4 tabs:

- Miscellaneous
- Columns
- Modules
- ALS

The following pages include a general description of the settings used in these tabs. Check the online **Help** for additional details.

Miscellaneo Pr essure	ous Columns Modules		e Config	uration				
psi	•		-	Valve Type		Name	Parameters	
Oven		•	1	Gas Sampling Valve	•	(Valve #1)	Loop Volume, mL: 1	
🔳 S	Slow Fan		2	Not Installed	•	(Valve #2)		
			3	Not Installed	•	(Valve #3)		
			4	Not Installed	•	(Valve #4)		
			5	Not Installed	•	(Valve #5)		
	Thermal Aux Type		6	Not Installed	•	(Valve #6)		
▶ 1	Not Installed		7	Not Installed	•	(Valve #7)		
2	MSD Transfer Line		8	Not Installed	•	(Valve #8)		
3	Not Installed							

Figure 6 Configuration panel

GC Configuration panel - Miscellaneous tab

Under the **Miscellaneous** tab you will define your method's pressure units, configure valve types and oven fan parameters (slow fan_), and view the thermal aux configuration.

Pressure Units psi 🔹	Valve Config					
Oven		Valve Type	_	Name	Parameters	
	▶ 1	Gas Sampling Valve	-	(Valve #1)	Loop Volume, mL: 1	
Slow Fan	2	Not Installed	-	(Valve #2)		
	3	Not Installed	-	(Valve #3)		
	4	Not Installed	-	(Valve #4)		
	5	Not Installed	-	(Valve #5)		
Thermal Aux Type	6	Not Installed	•	(Valve #6)		
1 Not Installed	7	Not Installed	•	(Valve #7)		
2 MSD Transfer Line	8	Not Installed	•	(Valve #8)		
3 Not Installed						

Figure 7 GC Configuration panel - Miscellaneous tab

GC Configuration panel - Columns tab

Under the **Configuration > Columns** tab you will define and configure a column for each position (1-6) in your GC. You can also calibrate a column, lock a column's configuration, describe how each column connects to GC devices, and tell the system how each column is heated.

		Columns Modules ALS		Catalog	Calibrate	Remove	
						Column Outlet Pres	ssure:
				1		0 psi	
∧∥		Column	Calibration Results	Inlet	Outlet	Heated By	
₽	1	Agilent 19091S-433: 12345 HP-5MS 5% Phenyl Methyl Silox -60 °C–325 °C (325 °C): 30 m x 250 μm x 0.25 μm	Uncalibrated	Front Inlet	MSD	Oven	•
	2	<not inventoried=""> -60 °C-450 °C (450 °C): 25 m x 320 µm x 0 µm</not>	Uncalibrated	Back Inlet	Back Detector	▼ Oven	•
[3	No Column Installed	Uncalibrated	Unspecified	▼ Other	▼ Oven	-
(4	No Column Installed	Uncalibrated	Unspecified	▼ Other	▼ Oven	•
1	5	No Column Installed	Uncalibrated	Unspecified	▼ Other	▼ Oven	•
		No Column Installed	Uncalibrated	Unspecified	▼ Other	▼ Oven	-

Figure 8 GC Configuration panel - Columns tab

GC Configuration panel - Modules tab

Under the **Configuration > Modules** tab you will define the gas types for your inlets, detectors, and any Aux EPC modules.

J GC Edit F	Parameters											- • •
ALS	Valves		Olumns	Oven	Detectors	LOS Aux Heaters	Events	 Signals	Configuration	1,2, Counters	Readiness	1
Miscellan	eous Colur		Front Inlet SS Inlet Back Inlet COC Inlet	t He	•							
			t Detector FID Makeup		•							
		Back	Affset with C Detector TCD		pard.							
			P/Reference EPC 4.5.6 Aux EPC 4 Aux EPC 5	4 N2	 							
			Aux EPC 6		▼ ▼							

Figure 9 GC Configuration panel - Modules tab

GC Configuration panel - ALS tab

If you have a front or back injector installed, under the **Configuration > ALS** tab you will see the installed injector type and current firmware revision.

From here you will set the configuration parameters to match your installed syringe and desired wash mode.

The configured syringe information must match the actual syringe to achieve accurate injection amounts.

Depending upon the installed injector and turret, these parameters may be available to configure multiple solvent wash bottles usage. If necessary, refer to your injector user documentation for details.

CAUTION

Some syringes are labeled so that the labeled syringe size reflects the maximum injectable volume, rather than the full syringe volume. The maximum injectable volume for a syringe installed in an Agilent injector is 50% of the full syringe volume. If the highest syringe volume marking is only halfway up the syringe barrel, enter double that value as the syringe size. Agilent systems calculate injection volume based on full plunger stroke.

ALS Valves Inlets Columns Over		N 1,2, = _
liscellaneous Columns Modules ALS		
Front Injector G2613A	Firmware rev: A.10.07	Tray G2614A Firmware rev.: A.02.01
	 A. B A-A2,B-B2 A-A3,B-B3 	Enable 3 of 9 barcode Enable 2 of 5 barcode Enable UPC barcode Enable Barcode Checksum
Back Injector G2913A	Firmware rev: A.11.03	
Syringe Size: 10 µL	Solvent Wash Mode	

Figure 10 GC Configuration panel - ALS tab

GC ALS panel

ALS - Front/Back Injector tab

Use the **Front/Back Injector** panels to configure injection parameters, washes and pumps settings, dwell time, plunger speed, sample depth, and the type of your injections.

Note that wash behavior varies depending on syringe size:

- For 100-uL and smaller syringes, the sampler draws the solvent volume specified in the Volume field. After the needle leaves the wash solvent, the injector draws the plunger up until the solvent slug rinses 80% of the syringe volume, then dispenses to waste.
- For 250-uL and larger syringes, the injector draws and dispenses the exact wash volume of solvent specified in the Volume field. The injector rinses only the volume specified.

GC Edit Parameters		
ALS Valves Inlets Columns Oven Detectors	Aux Heaters Events Signals Configuration Court	
Front Injector Back Injector Tray / Other		
In jection Syringe Size: 10 µL	Dwell Time Pre-Injection: 0 min Post-Injection: 0 min	
Injection Volume: $1 \mu L$ × $1 = 1 \mu L$ Multiple Injection Delay: 0 sec	Plunger Speed	
	Draw Dispense	
Washes and Pumps	Solvent Wash 300 μL/min 6000 μL/min	
Prelnj Postlnj Volume (µL)	Sample Wash 300 µL/min 6000 µL/min	
Solvent A Washes: 0 0 Max 🗸	Inject 6000 µL/min	
Solvent B Washes: 0 0 Max Sample Washes: 0 Max	Viscosity Delay: 7 💌 sec	
Sample Pumps: 1	Sample Depth	
	Enable 0 mm	
~~	Tower Fan	
	✓ Tower fan on	

Figure 11 ALS - Front/Back Injector parameters

ALS - Tray/Other tab

Use the **Tray/Other** tab to set the barcode reader, vial mixer, and vial heater parameters, if installed and supported on your system.

Sample overlap is also set on the Tray/Other tab. Sample overlap can increase throughput by allowing the ALS to begin processing the next sample before the current run finishes. ALS sample preparation does not have to be finished before the current runs ends.

To use Sample Overlap, select **Enable Sample Overlap**, then select the preferred timing for the overlap and enter a time (in minutes) as needed.

C GC Edit Parameters							
ALS Valves Inlets Columns Oven Detectors	Aux Heaters	Events	Signals	Configuration	1,2, Counters	Readiness	
Front Injector Back Injector Tray / Other							
Sample Overtap							
After the previous injection is completed							
Prepare sample Omin before end of GC run							
Prepare sample Omin after end of GC run							
ALS Errors: Pause for user interaction							

Figure 12 ALS - Tray/Other parameters

GC Valves panel

The **Valves** icon is available only if your GC and method configuration have installed and configured valves.

Refer to your GC documentation to determine the valve types and capabilities available with your GC type.

In a method you can specify the initial setting for valve parameters such as the On/Off state, Position, Load Time (min), and Inject Time (min) depending on the valves configured in your GC.

#1	Type Gas Sampling Valve	On	Position N/A	Load Time (min) 0.05	Inject Time (min) 0.05
#1	Not Installed		N/A	N/A	N/A
#2	Not Installed		N/A	N/A	N/A
#4	Not Installed		N/A	N/A	N/A
#5	Not Installed		N/A	N/A	N/A
#6	Not Installed		N/A	N/A	N/A
#7	Not Installed		N/A	N/A	N/A
#8	Not Installed		N/A	N/A	N/A

Figure 13 GC Valves panel

GC Inlets panel

Use the **Inlets** panel to set parameters for the front and back inlet installed in your GC. This example shows Split / Splitless (SSL) inlet parameters and setpoints. The column can be either pressure or flow controlled.

NOTE

Settings made in Columns Parameters automatically modify Pressure and Flow parameters in Inlet Parameters, and vice versa. For example, entering a Column panel Pressure of 30 psi sets Inlet panel Pressure to 30 psi.

The actual GC parameter value for each setpoint displays next to the setpoint field.

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. Gas Saver can be used in any column mode.

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.

🚥 GC Edit P	arameters											
ALS	()) Valves	⊣ Inlets	Ocolumns	(D) Oven	Detectors	Aux Heaters	Events	Signals	Configuration	1,2, n Counters	Readiness	
SSL - Fro	nt COC - Ba	ack										
Split-	Splitless	Inlet					Gas Saver:					
			Setpoint	t			Gas saver. ▼ On					
V H	leater:		250 °C]		20 mL/min		After:	3 min		
V F	Pressure:		1.1739	psi]							
т	otal Flow:		100.46	mL/min]							
S	Septum Purge	e Flow:	3 mL/m	nin]							
Septu	m Purge Flov	v Mode:	Standard	•								
Mod	de: Sol	litless	•	Purg	ge Flow to Split	Vent:						
		10000) mL/min		at 1 mir	ı				

Figure 14 GC Inlet panel

GC Columns panel

Use the **Columns** panel to control column flow and pressure behavior during the run.

Column parameters are available only if your GC and method configuration have installed and configured columns.

From the Selection box, select the desired column or auxiliary pressure control device for your method.

Click the **Control Mode** checkbox to enable the inlet EPC control, then configure the column Flow, Pressure, Average Velocity, and Holdup Time parameters.

Select a constant pressure, constant flow, ramped pressure, or ramped flow program. If you selected a ramped pressure or ramped flow program, configure the ramp table.

If desired, you can change an installed column using the Change Column option.

ALS Valves Inlets Columns Oven Detectors Au # Selection Aglent 19091S-433: 12345 FHP-5N5 5% Phenyl Methyl Silox Control M 1 Aglent 5% Phenyl Methyl Silox Control M Control M 1 -60 °C-325 °C (325 °C): 30 m x 250 µm x 0.25 µm Control M Control M 2 -60 °C-450 °C (450 °C): 25 m x 320 µm x 0 µm N: Back COC Inlet He Aux EPC 4 N2	Image: Signals Image
Agilent 19091S-433: 12345 HP-5MS 5% Phenyl Methyl Silox 1 -60 °C-325 °C (325 °C): 30 m x 250 μm x 0.25 μm In: Front SS Inlet He Out: MSD -60 °C-450 °C (450 °C): 25 m x 320 μm x 0 μm In: Back COC Inlet He Out: Back Detector TCD	Setpoint Flow 0.45587 mL/min Pressure 1.1739 psi Average Velocity 24.844 cm/sec
2 -60 °C-450 °C (450 °C): 25 m x 320 µm x 0 µm In: Back COC Inlet He Out: Back Detector TCD	Average Velocity 24.844 cm/sec (Initial): 0 min
Aux EPC 5 N2	Holdup Time 2.0125 min Out: MSD 30 m x 250 µm x 0.25 µm
Aux EPC 6 N2	Post Run: 0.57353 mL/min Column #1 Configuration Change Column Calibrate Column
<<< Only Show Columns >>>	

Figure 15 GC Columns panel

GC Oven panel

Use the **Oven** panel to control oven temperature parameters and to configure temperature ramps during and following a run.

If the current heater settings will adversely affect the columns you have specified for this method, they will be highlighted in yellow. Change the column selections, or your heater settings to resolve the problem before continuing.

Note that the oven total **Run Time** controls the maximum Run Time in all other flow, pressure, and temperature programs. For example, inlet and column program times cannot exceed the total oven Run Time.

Select **Override Column Max** (in °C) if you need to allow an oven temperature greater than the column maximum temperature setpoint. If the Maximum Oven Temperature is greater than the column maximum temperature, this label highlights.

The **Post Run** temperature value is the temperature at which the oven heats or cools to and holds for the specified time in the **Post Run Time** field. Set these if appropriate for your method.

GC Edit Parameters							
ALS Valves Inlets Columns		Aux Heaters	فی Events	Signals	1	A unters Readiness	
📝 Oven Temp On		Rate °C/mir		Value °C	Hold Time min	Run Time min]
70 °C	• (Initial)				70 1.5	1.5	
Equilibration Time	Ramp 1		16	2	00 0.5	10.125	
0.5 min	*						
325 °C							
		Post Run: (L				

Figure 16 GC Oven panel

GC Detector panel

Select the **Detectors** icon to open the Detectors panel and set parameters that control the front, back, and auxiliary detectors on your GC. The detector control parameters you see are based upon the type of detector you have installed and configured.

For example, if you have a Flame Ionization Detector (FID) detector, you would see a screen similar to this one.

The FID passes sample and carrier gas from the column through a hydrogen-air flame. The hydrogen-air flame alone creates few ions, but, when an organic compound is burned, there is an increase in ions produced. A polarizing voltage attracts these ions to a collector. The current produced is proportional to the amount of sample being burned. An electrometer senses the current, converts it to digital form, and sends the data as output.

Complete the Heater, Air Flow, H2 Flow, Makeup Flow settings as appropriate for your method. See the online Help for more details on each of these settings.

ALS Valves Inlets Columns Oven Detectors Aux Heaters Events	Signals Configuration Counters Readiness
Setpoint	FID Subtract from Signal: (a) (Nothing) (c) Column Compensation Curve #1 (c) Column Compensation Curve #2

Figure 17 Detector panel

GC Aux Heaters panel

Select the **Aux Heaters** icon to open the **Aux Heaters** panel and set parameters that enable or disable an auxiliary heated zone and control its temperature.

Typically, a Thermal Aux zone is used to control a heated valve box. Other uses include heated transfer lines for a mass spectrometer (MSD) or atomic emission detector (AED).

A given device connected to an auxiliary heated zone may have an upper limit in temperature above which damage could occur. Be sure to enter a temperature that is lower than the column maximum temperature and the temperature that would degrade the compounds you are trying to analyze.

0	GC Edit F	arameters											
	ALS	() Valves	⊣ Inlets	Columns	Oven	Detectors	Aux Heaters	فی Events	 Signals	Configuration	1,2, Counters	Readiness	1
	Ther	mal Aux	2 (MSD	Transfer	Line)								
	🔽 On												
	134 °C	:											
	L												

Figure 18 GC Aux Heaters panel

GC Events panel

Use **Events** panel to schedule events to occur automatically during a run. The events available depend on the hardware installed on your GC.

At the end of a run, the program automatically returns all setpoints to their original values, except for Switching Valve state changes. If you rotate a switching valve as a run time event, the program does not automatically return it to its initial setpoint position at the end of the run. You must specify this reset operation as a run time event.

For example, you could:

- Set a new detector fuel gas flow, or turn on/off (if applicable for the detector)
- Turn the valve On/Off
- Change an inlet's septum purge flow, or turn on/off (if applicable for the inlet)
- Use to change the source signal for Signal 1 and Signal 2 analog outputs

Please read online Help for more details on this option.

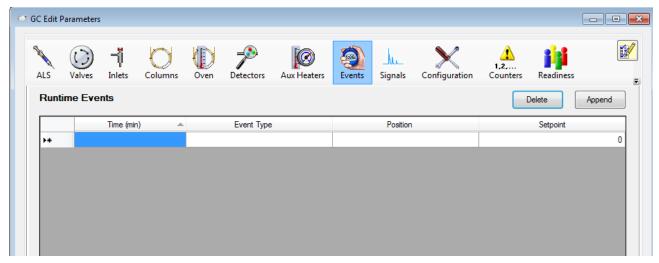


Figure 19 GC Events panel

GC Signals panel

On the **GC Signals panel**, you will identify the source of the signals and the data capture rate, plus what readings you want to display or save in a data file as output of the run.

For the Oven, for example, you can record the actual setpoint, the power, or the duty cycle of the oven. For the front inlet you can record the pressure and the actual setpoints or the inlet flow.

For every place that there are sensors recording data, you can elect to record that data. If you navigate through all of the possible settings here, you will see there are many variations from which to choose.

GC Edit Parameter	5											
ALS Valves	- T Inlets	Columns	Oven	Detectors	Aux He	aters	Events	Signals	Configuration	1,2, Counters	Readiness	
	Dual F B	Signal Source #1: Front Sig #2: Diagnos	gnal (FID)	lot		500 H	ate / Min F Hz / 0.0004 z / 0.004 m		Zero	Save		
	B None B Front Signal (FID)				•		lz / 0.0004 lz / 0.0004		• □ • □			
	Hide Dual	Back S	Signal (TCE ostics	L	 Test Plo 							
Delete Events	Signal Ev Si ▶*	ent Table gnal Source		Tin	Ambier Oven Front Ir Back In Aux 2 Column Front D Back Do Aux EP0	let (SS) let (CO) n etector	Inlet) C Inlet) (FID)	•	Actual Setpoint Power Duty Cycle	•		
Apply		ОК		Cancel		<u>H</u> el	p					

Figure 20 GC Signals panel

GC Counters panel

Use the **Counters** panel to identify the items you want to track as they are used each time this method is processed.

For example, if you are using the Front Inlet Liner and Front Inlet Gold Seal and you would like to keep track of how many times these have been used, you could check these items here. Then, each time this method is run, the total usage counters for these items is tracked by the GC.

🚥 GC Edi	it Parameter	5										
ALS	Valves	- j Inlets	Columns	(I) Oven	Detectors	LIO Aux Heaters	Events	 Signals	Configuration	1,2, Counters	Readiness	
EMF	F Counters											
	Indicate w	hich counte	ers should be m	onitored wh	ien this method	is run.						
		Front Inlet Back Inlet Back Inlet Back Inlet Back Inlet Back Inlet Front Dete Back Dete Column 1 Column 2 Column 3 Column 4 Column 6 Front Injec	Liner Gold Seal Split Vent Trap Top Weldment Septum Liner	oring coring r r yringe)								
	Apply		ОК		Cancel	<u>H</u> e	elp					

Figure 21 GC Counters panel

GC Readiness panel

Use the **Readiness** panel to select which instrument components your method requires to be *ready* before a run starts.

For example, if you are using the Oven and it needs to be at a specific temperature before the run starts, you should check the Oven checkbox here so the instrument will wait for the oven to reach the specified temperature before posting the **Ready** prompt.

This feature is useful if you wish to ignore the readiness state of hardware that is not used in your method. For example, if you use only the front detector, you do not need to wait for the back detector to reach temperature before starting the run, so you would leave the back detector checkbox unchecked.

🚥 GC Edit	Parameters	5										
ALS	() Valves	⊣ Inlets	Columns	(ID) Oven	Detectors	Aux Heaters	فی Events	Signals	Configuration	1,2, Counters	Readiness	(
			ents from			GC's Readi	iness S	tate				
	Bac Fro Bac Aup Aup	nt Inlet (SS ck Inlet (CC int Detector ck Detector x EPC 4 x EPC 5 x EPC 6	C Inlet) (FID)	r Line)								
	Chec	ck All										
A	pply		ОК		Cancel	<u>H</u> e	elp					

Figure 22 GC Readiness state panel

GC Calculators panel

You can use the **GC Calculator** panel to help you translate methods, pressure flows, solvent vent calculations, etc.

The calculations you receive here are for information purposes only. They are not saved as part of the method.



Figure 23 GC Calculators panel

5) Real-Time Plots for GC Dialog

When you have finished entering all your GC parameters, click **OK** to close the GC Edit Parameters window.

The next window that displays as part of the Edit Entire Method routine is the Real-Time Plots dialog.

Use the Real-Time Plots dialog to identify which GC signals you want displayed as real-time plots in the Instrument Control panel during the run.

Select **OK** to save the settings you make here, and close the dialog box. The MS Method Editor dialog displays next.

Real-Time Plots for GC 7890								
✓ Display Signal 1								
Display Signal 2								
Display Signal 3								
Display Signal 4								
Continuous GC Real-Time Plots								
OK Cancel Help								

Figure 24 GC Real-Time Plots dialog

6) MS Method Editor Dialog - Scan Method Setup

This dialog box is used to enter instrument parameters, select parameters to record during the run, and specify the curves to appear as real-time plots for the MS part of a method.

Sections of the MS Editor dialog

The screen capture shown below, shows three general areas:

- 1 Applies to all methods; Scan, SIM, or SIM/SCAN. (See "Sections to complete for all methods" on page 38.)
- 2 Applies to Scan methods only. (See "Settings for Scan Methods" on page 42)
- 3 Applies to SIM methods only. (See "Create a SIM Method MS Method Editor Dialog" on page 47).

In this example, we are creating a Scan method. So we will be completing the sections labeled 1 and 2.

Single Quadrupole MS Method Editor		×
Tune File		SIM Real-Time Plot Timed Events
ATUNE.U Browse	Bun Time 10.00 min	
Tune Type El	Solvent Delay 3.00 min	m/z Dwell Time Plot Ion → 74.10 100
Tune EMV 1200	Detector Setting	*
CI Gas Valve:	Trace Ion Detection	
CI Row: %	EM Setting: Gain Factor 💌	
Actual Setpoint	Gain Factor 1.000	
MS Source Offline 230 MS Quad Offline 150 Apply	Applied EM Voltage (V) 500	
MS Guad Offline 150		
Acquisition Type Scan	EM Saver Limit Sum Limit 1e8 (Default)	
Scan Time Segments		
Time Start End Mass Threshold Sca	n Speed (u/s) Frequency Cycle Time Step Size (scans/sec) (ms) (m/z)	
► 3.00 50.00 550.00 150	1,562 [N=2] ▼ 2.9 340.06 0.1	
SIM Time Segments		
Time Group Name Num	The Total Dwell Time Deschates Calculated	
3.00 1	1 100 5.9809 Low -	
*		
Method Last Saved: 11/4/2012 8:09:46 PM		OK Cancel Help



Sections to complete for all methods

Regardless of the type of method you are creating, SIM, Scan, or SIM/Scan, you will complete the:

Tune File group box	Detector Settings group box
Acquisition Type	Real-Time Plot tab
Run Time	Timed Events tab
Solvent Delay	

Each of these entries are described in this section.

Tune File group box

- The **Tune file name** displays the current tune file selected for the method. Autotune is a good choice. However, you may click **Browse** to select a different one.
- The **Tune Type** Displays the ion source and polarity configured when the tune file was obtained.
- **Tune EMV** Displays the EMV setting configured when the tune file was obtained.
- **CI Gas Valve** Displays the channel selected for reagent gas.
- **CI Flow** A read only field obtained from the method's tune file.
- **MS Source and MS Quad** Displays the MS Source and MS Quad setpoint values used during the method's tune and the current temperatures. Click **Apply** to send the MS Source and MS Quad temperature setpoints to the instrument for immediate control to these setpoint values.

Check online Help for more details on the Tune File.

Tune File ATUNE.U		D	Run Time	10.00	min	SI		leal-
		Browse	Solvent Delay	3.00				m
Tune Type	EI			3.00	min		►	74
Tune EMV	1200		Detector Setting				*	-
CI Gas Valve:			Trace lon Det	ection				
CI Flow:		%	M Setting:	Gain Factor	•			
A MS Source	Offline 230		Ciain Factor	1.000				
MS Quad	Offline 150	Apply	pplied EM Volta	ge (V) 500				

Figure 26 MS Method Editor dialog - Tune File group box

Acquisition Type

Under the **Acquisition Type** dropdown menu, select Scan (RAW) to create a Scan method. Scan stores all data.

Run Time

When the acquisition instrument is configured without a GC, the value entered in the Run time is the time span during which MS data is acquired. MS data is not collected during the solvent delay. If a GC is configured, its run time is used.

Solvent Delay

The solvent delay is the time in minutes after the start of the run when the mass spectrometer is turned on.

ATUNE.U		Browse	🔄 <u>R</u> un Time	10.00	min
Tune Type	El		Solvent Delay	3.00	min
Tune EMV	1200		Detector Setting		
CI Gas Valve:			Trace Ion Detection		
CI Flow:		%	EM Setting: Gain	Factor	•
MS Source	Actual Setpoint Offline 230		Gain Factor	1.000	
MS Quad	Offline 150	Apply	Applied EM Voltage (V)	500	

Figure 27 MS Method Editor dialog - Acquisition Type, Run Time, and Solvent Delay

Detector Settings

• Check the Trace Ion Detection checkbox to turn this feature ON.

Trace Ion Detection (TID) allows you to obtain lower Method Detection Limits (MDL's) during analysis. It decreases the noise content of Total and Extracted Ion Chromatograms.

The lower noise level results in more reproducible baselines for calculating the peak height and peak area for analyses and standards.

TID also reduces the number of peaks requiring manual integration in complex chromatograms.

Trace Ion Detection will be reported in Print Method.

- Under EM Setting, select one of the following:
 - Gain Factor The default and also the recommended EM.
 - Delta EMV Delta EMV is not recommended for most applications.
 - Absolute EMV

See online Help for more details on these settings.

• **Gain Factor** - If **Gain Factor** is selected in the **EM Setting** drop-down list, the Gain Factor can be specified here.

An EM gain factor adjusts the signal sensitivity of the detector. EM gain factors have the advantage of remaining constant as the multiplier ages. Therefore, the use of a gain factor produces much higher signal reproducibility for any instrument and better consistency between instruments.

- **Applied EM Voltage** is a read only field that displays the electron multiplier voltage reading of the detector.
- To use **EM Saver**, select this checkbox and then select a **Limit**. This feature is only available in SIM mode.

EM Saver is used to prevent a non-linear detector response at the upper range of a compound's calibration curve. This non-linear response can be caused by setting the gain value or dwell time too high on compounds with high ion concentrations. With EM saver, high gain values and dwell times can be used without saturating the EM.

EM Saver is used with SIM mode in a single quadrupole configuration and MRM mode in a triple quadrupole configuration. A benefit of using EM saver is a more consistent detector response and an extended EM life.

Tune Type	El		Solvenii Delay	3.00 Milli
Tune EMV	1200]	Detector Setting	
CI Gas Valve:]	Trace Ion Detection	'n
CI Flow:		%	EM Setting: Gai	in Factor
MS Source	Actual Setpoint Offline 230		Gain Factor	1.000
MS Quad	r	<u>A</u> pply	Applied EM Voltage (V) 500
Acquisition Type	Scan	•	EM Saver Lim	nit Sum Limit 1e8 (Default) 👻
Scan Time Segment	s			
Time	Start End Thre	shold S	can Speed (u/s)	ency Cycle Time Step Size

Figure 28 MS Method Editor dialog - Detector Settings

Real-Time Plot tab

Use the **Real-Time Plot** tab, to specify the Spectrum and Chromatogram for display in the real-time plots dialogs in Instrument Control view. Also specify Extracted Ion Chromatograms to display the EIC in the Instrument Control view Chromatogram panel with the label you specify here.

Timed Events tab

Use the Timed Events tab to schedule an event that you want to occur during a specified time in the data acquisition run.

SIM	Real-Time Plot Timed Eve	nts					
v	Total Ion Chromatogram						
V S	Spectrum						
	Base Peak Chromatogram						
Extra	acted Ion Chromatogram Dis	play	SIM F	leal-Time Pl	ot Timed Events	Parameter	
	Label	Mass or Mass Range					
•	Scan 1-1	50.00-550.00					
*							

Figure 29 MS Method Editor dialog - Real-Time Plot and Timed Events tabs

Settings for Scan Methods

.

When you are creating a Scan method, you will complete the sections labeled 1 and 2 of the MS Editor dialog (show in Figure 30).

- Items included in Section 1 were described in "Sections to complete for all methods" on page 38.
- The following describes how to complete the entries for Section 2, which apply to Scan methods.
- Section 3 is for creating SIM methods, and is discussed in Chapter 3, "Create a SIM Quantitation Method" on page 45.

	Quadrupole	e MS Meth	od Editor						_						×
Tun	e File									-	SIM	Real-Time Plot	Timed Events		
AT	UNE.U		Browse		Run Time		10.00 min				_				
Tu	ne Type	EI			olvent Delay		3.00 min				•	m/z 74.10	Dwell Time 100	Plot Ion	/
	ne EMV	120	0	D	etector Setting						*	74.10	100		
CI	Gas Valve:			[Trace Ion D	letection			_		*				
CI	Flow		%		EM Setting:	Gain Facto	r	•	_						
		Actual	Setpoint		Gain Factor		000	_							
MS	Source	Offline	230		Applied EM Vol			_							
MS	Quad	Offline	150 Apply		Abblied Fivi vol	tage (v) 3L	JU								
	_				EM Saver	Limit S	um Limit 1e8 (0)efault)	-						
		Scan	•												
Scan T	ime Segments		End To date			Frequency	Cycle Time	Step Size	-						
	Time	Mass	Mass	Scan Sp		(scans/sec)	(ms)	(m/z)							
•	3.00	50.00	550.00 150	1	562 [N=2] 🔻	2.	9 34	0.06	0.1						
SIM T															
	me Segmente														
	me Segments	-		Number	Total Dwall	Cycle		Gain	Colordated						
	me Segments Time	-	o Name	Number of lons	Total Dwell Time (ms)	Cycle Time (Hz)	Resolution	Gain Factor	Calculated EMV	1					
	Time	-) Name 1	Number of lons	Total Dwell Time (ms) 100	Time	Resolution	Gain Factor	Calculated						
*	Time	Group		of lons	Time (ms)	Time (Hz)		Factor	Calculated EMV						
	Time	Group		of lons	Time (ms)	Time (Hz)	Low -	Factor	Calculated						
	Time	Group		of lons	Time (ms)	Time (Hz)	Low -	Factor	Calculated						
	Time	Group		of lons	Time (ms)	Time (Hz)	Low -	Factor	Calculated EMV						
	Time	Group		of lons	Time (ms)	Time (Hz)	Low -	Factor	Calculated EMV						
	Time	Group		of lons	Time (ms)	Time (Hz)	Low -	Factor	Celoulated						
	Time	Group		of lons	Time (ms)	Time (Hz)	Low -	Factor	Caloulated						
	Time	Group		of lons	Time (ms)	Time (Hz)	Low -	Factor	Calculated S						
	Time	Group		of lons	Time (ms)	Time (Hz)	Low -	Factor	Calculated EMU						
	Time	Group		of lons	Time (ms)	Time (Hz)	Low -	Factor	Canolises EMV						

Figure 30 Sections of the MS Method Editor dialog

Scan Time Segments group box

In the **Scan Time Segments** group box (shown in Figure 31) you will define the time segments for the Scan run.

- The **Time** field displays what is entered in the **Solvent Delay** field. This the time at which the mass spec will turn on and start gathering data.
- In the **Start Mass** and **End Mass**, enter the mass range containing your ion of interest for this time segment.
- In the **Threshold** field, enter the abundance value below which data is considered noise, and should be ignored.
- From the **Scan Speed** dropdown menu select the atomic mass units you wish to scan in a second.

Click **OK** when you have entered your MS method settings, and the Select Monitors dialog box is displayed.

Acquisit	ion Type	Scan		•		EM Save	er	Limit Su	m Limit 1e8 (Defau	8 (Default)				
Scan Time	e Segments	s												
	Time	Start Mass	End Mass	Threshold	Scan	Speed (u/s)		Frequency (scans/sec)	Cycle Time (ms)	Step Size (m/z)				
•	3.00	50.00	550.00	150		1,562 [N=2]	•	2.9	340.06		0.1			

Figure 31 Scan Time Segments group box

7) Select Monitors Dialog

Use the **Select Monitors** dialog to identify the GC and MS monitors you wish to see displayed in the Instrument Control view.

After selecting the monitors you want to see, click **OK** to complete the process. The Save Method dialog box is automatically displayed.

🖳 Select Monitors		
Available Monitors		Selected Monitors
GC APC-1A Pressure GC APC-1B Pressure GC APC-1C Pressure GC APC-2A Pressure GC APC-2P Pressure GC APC-2C Pressure GC APC-3A Pressure GC APC-3B Pressure GC APC-3C Pressure GC AAC-3C Pressure GC Aux-1 Temperature GC Aux-3 Temperature GC Aux-3 Temperature GC Column-2 Flow Calc. GC Column-2 Flow Calc. GC Column-3 Flow Calc. GC Column-6 Flow Calc. GC Det-B Fuel Flow GC Det-B Temperature GC Det-B Temperature GC Det-B Temperature GC Det-B Temperature	<u>A</u> dd> < <u>R</u> emove Reset to <u>D</u> efault	GC Oven Temperature GC Inlet-F Temperature GC Column-1 Flow Calc. GC Aux-2 Temperature

Figure 32 Select Monitors dialog

8) Save The Method

This is the final step in the Edit The Entire Method process.

Type a name for your method and click **OK**.

This completes the Edit Entire Method process. Your method is now saved.

Save Method As	×
Method Path:	
D:\msdchem\1\METH0DS\	Browse
Method File :	
demoscan.M	
OK Cance	el Help

Figure 33 Save Method As dialog



Agilent MassHunter Data Acquisition Software for 5975/5977 Series GC/MSD Familiarization Guide

Create a SIM Quantitation Method

Introduction 46

Create a SIM Method - MS Method Editor Dialog 47 Simultaneously Acquire Scan and SIM Data (SIM/Scan Mode) 49 SIM/Scan Mode Cycle Frequency 50

This chapter describes how to create a SIM method by revising an existing Scan method.



Introduction

Selected ion monitoring (SIM) mode is a data acquisition technique where only selected ion fragments are monitored in order to obtain maximum sensitivity.

To find appropriate conditions for the SIM data acquisition, analyze your scan data for:

- **Ions** (*m*/*z*) **monitored for each peak** MS SIM parameters allow you to define up to 100 groups (SIM Time Segments) of up to 60 ions each for selected ion monitoring, however, Agilent recommends you use as few ions in a group as possible to maximize the signal to noise ratio.
- The best time to switch groups Agilent recommends that you choose a time to switch groups (Start a new Time Segment) where the peaks are well separated to avoid variations in retention time due to sample matrix effects.

Create a SIM Method - MS Method Editor Dialog

When you create a SIM method, you will complete all the common settings (labeled as 1 in Figure 25 on page 37), plus the SIM Time Segments settings (labeled as 3 in Figure 25 on page 37), and described here.

Previously we accessed the Single Quadrupole Method Editor dialog automatically during the Edit an Entire Method procedure. This time we will access this dialog directly since we are not changing other parts of the method.

To begin the process:

1 Click the Load Method icon or select Method/Load Method.



- 2 Navigate to and select the method you want to start with (e.g., the Scan method created in Chapter 2), and click **OK**.
- 3 Click the MS Instrument Parameters icon, or select Instrument/MS Edit Parameters... to open the Single Quadrupole Method Editor dialog.



- 4 See "Sections to complete for all methods" on page 38 for details on filling out the general method settings (those that are common to both SIM and Scan).
- **5** Under the **Acquisition Type** dropdown menu select SIM and then specify the SIM parameters for each time segment that you define in the table below.
- **6** In the SIM Time Segments group box enter the SIM parameters for the run's first time segment when the Acquisition type is set to SIM or SIM and Scan analysis.

	Time	Start Mass	End Mass	Threshold	Scan Spe	eed (u/s)	Frequency (scans/sec)	Cycle Tin (ms)	е	Step Size (m/z)		
	3.00	50.00	550.00	150	1,	562 [N=2] 🔻	2.9	3 3	40.06		0.1	
SIM Tin	e Segments											
	Time	Grou	ıp Name		Number of lons	Total Dwell Time (ms)	Cycle Time (Hz)	Resolution	Ga Fa		Calculated EMV	
	2	00		1	3	400	2.3719	Low	•		5	00
▶	э.											
▶ *									-			
	3.								•			

Figure 34 MS Method Editor dialog- SIM Time Segments

Assign a Group Name for this time segment, select a Resolution of High or Low, and if needed enter a different value for the specified EM Setting (Gain Factor, Absolute EMV, Delta EM) for this time segment only. If you do not enter a value here the EM Setting specified in the Detector Settings area located in labeled area 1 is used. Next specify the ions to acquire in this time segment.

7 Select the SIM tab and specify each ion to acquire for this time segment. For each ion, in the Dwell Time column enter the time in ms to acquire the ion's abundance. Select Plot to have the EIC displayed in the Instrument Control view Chromatogram panel labeled with the ion m/z.

			. 0	-
	SIM	Real-Time Plot T	imed Events	
min				
min		m/z	Dwell Time	Plot Ion
		74.10	100	
		128.00	100	
	1	312.00	100	
•	*			
3 (Default)				
me Step Size				

Figure 35 MS Method Editor dialog- SIM tab

8 To add additional SIM time segments, right-click within the SIM Time Segments area and from the context menu select Add. In the new time segments Time column enter the starting time for this segment which is also the ending time for the previous time segment.

Enter the acquisition parameters that define this time segment and enter the ions to acquire as above.

9 Exit the Single Quadrupole Method Editor dialog by clicking OD and then save the method.

Simultaneously Acquire Scan and SIM Data (SIM/Scan Mode)

An MSD can simultaneously acquire SIM and Scan data if it equipped with fast electronics like the Agilent 5977 MSD and 5975 MSD (fast electronics model). The cycle time displayed for both Scan and SIM are not corrected for simultaneous acquisition. See "SIM/Scan Mode Cycle Frequency" on page 50.

- 1 Open the Single Quadrupole Method Editor dialog.
- 2 From the Acquisition Type dropdown list, select SIM and Scan and notice that the areas for entering both the SIM data and the Scan data are in edit mode..

Tune	File										SI	MF	Real-Time Plot	imed Events	
ATUN	IE.U			Browse		<u>R</u> un Time		10.00 min							
Tune	Type	EI			S	olvent Delay		3.00 min					m/z	Dwell Time	Plot Ion
Tune		12	00		⊂ De	etector Setting					_	▶	74.10	100	
	s Valve:	-		_		Trace Ion D	stastian						128.00	100	V
									_				312.00	100	
CI Flo	W:		-	%	E	EM Setting:	Gain Facto	r	•			*			
	_	Actual	Setpoint		G	ain Factor	1.0)							
MS S	ource	Offline	230	Apply	_		age (V) 50	0							
MS G	luad	Offline	150	Дрріу		pplied EM Volt	age (v) ou	U							
Acquisit	tion Type	SIM and	Scan	•	Ľ	EM Saver	Limit Su	um Limit 1e8 (De	fault)		<u> </u>				
ican Tim	e Segments														
	Time	Start Mass	End Mass	Threshold	Scan Spe	ed (u/s)	Frequency (scans/sec)	Cycle Time (ms)	Step Size (m/z)						
	3.00	50.00	550.00	150	1,5	562 [N=2] 🔻	2.9	ə 340.)6	0.1					
SIM Time	e Segments														
	Time	Grou	ıp Name		Number of lons	Total Dwell Time (ms)	Cycle Time (Hz)	Resolution	Gain Factor	Calculated EMV					
•	3	.00		1	3	300	3.1095	Low 🔻		500					
*															

Figure 36 Scan and SIM data entry both active

- Edit the Scan and SIM acquisition parameters, as needed. Refer to "6) MS Method Editor Dialog - Scan Method Setup" on page 37 and "Create a SIM Method - MS Method Editor Dialog" on page 47.
- **4** At a time during the run where you require the number of peak data points generated, write down both the Scan and SIM cycle times in the time segments that bracket this time.

In SIM/Scan mode the number of data points taken in each mode is reduced and we will see how that impacts the total cycle frequency in "SIM/Scan Mode Cycle Frequency" on page 50.

5 Save the method.

3 Create a SIM Quantitation Method

SIM/Scan Mode Cycle Frequency

In SIM/Scan mode, to complete one cycle the MSD acquires a single group of SIM data followed by a single group of Scan data. It may be necessary to increase the Scan speed or decrease the SIM dwell time to achieve the desired number of data points for effective chromatographic integration. See Figure 37.

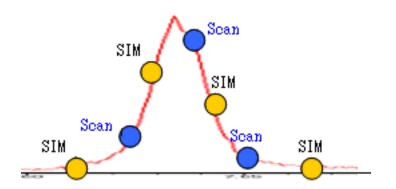
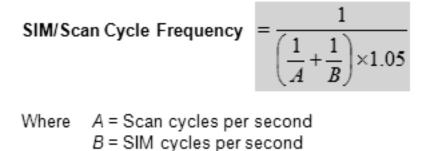


Figure 37 SIM/Scan mode

Actual cycle frequency is calculated with the equation in Figure 38.



2

Figure 38 SIM/Scan cycle

When switching from the SIM data acquisition mode to the Scan mode, about 5% of the available run time will be consumed.

For our example, Scan = 2.44 cycles/sec and SIM = 1.97 which results in an actual cycle time of 1.04 cycles/sec. To improve the number of data points, we could reduce the SIM dwell time, and increase the scan speed.



Agilent MassHunter Data Acquisition Software for 5975/5977 Series GC/MSD Familiarization Guide

Running Samples

Running a Single Sample 52 Running a Sequence 55



Running a Single Sample

The following describes how to run a single sample in MassHunter Data Acquisition.

Load the Method

1 From the PC desktop, click the MassHunter shortcut icon. The **Instrument Control** window below opens.



2 Click the Load Method icon (red box 1) to open the Load Method dialog and select the method you want to use to acquire data. Click OK to load the method and close the dialog. The method name is displayed in the title bar of the Instrument Control window (red box 4).

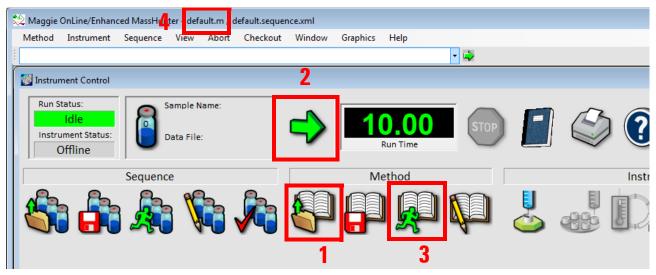


Figure 39 Instrument Control window

Run the Method

For an automated injection, with your method loaded and a sample vial loaded in the ALS, begin the run as follows:

- 1 Click the **Run Method** icon (red box 1 or 3). The **Start Run** dialog box opens.
- 2 Enter the method parameters in the start run dialog for this sample run.

Basic Tab

The top part of the dialog displays the parameters specified by the method (See Figure 40 on page 53). These are read-only fields. To modify these entries you need to edit the method. Included are the:

- Current Method Inject Style
- Inlet Location
- MS Connected To

nlet Location	Rear	Dual		MS Connected to:	Front Inlet	Rear	Inlet
	<u>O</u> perator Name: Data <u>P</u> ath:	John Smith C:\MassHunter\GCMS\2\				Browse	
Sample	Data <u>r</u> atri.	C. (Masshuniter (dCM3 (2	DATA			browse	
Data <u>F</u> ile Name:	Maggie OnLine_(001.D	Browse	Data <u>F</u> ile Name:	EVALDEMO.D		Browse
Sample <u>N</u> ame: Misc. <u>I</u> nfo:				Sample <u>N</u> ame: Misc. <u>I</u> nfo:			
Expected Barcode:				Expected Barcode:			
Sample Amount:		0		Sample Amount:		0	
<u>M</u> ultiplier:		1		<u>M</u> ultiplier:		1	
<u>V</u> ial Number:	1			Vial Number:			
Tray Name:				 <u>T</u> ray Name:			T
Injection Volume:				Injection Volume:			
Curr	ent Method	μ		Cum	ent Method	μL	
Ove	rride using 1	μL		Over	rride using	μL	

Figure 40 Start run dialog

Operator Name - Optional. Enter the name of the person performing the run. This name will be stored in the data file.

Data Path - The current data path is displayed. If you wish to have data files placed in a different data file directory, click the Browse button and select the new directory.

Data File Name - Required. The file used for data storage. You can also click the Browse button to select a different data file name.

Sample Name - Optional. This is the name you give to your sample. This field is informational only and is stored in the data file.

Misc Info - Optional. Enter any additional information about the sample or the method. This field is stored in the data file.

Expected Barcode - Optional. Enter the barcode for the current sample. This is greyed out if a barcode reader is not installed.

Sample Amount - A divisor to convert the absolute amounts of compounds to a percentage of the original sample. If you are generating a quantitative report, this item may be needed.

Multiplier - A multiplier to correct for dilution or other sample handling adjustments. If you are generating a quantitative report, this item may be needed.

Vial Number - This is the vial number containing your sample.

Tray Name - Some ALS models have multiple trays. Select a tray name from the drop-down list if configured.

Injection Volume - Click the injection volume option. You may select the volume from the current method, or specify a sample volume by clicking the Override option.

Method Sections to Run - This section allows you to specify whether you want to run a Data Acquisition method, a Data Analysis method, or both.

When the instrument is in a ready state as shown by a green
 Ready indicator in the instrument status, click OK and Run
 Method to close the dialog and start the run. The ready state indicator changes to Run.

Running a Sequence

A sequence is a list of samples to be analyzed automatically without operator intervention. Each sample is assigned a method to be used for analysis.

To begin the process you must first create a sequence.

Create the Sequence

1 Click the **Edit Sequence** icon



opens. This is where you will create the list of samples to be analyzed and designate the method to be used for each analysis.

- 2 To select the cells you wish to edit in the Sequence Table:
 - Left-click in a cell to select it
 - Click and drag to select multiple cells
 - Select a series of cells by left-clicking the first cell, holding **Shift**, and left-clicking the final cell
 - Select specific multiple cells by holding the Ctrl key while left-clicking each cell
 - Select a rows of cells by left-clicking in the grey column on the left
- 3 To add lines to the table, with a line in the table selected, click the New Sample(s) button. From the drop down menu that is displayed, select 1 Sample to insert one new sample or 5 Samples to insert 5 new samples at the bottom of the table, or select N Samples to specify the number of samples to add to the table. For this example, we will just use the 3 default lines provided.

	lew Sample(s) 👻 🗙 🛛 🔤	To	ols 👻 Method File	Data File	Туре		Level	Dil.		Comme
1	5 Samples	1	default.m		Sample	-			1	
2	N Samples	1	default.m	 Ì	Sample	-			1	
3	Insert Sample	1	default.m		Sample	-			1	
4		<i>.</i>				-				

Figure 41 Sequence Table with default entries

- 4 In the **Name** column, type the name for your sample.
- **5** To increment this value down through all the subsequent lines in this table, select the cell with the information you want to increment, and click the **Increment** icon.



- 6 Under the Vial column, enter the location of the sample(s) in the ALS tray. You can use the **Increment** icon here too.
- 7 Under the **Method File** column, select the ellipses and browse to the method you want to use to acquire the data from this sample.



8 To copy this method name down to all the subsequent cells, select the cell and click the Copy Down icon.



- **9** In the **Data File** column, enter the name you want to be used for the data collected from this sample. Use the **Increment** icon here, if desired.
- 10 From the **Type** drop down box, select the applicable sample type for each line in your table. This entry identifies how the sample is processed by the MassHunter Data Analysis programs. For this example, we are using the type called **Sample**.

Туре
Sample -
- Sample
Blank
Cal QC
Keyword
TuneCheck MatrixBlank
MatrixSpike
MatrixSpikeDup DoubleBlank
CC Remove Charle
ResponseCheck

	New Sample(s)	Vial	Method File	Data File	Туре		Level	Dil.		Com
1	Benzo021409_1		0	Benz02140		-	Level	24.	1	Com
-	Benzo021409_2			Benz02140		-			1	
3	Benzo021409_3	3	default.m	Benz02140	9_3 Sample	-			1	

Figure 42

11 When you have finished entering all the samples you want to run in this sequence, click the **OK** button to close the Sequence table. You are returned to the main MassHunter Data Acquisition window.

Save the Sequence

- Select the Save Sequence As... icon
 The Save Sequence dialog box opens.
- 2 In the **File name** field, type a name for your sequence.
- 3 Click **Save**. The dialog box closes and the sequence is saved.

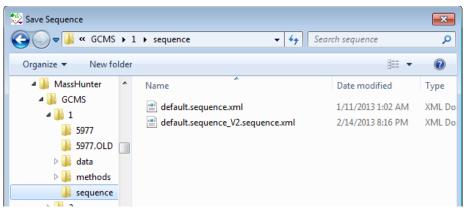


Figure 43 Save Sequence

Load the Sequence

- 1 Select the Load Sequence icon 🗁
- 2 Navigate to and select the sequence you want to load, or type the name in the **File Name** field.
- **3** Click **Open** to close the dialog box and load the sequence.

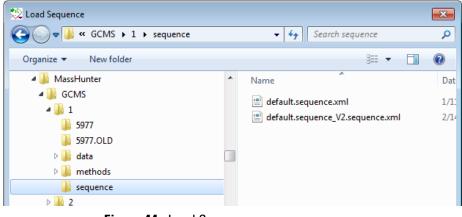


Figure 44 Load Sequence

Run the Sequence

- Click the Run Sequence icon The Start Sequence dialog box opens. This dialog is used to set some general parameters to control the sequence process.
- 2 In the **Sequence Comment** field, enter a description of the sequence.
- 3 In the **Operator Name** field, enter your name.
- 4 In the **Data File Directory** field, accept the default location for this data file, or click **Browse** to select a new path.
- **5** The **Pre-Sequence** and **Post Sequence Macros/Commands** options let you specify data acquisition or data analysis marcos or commands to run before or after the sequence.

tart Sequence default.sequence.xm	I Last Modified: Tue Jan 1 00:00	:01 2013	x
 Method Sections to Run Full Method 		Sequence Barcode Options Disable barcode for this sequence. On mismatch, inject anyway. On mismatch, don't inject; continue the sequence. On mismatch, don't inject; stop the sequence. 	
Overwrite Existing Date	a Files		
Sequence Comment:			
Operator Name:	TWI\jjt		
Data File Directory:	C:\MassHunter\GCMS\2\DATA\	Browse	
Pre-Sequence Macros/Comma	inds		
Acquisition:		Browse	
Data Analysis:		Browse	
Post-Sequence Macros/Comm	ands		
Acquisition:		Browse	
Data Analysis:		Browse	
Inject anyway, do not generate	an error or stop the sequence		
<u>B</u> un Sea	Quence OK	Cancel <u>H</u> elp	

Figure 45 Start Sequence dialog

6 When you have completed your selections, click **Run** Sequence.

The **Sequence Status** bar is displayed. During the sequence run, you can monitor the number of the samples run, the number of samples remaining, and the current sample vial being processed. Use the controls on the bar to pause the sequence, access data analysis, or edit sequence sample entries that have not yet run.

l	Sequence default	.sequence.x	ml is running			
					- 🛶	
	Running 1	of 3	Vial 1	C:\MassHunter\GCMS\2\DATA\00101001.D	→ E	dit Data Analysis Pause

Figure 46 The sequence status bar

Print the Sequence Log

- Select the Print button, Line Select Items to Print dialog box opens.
- 2 Mark the **Sequence Log** checkbox.

Select Items to print
Sequence Log
Current Sequence
Instrument Parameters
🗖 Data Analysis Parameters
Detailed Data Analysis Parameters
OK Cancel

Figure 47 Select Items to print

3 Select **OK**. The **Sequence log** is displayed for printing.

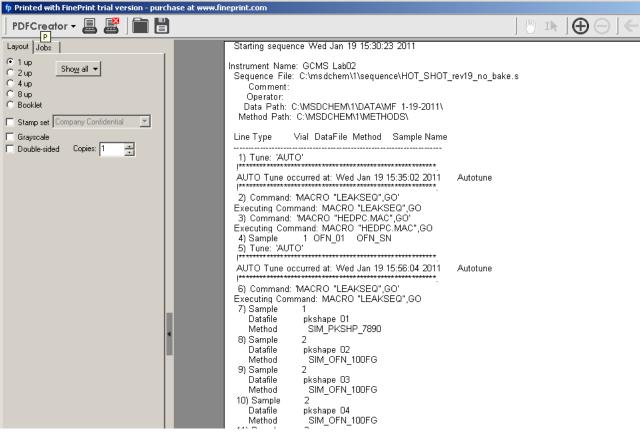


Figure 48 Printed sequence log



Agilent MassHunter Data Acquisition Software for 5975/5977 Series GC/MSD Familiarization Guide

General Information

Editing Individual GC Parameters62Add a Column to Your Local Column Inventory63Upload Parameters from the 7890X GC66Customize the Status Panel View66



Editing Individual GC Parameters

Although a good way to edit a method is use the Edit Entire Method option, as described in Chapter 2, "Create a Scan Method", you may edit any single part, outside the Edit Entire Method option, using the following procedure.

1 From Instrument Control select the GC Parameters icon to display the GC Edit Parameters window.



2 Click on any icon to open the corresponding dialog and enter changes as required.

iscellane ^p ressure psi	eous Columns Modules AL Units		ve Config	juration				
				Valve Type		Name	Parameters	
Oven		+	1	Gas Sampling Valve	-	(Valve #1)	Loop Volume, mL: 1	_
S	Slow Fan		2	Not Installed	-	(Valve #2)		_
			3	Not Installed	-	(Valve #3)		_
			4	Not Installed	-	(Valve #4)		
			5	Not Installed	-	(Valve #5)		
	Thermal Aux Type		6	Not Installed	-	(Valve #6)		
▶ 1	Not Installed		7	Not Installed	-	(Valve #7)		
2	MSD Transfer Line		8	Not Installed	-	(Valve #8)		

Figure 49 GC Edit Parameters window

3 Apply or cancel your changes as needed. See Table 1 on page 63 for a description of the **GC Edit Parameters** window buttons.

Button	Action
Apply	Downloads any settings that have been changed to the GC.
OK	Downloads any settings that have been changed to the GC and closes the GC Edit Parameters window.
Cancel	Discards any settings that have been changed and closes the GC Edit Parameters window.
Help	Displays help topics for the current parameter.

 Table 1
 GC Edit Parameters window buttons

Add a Column to Your Local Column Inventory

Use the **Catalog** option to select a column from the **Column Catalog** and add it to your **Local Column Inventory**.

1 Select the **Configuration** icon, then the **Columns** tab to display the columns configured for the instrument.

		1					Column Outlet Pressu 0 psi
↑ ↓	1	Column Agilent 19091S-433: 12345 HP-5MS 5% Phenyl Methyl Silox -60 °C-325 °C (325 °C): 30 m x 250 μm x 0	1.25.um	Calibration Results Uncalibrated	Front Inlet	Outlet MSD	Heated By
	2	<not inventoried=""> -60 °C-450 °C (450 °C): 25 m x 320 µm x 0</not>		Uncalibrated	Back Inlet	Back Detector	Oven
	3	No Column Installed	- F arr	Uncalibrated	Unspecified 🔻	Other -	Oven
Ī	4	No Column Installed		Uncalibrated	Unspecified 💌	Other 🔻	Oven
	5	No Column Installed		Uncalibrated	Unspecified 💌	Other 🔻	Oven
0	6	No Column Installed		Uncalibrated	Unspecified 💌	Other 🔻	Oven
	6	No Column Installed		Uncalibrated	Unspecified •	Other 🗸 🔻	Oven

Figure 50 Columns configured for the instrument

- 2 Click **Catalog** button to display a local database that is shared across all instrument sessions on your data system. The database contains popular column models, plus any custom columns entered.
- **3** Use the GC Column Catalog to select a column model to add to your Column Inventory, or to select a column model already entered in your inventory.

						▼ Fin	d	Clear						
aı	nufacturer 🔺			Lang	Diama	Film	Phase	Min	Max	Max	Farm			
	Part Number	Description	Favo	Leng m	Diame µm	Thick-	Ratio	Temp,	Temp,	Max Prog	Form Factor	Keywords	Comments	Time Stam
	± 19091S-433	HP-5ms		30	250	0.25	250	-60	325	350	7-inch	HP-5ms		11/26/12.
	19091S-433E	HP-5MS		30	250	0.25	250	-60	350	350	5-inch	HP-5ms		11/26/12.
	19091S-433I	HP-5msi		30	250	0.25	250	-60	325	340	7-inch	HP-5ms		11/26/12.
	19091S-433LTM	HP-5ms		30	250	0.25	250	-60	325	350	LTM	HP-5ms		11/26/12.
	19091S-433UI	HP-5ms U		30	250	0.25	250	-60	325	350	7-inch	HP-5ms Ultra Inert		11/26/12.
	19091S-433UIE	HP-5MS		30	250	0.25	250	-60	325	350	5-inch	HP-5ms Ultra Inert		11/26/12.
		HP-5ms U		30	250	0.25	250	-60	325	350	LTM	HP-5ms Ultra Inert		11/26/12.
	19091S-436	HP-5MS		60	250	0.25	250	-60	325	350	7-inch	HP-5ms		11/26/12.
	19091S-436E	HP-5MS		60	250	0.25	250	-60	325	350	5-inch	HP-5ms		11/26/12.
	19091S-436UI	HP-5MS		60	250	0.25	250	-60	325	350	7-inch	HP-5ms Ultra Inert		11/26/12.
	19091S-510	Blood OH		7.5	320	2	40	-60	270	290	7-inch	HP-Blood Alcohol		11/26/12.
	19091S-510E	Blood OH		7.5	320	2	40	-60	270	290	5-inch	HP-Blood Alcohol		11/26/12.
	19091S-510LTM	HP-Blood		7.5	320	20	4	-60	270	290	LTM	HP-Blood Alcohol		11/26/12.
	19091S-577	HP-5MS		20	180	0.18	250	-60	325	350	7-inch	HP-5ms; High Eff		11/26/12.
	19091S-577E	HP-5MS		20	180	0.18	250	-60	325	350	5-inch	HP-5ms		11/26/12.
	19091S-577LTM	HP-5ms		20	180	0.18	250	-60	325	350	LTM	HP-5ms		11/26/12.
	🗄 19091S-577UI	HP-5ms U		20	180	0.18	250	-60	325	350	7-inch	HP-5ms Ultra Ine		11/26/12.
	⊞ 19091S-577UI	HP-5ms U		20	180	0.18	250	-60	325	350	LTM	HP-5ms Ultra Inert		11/26/12.
	19091S-602	HP-1MS		25	200	0.33	152	-60	325	350	7-inch	HP-1ms		11/26/12.
	19091S-602E	HP-1MS		25	200	0.33	152	-60	325	350	5-inch	HP-1ms		11/26/12.
	19091S-602LTM	HP-1ms		25	200	0.33	152	-60	325	350	LTM	HP-1ms		11/26/12.
	· 19091S-612	HP-1MS		25	320	0.52	154	-60	325	350	7-inch	HP-1ms		11/26/12.
	19091S-612E	HP-1MS		25	320	0.52	154	-60	325	350		No Longer Available		11/26/12.

Figure 51 Column catalog

4 Click **Actions Menu** in the upper left corner of the screen, to display the actions available in this catalog.

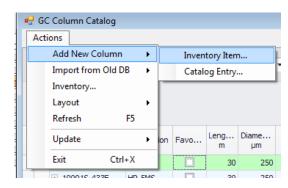


Figure 52 GC Column Catalog Action menu

5 Once you define a column, the column information displays in your method editor, the GC actuals, and in the report following a run.

Refer to online **Help** for details on how to complete the actions shown here.

Upload Parameters from the 7890X GC

- 1 On the **Instrument > GC Edit Parameters** screen, right-click in the blank area.
- 2 From the shortcut menu, select Upload Method from GC.

Customize the Status Panel View

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



Status Items Select Status Items to Display	×
Status Items GC Information Sun Information Front Inlet Sack Inlet Front Detector Thermal Aux QQQ> Columns Valves	↑ ↓ Select All Clear All
Help	Save Cancel

Figure 53

- 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.



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