

## Agilent MassHunter EnviroQuant (EPA) Mode Using Quantitative Analysis

Workflow Guide



#### Notices

© Agilent Technologies, Inc. 2014

No part of this manual may be reproduced in any form or by any means (including electronic storage and retrieval or translation into a foreign language) without prior agreement and written consent from Agilent Technologies, Inc. as governed by United States and international copyright laws.

#### **Manual Part Number**

G6845-90030

#### **Edition**

First edition, August 2014

Printed in USA

Agilent Technologies, Inc. 5301 Stevens Creek Boulevard Santa Clara, CA 95051 USA

#### Warranty

The material contained in this document is provided "as is," and is subject to being changed, without notice, in future editions. Further, to the maximum extent permitted by applicable law, Agilent disclaims all warranties, either express or implied, with regard to this manual and any information contained herein, including but not limited to the implied warranties of merchantability and fitness for a particular purpose. Agilent shall not be liable for errors or for incidental or consequential damages in connection with the furnishing, use, or performance of this document or of any information contained herein. Should Agilent and the user have a separate written agreement with warranty terms covering the material in this document that conflict with these terms, the warranty terms in the separate agreement shall control.

#### **Technology Licenses**

The hardware and/or software described in this document are furnished under a license and may be used or copied only in accordance with the terms of such license.

#### **Restricted Rights Legend**

If software is for use in the performance of a U.S. Government prime contract or subcontract. Software is delivered and licensed as "Commercial computer software" as defined in DFAR 252.227-7014 (June 1995), or as a "commercial item" as defined in FAR 2.101(a) or as "Restricted computer software" as defined in FAR 52.227-19 (June 1987) or any equivalent agency regulation or contract clause. Use, duplication or disclosure of Software is subject to Agilent Technologies' standard commercial license terms, and non-DOD Departments and Agencies of the U.S. Government will receive no greater than **Restricted Rights as defined in FAR** 52.227-19(c)(1-2) (June 1987). U.S. Government users will receive no greater than Limited Rights as defined in FAR 52.227-14

(June 1987) or DFAR 252.227-7015 (b)(2) (November 1995), as applicable in any technical data.

#### **Safety Notices**

#### CAUTION

A **CAUTION** notice denotes a hazard. It calls attention to an operating procedure, practice, or the like that, if not correctly performed or adhered to, could result in damage to the product or loss of important data. Do not proceed beyond a **CAUTION** notice until the indicated conditions are fully understood and met.

#### WARNING

A WARNING notice denotes a hazard. It calls attention to an operating procedure, practice, or the like that, if not correctly performed or adhered to, could result in personal injury or death. Do not proceed beyond a WARNING notice until the indicated conditions are fully understood and met.

In This Guide	
	This Workflow describes how to use MassHunter EnviroQuant to create a database of compounds, qualifiers, their calibration curves, and specify quality control parameters to comply with EPA regulations. The example used here is EPA Method 8270. A similar process would be use for other EPA methods.
	More common operations, not directly associated with the EnviroQuant Workflow mode, are briefly discussed here, but are covered in more detail in both online Help and Familiarization Guides. Please refer to the online Help for more details on these topics and for links to unabridged versions MassHunter Familiarization Guides specific to your instrument.
	A brief summary of chapter contents for this Workflow Guide follows.
1 Before You Begin	Chapter 1 describes how to set up your MassHunter GCMS Acquisition and MassHunter Quantitative Data Analysis programs for using the EnviroQuant (EPA) Workflow Mode user interface (UI).
2 Create the Data Acquisition Method	Chapter 2 describes how to set up a method for data acquisition. A Data Acquisition method must exist prior to the creation of a Quantitative Data Analysis method.
3 Create a Quantitation Method	Chapter 3 describes how to create a basic MassHunter Quantitation method from a ChemStation Quant database. Alternate instructions are included for creating a quantitation method from a calibration sample data file if you are not interested in converting ChemStation methods.
4 Run Samples for Quant Method Creation	This chapter explains how to create a sequence, that when run, will generate a batch containing the analyzed results of samples used to update the compound calibration curves in the quantitation method. You will also use these samples to create the Tune Evaluation Method (tunevaluation.xml), create the Reference Library, and initialize the CC sample response.
5 Enter EnviroQuant Parameters in the Method	Chapter 5 explains how to add outliers to a quantitative method that monitor compound properties and instrument performance as specified by the EPA or your laboratory requirements (for example EPA Method 8270).

6 Create Report Methods	Chapter 6 explains how to create report methods that enable you to save report parameters, including multiple report templates, to a file than can be applied to a sample or group of samples. These methods can be used both interactively in EnviroQuant or used to generate a report automatically when samples are run from an automated sequence.
7 Run Samples	Chapter 7 describes a workflow for running initial calibrations and a workflow for running daily fields samples.
Where to Find More Information	<ul> <li>Accompanying your hardware and software is a comprehensive collection of manuals, videos, user applications, and method development tools. These are located on the:</li> <li>Agilent GC and GC/MS Manuals and Tools DVD set</li> <li>Agilent GC/MS Software Information and Manuals memory stick</li> </ul>
	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 Insert the memory stick into a USB port and follow the prompts. This can be installed by anyone who has authority to copy information onto the receiving computer.

## Contents

#### 1 Before You Begin

Configure MassHunter GCMS Acquisition for EnviroQuant (EPA) 8 Configure MassHunter Quant for Environmental Analysis Mode 9 Understand the Directory Structure 10

#### 2 Create the Data Acquisition Method

Step 1: Load the data acquisition method. 12

- Step 2: Select the parts of the method to edit. 12
- Step 3: Describe the method and where it is saved. 13
- Step 4: Review what is coming next. 14
- Step 5: Complete the Inlet and Injection Parameters dialog. 14
- Step 6: Complete the GC Edit Parameters dialogs. 15
- Step 7: Skip the Real Time Plot displays. 18
- Step 8: Edit the MS Method parameters. 18
- Step 9: Select the monitors. 19
- Step 10: Save the method. 19
- Step 11: Create the basic quantitation method. 19

#### **3** Create a Quantitation Method

- Introduction 22 Step 1: Convert an MSD ChemStation method. 22 Step 2: Examine the method. 24 Step 3: Review the Retention Times. 26 Step 4: Review the ISTDs. 27 Step 5: Review the Concentrations. 28 Step 6: Review the Qualifiers. 29 Step 7: Review the Calibration Curve Settings. 30 Step 8: Set up the Integrator. 31 Step 9: Save the method. 32
- Step 10: Run Samples. 32

#### 4 Run Samples for Quant Method Creation

Introduction 34 Step 1: Create a batch. 34 Step 2: Complete the Tune Evaluation criteria. 35 Step 3: Complete the GC Performance Evaluation criteria. 38 Step 4: Review the tune evaluation results. 39 Step 5: Create a Reference library. 43 Step 6: Initialize the Continuing Calibration response. 44 Step 7: Save the Method. 45 Step 8: Complete the quantitation method. 46

#### 5 Enter EnviroQuant Parameters in the Method

- Introduction 48
- Step 1: Open the batch. 48
- Step 2: Specify the surrogates and matrix spikes. 49
- Step 3: Set up the CC Maximum Elapsed Time to 12 hours. 51
- Step 4: Set up outlier limits for the EPA method criteria. 52
- Step 5: Save the method. 66
- Step 6: Create report methods. 66

#### **6** Create Report Methods

- Introduction 68
- Step 1: Generate an interactive report. 68
- Step 2: Create an Initial Calibration Report Method. 72
- Step 3: Create a Quant Report Method. 75
- Step 4: Create a Continuing Calibration Report Method. 80
- Step 5: Create a Matrix Spike Duplicate Report Method. 83
- Step 6: Create a QA Check Report Method. 86
- Step 7: Run samples. 88

#### 7 **Run Samples**

Introduction 90

- Step 1: Run a calibration of the instrument. 90
- Step 2: Run daily unknown samples. 95
- Step 3: Perform Data Analysis Interactively. 101

## 1 Before You Begin

Configure MassHunter GCMS Acquisition for EnviroQuant (EPA) 8 Configure MassHunter Quant for Environmental Analysis Mode 9 Understand the Directory Structure 10

**Agilent Technologies** 

#### Configure MassHunter GCMS Acquisition for EnviroQuant (EPA)

#### Configure MassHunter GCMS Acquisition for EnviroQuant (EPA)

- 1. Double-click the GCMS Configuration desktop icon to launch the Agilent GC/MS Configuration program.
- 2. Select the instrument name that you will be running to acquire the data. Instrument **1** is selected in this example.
- 3. Select the EnviroQuant (EPA) Workflow Mode and click OK to close the dialog.

4. Click **Yes** to confirm the configuration and exit the Agilent GC/MS Configuration program. Depending on your instrument, MassHunter GCMS Acquisition and MassHunter Quantitative Analysis may be set up to run in several Workflow Modes, including:

- Enhanced
- Drug Quant
- EnviroQuant (EPA)
- Aromatics in Gasoline

Here we are going to be using the **EnviroQuant (EPA)** Workflow Mode. So, before doing anything else, you must set up the MassHunter GCMS Acquisition program and the MassHunter Quantitative Analysis program to run in the EnviroQuant Workflow Mode.

To reconfigure an existing GC/MSD instrument to work in the EnviroQuant Mode:



Ag	ilent G	GC/MS Instrument C	onfiguratio	n						
File	Co	nfigure Help								
1	2 3	4 8								
						- Ex	ecute			
_					Current Agilent	GC/MS Instru	ument Con	figuration		
Γ		Name	Offine	MS	MS IP	Available Sources	GC	GC IP	Workflow Mode	Laboratory ID Number
	• 1	Komit			192.168.1.201		7890 GC	192.168.1.203	EnviroQuant (EPA)	
4	2	Grover		/000	192.168.1.55	EXEX	7890 GC	192.168.1.203	Enviroquant (EPA)	201
	3	Miss Piggy	V	7200	192.168.1.55	Elris	7890 GC	192.168.1.203	EnviroQuant (EPA)	201

1 A A A A A A A A A A A A A A A A A A A	Kermit	
Instrument Name	Nermit	
Laboratory ID Number	201	
Offline Instrument		
Mass Spectrometer		
<u>M</u> odel	DC Polarity	
5977 🔹	<u>     Positive (+)   </u>	
Address	Negative (-)	
192.168.1.201		
Mo <u>d</u> el 7890 GC Add <u>r</u> ess	Use a PAL Sampler	Configure PAL Sampler
192.168.1.203	Headspace Type	Headspace Address
102.100.1.200	<none> ~</none>	
Enable Direct Communication between instruments		

#### 1. Before You Begin

Acquisition.

5.

Configure MassHunter Quant for Environmental Analysis Mode



#### Configure MassHunter Quant for Environmental Analysis Mode

Double-click the Instrument icon to launch MassHunter GCMS

#### **Check for the Startup icon**

#### Add a startup icon

- 1. From the windows Start menu select Agilent \MassHunter Workstation \Quant Tools \Setup Desktop Icons.
- 2. Check the **Environmental Analysis** mode for your instrument(s).
- 3. Click **OK** to close the dialog and add your newly selected startup icon(s) to the desktop.

When MassHunter Quantitative Analysis is installed, a group of icons used for starting Quantitative Analysis, is placed on the desktop.

To begin MassHunter Quantitative Analysis, double-click the applicable icon.

For example, to start a Quantitative Analysis session for single quadrupole data in the EnviroQuant workflow mode you would click the desktop icon labeled **Environmental Quant (MS)**. The Quant program is then optimized for single quadrupole data in the EnviroQuant workflow mode.

If you do not see a desktop icon labeled **Environmental Quant (MS)** for your instrument, add it from the Setup Desktop Icons tool.

Choose Icons -	Quantitative Analysis			X
Please choose icons to appear on your desktop				
			Application	
		Standard	Drug Analysis	Environmental Analysis
	MS (single quadrupole)	V		
	QQQ (triple quadrupole)			
	TOF (time-of-flight)			
Q-TOF	(quadrupole time-of-flight)			
				OK Cancel

In this example, both the Standard and Environmental Analysis modes are selected for the MS, single quadrupole instrument.

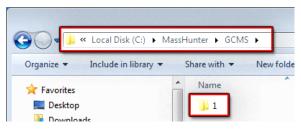
## Understand the Directory Structure

1. Locate the instrument directories.

2. Review the default data, methods, and sequence directories. You can configure and run up to four instruments with MassHunter GCMS Acquisition.

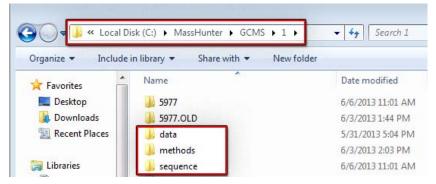
For each instrument you configure, MassHunter GCMS Acquisition will create a numbered directory corresponding to the instrument number;

*drive*:\MassHunter\GCMS\1 for example. Although drive C is shown here, Agilent supplied PCs with MassHunter factory installed store an instrument's data on the D drive.



Under each instrument directory (**1** shown here), you will see a default data, methods, and sequence subdirectory, as shown in the next example.

These are the recommended and default locations for your data, methods, and sequences. Your files can be located here or you can locate these files anywhere that is accessible to the MassHunter programs.



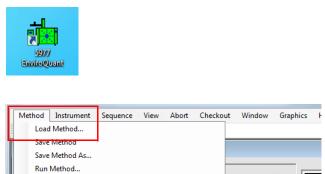
- The data directory contains the data files from each batch, stored in a user named batch directory specified at the beginning of a run.
- **The methods directory** contains your master methods. Each method has a user defined file name with a file extension of m. Master methods in the sequence get updated when sample types such as CAL are included in the batch.
- **The sequence directory** contains all of your sequence files. Each sequence has a user defined file name with a file (.sequence.xml) extension.

2

Step 1: Load the data acquisition method. 12
Step 2: Select the parts of the method to edit. 12
Step 3: Describe the method and where it is saved. 13
Step 4: Review what is coming next. 14
Step 5: Complete the Inlet and Injection Parameters dialog. 14
Step 6: Complete the GC Edit Parameters dialogs. 15
Step 7: Skip the Real Time Plot displays. 18
Step 8: Edit the MS Method parameters. 18
Step 9: Select the monitors. 19
Step 10: Save the method. 19
Step 11: Create the basic quantitation method. 19



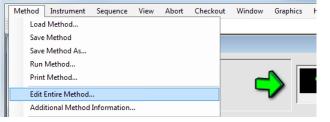
The following describes how to create a data acquisition method to acquire sample data for environmental analysis. Here we will be showing the acquisition parameters in a demonstration method named bnalist.m. This method is located in the Envdemo folder provided with the Agilent GC/MS Productivity ChemStation.



GC/MS Methods created in MSD Productivity ChemStation can be opened directly in MassHunter and used. It might be good practice to save as a new name to maintain compatibility with older systems if you are not moving every instrument to MassHunter.

You can load the bnalist.m from the Productivity ChemStation, if available, or another similar method instead of using the default method as a starting point.

During this process we will cover the parts of a data acquisition method that are related to environmental analysis.



Check Method Sections to Edit:	
Method Information	
☑ Instrument/Acquisition	

#### Step 3: Describe the method and where it is saved.

#### Step 3: Describe the method and where it is saved.

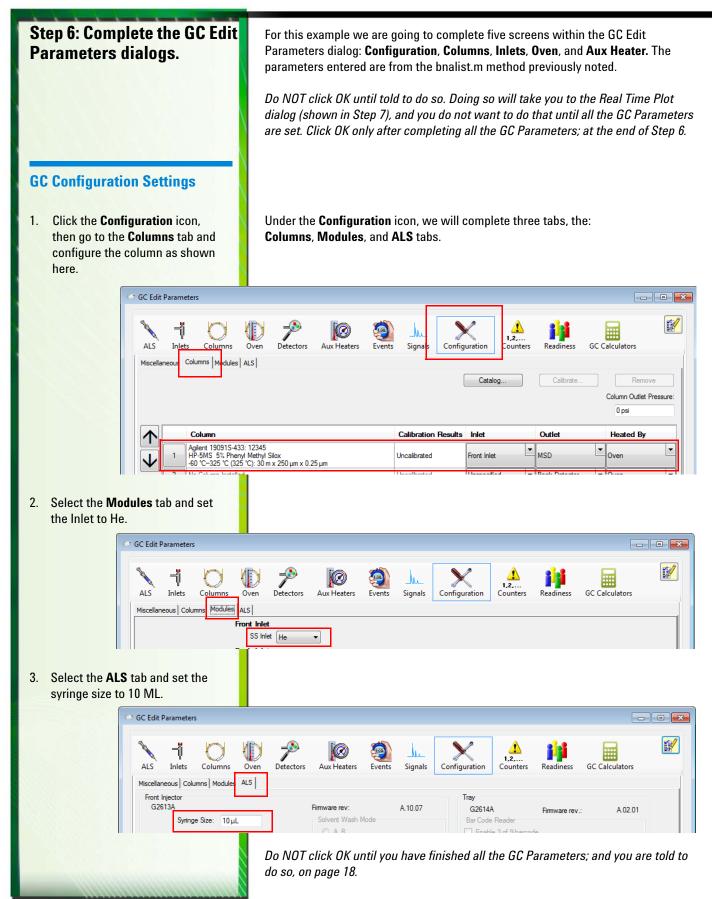
- 1. Provide a description of the method in **Method Comments**.
- 2. Decide whether or not to save a copy of this method with the data file.
- 3. Select **Data Acquisition** and **Data Analysis** for the run. Although the MassHunter Quantitative Analysis method does not yet exist, you will want to run the data analysis portion of the method when it is available.
- 4. Click **OK** to continue.

od Information			
Method <u>C</u> omments:			
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
ОК	Cancel	Help	

**Note** – In MassHunter the data analysis method cannot be edited in the Data Acquisition program. The data analysis method can only be created or edited in the MassHunter Quantitative Analysis program. See Chapter 3, "Create a Quantitation Method" for more details.

Step 4: Review what is coming next.	<ul> <li>During this process you will be presented with the following 5 Instrument Acquisition parameter dialog boxes. Complete each one as shown in the examples on the following pages and click OK to continue. Each time you click OK the next dialog is opened automatically.</li> <li>Note: These dialogs are completed in the exactly the same way for all Workflow Modes (i.e., Enhanced, EnviroQuant (EPA), Gasoline, etc.), and are described in detail the MassHunter Familiarization guide and in online Help. Please refer to that documentation for more details.</li> <li>Inlet and Injection Parameters dialog - Used to select the sample type, inlet, and injection source.</li> <li>GC Edit Parameters dialog - Used to define the settings for your GC. Here you will click each icon to display and complete the corresponding window for each component.</li> <li>Real-Time Plots dialog - Used to select which signals you want displayed.</li> <li>MS Method Editor dialog - Used to define the Tune File, SCAN, Real-Time Plots dialog - Used to define the Tune File, SCAN, Real-Time</li> </ul>
	Plot, and Timed Events, settings, using the single quadrupole or triple quadrupole method editor. Monitors dialog - Used to define the MS monitors you wish to display. Available Monitors
Step 5: Complete the Inlet	Select the inlet, injection source, Use MS, inlet location, and MS Connected to.
and Injection Parameters dialog.	Inlet and Injection Parameters
	Injection Source GC ALS
	✓ Use <u>M</u> S
	Inlet Location
	MS Connected to:
	Click <b>OK</b> when you are finished, and the <b>GC Edit Parameters</b> dialog is displayed.

#### Step 6: Complete the GC Edit Parameters dialogs.



GC Method Parameters Next we w Heater.			Next we will complete the settings for the <b>ALS, Columns, Inlets, Oven</b> , and <b>Heater.</b>	Aux
1.		i icon and edit the ers appropriate to		
		GC Edit Parameters		
		ALS Inlets Columns Front Injector Back Injector Tray Injection Syringe Size: 10 µL Injection Volume: 1µL Multiple Injection Delay: 0 sec Washes and Pumps Solvent A Washes: 0 Solvent B Washes: 0 Sample Pumps: 6	Dwell Time Pre-Injection: 0 min Post-Injection: 0 min Plunger Speed ● Fast ● Slow ● Variable	
2.	the Column p	o your method.	Because settings made in the <b>Columns</b> parameters dialog automatically mo Pressure and Flow parameters in the Inlet Parameters tab, and vice versa, in good idea to set the <b>Columns</b> settings before the <b>Inlets</b> settings. Therefore, enter the column settings first and the Inlet settings next.	t is a , we will
		GC Edit Parameters		
			Image: Control Mode       Image: Control Mode       Image: Control Mode         Image: Control Mode       Image: Control Mode       Image: Control Mode         Image: Control Mode       Image: Control Mode       Image: Control Mode         Image: Control Mode       Image: Control Mode       Image: Control Mode         Image: Control Mode       Image: Control Mode       Image: Control Mode         Image: Control Mode       Image: Control Mode       Image: Control Mode         Image: Control Mode       Image: Control Mode       Image: Control Mode         Image: Control Mode       Image: Control Mode       Image: Control Mode         Image: Control Mode       Image: Control Mode       Image: Control Mode         Image: Control Mode       Image: Control Mode       Image: Control Mode         Image: Control Mode       Image: Control Mode       Image: Control Mode         Image: Control Mode       Image: Control Mode       Image: Control Mode         Image: Control Mode       Image: Control Mode       Image: Control Mode         Image: Control Mode       Image: Control Mode       Image: Control Mode         Image: Control Mode       Image: Control Mode       Image: Control Mode         Image: Control Mode       Image: Control Mode       Image: Control Mode         Image: Control Mode	

3.		ets icon and edit the ters appropriate to
	your method	
		GC Edit Parameters
		ALS       Inlets       Oven       P       Detectors       Aux Heaters       Events       Signals       Configuration       Image: Configuration of the configuration of th
		Setpoint     Gas Saver:       I Heater:     250 °C       I Pressure:     8.8085 psi       Total Row:     54 mL/min       I Septum Purge Row:     3 mL/min       Septum Purge Row Mode:     Standard
		Mode:     Purge Flow to Split Vent:       Splitless     50 mL/min   at 2 min
4.		en icon and edit the eters appropriate to
		GC Edit Parameters
		ALS Inlets Columns Oven Aux Heaters Events Signals Configuration Backflush Readiness GC Calculators
		Image: Work Temp On     Rate °C/min     Value °C     Hold Time min     Run Time min       70 °C     (Initial)     70     2     2       Ramp 1     4     230     5     47
		0.5 min
		Maximum Oven Temperature 325 °C Override Column Max: 325 °C
		Post Run: 70 °C
		Post Run Time: 0 min
-		

5. Click the <b>Aux Heaters</b> icon and edit the Aux Heaters parameters appropriate to your method, then click <b>OK</b> .	The MS Transfer line temperature is set via the GC.
GC Edit Parameters	
ALS Inlets Columns Thermal Aux 2 (MSD Tra On 2010	Oven       P
Stor 7: Chin the Deal Time	When you click <b>OK</b> , the Real Time Plot dialog displays.
Step 7: Skip the Real Time Plot displays.	For this example, leave these entries blank, and click <b>OK</b> to continue.
	Real-Time Plots for GC
	Display Signal 1
	Display Signal 2
	Display Signal 3
	Display Signal 4
Step 8: Edit the MS Method parameters.	When done, click <b>OK</b> to continue.
🖳 Single Quadrupole MS Method Editor	
Tune File	SIM Real-Time Plot Timed Events
Tune Type El Tune EMV 1200	Solvent Delay 3.00 min I Iotal Ion Chromatogram Detector Setting I Spectrum
Tune EMV         1200           CI Gas Valve	Trace Ion Detection     Base Peak Chromatogram
CI Flow	EM Setting Gain Factor  Gain Factor  1.000
MS Source Offline 230 MS Quad Offline 150 Apply Acquisition Type Scan	Applied EM Voltage (V) 500 EM Saver Limit Sum Limit 1e8 (Default)   Label Mass or Mass Range Scan 1-1 50.00-550.00
Scan Time Segments Time Start Mass End Mass Threat Scan Time Start Mass End Mass Threat Time Start Mass End Mass Threat Scan Time Start Mass Threat Scan Time St	hold         Scan Speed (u/s)         Frequency (scans/sec)         Cycle Time (ms)         Step Size (m/z)           150         1.562 [N=2]         2.9         342.63         0.1
	N

Step 9: Select the monitors.	In the Monitors dialog, select the monitors you want to see and click <b>OK</b> to
	continue.
	Available Monitors
	GC APC-1A Pressure GC Oven Temperature GC Inlet-F Temperature
	GC         APC-1C Pressure         Add>         GC         Column-1 Flow Calc.           GC         APC-2A Pressure         GC         Aux-2 Temperature           GC         APC-2B Pressure         MS         MS Source
	GC_APC-2C Pressure C C Bemove MS_MS Quad
Step 10: Save the method.	Save the method as C:\MassHunter\GCMS\1\METHODS\bnalist.m and click <b>OK</b> to continue. Although drive C is shown here, Agilent supplied PCs with MassHunter
	factory installed store an instrument's data on the D drive.
	Save Method As Method Path:
	C:\MassHunter\GCMS\1\METHODS Browse Method File:
	bnalist.M
	OK Cancel Help
	This completes the Edit Entire Method process. Your method is now saved.
	You are now ready to continue by creating a EnviroQuant Data Analysis method.
Step 11: Create the basic quantitation method.	See Chapter 3, "Create a Quantitation Method".

3

## **Create a Quantitation Method**

#### Introduction 22 Step 1: Convert an MSD ChemStation method. 22 Step 2: Examine the method. 24 Step 3: Review the Retention Times. 26 Step 4: Review the Retention Times. 26 Step 5: Review the ISTDs. 27 Step 5: Review the Concentrations. 28 Step 6: Review the Qualifiers. 29 Step 7: Review the Calibration Curve Settings. 30 Step 8: Set up the Integrator. 31 Step 9: Save the method. 32

**Agilent Technologies** 

In	troduction	In step 1 of this chapter you will learn how to create a basic MassHunter Quantitation method from an MSD ChemStation quant database.
		An alternative would be to create a quantitation method from an existing scan data file. This is documented in the MassHunter Quantitative Analysis for GC/MSD Familiarization Guide G3335-90200 provided with your MassHunter software documentation for the 5977 MSD and available for download from the Agilent website.
		Once you have a Quantitation database developed, using either of the above procedures, you can complete the quantitation method as described in Chapter 5, "Enter EnviroQuant Parameters in the Method". In that chapter you will see how to edit the method's parameters with EPA specific outliers, add a Tune Check method, and initialize a compound's continuing calibration concentration to monitor compliance with EPA Method 8270.
	ep 1: Convert an MSD nemStation method.	This step describes how to convert an existing MSD ChemStation method to a MassHunter Quantitative Analysis method using the <b>GC MSD Translator</b> tool.
		For this example we are using a sample SCAN method bnalist.m. This is an environmental demonstration method installed in <b>C:\envdemo\bnalist.m</b> . during a ChemStation installation.
		The quantitation database in this demo method was set up for EPA method 8270. This is a good starting point for creating a Quantitative method for your analysis.
1.	Start the GC MSD ChemStation Translator tool.	CC WED ChemStatica Quanti Widthod Transistor
2.	Select Translate Quantitation	Select Translation Task
	Databases.	Please choose a GC/MS Translator Option
		MSD ChemStation
		Translate Data Files
		Translate Quantitation Databases

#### Step 1: Convert an MSD ChemStation method.

3.	Select the <b>bnalist.m</b> method.	Export MSD ChemStation Quant Database	?
		Options	
		Input MSD ChemStation Method Containing Quant Database	
		C:\envdemo\bnalist.m	Choose Folder
4.	Click Export to MassHunter Quantitation Method.	The method is converted in place. When the process is <b>Translation was successful</b> at the bottom of the screer assigned ISTDs which can be expanded to see the list or ISTD.	n. The tool shows the
		Export MSD ChemStation Quant Database	? 💌
		Options	
		Input MSD ChemStation Method Containing Quant Database	
		C:\envdemo\bnalist.m	Choose Folder
		Input Quant Database File:	
		C:\envdemo\bnalist.m\qdb.mth	
		Output MassHunter Quantitation Method	
		C:\envdemo\bnalist.m\DAMethod\Quant\quantitative.xml	
		<ul> <li>P. 1.4-Dicklorobenzene-34 (Internal Standard #1)</li> <li>Naphthalene-d8 (Internal Standard #2)</li> <li>Acenaphthene-d10 (Internal Standard #3)</li> <li>Phenanthrene-d10 (Internal Standard #4)</li> <li>Cruysene-d12 (Internal Standard #5)</li> <li>Perylene-d12 (Internal Standard #6)</li> </ul>	
		Export to MassHunter Quantitation Method	
			Close
		MassHunter GC/MS Translator B.07.02 1848 09-May-2014 Translation was successful.	
5.	Copy the converted method to your master method directory.	Here we are using instrument 1's method directory as o	ur master method directory
		A state of the state of	← Search metho
		Organize ▼ 😭 Open Include in library ▼ Share with ▼ New folde	r
		★ Favorites	

★ Favorites
 ■ Desktop
 Downloads
 ▲ OneDrive

📃 Recent Places

鷆 BFB.m

퉬 bnalist.m

퉬 checkout

CheckTune.m

....

#### Step 2: Examine the method.

#### Step 2: Examine the method.

 In MassHunter Quantitative Analysis, select Method > Open Method from Existing File.

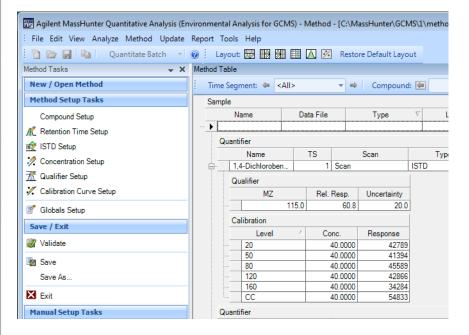
 Select the C:\MassHunter\GCMS\1\ METHODS\bnalist.m file that you converted in the last section and click OK.

3. Select Compound Setup.

The converted method contains the quantitation database with all compounds, qualifiers, and calibration curves but the ChemStation's EPA monitoring parameters are not converted. In later steps we will enter the EPA monitoring parameters.

📅 Agilent MassHunter Quar	ntitati	ve Analysis						
Edit View Analyze	Met	hod Update	Report	Tools	Help		_	
🗄 🛅 🗁 📕 🖬 💭 A		New				•	$\overline{\Lambda}$	Restore Default Layout
Batch Table		Open				•	B	Open Method from Existing File
Sample: 😭		Append Edit				•		Open Method from Existing Batch
Sa	P					F10		Open and Apply from Existing File
V Name Data File		Validate						~
	Fin	Save						

The EnviroQuant Method Editor opens with the converted method loaded. Although drive C is shown here, Agilent supplied PCs with MassHunter factory installed store an instrument's data on the D drive.





A. Review the newly imported list of The	compound parameter	s are disp	layed and	may be edit	ed. When	first opened, the
	s sorted by retention t				method's	compound <b>Type</b> ,
mz,	RT, and identity Criter	<b>ia</b> are coi	rectly cor	nverted.		
	Agilent MassHunter Quantitative Ar				d - <c:\masshu< td=""><td>unter\GCMS</td></c:\masshu<>	unter\GCMS
	ile Edit View Analyze Method ) 🗁 📕 🗈 🛛 Quantitate Bat				Restore Def	ault Lavout
	nod Table					
	Time Segment: 🖛 <all></all>	▼ ➡ Co	ompound: 🔙	Benzo[g,h,i]per 🔻	📦 🛛 Reset T	able View
	Sample Name Data File Type	e Level Acq. N	Nethod File	Acq. Date-Time		
	Continuing Cal CC.d CC	CC bnalis		2014 6:45 PM		
	Quantifier Name	TS Scan	Туре	MZ RT 4	Ion Polarity	Criteria
	2-Fluorophenol	1 Scan	Target	112.0 8.255	Positive	Close RT with Qualif
	bis(2-Chloroethyl)ether Phenol-d5	1 Scan 1 Scan	Target Target		Positive Positive	Close RT with Qualif Close RT with Qualif
	Phenol	1 Scan	Target	94.0 11.04	Positive	Close RT with Qualif
	2-Chlorophenol 1,3-Dichlorobenzene	1 Scan 1 Scan	Target Target	128.0 11.08		Close RT with Qualif Close RT with Qualif
	1,4-Dichlorobenzene-d4	1 Scan	ISTD		7 Positive	Greatest Response
	1,4-Dichlorobenzene	1 Scan	Target	146.0 11.54	B Positive	Close RT with Qualif
	1,2-Dichlorobenzene	1 Scan	Target		7 Positive Resitive	Close RT with Qualif
	Benzyl alcohol bis(2-chloroisopropyl)ether	1 Scan 1 Scan	Target Target	45.0 12.56		Close RT with Qualif Close RT with Qualif
	2-Methylphenol	1 Scan	Target	108.0 12.68		Close RT with Qualif
	Hexachloroethane	1 Scan	Target	117.0 12.95	2 Positive	Close RT with Qualif
	N-Nitroso-di-n-propylamine	1 Scan 1 Scan	Target		B Positive D Positive	Close RT with Qualif Close RT with Qualif
	4-Methylphenol Nitrobenzene-d5	1 Scan 1 Scan	Target Target	82.0 13.25		Close RT with Qualif
	Nitrobenzene	1 Scan	Target		8 Positive	Close RT with Qualif
	Isophorone	1 Scan	Target		) Positive	Close RT with Qualif
	2-Nitrophenol 2,4-Dimethylphenol	1 Scan 1 Scan	Target Target	139.0 14.27	Positive Positive	Close RT with Qualif Close RT with Qualif
	bis(2-Chloroethoxy)metha	1 Scan	Target	93.0 14.86		Close RT with Qualif
	2,4-Dichlorophenol	1 Scan	Target		7 Positive	Close RT with Qualif
	1,2,4-Trichlorobenzene Naphthalene-d8	1 Scan 1 Scan	Target ISTD	180.0 15.24	Positive Positive	Close RT with Qualif Greatest Response
	Naphthalene	1 Scan	Target	128.0 15.39		Close RT with Qualif
	4-Chloroaniline	1 Scan	Target	127.0 15.71		Close RT with Qualif
	Hexachlorobutadiene	1 Scan	Target		B Positive	Close RT with Qualif
	4-Chloro-3-methylphenol 2-Methylnaphthalene	1 Scan 1 Scan	Target Target		Positive Positive	Close RT with Qualif Close RT with Qualif
	Hexachlorocyclopentadiene	1 Scan	Target		B Positive	Close RT with Qualif
	2,4,6-Trichlorophenol	1 Scan	Target		4 Positive	Close RT with Qualif
	2,4,5-Trichlorophenol	1 Scan	Target		7 Positive	Close RT with Qualif
	2-Fluorobiphenyl 2-Chloronaphthalene	1 Scan 1 Scan	Target Target		Positive Positive	Close RT with Qualif Close RT with Qualif
		1 Scan	Target		) Positive	Close RT with Qualif
	Dimethylphthalate	1 Scan	Target		2 Positive	Close RT with Qualif
	Acenaphthylene 2,6-Dinitrotoluene	1 Scan 1 Scan	Target Target		Positive Positive	Close RT with Qualif Close RT with Qualif
	Acenaphthene-d10	1 Scan	ISTD		Positive	Greatest Response
	3-Nitroaniline	1 Scan	Target		2 Positive	Close RT with Qualif
	Acenaphthene 2,4-Dinitrophenol	1 Scan 1 Scan	Target Target		B Positive B Positive	Close RT with Qualif Close RT with Qualif
	Dibenzofuran	1 Scan 1 Scan	Target		Positive	Close RT with Qualif
	2,4-Dinitrotoluene	1 Scan	Target	165.0 21.69	6 Positive	Close RT with Qualif
	4-Nitrophenol	1 Scan 1 Scan	Target		7 Positive	Close RT with Qualif
	Fluorene 4-Chlorophenyl-phenylether	1 Scan 1 Scan	Target Target		Positive Positive	Close RT with Qualif Close RT with Qualif
	Diethylphthalate	1 Scan	Target	149.0 22.61	1 Positive	Close RT with Qualif
	4-Nitroaniline	1 Scan	Target	138.0 22.91	6 Positive	Close RT with Qualif
	4,6-Dinitro-2-methylphenol n-Nitrosodiphenylamine	1 Scan 1 Scan	Target Target		Positive Positive	Close RT with Qualif Close RT with Qualif
	2,4,6-Tribromophenol	1 Scan 1 Scan	Target Target		Positive Positive	Close RT with Qualif
	4-Bromophenyl-phenylether	1 Scan	Target	248.0 24.09	6 Positive	Close RT with Qualif
	Hexachlorobenzene	1 Scan	Target		B Positive	Close RT with Qualif
	Pentachlorophenol Phenanthrene-d10	1 Scan 1 Scan	Target ISTD		Positive Positive	Close RT with Qualif Greatest Response
	Phenanthrene	1 Scan	Target	178.0 25.52	Positive	Close RT with Qualif
	Anthracene	1 Scan	Target	178.0 25.66	2 Positive	Close RT with Qualif
	Di-n-butylphthalate	1 Scan	Target Target		Positive Regitive	Close RT with Qualif
	Fluoranthene Pyrene	1 Scan 1 Scan	Target Target		Positive Positive	Close RT with Qualif Close RT with Qualif
	Terphenyl-d14	1 Scan	Target		Positive	Close RT with Qualif
	Butylbenzylphthalate	1 Scan	Target	149.0 32.33	5 Positive	Close RT with Qualif
	Benzo[a]anthracene	1 Scan	Target		Positive Resitive	Close RT with Qualif
	Chrysene-d12 3,3'-Dichlorobenzidine	1 Scan 1 Scan	ISTD Target		Positive Positive	Greatest Response Close RT with Qualif
	Chrysene	1 Scan	Target		2 Positive	Close RT with Qualif
	Chrysene	1   Scan	larget	228.0 33.92	2  Positive	Close RT with Qualif

St Re	ep 3: Review the etention Times.
1.	Select Retention Time Setup.
2.	Review the converted retention times.

Method Setup Tasks
Compound Setup
K Retention Time Setup
ISTD Setup Retention Time Setup
🛣 Qualifier Setup
🛠 Calibration Curve Setup
Globals Setup

# The compound parameters are displayed and may be edited. Notice that the converted method's Left RT Delta, Right RT Delta, and RT Delta Units are correctly converted.

im	ne Segment: 🛛 🖛	<all></all>		-	Compound:	4		🕶 📄 🛛 Reset	Table View
an	nple	1							
	Name	Data File			Туре	V	Level	Acq. Method File	Acq. Date-Time
- [		I		1		Ť	ľ		
Ĩ	Quantifier								1
		01746		_	1 -				
		me	TS	Scan	Туре /	RT	Left RT Delta		
	1,4-Dichloro		1	Scan	ISTD	11.487	0.500	0.500	Minutes
	Naphthalene		1	Scan	ISTD	15.331	0.500	0.500	Minutes
	Acenaphthen		1	Scan	ISTD	20.821	0.500	0.500	Minutes
	Phenanthren		1	Scan	ISTD	25.438	0.500	0.500	Minutes
	Chrysene-d1		1	Scan	ISTD	33.841	0.500	0.500	Minutes
	Perylene-d12		1	Scan	ISTD	37.983	0.500	0.500	Minutes
	2-Fluoropher		1	Scan	Target	8.255	0.500	0.500	Minutes
	bis(2-Chloro	ethyl)ether	1	Scan	Target	10.979	0.500	0.500	Minutes
	Phenol-d5		1	Scan	Target	11.019	0.500	0.500	Minutes
	Phenol		1	Scan	Target	11.040	0.500	0.500	Minutes
	2-Chlorophe		1	Scan	Target	11.080	0.500	0.500	
	1,3-Dichloro		1	Scan	Target	11.386	0.500	0.500	
	1,4-Dichloro		1	Scan	Target	11.548	0.500	0.500	Minutes
	1,2-Dichloro		1	Scan	Target	12.077	0.500	0.500	Minutes
	Benzyl alcoh		1	Scan	Target	12.179	0.500	0.500	Minutes
		isopropyl)ether	1	Scan	Target	12.565	0.500	0.500	Minutes
	2-Methylphe		1	Scan	Target	12.687	0.500	0.500	Minutes
	Hexachloroe		1	Scan	Target	12.952	0.500	0.500	Minutes
		-n-propylamine	1	Scan	Target	13.053	0.500	0.500	Minutes
1	4-Methylphe		1	Scan	Target	13.155	0.500	0.500	Minutes
	Nitrobenzen		1	Scan	Target	13.257	0.500	0.500	Minutes
	Nitrobenzen	e	1	Scan	Target	13.318	0.500	0.500	
	Isophorone		1	Scan	Target	14.090	0.500	0.500	
	2-Nitropheno		1	Scan	Target	14.273	0.500	0.500	
	2,4-Dimethyl		1	Scan	Target	14.680	0.500	0.500	Minutes
		ethoxy)methane	1	Scan	Target	14.863	0.500	0.500	Minutes
	2,4-Dichloro		1	Scan	Target	15.107	0.500	0.500	Minutes
	1,2,4-Trichlo		1	Scan	Target	15.249	0.500	0.500	Minutes
	Naphthalene		1	Scan	Target	15.392	0.500	0.500	Minutes
	4-Chloroanil		1	Scan	Target	15.717	0.500	0.500	Minutes
	Hexachlorob	and the second se	1	Scan	Target	16.023	0.500	0.500	Minutes
	4-Chloro-3-n		1	Scan	Target	17.465	0.500	0.500	Minutes
	2-Methylnap		1	Scan	Target	17.526	0.500	0.500	
-		cyclopentadiene	1	Scan	Target	18.258	0.500	0.500	
	2,4,6-Trichlo		1	Scan	Target	18.624	0.500	0.500	
	2,4,5-Trichlo		1	Scan	Target	18.787	0.500	0.500	
	2-Fluorobiph		1	Scan	Target	18.828	0.500	0.500	
	2-Chloronap		1	Scan	Target	19.032	0.500	0.500	
	2-Nitroanilin		1	Scan	Target	19.580	0.500	0.500	Minutes
	Acenaphthyle	ene	1	Scan	Target	20.333	0.500	0.500	Minutes

40,0000

40.0000

40.0000

40.0000

40.0000

40.0000

-1.0000

-1 0000

-1.0000

-1.0000

-1.0000

-1.0000

-1.0000

-1.0000

-1.0000

-1.0000

-1.0000

-1.0000

-1 0000

-1.0000

-1.0000

-1.0000

-1.0000

-1.0000

-1.0000

-1.0000

-1,0000

-1.0000

-1.0000

-1.0000

-1.0000

-1.0000

-1.0000

-1.0000

-1.0000

-1.0000

-1.0000

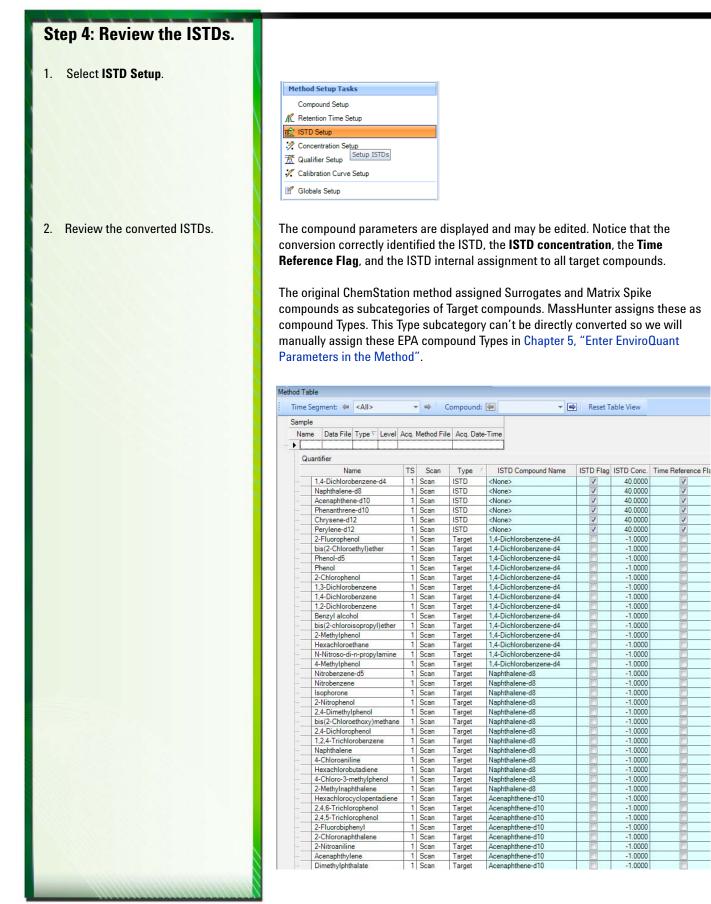
-1.0000

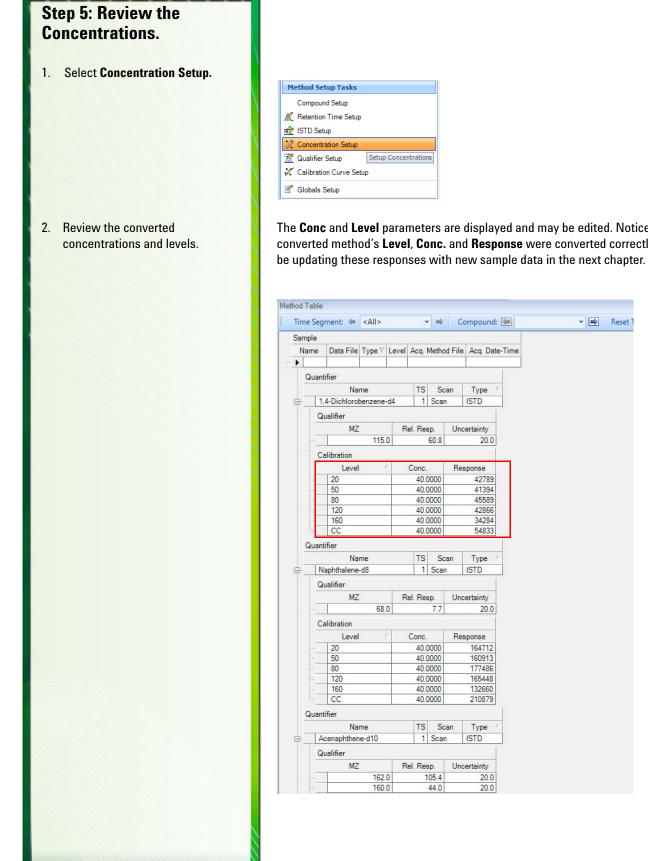
-1.0000

-1.0000

-1.0000

1





The **Conc** and **Level** parameters are displayed and may be edited. Notice that the converted method's Level, Conc. and Response were converted correctly. We will

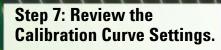
	gment: 🖛 <all></all>			-	C		4	 	
ample							-		
Name	Data File Type ∇	Level	Acq. I	Method	I File	Acq. Dat	e-lime		
•						1			
Quar	ntifier								
	Name		TS	Sca	n	Туре	5		
- 1	1,4-Dichlorobenzene-	14	1	Scan		ISTD			
G	Qualifier								
-	MZ		el. Res	SD.	Unc	ertainty			
	115.0			60.8	0110	20.0			
Ē	Charles and a second	-				20.0			
	Calibration		1.20000				_		
	Level /		Conc.	<u>e</u>	Res	sponse			
	20	-		0000		42789			
-	50 80	-		0000		41394 45589			
-	120	-		_	40005				
-	160	-	40.0000		34284				
	CC	-		0000		54833			
0	ntifier	-							
Qual	Name		TS	Sca	-	T	20		
	Name Naphthalene-d8		15	Scan	an	Type ISTD			
			1 1	Scan		1510			
	Qualifier				100 00000000000				
	MZ		Rel. Res						
Ī			el. Res		Unc	ertainty			
	MZ 68.0		el. Res	sp. 7.7	Unc	ertainty 20.0			
			el. Res		Unc				
	68.0	)	el. Res Conc.	7.7		20.0			
	68.0 Calibration	)	Conc.	7.7					
	Calibration	)	Conc. 40.0	7.7		20.0 sponse			
	Calibration Level / 20	)	Conc. 40.0 40.0	7.7		20.0 sponse 164712 160913 177486			
	68.0 Calibration Level / 20 50 80 120	)	Conc. 40.0 40.0 40.0 40.0	7.7		20.0 sponse 164712 160913 177486 165448			
	68.0 Calibration 20 50 80 120 160	)	Conc. 40.0 40.0 40.0 40.0 40.0	7.7 0000 0000 0000 0000 0000		20.0 sponse 164712 160913 177486 165448 132660			
	68.0 Calibration Level / 20 50 80 120	)	Conc. 40.0 40.0 40.0 40.0 40.0	7.7		20.0 sponse 164712 160913 177486 165448			
	68.0 Calibration 20 50 80 120 160	)	Conc. 40.0 40.0 40.0 40.0 40.0	7.7 0000 0000 0000 0000 0000		20.0 sponse 164712 160913 177486 165448 132660			
	68.0           Level         /           20         /           50         80           120         160           CC	)	Conc. 40.0 40.0 40.0 40.0 40.0	7.7 0000 0000 0000 0000 0000	Res	20.0 sponse 164712 160913 177486 165448 132660			
	68.0           Level         /           20         /           50         80           120         160           CC	)	Conc. 40.0 40.0 40.0 40.0 40.0 40.0 7S	7.7	Res	20.0 sponse 164712 160913 177486 165448 132660 210879			
Quar	68.0           Calibration           Level         /           20         /           50         80           120         160           CC         .           ntifier         Name           Accenaphthene-d10	)	Conc. 40.0 40.0 40.0 40.0 40.0 40.0 7S	7.7 0000 0000 0000 0000 0000 0000 0000	Res	20.0 sponse 164712 160913 177486 165448 132660 210879 Type			
Quar	68.0           Calibration           Level         /           20         /           50         80           120         160           CC         .           ntifier         Name           Accenaphthene-d10         Qualifier		Conc. 40.0 40.0 40.0 40.0 40.0 40.0 1 5 1	7.7 0000 0000 0000 0000 0000 0000 0000	Res	20.0 sponse 164712 160913 177486 155448 132660 210879 Type ISTD			
Quar	68.0           Calibration           Level         /           20         /           50         80           120         160           CC         .           ntifier         Name           Accenaphthene-d10	R	Conc. 40.0 40.0 40.0 40.0 40.0 40.0 40.0 40	7.7 0000 0000 0000 0000 0000 0000 0000	Res	20.0 sponse 164712 160913 177486 165448 132660 210879 Type			

	tep 6: Review the ualifiers.
1	Select Qualifier Setup.
	Select Qualitier Setup.
2.	Review the converted qualifiers.

Method Setup Tasks
Compound Setup
K Retention Time Setup
<u>is</u> ∕ ISTD Setup
🪀 Concentration Setup
Ҟ Qualifier Setup
Calibration Setup Qualifiers
I Globals Setup

The compound parameters are displayed and may be edited. Notice that the converted method's mz, Rel Resp, Uncertainty, and Area Sum state were converted correctly.

-	Segment: 🖛 <all></all>		_			ompound		
Samp	le							
Nan	ne Data File Type V	Level	Acq.	Metho	od File	Acq. Dat	e-Time	
Q	uantifier							
	Name		TS		can	Туре	MZ	Uncertaint
	1,4-Dichlorobenzene	-d4	1	Sca	n	ISTD	15	2.0 Absolute
	Qualifier							
	MZ	Re	I. Re	sp.	Un	certainty	Area Su	n
	115	.0		60.8		20.0		
Q	uantifier							
	Name		TS	So	an	Туре	MZ	Uncertaint
5	Naphthalene-d8		1	Sca	n	ISTD	13	5.0 Absolute
	Qualifier							
	MZ	Re	I. Re	SD.	Un	certainty	Area Su	n
	68			7.7		20.0		
0	uantifier							
-	Name		TS	Se	can	Туре	MZ	Uncertaint
	Acenaphthene-d10		1.1.2	Sca		ISTD	1000	4.0 Absolute
Π	Qualifier	1	-					
	MZ	Re	I. Re:	an an	Un	certainty	Area Su	n
	162			05.4	OIN	20.0		
	160			44.0		20.0	(177)	
Q	uantifier							
	Name		TS	Se	an	Туре	MZ	Uncertaint
	Phenanthrene-d10		1	Sca	n	ISTD	18	3.0 Absolute
	Qualifier							
	MZ	Re	I. Re	an a	Un	certainty	Area Su	n
	94	11/10/08		12.7	0	20.0		
0	uantifier							
4	Name		TS	0	can	Туре	MZ	Uncertaint
	Chrysene-d12		13	Sca		ISTD	- 10 S	0.0 Absolute
	Qualifier						24	, and the second to
	MZ		I. Re		11-		A C	-
	120		I. Re	sp. 15.6	Une	certainty 20.0	Area Su	n
	236			22.3		20.0		-
0	uantifier		_					
4	Name		TS	C.	can	Туре	MZ	Uncertaint
	Perylene-d12		10.00	Sca		ISTD	26	2000 CONTRACTOR
ΤT	Sector Contractor		1.1	500		1010	20	Ausointe
	Qualifier			-				
	MZ		I. Re		Un	certainty	Area Su	n
	260		-	20.5		20.0		_
	265			13.2		20.01		



1. Select Calibration Curve Setup.

2. Review the converted Calibration curve.

The compound parameters are displayed and may be edited. Notice that the Curve Fit (**CF**), **CF Origin**, and **CF Weight** were correctly converted.

Time	Segment: 🖛	<all></all>			- 📫 C	ompound:	4	*	Reset Table V	iew
Sampl	le			_		-/-0				
Nam	ne Data File	Tvpe ∇	Level	Aca.	Method File	Acq. Date	Time			
•		1								
· •										
Q	uantifier			TS						-
	Name 1,4-Dichlorobenzene-d4				Scan	Туре	(	CF	CF Origin	CF Weigh
					Scan	ISTD	Average of Resp		Ignore	None
<u></u>	Naphthalene-d8 Acenaphthene-d10			1		ISTD	Average of Resp		Ignore	None
<u></u>				1		ISTD	Average of Resp		Ignore	None
-	Phenanthren			1		ISTD	Average of Resp		Ignore	None
<u></u>	Chrysene-d			1		ISTD	Average of Resp		Ignore	None
-	Perylene-d1			1		ISTD	Average of Resp		Ignore	None
	2-Fluorophe			1		Target	Average of Resp		Ignore	None
	bis(2-Chloro	ethyl)eth	er	1		Target	Average of Resp		Ignore	None
-	Phenol-d5			1		Target	Average of Resp		Ignore	None
	Phenol			1		Target	Average of Resp		Ignore	None
<u></u>	2-Chlorophe			1		Target	Average of Resp		Ignore	None
	1,3-Dichloro			1		Target	Average of Resp	and the second se	Ignore	None
-	1,4-Dichloro			1		Target	Average of Resp		Ignore	None
h	1,2-Dichloro			1		Target	Average of Resp		Ignore	None
	Benzyl alcoh	lor		1		Target	Average of Resp	onse Factors	Ignore	None
	bis(2-chloro		)ether	1		Target	Average of Resp	and the second se	Ignore	None
-	2-Methylphe			1		Target	Average of Resp		Ignore	None
<u></u>	Hexachloroe			1		Target	Average of Resp		Ignore	None
	N-Nitroso-di	-n-propyl	amine	1		Target	Average of Resp		Ignore	None
<u></u>	4-Methylphe			1		Target	Average of Resp	and the second se	Ignore	None
	Nitrobenzen	e-d5		1		Target	Average of Resp	onse Factors	Ignore	None
	Nitrobenzen	е		1	Scan	Target	Average of Resp	onse Factors	Ignore	None
-	Isophorone			1	Scan	Target	Average of Resp	onse Factors	Ignore	None
-	2-Nitrophene			1		Target	Average of Resp		Ignore	None
-	2,4-Dimethy	Iphenol		1	Scan	Target	Average of Resp	onse Factors	Ignore	None
-	bis(2-Chloro	ethoxy)n	nethane	1	Scan	Target	Average of Resp	onse Factors	Ignore	None
-	2,4-Dichloro	phenol		1	Scan	Target	Average of Resp	onse Factors	Ignore	None
-	1,2,4-Trichle	probenzei	ne	1	Scan	Target	Average of Resp		Ignore	None
	Naphthalene			1	Scan	Target	Average of Resp	onse Factors	Ignore	None
-	4-Chloroanil	ine		1	Scan	Target	Average of Resp	onse Factors	Ignore	None
-	Hexachlorob	outadiene		1	Scan	Target	Average of Resp	onse Factors	Ignore	None
-	4-Chloro-3-r	nethylphe	enol	1		Target	Average of Resp	onse Factors	Ignore	None
-	2-Methylnap	hthalene	1.0	1		Target	Average of Resp	onse Factors	Ignore	None
-	Hexachloroc			1		Target	Average of Resp		Ignore	None
-	2,4,6-Trichlo			1		Target	Average of Resp	onse Factors	Ignore	None
-	2,4,5-Trichlo	prophenol		1		Target	Average of Resp	onse Factors	Ignore	None
-	2-Fluorobiph	nenyl		1	Scan	Target	Average of Resp	onse Factors	Ignore	None
	2-Chloronap	hthalene		1	Scan	Target	Average of Resp	onse Factors	Ignore	None
	2-Nitroanilin	e		1	Scan	Target	Average of Resp	onse Factors	Ignore	None
	Acenaphthyl	ene		1	Scan	Target	Average of Resp	onse Factors	Ignore	None
	Dimethylpht	halate		1	Scan	Target	Average of Resp	onse Factors	Ignore	None
	2,6-Dinitroto	luene		1	Scan	Target	Average of Resp	onse Factors	Ignore	None

#### Step 8: Set up the Integrator.

- 1. In the Advanced Tasks area, select Integration Parameters Setup.
- 2. Review the integrator used.
- 3. To change to the type of integrator used in the ChemStation method, select **General** for the first quantifier then select **Fill Down** from the context menu.

4. Select **Int. Parms.** in the Method Table for the first quantifier and edit the integration parameters to suit your method then select **Fill Down** from the context menu.

Advanced Tasks								
Integration Parameters Setup								
Signal to Noise Setup Smoothing Setup								
III Mass Extraction Setup Spectrum Extraction Setup Isotopic Dilution Setup								

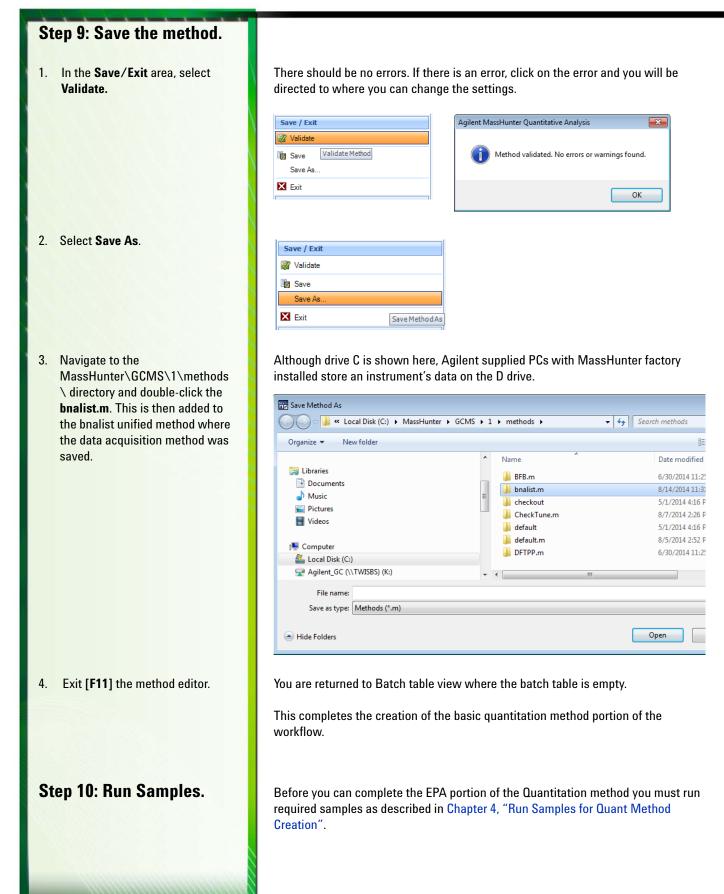
During the ChemStation method conversion the MassHunter parameterless **Agile** integrator was substituted for the ChemStation specified integrator.

All quantifiers now use the **General** integrator originally used in the ChemStation method.

c.,	mole	mple												
_	· · · · · · · · · · · · · · · · · · ·			Acq. Method File			Aca Date	Time						
		e Data i lie	Type	Lever	AUQ.	Metho	u i lie	Acy. Date	TIME					
	Qu	Quantifier												
	Name					TS Scan		Туре	RT Int			Int. Parms.		
ė	•	1,4-Dichlorobenzene-d4				Scar	1	ISTD	11.487	Agile				
	Qualifier													
		MZ Re		el. Re	sp.	Unc	ertainty	Int. I	Parms.					
		115.0			-	60.8		20.0						
	Quantifier													
		Na	TS	TS Scan		Туре	RT In			Int. Parms.				
-		Naphthalene-d8				1 Scan		ISTD	15.331	Agile				
	Qualifier													
		MZ	<u>.</u>	R	el. Res	sp.	Unc	ertainty	Int. I	Parms.				
			68.	0		7.7		20.0						
	Quantifier													
		Na	TS	Scan		Type /	RT	Int.		Int. Parms.				
		Acenaphthene-d10				1000		and the second second						

By default, the qualifiers are assigned the same integration parameters as the quantifier but this can be overridden by selecting the **Int Params** for the qualifiers.

ntegrator General Universal Spe	ectrum Summation Peak Filt	er		
Data point sampling: 1	Start three	hold:	0.2	
Smoothing	Stop thres	0		
Detection filtering: 5 point	✓ Peak loca	ation:	Тор	-
	If leading or trailing edge <	100		%
Baseline preference:	Tangent skim else drop			•



# •

4

## Run Samples for Quant Method Creation

Introduction 34 Step 1: Create a batch. 34 Step 2: Complete the Tune Evaluation criteria. 35 Step 3: Complete the GC Performance Evaluation criteria. 38 Step 4: Review the tune evaluation results. 39 Step 5: Create a Reference library. 43 Step 6: Initialize the Continuing Calibration response. 44 Step 7: Save the Method. 45 Step 8: Complete the quantitation method. 46

**Agilent Technologies** 

#### Introduction

#### Step 1: Create a batch.

- 1. Double-click the Instrument icon to launch MassHunter GCMS Acquisition.
- 2. Load a default sequence.
- Select Sequence > Edit Sequence, complete the entries similar to those shown here, then click OK.

4. Select Sequence > Save Sequence As... and save the sequence as QuantSetup. This chapter explains how to create a sequence, that when run, will generate a batch containing the analyzed results of samples used to update the compound calibration curves in the quantitation method. You will also use these samples to create the Tune Evaluation Method (tunevaluation.xml), create the Reference Library, and initialize the CC sample response.



The first sample in this sequence should contain compounds that are representative of what will be analyzed (e.g., Pentachlorophenol, DFTPP, Benzidine, and DDT for EPA method 8270).

The next 5 sample are calibration samples that will be used to create the calibration curves for all compounds in the method.

The last column, **Update Response Factor**, is specifying that the current response factors in the method should be replaced with the response factors from these 5 CAL samples.

Also, one of these samples will be used to create a Reference Library.

The Continuing Cal sample's compound responses will be manually entered into the method to initialize future CC's.

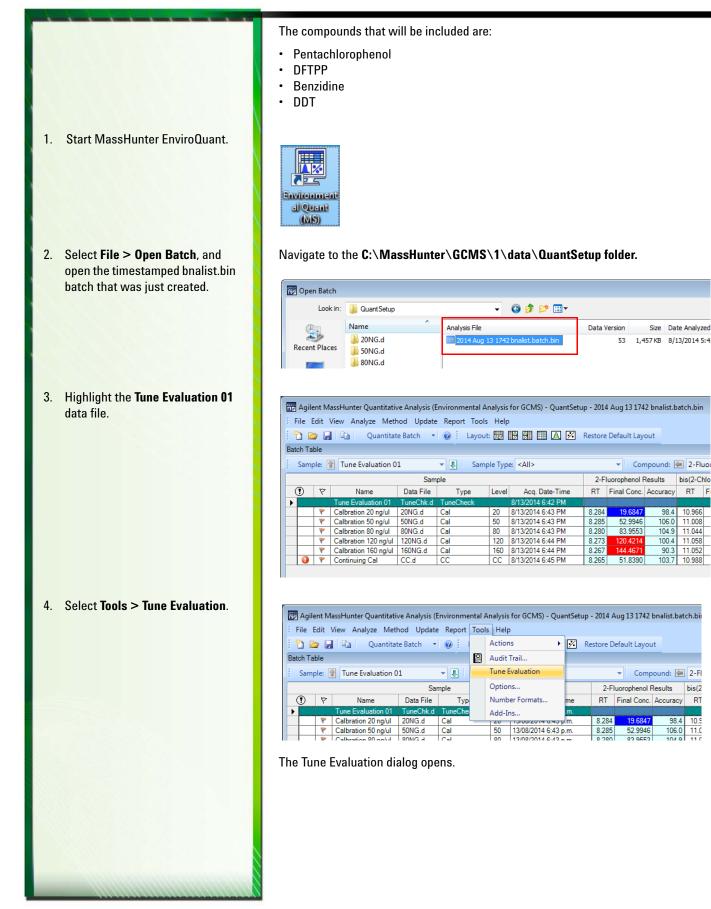
il.	New Sample(s) 🔻		Tool	5 •					
	Name	Vial	Туре		Level	Data File	Method File	Update Response Factor	r
1	Tune Evaluation 01	10	TuneCheck	-		TuneChk.d	bnalist.m		
2	Calbration 20 ng/ul	11	Cal	-	20	20NG.d	bnalist.m	 Replace	•
3	Calbration 50 ng/ul	12	Cal	-	50	50NG.d	bnalist.m	 Replace	•
4	Calbration 80 ng/ul	13	Cal	-	80	80NG.d	bnalist.m	 Replace	•
5	Calbration 120 ng/ul	14	Cal	-	120	120NG.d	bnalist.m	 Replace	•
6	Calbration 160 ng/ul	15	Cal	-	160	160NG.d	bnalist.m	 Replace	•
7	Continuing Call	16	CC	-	CC	CC.d	bnalist.m	 No Update	•

### 4. Run Samples for Quant Method Creation

<ol> <li>Select Sequence &gt; Run Sequence, and complete t dialog as shown here.</li> </ol>	the							
Star	t Sequence QuantSetup.sequence.xml Last Modified:	Fri Aug 08 14:54:33 2014						
	- Method Sections to Run	Sequence Barcode Options						
	Full Method	<ul> <li>Disable barcode for this sequence.</li> </ul>						
		<ul> <li>On mismatch, inject anyway.</li> <li>On mismatch, don't inject; continue the sequence.</li> </ul>						
		<ul> <li>On mismatch, don't inject; stop the sequence.</li> </ul>						
	Verwrite Existing Data Files							
	Sequence Comment:							
	Operator Name:	int						
	Data File Directory:	C:\MassHunter\GCMS\1\data\QuantSetup\ Browse						
	Pre-Sequence Macros/Commands							
	Acquisition: Data Analysis:	Browse						
	Post-Sequence Macros/Commands							
	Acquisition: Data Analysis:	Browse						
	Inject anyway, do not generate an error or stop the seque							
	<u>R</u> un Sequence	OK Cancel <u>H</u> elp						
<ol> <li>Click Run Sequence when finished.</li> <li>Step 2: Complete the Evaluation criteria.</li> </ol>	data files and sav         this case: C:\Max         The method's res         The Tune         The Tune Evaluati         required analyzer         and saved (as tun)         In practice, the tu         During processing	Acquisition will automatically create a batch containing these e it in the MassHunter folder specified in the Sequence table. In ssHunter\GCMS\1\data\QuantSetup. ponse factors for the 5 CAL samples are automatically updated. ion Tool in MassHunter EnviroQuant makes it easy to enter EPA tune and GC performance criteria. Once the criteria are entered <i>vevaluation.xml</i> ), they become part of the unified method. ne evaluation sample is processed as the first sample in the batch. g, if the tune evaluation sample fails to comply with the criteria une Evaluation method (which is one part of the unified method),						
	the sequence will running on an ins The following des ( <i>tunevaluation.xm</i> EPA method 8270	automatically stop to prevent the remaining samples from trument that requires tuning. scribes how to build the tune evaluation method n/). The example shown here includes the criteria for D. Entries for other EPA methods are entered in a similar manner. The process describes how to set up a Reference Library.						

#### 4. Run Samples for Quant Method Creation

#### Step 2: Complete the Tune Evaluation criteria.



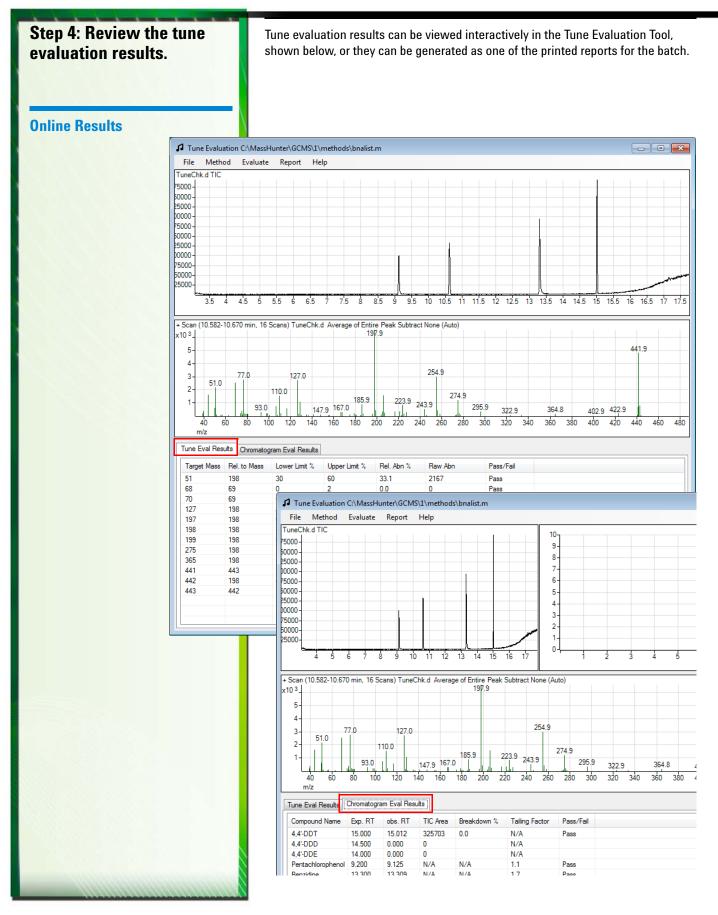
## Step 2: Complete the Tune Evaluation criteria.

		J Tune Evaluation						
1.1.1.1.1		File Method Evaluate	Report Hel	P				
		35 4 45 5	5.5 6 6.5	7 7.5 8 8.5	9 95 10 10.5 11 1	1.5 12 12.5 13 13.5	14 14.5 15 15.5 16 16	5 17 175
	No. Contraction of the	10						
		5- 0- 0.5 1 1.	5 2 2	25 3 35 4	4 4.5 5 5.5	é 6.5 7	7.5 8 8.5 9	9.5
		Tune Eval Results Chromatogra Target Mass Rel. to Mass		Upper Limit % Rel. Abr	n % Raw Abn I	Pass/Fail		
		<u>(</u>						
5. Select Method	l > Edit Method.	J Tune Evaluation	n					
		File Method	Evaluate	Report He	lp			
			Method I Method					
		25000 - Save	Method A	.s				
		75000 -						
6. Complete the	Tune Evaluation.	For FPA meth	od 827	70 vou woi	uld complet	te this scre	en similar to	the one shown
o. complete the		here.	.04 02	e you not				
	Time Evaluation Method							×
	Tune Evaluation GC Performance Evalua	tion						
	Tune Evaluation		Criteria	MZ 198	٨4	emate Base MZ		
			Dase	100	AU	en late base MZ		
	Method Title DFTPP			Mass	Rel. To MZ	% Low	% High	Alt. Base OK
	Method Title DFTPP Spectral Evaluation		)					Alt. Base OK
	Spectral Evaluation			Mass 51 68 70	Rel. To MZ 198 69 69	% Low 30 0 0	% High 60 2 2	
				Mass 51 68 70 127	Rel. To MZ 198 69 69 198	% Low 30 0 0 40	% High 60 2 2 60	
	Spectral Evaluation			Mass 51 68 70 127 197	Rel. To MZ 198 69 69 198 198	% Low 30 0 0 40 0	% High 60 2 2 60 1	
	Spectral Evaluation <ul> <li>Manual</li> <li>Manual</li> <li>Manual Options</li> </ul>			Mass 51 68 70 127	Rel. To MZ 198 69 69 198	% Low 30 0 0 40	% High 60 2 2 60	
	Spectral Evaluation Manual   Auto			Mass 51 68 70 127 197 198	Rel. To MZ           198           69           69           198           198           198           198           198           198           198	% Low 30 0 0 40 0 100	% High 60 2 2 60 1 100	
	Spectral Evaluation          Manual       Auto         Manual Options       Spectrum Extraction         Apex			Mass 51 68 70 127 197 198 199 275 365	Rel. To MZ           198           69           198           198           198           198           198           198           198           198           198           198           198           198           198           198           198	% Low           30           0           0           40           0           100           5           10           1	% High           60           2           60           1           100           9           30           100	
	Spectral Evaluation           Manual         Auto           Manual Options         Spectrum Extraction			Mass 51 68 70 127 197 198 199 275 365 441	Rel. To MZ           198           69           198	% Low         30           0         0           0         0           40         0           100         5           10         1           1E-10         1	% High           60           2           2           60           1           100           9           30           100           100	
	Spectral Evaluation          Manual       Auto         Manual Options       Spectrum Extraction         Apex       Background Subtraction         None       *			Mass           51           68           70           127           197           198           199           275           365           441           442	Rel. To MZ           198           69           198           198           198           198           198           198           198           198           198           198           198           198           198           198           198           198           198           198	% Low         30           30         0           0         0           40         0           100         5           10         1           1E-10         40	% High           60           2           2           60           1           100           9           30           100           100           100           100           100           100	
	Spectral Evaluation          Manual       Auto         Manual Options       Spectrum Extraction         Apex       Background Subtraction			Mass 51 68 70 127 197 198 199 275 365 441	Rel. To MZ           198           69           198	% Low         30           0         0           0         0           40         0           100         5           10         1           1E-10         1	% High           60           2           2           60           1           100           9           30           100           100	
	Spectral Evaluation          Manual       Auto         Manual Options       Spectrum Extraction         Apex       Background Subtraction         None       *		•	Mass           51           68           70           127           197           198           199           275           365           441           442	Rel. To MZ           198           69           198           198           198           198           198           198           198           198           198           198           198           198           198           198           198           198           198           198	% Low         30           30         0           0         0           40         0           100         5           10         1           1E-10         40	% High           60           2           2           60           1           100           9           30           100           100           100           100           100           100	
	Spectral Evaluation          Manual       Auto         Manual Options       Spectrum Extraction         Apex       Background Subtraction         None       *	+ 20 Scans	*	Mass 51 68 70 127 197 198 199 275 365 441 442 443	Rel. To MZ           198           69           69           198           198           198           198           198           198           198           198           198           198           198           198           198           198           198           198           198           198           443           198           442	% Low           30           0           0           0           0           100           5           10           1           1E-10           40           17	% High           60           2           2           60           1           100           9           30           100           100           100           100           100           100	
	Spectral Evaluation          Manual       Auto         Manual Options       Spectrum Extraction         Apex       Background Subtraction         None       *		*	Mass           51           68           70           127           197           198           199           275           365           441           442	Rel. To MZ           198           69           69           198           198           198           198           198           198           198           198           198           198           198           198           198           198           198           198           198           198           443           198           442	% Low           30           0           40           0           100           5           10           1           1E-10           40           17	% High           60           2           2           60           1           100           9           30           100           100           100           100           100           100	
	Spectral Evaluation          Manual       Auto         Manual Options       Spectrum Extraction         Apex       Background Subtraction         None       *	+ 20 Scans	+ + 	Mass 51 68 70 127 197 198 199 275 365 441 442 443 Cancel Jto, as sho	Rel. To MZ         198         69         69         198         199         198         199         199         199         199         199         199         199         199         199         199         199        <	% Low       30       0       0       40       0       100       5       10       1       1E-10       40       17       III	% High         60         2         2         60         1         100         9         30         100         100         23	

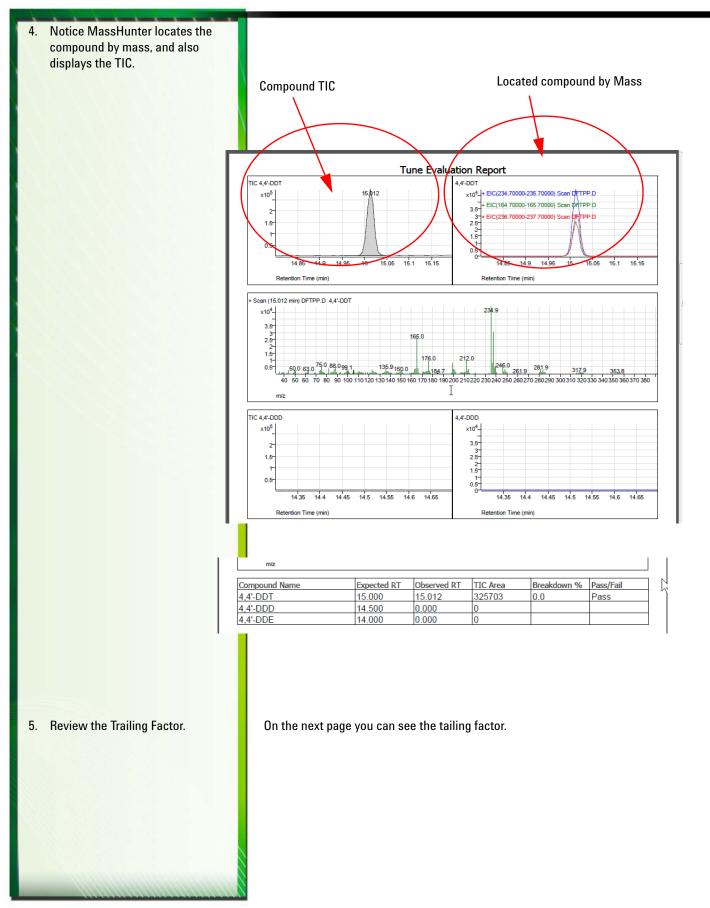
#### Step 3: Complete the GC Performance Evaluation criteria.

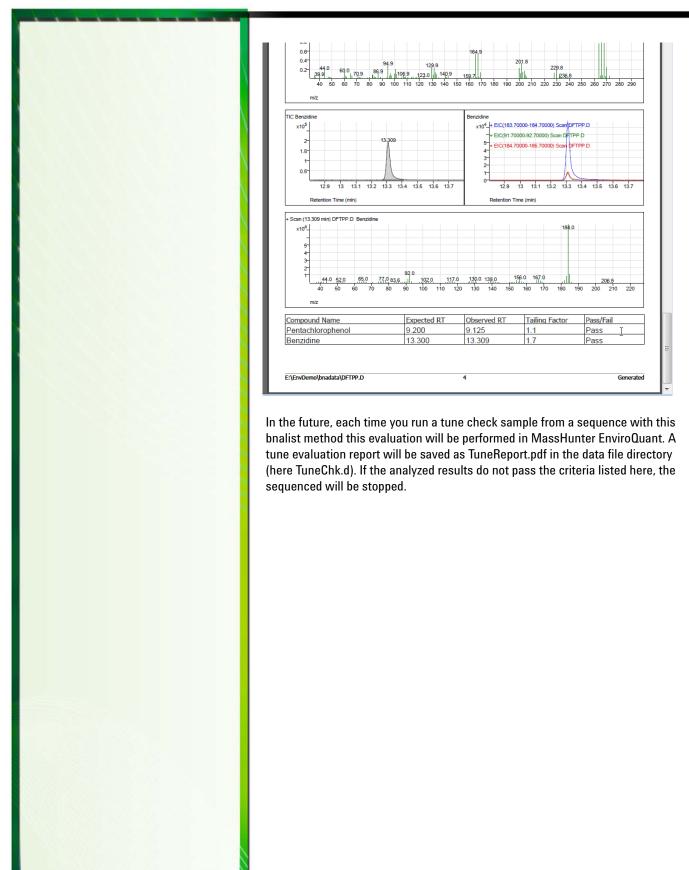
#### **Step 3: Complete the GC** For EPA method 8270, we will enter degradation of DDT, DDD, and DDE, and tailing **Performance Evaluation** for Pentachlorophenol and Benzidine. Notice that here we are finding the compounds by mass, however, the evaluation is done on the total ion criteria. chromatogram for the method. Click the GC Performance Enter the parameters for the degradation of DDT, DDD, and DDE as shown here. 1. **Evaluation** tab, select Breakdown to enable the test and enter the Breakdown parameters. Tune Evaluation Method Tune Evaluation GC Performance Evaluation Breakdown Compound Name Parent Breakdown Expected RT Delta RT Qual lons Parent Compound Quant Ion CompoundName Limit 15 0.2 V 4,4'-DDT 235 165.237 15 4,4'-DD 4,4'-DDD 14.5 0.2 4,4'-DDT 235 237,165 15 4 4'-DDF 14 02 4 4'-DDT 246 248 176 15 2. Select Tailing Factor to enable Enter tailing factor parameters for Pentachlorophenol and Benzidine. the test and enter the Tailing Factor parameters. ☑ Tailing Factor Compound Name Tailing Factor ExpectedRT Delta RT Quant Ion Qual lons Limit 9.2 0.5 266 264,268 5 Pentachl Benzidine 13.3 0.5 184 92,185 3 Apply the criteria. Click Apply, when ready, and the results are displayed online. See "Step 4: Review 3. the tune evaluation results." on page 39. Select Method > Save Method MassHunter saves this as the **tunevaluation.xml** method in the DAMethod\Quant\ 4. As, and save this to: sub-directory of the bnalist.m method. MassHunter\GCMS\1 \Methods\bnalist.m. Save a Tune Evaluation Method File Computer → Local Disk (C:) → MassHunter → GCMS → 1 → methods → ✓ 4 Search method Organize 🔻 New folder Recent Places Name Date modified 📗 BFB.m 6/30/2014 11:2 🔚 Libraries 8/14/2014 5:40 bnalist.m Documents 5/1/2014 4.16 chockout 5. Reply Yes when asked to Once the criteria are entered and saved, they become part of the bnalist method overwrite the existing method. which now contains method parameters for data acquisition, quantitative analysis, and Tune Evaluation.

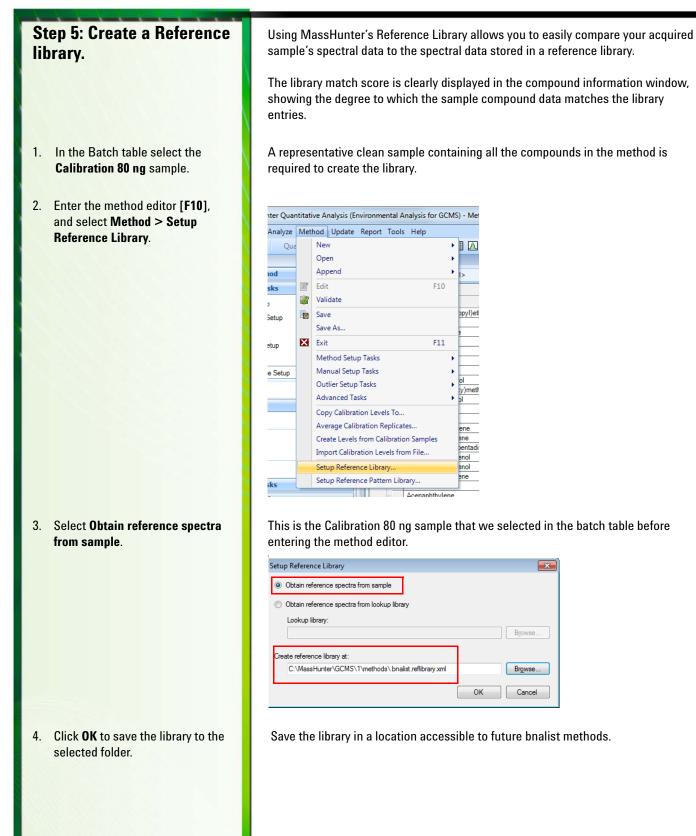
#### Step 4: Review the tune evaluation results.



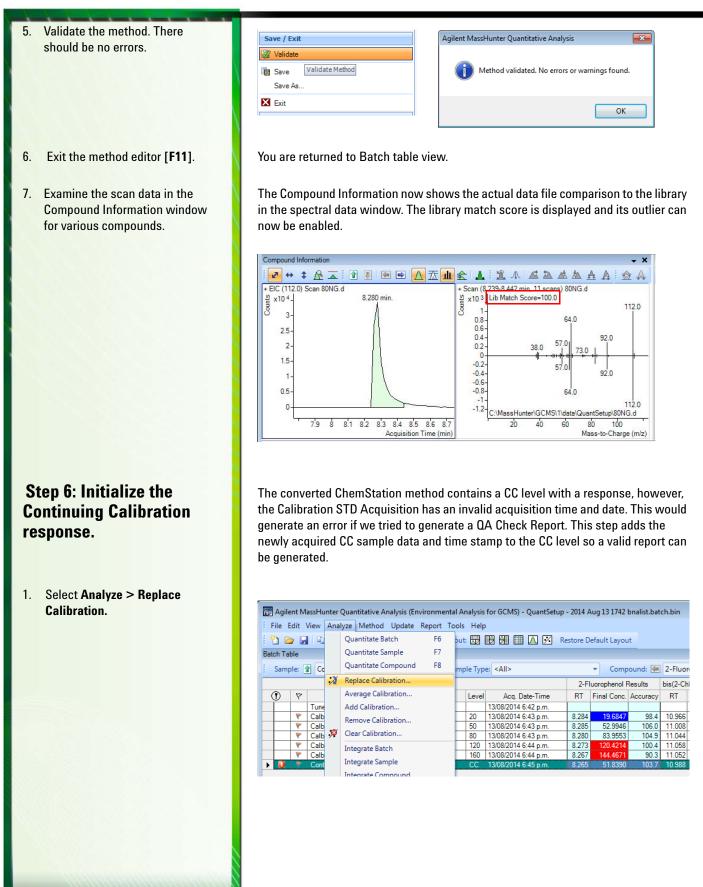
-	ine Evaluation PDF Report	
10		
1.	Click <b>Report</b> in Tune Evaluation.	Tune Evaluation C:\MassHunter\GCMS\1\methods\bnalist.m File Method Evaluate Report Help 50NG.d TIC 20000 1
2.	Accept the default location and name for the PDF report.	Save Report As         Image: Save Report As         Image
3.	Review the Pass/Fail condition for the first compound.	The PDF is generated and opened in Acrobat.
		<text><text><text><text><text><figure></figure></text></text></text></text></text>





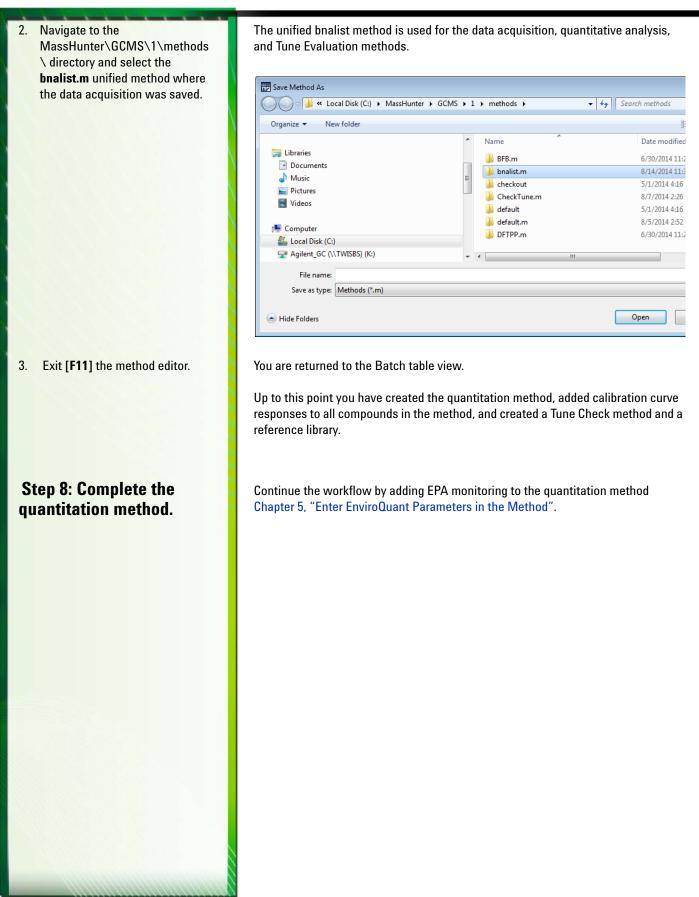


#### Step 6: Initialize the Continuing Calibration response.



1								
2.	In the Select Compounds tab,						1	
	click Select All then click Select	Replace Calibration					×	
		Select Compounds	Select Sample					
	Samples tab.	J Select Compounds	Select Sample					
			TO	DT ICTO		_		
		Name	TS		) Flag Cmpd. Gro	up	Â	
		2-Fluorophenol		1 8.255				
		bis(2-Chloroethyl)e		1 10.979				
		Phenol-d5		1 11.019				
		Phenol		1 11.040				
		2-Chlorophenol		1 11.080				
		1,3-Dichlorobenze		1 11.386	T		-	
		Select All				ОКС	ancel	
							.11	
3.	On the Select Samples tab, select	(						
	the Continuing Cal sample and	Replace Calibration					×	
	click <b>OK</b> .	Select Compounds	Select Samples	1				
	CIICK UK.		,				-	
		Name	Data File	Туре	Level	Sample Group		
		Calbration 20 ng/ul		Calibration	20			
		Calbration 50 ng/ul		Calibration	50			
		Calbration 80 ng/ul		Calibration	80			
		Calbration 120 ng		Calibration	120			
		Calbration 160 ng		Calibration	160 CC			
		Continuing Cal	CC.d	CC				
			_					
		Select All				OK Cancel		
							H.	
		The responses			libration co	ompounds are	replaced	with the
		responses in t	he data file					
St	ep 7: Save the Method.							
	op 7. ouve the wrethou.							
1.	Select Save As.							
		Save / Exit						
		📓 Validate						
		validate						
		📳 Save						
		Save As						
		X Exit	Eave	MathadAa				
			Save	e Method As				
	28.8 5.57							

#### Step 8: Complete the quantitation method.



# 5

## **Enter EnviroQuant Parameters in the** Method

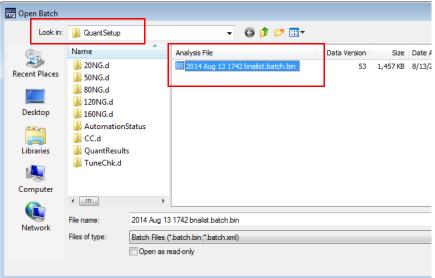
## Introduction 48 Step 1: Open the batch. 48 Step 2: Specify the surrogates and matrix spikes. 49 Step 3: Set up the CC Maximum Elapsed Time to 12 hours. 51 Step 4: Set up outlier limits for the EPA method criteria. 52 Step 5: Save the method. 66 Step 6: Create report methods. 66

**Agilent Technologies** 

## Introduction In this chapter you will learn how to add outliers to a quantitative method that Method 8270. Step 1: Open the batch. already open, skip this step. 1. In MassHunter EnviroQuant select File > Open Batch. 📅 Open Batch Look in: 📗 Quant Setup Name 9 20NG.d Recent Places 퉬 50NG.d 80NG.d 퉬 120NG.d Desktop 칠 160NG.d AutomationStatus 📕 CC.d 퉬 QuantResults Libraries 퉬 TuneChk.d Computer < III | Þ File name: Network Files of type: 2. Navigate to the QuantSetup folder, select the bnalist batch, and click **Open**.

monitor compound properties and instrument performance as specified by EPA

If the bnalist batch saved in the in the QuantSetup folder in the previous chapter is



#### The batch table opens with all samples quantitated.

File	Edit	View Analyze Metł	nod Update	e Report Tools	Help	•			
b I	<u>&gt;</u>	Quantitat	e Batch 🔹	🕜 🕴 Layout			Restore	Default Lay	out
itch T	able								
San	nple:	Calbration 20 ng/	ul	👻 🌉 🛛 Samp	ole Typ	e: <all></all>		▼ Con	npound: [
			Sam	ple			2-FI	uorophenol F	Results
•	7	Name	Data File	Туре	Level	Acq. Date-Time	RT	Final Conc.	Accuracy
		Tune Evaluation 01	TuneChk.d	TuneCheck		8/13/2014 6:42 PM			
	*	Calbration 20 ng/ul	20NG.d	Cal	20	8/13/2014 6:43 PM	8.284	19.6847	98.4
	٣	Calbration 50 ng/ul	50NG.d	Cal	50	8/13/2014 6:43 PM	8.285	52.9946	106.0
	*	Calbration 80 ng/ul	80NG.d	Cal	80	8/13/2014 6:43 PM	8.280	83.9553	104.9
	8	Calbration 120 ng/ul	120NG.d	Cal	120	8/13/2014 6:44 PM	8.273	120.4214	100.4
	10r	Calbration 160 ng/ul	160NG.d	Cal	160	8/13/2014 6:44 PM	8.267	144.4671	90.3
H	<b>Y</b>	Calbration 160 fig/ul	i loona.a						

Step 2: Specify the surrogates and matrix spikes.	Surrogates and matrix s in ChemStation, here in	-			
1. Open the method editor [ <b>F10</b> ]	L N				
2. Select Compound Setup.					
	File Edit View Analyze Method Update R				
		) Layout: 🕎 😰 🔛		Restore Default Lay	out
	Method Tasks 🗸 🗸	Method Table			
	New / Open Method	Time Segment: 🖛 <all></all>		👻 🔿 🛛 Compo	und: 🔄 2-Fluorophenol
	Method Setup Tasks	Quantifier			
	Compound Setup	Name	TS	Scan	Туре 🗠
	Retention Time Setup Setup Compounds	2-Fluorophenol		Scan	Surrogate
	IC Retention Time Setup Setup Compounds ISTD Setup	Phenol-d5 Nitrobenzene-d5	1	Scan Scan	Surrogate Surrogate
	Concentration Setup	2-Fluorobiphenyl	1		Surrogate
		2,4,6-Tribromop	1		Surrogate
	K Qualifier Setup	Terphenyl-d14	1		Surrogate
	K Calibration Curve Setup	bis(2-Chloroethy 1,3-Dichloroben	1		Target Target
	If Globals Setup	1,2-Dichloroben	1		Target
	Save / Exit	Benzyl alcohol	1		Target
		bis(2-chloroisopr	1	Scan	Target
4. Compare your edits with this example.	2-Fluorophenol Phenol-d5 Nitrobenzene-d5 2-Fluorobiphenyl 2,4,6-Tribromophenol Terphenyl-d14 After editing these com scroll to the Surrogate c		to sort	the compoun	ds by type and
	File Edit View Analyze Method Update Repor	Layout: 🔜 🔛 🔠 🛄 💽	Pertero (	Defecult Lavaut	
	i D D L Quantitate Batch V V i Method Tasks V Me		- Nestore i		
	New / Open Method	Time Segment: 🖛 <all></all>	-	Compound: 4	-Fluorophenol 👻 📑 Re
	Method Setup Tasks	Quantifier			
	Compound Setup	Name TS		Scan	Type 🛆 MZ
		- 2-Fluorophenol	1 Scan	Surroga	ate 1
	Retention Time Setup Setup Compounds	Phenol-d5 Nitrobenzene-d5	1 Scan	Surroga	
	152 ISTD Setup	2-Fluorobiphenyl	1 Scan 1 Scan	Surroga Surroga	
		2,4,6-Tribromop	1 Scan	Surroga	ate 3
	Calibration Curve Setup	Terphenyl-d14 bis(2 Chloroethy	1 Scan 1 Scan	Surroga Target	ate 2
		1,3-Dichloroben	1 Scan	Target	1
	I Globals Setup	1,2-Dichloroben Benzyl alcohol	1 Scan 1 Scan	Target Target	1
	Save / Frit			ruge	

5. Specify **Matrix Spike** as the **Type** for these compounds.

In the Quantifier table set the compound **Type** for each of these 11 compounds to Matrix Spike.

#### Phenol

- 2-Chlorophenol 1,4-Dichlorobenzene N-Nitroso-di-n-propylamine 1,2,4-Trichlorobenzene 4-Chloro-3-methylphenol Acenaphthene 2-4-Dinitrotoluene 4-Nitrophenol Pentachlorophenol Pyrene
- 6. Compare your edits with this example.

After editing these compounds, click on **Type** to sort compounds by type and scroll to the Matrix Spike compound Types.

Layou	t: 🔙 🛛 🖓 🛄		Restore <u>D</u> efault Layou	it			
thod Tab	ole						
Time S	Gegment: 🖛 <all></all>		▼ 🔿 Compour	nd: 🔄 Pyrene	▼ 🛃 🛛 <u>R</u> eset Tab	ole View	
Qu	antifier						
	Name	TS	Scan	Type 🗠	MZ	RT	lon f
_	Phenol	1	Scan	Matrix Spike	94.0	11.040	Positive
npounds	2-Chlorophenol	1	Scan	Matrix Spike	128.0	11.080	Positive
	1,4-Dichloroben	1	Scan	Matrix Spike	146.0	11.548	Positive
	N-Nitroso-di-n-pr	1	Scan	Matrix Spike	70.0	13.053	Positive
	1,2,4-Trichlorob	1	Scan	Matrix Spike	180.0	15.249	Positive
	4-Chloro-3-meth	1	Scan	Matrix Spike	107.0	17.465	Positive
	Acenaphthene	1	Scan	Matrix Spike	153.0	20.943	Positive
	2,4-Dinitrotoluene	1	Scan	Matrix Spike	165.0	21.696	Positive
·····	4-Nitrophenol	1	Scan	Matrix Spike	109.0	21.777	Positive
	Pentachlorophe	1	Scan	Matrix Spike	266.0	25.174	Positive
•••• •	Pyrene	1	Scan	Matrix Spike	202.0	29.933	Positive
	2-Fluorophenol	1	Scan	Surrogate	112.0	8 255	Positive

## 5. Enter EnviroQuant Parameters in the Method Step 3: Set up the CC Maximum Elapsed Time to 12 hours.

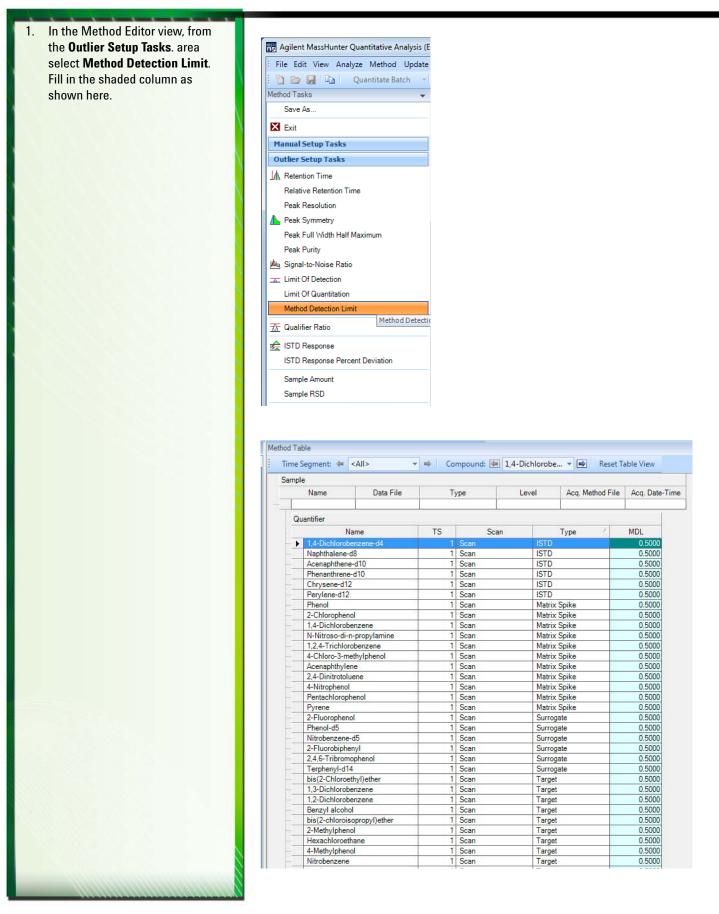
## Step 3: Set up the CC Maximum Elapsed Time to 12 hours.

- 1. In the Method Setup Tasks area, select **Globals Setup**.
- 2. Set the CC Maximum Elapsed Time in Hours to 12.000.

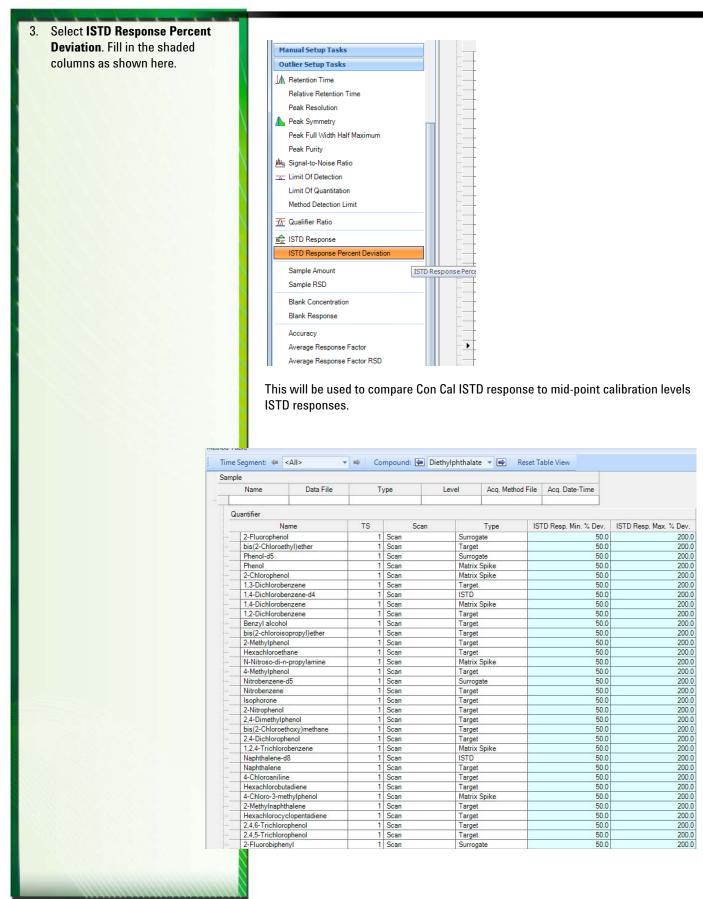
This global parameter sets the maximum amount of time that samples can be run without performing another continuous calibration. For EPA method 8270 that time is 12 hours. The QA Check Report uses this value when reporting if all samples in a batch were run before this time elapsed.

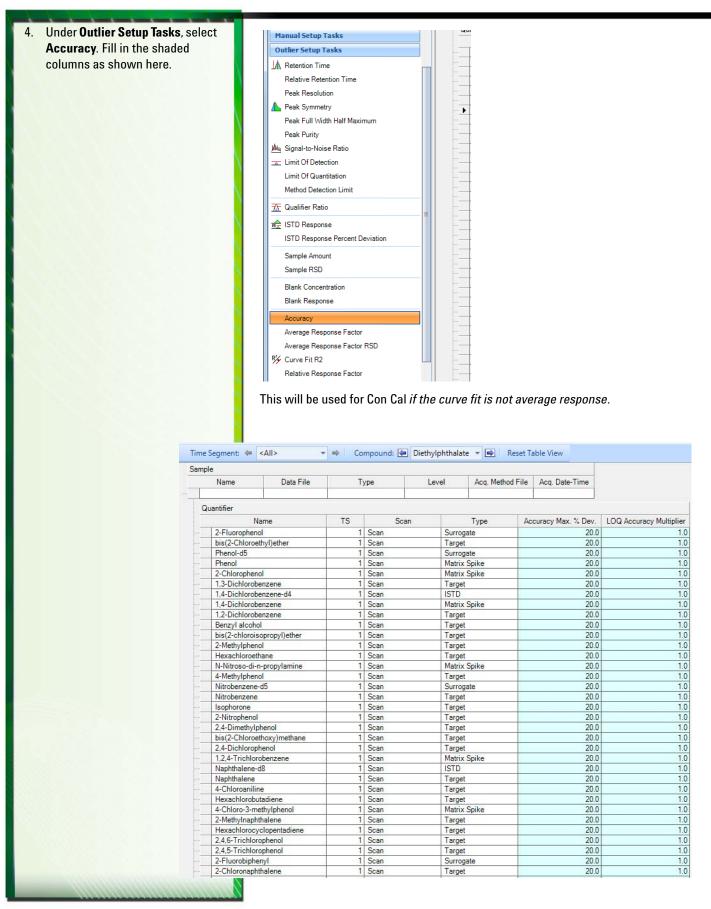
Method Tasks 🗸 🗸 🗸	C N	lethoo	d Table					
New / Open Method		Ti	me Segment: 🖛 🔸	All> 👻	⇒ [	Compound: 🔄	2-Flu	orophen
Method Setup Tasks		Sa	mple					
Compound Setup			Name	Data File		Туре	Ŀ	evel
Retention Time Setup			Calibration 120n	clwb120.d	Cal		120	
if ISTD Setup			Globals					
Concentration Setup								
Rualifier Setup			Apply Multiplier to	ISTD			1	
			Apply Multiplier to	Matrix Spike	1	<b>V</b>		
🛠 Calibration Curve Setup			Apply Multiplier to	Surrogate		$\checkmark$		
🖆 Globals Setup			Apply Multiplier to	Target		$\checkmark$		
Save / Exit Setup Globals		Г	Bracketing Type		Non		<u>+ </u>	
-				sed Time In Hours		12.000		
🥁 Validate			Correlation Windo			2.000		
I Save			Dynamic Backgrou Ignore Peaks Not I		-			
Save As			Non Reference Wi			200.000		
	-11		Non Reference Wi		Perc		-	
X Exit			Reference Library	/	C:\M	lassHibrary.xml	-	
Manual Setup Tasks			Reference Pattern	Library				
Outlier Setup Tasks			Reference Window	/		80.000	)	
Advanced Tasks			Reference Window	/ Туре	Perc	ent		
Advalleed Tasks			Relative ISTD				_	
			Standard Addition					

Step 4: Set up outlier limits for the EPA method criteria.	In this section you will set outlier criteria for monitoring compounds and instrument performance as required by EPA Method 8270, including the:
	Method Detection Limit
	<ul> <li>Surrogate Concentration, Percent recovery min and max</li> </ul>
	<ul> <li>ISTD Response Min and Max Percent Deviation - to compare the Con Cal ISTD response to the Mid-point calibration levels ISTD responses.</li> </ul>
	<ul> <li>Accuracy max percent deviation for Con Cal if the curve fit is not average response</li> </ul>
	Average Response Factor - for the ICal Report Minimum RF
	Average Response Factor RSD - for the ICal Report RSD
	• Curve Fit R2 - for the ICal Report curve fits other than Average Response Factor
	CC Relative Response - for the Minimum CC Response Factor
	<ul> <li>CC Average Response Factor - Con Cal report if the curve fit is average response factor</li> </ul>
	Matrix Spike Percent Difference
	Matrix Spike Percent Recovery
	Matrix Spike Group Recovery
	Surrogate Percent Recovery
	Library Match Score
	Once these outliers are set they can be displayed as color coded cells in the Batch Table and Compounds-at-a-Glance.

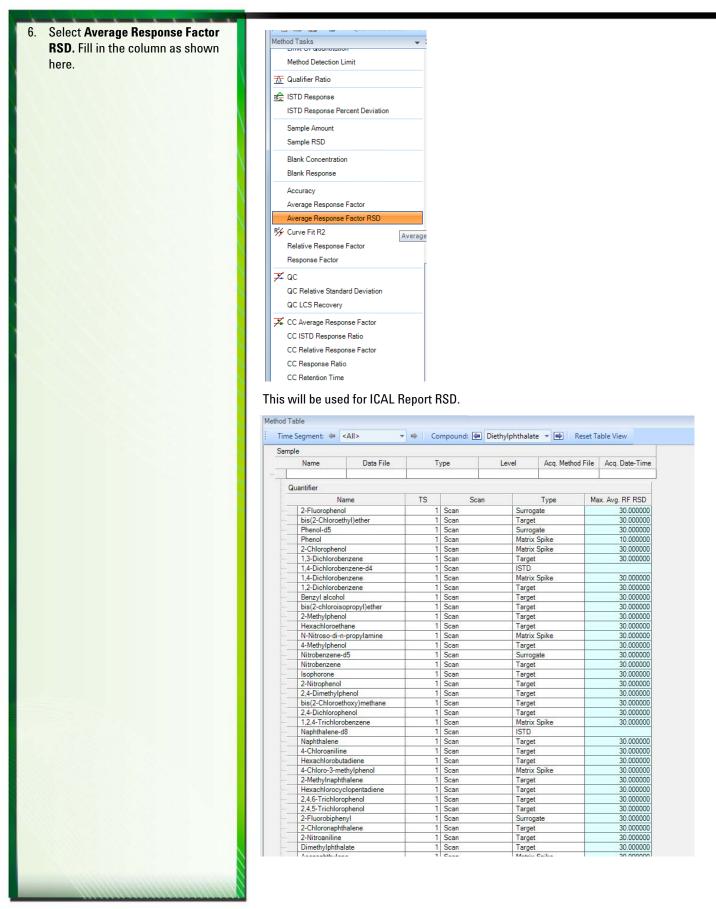


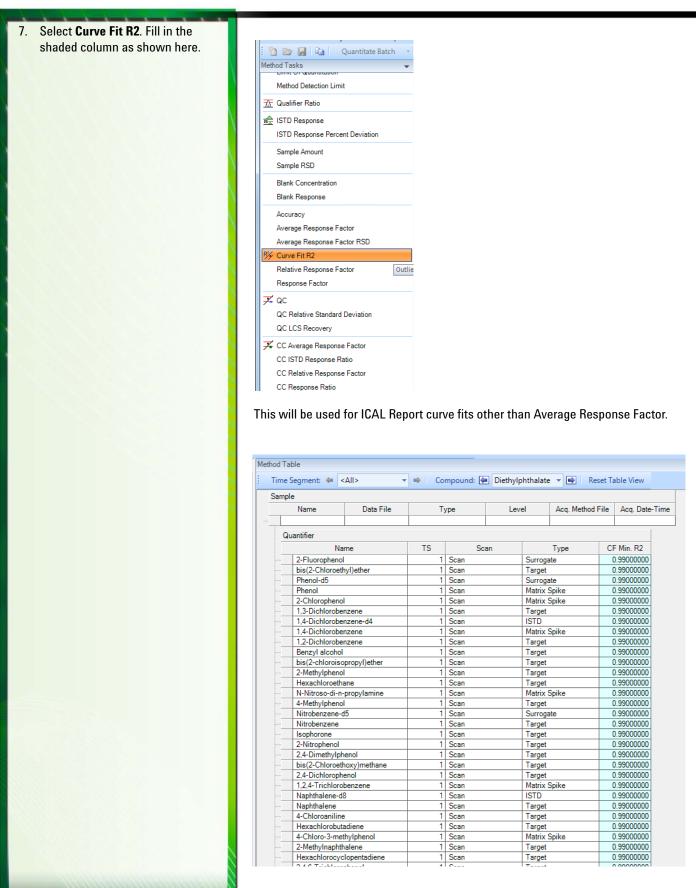
2. Scroll down the list of Outliers	
and select Qualifier Ratio. Fill in	Outlier Setup Tasks
the shaded columns as shown	JM Retention Time
here.	Relative Retention Time
liere.	Peak Resolution
	A Peak Symmetry
N	Peak Full Width Half Maximum
	Peak Purity
	Wu Signal-to-Noise Ratio
	Limit of Detection
	Method Detection Limit
N	
	Qualifier Ratio
	ISID Response
	ISTD Response Percent Deviation
	Sample Amount
	Sample RSD
	Blank Concentration
	Blank Response
	Accuracy
	Average Response Factor
	Average Response Factor RSD
	₿ <sup>™</sup> Curve Fit R2
	Relative Response Factor
	Response Factor
	Image: Time Segment:     Image: All > Image: Provide the Segment of Compound:     Image: Diethylphthalate     Image: Reset Table View       Sample     Image: Segment of Compound:     Image: Segment of Compound:     Image: Segment of Compound:     Image: Segment of Compound:
	Name         Data File         Type         Level         Acq. Method File         Acq. Date-Time
	Quantifier         TS         Scan         Type         Uncertainty
	Quantifier       Name     TS     Scan       2-Fluorophenol     1     Scan   Surrogate
	Quantifier         TS         Scan         Type         Uncertainty
	Quantifier     TS     Scan     Type     Uncertainty       2-Fluorophenol     1     Scan     Surrogate     Absolute       Qualifier     MZ     Rel. Resp.     Uncertainty       64.0     70.1     20.0       Quantifier     TS     Scan     Type       Uncertainty     64.0     70.1     20.0
	Quantifier     TS     Scan     Type     Uncertainty       2-Fluorophenol     1     Scan     Surrogate     Absolute       Qualifier     MZ     Rel. Resp.     Uncertainty       64.0     70.1     20.0       Quantifier     Image: Comparison of the second sec
	Quantifier     TS     Scan     Type     Uncertainty       Qualifier     1     Scan     Surrogate     Absolute       Qualifier     0.0     0.1     20.0       Quantifier     0.0     0.0     0.0       Quantifier     1     Scan     Type       Uncertainty     64.0     70.1     20.0       Quantifier     1     Scan     Type       bis(2-Chloroethyl)ether     1     Scan     Target       Qualifier     1     Scan     Target       Qualifier     1     Scan     Target
	Quantifier       TS       Scan       Type       Uncertainty         2-Fluorophenol       1       Scan       Surrogate       Absolute         Qualifier
	Quantifier     TS     Scan     Type     Uncertainty       Qualifier     1     Scan     Surrogate     Absolute       Qualifier     0.0     0.1     20.0       Quantifier     0.0     0.0     0.0       Quantifier     1     Scan     Type       Uncertainty     64.0     70.1     20.0       Quantifier     1     Scan     Type       bis(2-Chloroethyl)ether     1     Scan     Target       Qualifier     1     Scan     Target       Qualifier     1     Scan     Target
	Quantifier     TS     Scan     Type     Uncertainty       2-Fluorophenol     1     Scan     Surrogate     Absolute       Qualifier     MZ     Rel. Resp.     Uncertainty       64.0     70.1     20.0       Quantifier     Iscan     Type       Uncertainty     64.0     70.1       0     64.0     70.1     20.0       Quantifier     Iscan     Target       bis(2-Chloroethyl)ether     1     Scan       Qualifier     Iscan     Target       MZ     Rel. Resp.     Uncertainty       63.0     72.5     20.0       Quantifier     Iscan     Type       MZ     Rel. Resp.     Uncertainty       63.0     72.5     20.0       Quantifier     Iscan     Type       Mame     TS     Scan
	Quantifier       TS       Scan       Type       Uncertainty         2-Fluorophenol       1       Scan       Surrogate       Absolute         Qualifier       MZ       Rel. Resp.       Uncertainty         64.0       70.1       20.0         Quantifier       1       Scan       Type         Uncertainty       64.0       70.1       20.0         Quantifier       1       Scan       Type       Uncertainty         bis(2-Chloroethyl)ether       1       Scan       Target       Absolute         Qualifier       Uncertainty       63.0       72.5       20.0         Quantifier       0.0       95.0       30.9       20.0         Quantifier       TS       Scan       Type       Uncertainty         95.0       30.9       20.0       20.0       20.0         Quantifier       TS       Scan       Type       Uncertainty         Phenol-d5       1       Scan       Scan       Type       Uncertainty
	Quantifier     TS     Scan     Type     Uncertainty       2-Fluorophenol     1     Scan     Surrogate     Absolute       Qualifier     MZ     Rel. Resp.     Uncertainty       64.0     70.1     20.0       Quantifier     Iscan     Type       Uncertainty     64.0     70.1       0     64.0     70.1     20.0       Quantifier     Iscan     Target       bis(2-Chloroethyl)ether     1     Scan       Qualifier     Iscan     Target       MZ     Rel. Resp.     Uncertainty       63.0     72.5     20.0       Quantifier     Iscan     Type       MZ     Rel. Resp.     Uncertainty       63.0     72.5     20.0       Quantifier     Iscan     Type       Mame     TS     Scan
	Quantifier       TS       Scan       Type       Uncertainty         2-Fluorophenol       1       Scan       Surrogate       Absolute         Qualifier
	Quantifier       TS       Scan       Type       Uncertainty         2-Fluorophenol       1       Scan       Surrogate       Absolute         Qualifier       MZ       Rel. Resp.       Uncertainty         64.0       70.1       20.0         Quantifier       Iscan       Target       Absolute         Qualifier       Iscan       Type       Uncertainty         63.0       72.5       20.0       20.0         Qualifier       Iscan       Surrogate       Absolute         Phenol-d5       1       Scan       Surrogate       Absolute         Qualifier       MZ       Rel. Resp.       Uncertainty       Absolute       Incertainty         Phenol-d5       1       Scan       Surrogate       Absolute       Incertainty
	Quantifier       TS       Scan       Type       Uncertainty         2-Fluorophenol       1       Scan       Surrogate       Absolute         Qualifier
	Quantifier       TS       Scan       Type       Uncertainty         2-Fluorophenol       1       Scan       Surrogate       Absolute         Qualifier
	Quantifier       TS       Scan       Type       Uncertainty         Qualifier       1       Scan       Surrogate       Absolute         Qualifier       MZ       Rel. Resp.       Uncertainty         64:0       70:1       20:0         Quantifier       Uncertainty         bis(2-Chloroethyl)ether       1       Scan         Visite       Visite       Visite         Qualifier       Uncertainty         Qualifier       Visite       Visite         Qualifier       1       Scan       Target         Qualifier       Visite       1       Scan       Scan         Qualifier       Visite       1       Scan       Scan       Visite         Qualifier       Visite       1       Scan       Target       Absolute         Qualifier       Visite       Visite       Visite       Abs
	Quantifier       TS       Scan       Type       Uncertainty         Qualifier       1       Scan       Surrogate       Absolute         Qualifier       MZ       Rel. Resp.       Uncertainty         G4.0       70.1       20.0         Quantifier       1       Scan       Type         Uncertainty       64.0       70.1       20.0         Quantifier       1       Scan       Type       Uncertainty         bis(2-Chloroethyl)ether       1       Scan       Target       Absolute         Qualifier       0       0.0       30.9       20.0         Quantifier       MZ       Rel. Resp.       Uncertainty         63.0       72.5       20.0       20.0         Quantifier       1       Scan       Type       Uncertainty         Phenol-d5       1       Scan       Type       Uncertainty         Qualifier       0       1       Scan       Surrogate       Absolute         Qualifier       0       1       Scan       Type       Uncertainty         42.0       21.2       20.0       20.0       20.0       20.0         Quantifier       1       Scan       <
	Quantifier       TS       Scan       Type       Uncertainty         2.Fluorophenol       1       Scan       Surrogate       Absolute         Qualifier
	Quantifier       TS       Scan       Type       Uncertainty         2-Fluorophenol       1       Scan       Surrogate       Absolute         Qualifier       MZ       Rel. Resp.       Uncertainty         64.0       70.1       20.0         Quantifier       1       Scan       Type         Uncertainty       64.0       70.1       20.0         Quantifier       1       Scan       Type       Uncertainty         bis(2-Chloroethyl)ether       1       Scan       Type       Uncertainty         MZ       Rel. Resp.       Uncertainty       Absolute       Qualifier         Qualifier       MZ       Rel. Resp.       Uncertainty       Absolute         Phenol-d5       1       Scan       Type       Uncertainty         Phenol-d5       1       Scan       Surrogate       Absolute         Qualifier       MZ       Rel. Resp.       Uncertainty       Absolute         Qualifier       MZ       Scan       Type       Uncertainty         42.0       21.2       20.0       20.0       20.0       20.0         Qualifier       MZ       Rel. Resp.       Uncertainty       Absolute       20.0
	Quantifier       Name       TS       Scan       Type       Uncertainty         Qualifier       MZ       Rel. Resp.       Uncertainty       Absolute         Qualifier       MZ       Rel. Resp.       Uncertainty         64.0       70.1       20.0         Quantifier       1       Scan       Type       Uncertainty         64.0       70.1       20.0       Quantifier       Uncertainty         0       bis(2-Chloroethyl)ether       1       Scan       Type       Uncertainty         0       63.0       72.5       20.0       Qualifier       Absolute       Qualifier         0       95.0       30.3       20.0       Qualifier       Absolute       Qualifier         0       Qualifier       1       Scan       Surrogate       Absolute         Qualifier       1       Scan       Surrogate       Absolute         0       71.0       37.6       20.0       Quantifier       Absolute         0       0       71.0       37.6       20.0       Quantifier       Absolute         0       0       1       Scan       Type       Uncertainty       Qualifier       Absolute       Qualifier
	Quantifier       Image: TS       Scan       Type       Uncertainty         Qualifier       1       Scan       Surrogate       Absolute         Qualifier       MZ       Rel. Resp.       Uncertainty         Guantifier       MZ       Rel. Resp.       Uncertainty         Uncertainty       64.0       70.1       20.0         Quantifier       MZ       Rel. Resp.       Uncertainty         Usi(2-Chloroethyl)ether       1       Scan       Type       Uncertainty         Usi(2-Chloroethyl)ether       1       Scan       Type       Uncertainty         Guantifier       MZ       Rel. Resp.       Uncertainty       Uncertainty         Guantifier       MZ       Rel. Resp.       Uncertainty         Phenol-d5       1       Scan       Surrogate       Absolute         Qualifier       MZ       Rel. Resp.       Uncertainty         42.0       21.2       20.0       Quantifier       MZ       Absolute         Qualifier       MZ       Rel. Resp.       Uncertainty       MZ       Absolute         Qualifier       MZ       Scan       Type       Uncertainty         Phenol       1       Scan       Matrix Spike

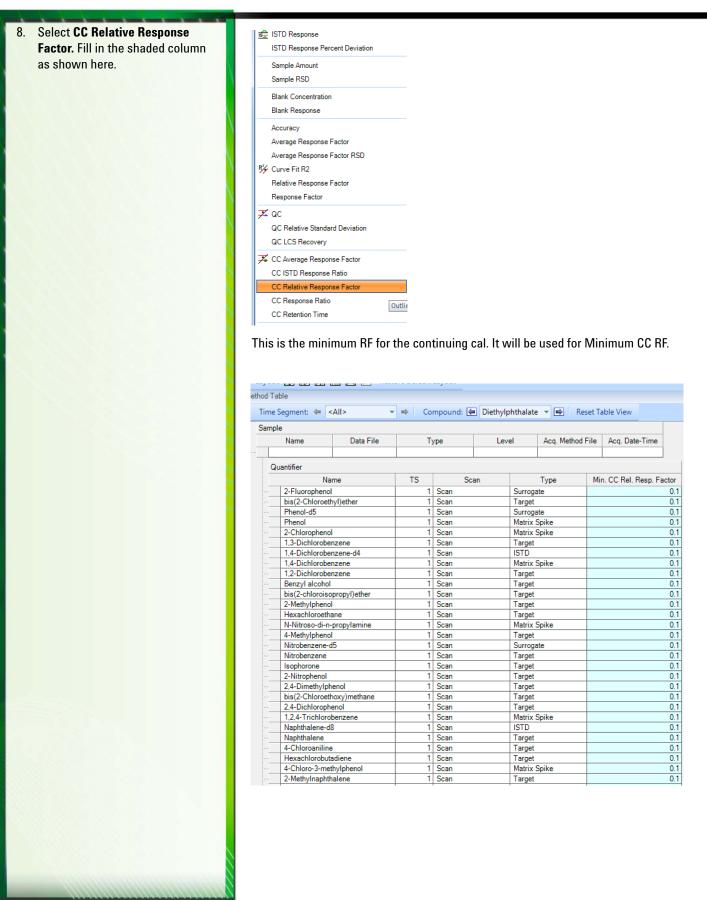


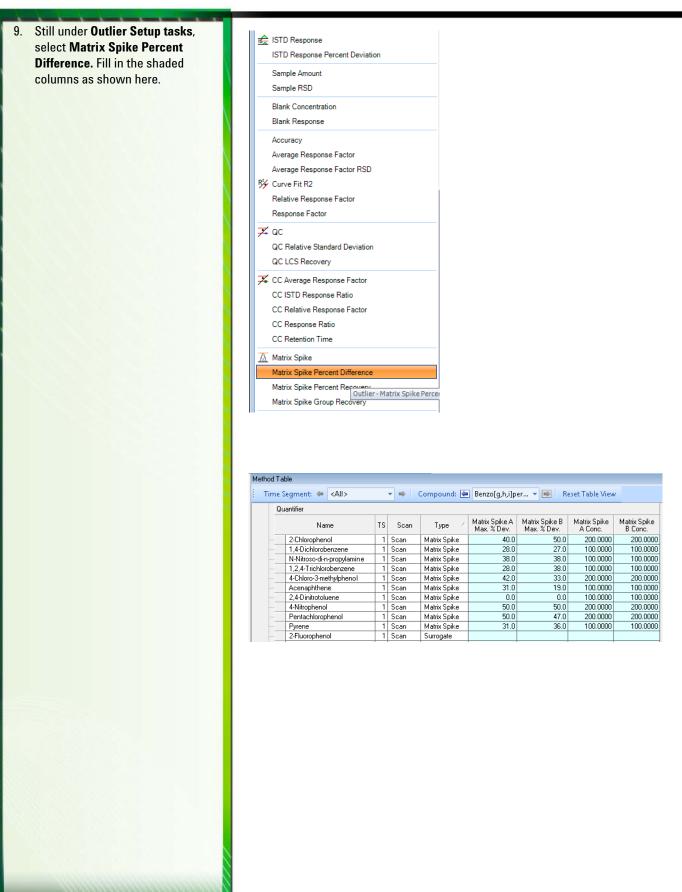


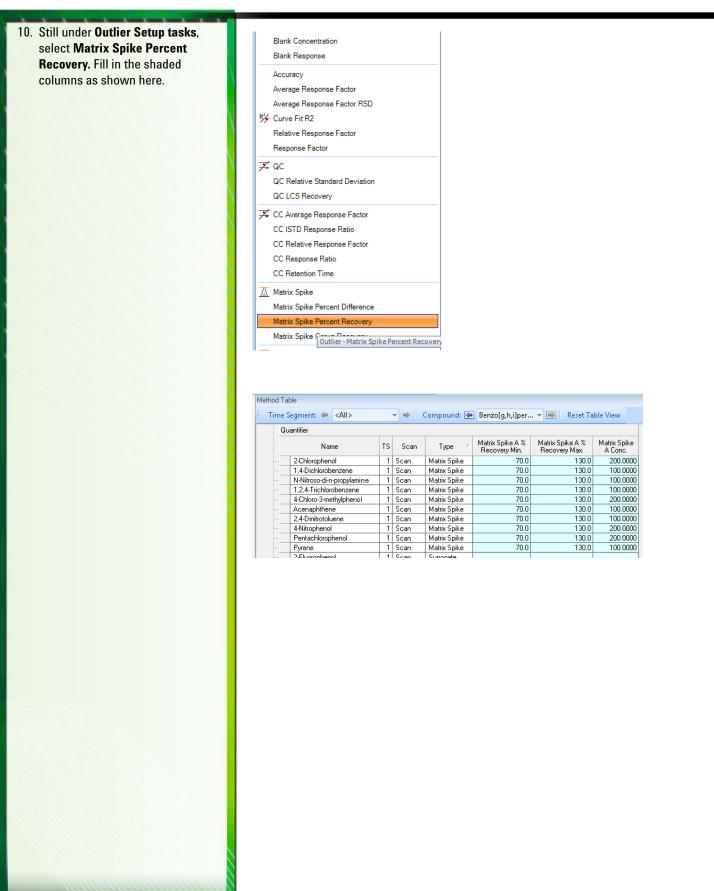
5.									
		Outlier	Setup Tasks						
	Fill in the shaded column as	A Rete	ntion Time						
	shown here.		tive Retention Tin	ne					
			Resolution						
		A Peak	Symmetry						
			Full Width Half N	/laximum					
		Peak	Purity						
		Mu, Signa	al-to-Noise Ratio						
		TT Limit	Of Detection						
		Limit	Of Quantitation						
		Meth	od Detection Limi	it					
		TT Qual	ifier Ratio						
			Response Response Perce	at Deviation					
				ant Deviation					
			ple Amount						
		Sam	ple RSD						
		Blan	k Concentration						
		Blan	k Response						
		Accu	iracy						
		Aver	age Response Fa	ictor					
		Aver	age Response Ea	ector RSD	a Fa				
		₿∛⁄y Curv	e Fit R2	er - Average Respon	se⊨a				
		Relat	tive Response Fa	ctor					
		Resp	oonse Factor						
		This w	ill be used	for ICAL Rep	ort min	imum RF.			
		Method T							
			Segment: 🖛	<all></all>	🚽 🖬 🕹 Co	ompound: 🔄	Diethylpht	halate 🔻 📑 🛛 Re	eset Table View
		Samp	Name	Data File					
			Name	Data File			l aval	Aca Method	File Aca Date-Time
						уре	Level	Acq. Method	File Acq. Date-Time
		G	uantifier			уре	Level	Acq. Method	File Acq. Date-Time
			Na	ame	TS	Scar	1	Туре	File Acq. Date-Time
			Na 2-Fluoropheno	d	TS 1	Scan	ו א	Type	Min. Avg. RF 0.1000
			Na	d	TS	Scan Scan	n S	Туре	Min. Avg. RF
			Na 2-Fluoropheno bis(2-Chloroet Phenol-d5 Phenol	l hyl)ether	TS 1 1 1	Scan Scan Scan Scan Scan	n S T S M	Type urrogate arget urrogate latrix Spike	Min. Avg. RF 0.1000 0.1000 0.1000 0.1000
			Na 2-Fluoropheno bis(2-Chloroet Phenol-d5	l hyl)ether bl	TS	Scan Scan Scan Scan Scan Scan	n S T S N N	Type urrogate arget urrogate	Min. Avg. RF 0.1000 0.1000 0.1000
			Na 2-Fluoropheno bis(2-Chloroet Phenol-d5 Phenol 2-Chloropheno 1,3-Dichlorobe 1,4-Dichlorobe	l hyl)ether ol enzene enzene-d4	TS	Scan Scan Scan Scan Scan Scan Scan Scan	n S T S M M T	Type urrogate arget urrogate latrix Spike latrix Spike arget STD	Min. Avg. RF 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000
			Na 2-Fluoropheno bis(2-Chloroet Phenol-d5 Phenol 2-Chloropheno 1,3-Dichlorobe 1,4-Dichlorobe 1,4-Dichlorobe	N hyl)ether ol enzene enzene-d4 enzene	TS	Scan Scan Scan Scan Scan Scan Scan Scan	n S T S M M T I S N N N	Type urrogate arget urrogate latrix Spike latrix Spike arget STD latrix Spike	Min. Avg. RF 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000
			Na 2-Fluoropheno bis(2-Chloroet Phenol-d5 Phenol 2-Chloropheno 1,3-Dichlorobe 1,4-Dichlorobe 1,4-Dichlorobe 1,2-Dichlorobe Benzyl alcohol	N hyl)ether sinzene sinzene-d4 sinzene sinzene I	TS 1	Scan Scan Scan Scan Scan Scan Scan Scan	N S T S N N T I S N T T T T	Type urrogate arget urrogate latrix Spike latrix Spike arget STD latrix Spike arget arget arget	Min. Avg. RF 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000
			Na 2-Fluoropheno bis(2-Chloroet Phenol-d5 Phenol 2-Chloropheno 1,3-Dichlorobe 1,4-Dichlorobe 1,2-Dichlorobe Benzyl alcohol bis(2-chloroist	N hyl)ether Inzene Inzene Inzene Inzene Inzene Inzene Inzene	TS 1	Scan Scan Scan Scan Scan Scan Scan Scan	n S T S M M T I S N T T T T	Type urrogate arget urrogate latrix Spike latrix Spike arget STD latrix Spike arget arget arget arget arget	Min. Avg. RF 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000
			Na 2-Fluoropheno bis(2-Chloroet Phenol-d5 Phenol 2-Chloropheno 1.4-Dichlorobe 1.4-Dichlorobe 1.2-Dichlorobe Benzyl alcoho bis(2-chlorois 2-Methylpheno Hexachloroeth	N hyl)ether mzene mzene snzene snzene mzene b propyl)ether snzene l spropyl)ether snzene	TS	Scan Scan Scan Scan Scan Scan Scan Scan	n S T S N M T I S N T T T T T T T T	Type urrogate arget urrogate latrix Spike latrix Spike arget 3TD latrix Spike arget arget arget arget arget arget arget arget	Min. Avg. RF 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000
			Na 2-Fluoropheno bis(2-Chloroet Phenol-d5 Phenol 2-Chloropheno 1,3-Dichlorobe 1,4-Dichlorobe 1,2-Dichlorobe Benzyl alcohol bis(2-chlorois 2-Methylpheno Hexachloroett N-Nitroso-di-n	N hyl)ether enzene enzene-d4 enzene nzene nzene popopyl)ether ol ane -propylamine	TS	Scan Scan Scan Scan Scan Scan Scan Scan	n S S S N M T T I S N T T T T T T T T	Type urrogate arget urrogate latrix Spike latrix Spike latrix Spike arget arget arget arget arget arget latrix Spike	Min. Avg. RF 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000 0.1000
			Na 2-Fluoropheno bis(2-Chloroet Phenol-d5 Phenol 2-Chloropheno 1.4-Dichlorobe 1.4-Dichlorobe 1.4-Dichlorobe 1.2-Dichlorobe bis(2-chloroist 2-Methylpheno Hexachloroeth N-Nitroso-dirn 4-Methylpheno Nitrobenzene-	N hyl)ether enzene enzene-d4 enzene snzene l popropyl)ether of ene -propylamine ol	TS 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	Scan Scan Scan Scan Scan Scan Scan Scan	n S T S N N T IS N T T T T T T T T T S S	Type urrogate arget latrix Spike latrix Spike latrix Spike arget 3TD latrix Spike arget arget arget arget latrix Spike arget arget arget urrogate	Min. Avg. RF 0.1000
			Na 2-Fluoropheno bis(2-Chloroet Phenol-d5 Phenol 2-Chloropheno 1.4-Dichlorobe 1.4-Dichlorobe 1.4-Dichlorobe Benzyl alcoho bis(2-chlorois 2-Methylpheno Hexachloroeth N-Nitroso-di-n 4-Methylpheno Nitrobenzene- Nitrobenzene	N hyl)ether enzene enzene-d4 enzene snzene l popropyl)ether of ene -propylamine ol	TS	Scan Scan Scan Scan Scan Scan Scan Scan	n S T S N M T T T T T T T T T T T T T T T T	Type urrogate arget urrogate latrix Spike latrix Spike latrix Spike arget arget arget arget arget arget arget latrix Spike arget urrogate arget	Min. Avg. RF 0.1000
			Na 2-Fluoropheno bis(2-Chloroet Phenol-d5 Phenol 2-Chloropheno 1.4-Dichlorobe 1.4-Dichlorobe 1.4-Dichlorobe 1.2-Dichlorobe bis(2-chloroist 2-Methylpheno Hexachloroeth N-Nitroso-dirn 4-Methylpheno Nitrobenzene-	N hyl)ether enzene enzene-d4 enzene snzene l popropyl)ether of ene -propylamine ol	TS 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	Scan Scan Scan Scan Scan Scan Scan Scan	1 S 5 S 1 T 5 S 1 M 1 M 1 M 1 T 1 T 1 T 1 T 1 T 1 S 5 S 1 T 1 T 1 T 1 T 1 T 1 T 1 T 1 T	Type urrogate arget latrix Spike latrix Spike latrix Spike arget 3TD latrix Spike arget arget arget arget latrix Spike arget arget arget urrogate	Min. Avg. RF 0.1000
			Na 2-Fluoropheno bis(2-Chloroet Phenol-d5 Phenol 2-Chloropheno 1.4-Dichlorobe 1.4-Dichlorobe 1.4-Dichlorobe 1.2-Dichlorobe bis(2-chloroist 2-Methylpheno Hexachloroeth N-Nitrose-di-n 4-Methylpheno Nitrobenzene- Nitrobenzene Nitrobenzene Sophorone 2-Nitrophenol 2.4-Dimethylpheno	M hyl)ether enzene enzene enzene enzene l opropyl)ether d l enne -propylamine d d f henol	TS	Scan Scan Scan Scan Scan Scan Scan Scan	n S S N N N T I S S S T T T T T T T T T T T	Type urrogate arget urrogate latrix Spike latrix Spike latrix Spike arget TD latrix Spike arget arget arget arget arget arget urrogate arget arg	Min. Avg. RF 0.1000
			Na 2-Fluoropheno bis(2-Chloroet Phenol-d5 Phenol 2-Chloropheno 1.4-Dichlorobe 1.4-Dichlorobe 1.4-Dichlorobe 1.2-Dichlorobe bis(2-chloroist 2-Methylpheno Hexachloroeth N-Nitrose-di-n 4-Methylpheno Nitrobenzene- Nitrobenzene Nitrobenzene Sophorone 2-Nitrophenol 2.4-Dimethylpheno	M hyl)ether enzene enzene enzene enzene propyl)ether propyl)ether d5 henol hoxy)methane	TS	Scan Scan Scan Scan Scan Scan Scan Scan	1         S           T         S           N         N           T         S           IS         N           N         N           T         T           T         T           T         T           T         T           T         T           T         T           T         T           T         T           T         T           T         T           T         T           T         T           T         T           T         T	Type urrogate arget urrogate latrix Spike latrix Spike latrix Spike arget arget arget arget arget arget latrix Spike arget arget urrogate arget	Min. Avg. RF 0.1000
			Na 2-Fluoropheno bis(2-Chloroet Phenol-d5 Phenol-d5 Phenol 2-Chloropheno 1,3-Dichlorobe 1,4-Dichlorobe Benzyl alcohol bis(2-chloroise 2-Methylpheno Nitrobenzene- Nitrobenzene- Nitrobenzene- Nitrobenzene- 2-Nitrophenol 2,4-Dichlorophenol 2,4-Dichlorophenol 2,4-Dichlorophenol 2,4-Dichlorophenol 2,4-Dichlorophenol 2,4-Dichlorophenol 2,4-Dichlorophenol 2,4-Dichlorophenol 2,4-Dichlorophenol 2,4-Dichlorophenol 1,2,4-Trichlorophenol 1,3,4-Trichlorophenol 1,4-Trichlorophenol 1,4-Trichlorophenol 1,4-Trichlorophenol 1,4-Trichlorophenol 1,4-Trichlorophenol 1,4-Trichlorophenol 1,4-Trichlorophenol 1,4-Trichlorophenol 1,4-Trichlorophenol 1,4-Trichlorophenol 1,4-Trichlorophenol 1,4-Trichlorophenol 1,	M hyl)ether hyl)ether hyl)ether hyl enzene enzene-d4 enzene popropyl)ether hane propylamine d5 henol hoxy)methane enol bebenzene	TS	Scan Scan Scan Scan Scan Scan Scan Scan	n S S N N N T T T T T T T T T T T T T T T T	Type urrogate arget latrix Spike latrix Spike arget STD latrix Spike arget arget arget arget arget latrix Spike arget ar	Min. Avg. RF           0.1000
			Na 2-Fluoropheno bis(2-Chloroet Phenol-d5 Phenol 2-Chloropheno 1.3-Dichlorobe 1.4-Dichlorobe 1.4-Dichlorobe 1.4-Dichlorobe 1.2-Dichlorobe bis(2-chlorois 2-Methylpheno Hexachloroeth Nitrobenzene- Nitrobenzene Sophorone 2-Nitrophenol 2.4-Direthylphenol 2.4-Direthylphenol 2.4-Direthylphenol 1.2-Chloroett 2.4-Direthylphenol 1.2-Dichlorope 1.2.4-Direthylphenol 1.3.4-Direthylphenol 1.3.4-Direthylphenol 1.3.4-Direthylphenol 1.3.4-Direthylphenol 1.3.4-Direthylphenol 1.3.4-Direthylphenol 1.3.4-Direthylphenol 1.3.4-Direthylphenol 1.3.4-Direthylphenol 1.3.4-Direthylphenol 1.3.4-Direthylphenol 1.3.4-Direthylphenol 1.3.4-Direthy	M hyl)ether hyl)ether hyl)ether hyl enzene enzene-d4 enzene popropyl)ether hane propylamine d5 henol hoxy)methane enol bebenzene	TS TS TS TI	Scan Scan Scan Scan Scan Scan Scan Scan	1 S S N N N T S S N N T T T T T T T T T T	Type urrogate arget urrogate latrix Spike latrix Spike latrix Spike arget 3TD latrix Spike arget arget arget arget arget arget urrogate arget ar	Min. Avg. RF           0.1000
			Na 2-Fluoropheno bis(2-Chloroet Phenol-d5 Phenol 2-Chloropheno 1,3-Dichlorobe 1,4-Dichlorobe 1,2-Dichlorobe Benzyl alcoho bis(2-chlorosis 2-Methylpheno Hexachloroeth N-Nitrose-di-n 4-Methylpheno Nitrobenzene Isophorone 2-Nitrophenol 2-Nitrophenol 2-Alicophorone 2-Nitrophenol 2-Alicophorone 2-Nitrophenol 2-4-Dichloropt 1,2-4-Trichloro Naphthalene 4-Chloroanilin	M hyl)ether hyl)ether hyl)ether snzene nzene-d4 snzene nzene l propyl)ether l snzen l snzen l snzene l snzene l snze l sn	TS	Scan Scan Scan Scan Scan Scan Scan Scan	N         S           T         S           N         M           T         S           IS         N           N         T           T         T           T         T           T         T           T         T           T         T           T         T           T         T           T         T           T         T           T         T           T         T           T         T           T         T           T         T           T         T           T         T           T         T           T         T	Type urrogate arget urrogate arget atrix Spike latrix Spike arget	Min. Avg. RF 0.1000
			Na 2-Fluoropheno bis(2-Chloroet Phenol-d5 Phenol 2-Chloropheno 1,4-Dichlorobe 1,4-Dichlorobe 1,2-Dichlorobe 1,2-Dichlorobe 1,2-Dichlorobe bis(2-chloroist 2-Methylpheno Hexachloroeth N-Nitrobenzene Isophorone 2,4-Direhtylpheno 2,4-Direhtylpheno 2,4-Direhtylpheno 2,4-Direhtylpheno 2,4-Direhtylpheno 1,2,4-Tichloro Naphthalene- Maphthalene- Naphthalene- A-Chloroaniim Hexachlorobut	M hyl)ether hyl)ether hyl)ether enzene-d4 enzene-d4 enzene l popropyl)ether l ane propylamine d5 hoxy)methane enol bebenzene l8 e e tadiene	TS	Scan Scan Scan Scan Scan Scan Scan Scan	n S S N N N T T T T T T T T T T T T T T T	Type urrogate arget latrix Spike latrix Spike latrix Spike arget arget arget arget arget arget latrix Spike arget arget latrix Spike arget arget arget latrix Spike arget latrix Spike arget latrix Spike arget latrix Spike arget	Min. Avg. RF 0.1000
			Na 2-Fluorophenc bis(2-Chloroet Phenol-d5 Phenol 2-Chlorophenc 1,3-Dichlorobe 1,4-Dichlorobe 1,4-Dichlorobe 1,2-Dichlorobe 1,2-Dichlorobe 1,2-Dichlorobe 1,2-Dichlorobe 1,2-Chlorois 2-Methylphenc Hexachloroeth Nitrobenzene- Nit	M hyl)ether hyl)ether hyl)ether nzene-d4 nzene encend nzene encend propyl)ether hane propylamine d5 henol hoxy)methane henol k8 e e tadiene ttylphenol halene	TS	Scan Scan Scan Scan Scan Scan Scan Scan	N         S           T         S           N         N           N         N           T         T	Type urrogate arget urrogate latrix Spike latrix Spike latrix Spike arget STD latrix Spike arget	Min. Avg. RF 0,1000
			Na 2-Fluorophenc bis(2-Chloroet Phenol-d5 Phenol 2-Chlorophenc 1.3-Dichlorobe 1.4-Dichlorobe Benzyl alcohol bis(2-chlorois) 2-Methylphenc Hexachloroeth N-Nitrose-di-n 4-Methylphenc Nitrobenzene Isophorone 2-Nitrophenol 2.4-Dichloroph 2.4-Dichloroph 2.4-Dichloroph 2.4-Dichloroph 2.4-Dichloroph 2.4-Dichloroph 2.4-Dichloroph 1.2.4-Trichloro Naphthalened 4-Chloro-3-me 4-Chloro-a-milin Hexachlorobul 4-Chlor	M hyl)ether hyl)ether hyl)ether hyl)ether hyle hyle hyle her hyl	TS	Scan Scan Scan Scan Scan Scan Scan Scan	n         S           T         S           N         M           T         S           N         N           T         T           T         T           T         T           T         T           T         T           T         T           T         T           T         T           T         T           T         T           T         T           T         T           T         T           N         IS           IS         S           T         T           T         T           T         T           T         T	Type urrogate arget urrogate arget atrix Spike latrix Spike arget	Min. Avg. RF 0.1000
			Na 2-Fluorophenc bis(2-Chloroet Phenol-d5 Phenol 2-Chlorophenc 1,3-Dichlorobe 1,4-Dichlorobe 1,4-Dichlorobe 1,2-Dichlorobe 1,2-Dichlorobe 1,2-Dichlorobe 1,2-Dichlorobe 1,2-Chlorois 2-Methylphenc Hexachloroeth Nitrobenzene- Nit	M hyl)ether hyl)ether hyl)ether nzene nzene enzene nzene enzene l opropyl)ether ol hoxy)methane enol benzene l8 e thylphenol halene clopentadiene pohenol	TS	Scan Scan Scan Scan Scan Scan Scan Scan	S           N           N           N           N           N           N           T           N           S           T           T           T           T           N           T           N           T           T           T           T           T           T           T           T	Type urrogate arget urrogate latrix Spike latrix Spike latrix Spike arget STD latrix Spike arget	Min. Avg. RF 0,1000
			Na 2-Fluoropheno bis(2-Chloroet Phenol-d5 Phenol 2-Chloropheno 1.3-Dichlorobe 1.4-Dichlorobe 1.4-Dichlorobe 1.2-Dichlorobe 1.2-Dichlorobe bis(2-chloroisi 2-Methylpheno Hexachloroeth N-Nitrobenzene- 2-Nitrophenol 2.4-Direnthylp bis(2-Chloroethylphenol 2.4-Direnthylphenol 4-Chloroa-there 4-Chloroa-there 4-Chloroa-there 4-Chloroa-there 2.4-Direchlorobut 4-Chloroa-there 2.4-Direchlorobut 4-Chloroa-there 2.4-Direchlorobut 4-Chloroa-there 2.4-Direchlorobut 4-Chloroa-there 2.4-Direchlorobut 4-Chloroa-there 2.4-Direchlorobut 4-Chloroa-there 2.4-Direchlorobut 4-Chloroa-there 2.4-Direchlorobut 4-Chloroa-there 2.4-Direchlorobut 4-Chloroa-there 2.4-Direchlorobut 4-Chloroa-there 2.4-Direchlorobut 4-Chloroa-there 2.4-Direchlorobut 4-Chloroa-there 2.4-Direchlorobut 4-Chloroa-there 2.4-Direchlorobut 4-Chloroa-there 2.4-Direchlorobut 4-Chloroa-there 1-	M hyl)ether hyl)ether hyl)ether nzene nzene enzene nzene enzene l opropyl)ether ol hoxy)methane enol benzene l8 e thylphenol halene clopentadiene pohenol	TS	Scan Scan Scan Scan Scan Scan Scan Scan	S           N           N           N           N           N           N           T           N           S           T           T           T           T           N           T           N           T           T           T           T           T           T           T           T	Type urrogate arget latrix Spike latrix Spike latrix Spike arget arget arget arget arget arget latrix Spike arget	Min. Avg. RF 0.1000

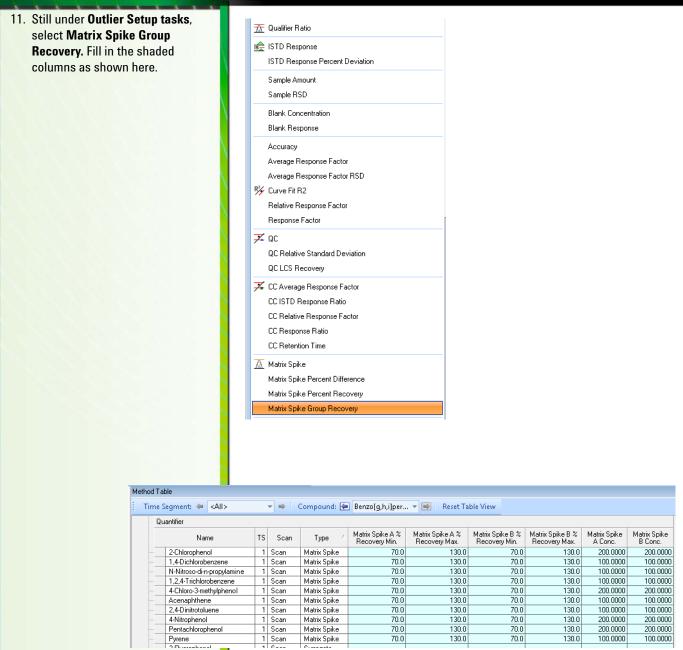




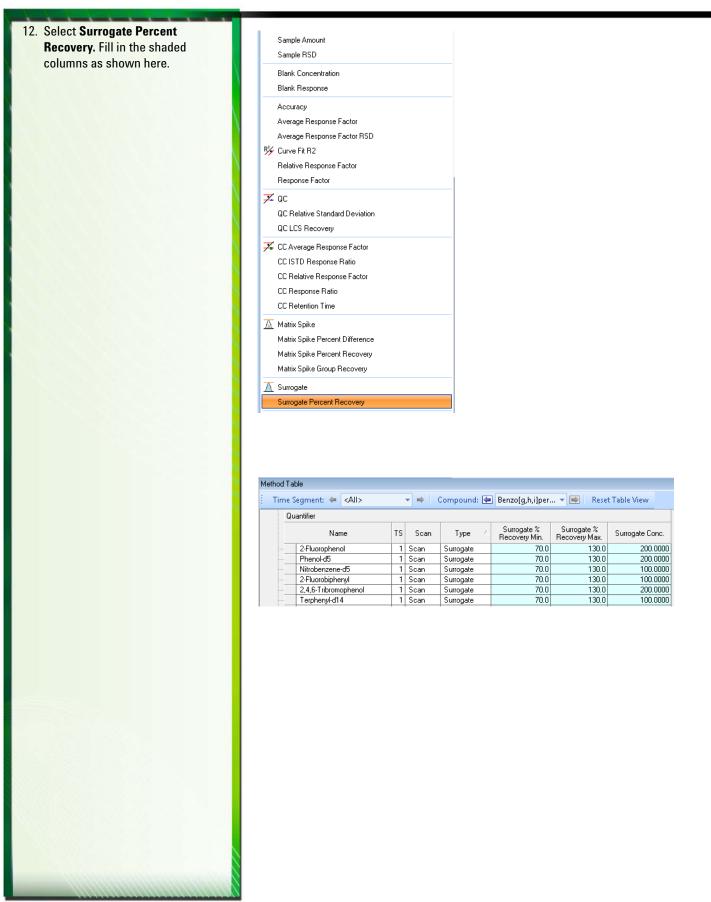


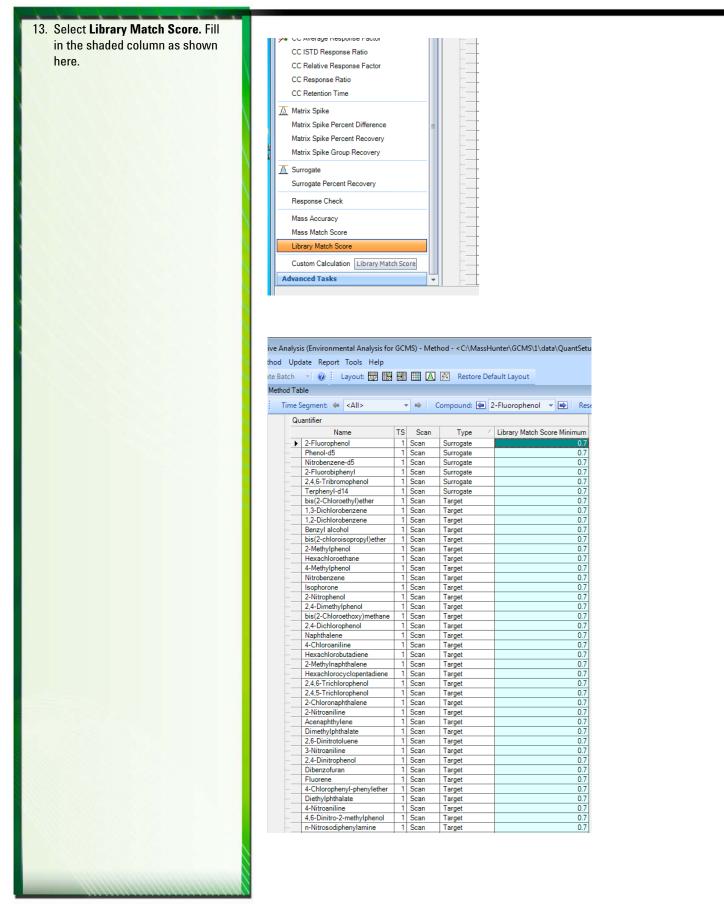


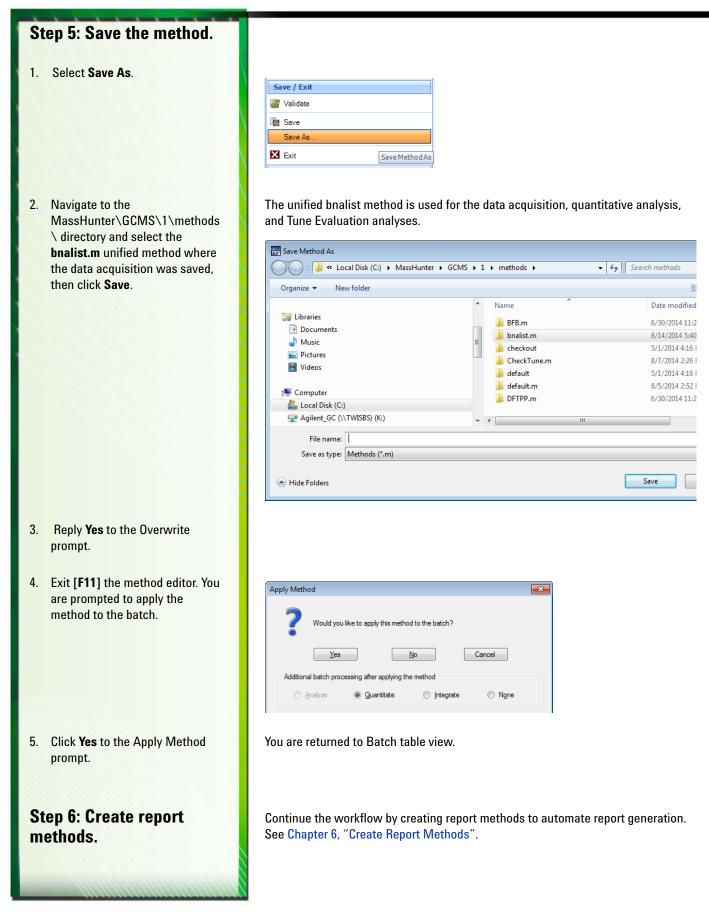












# 6

## **Create Report Methods**

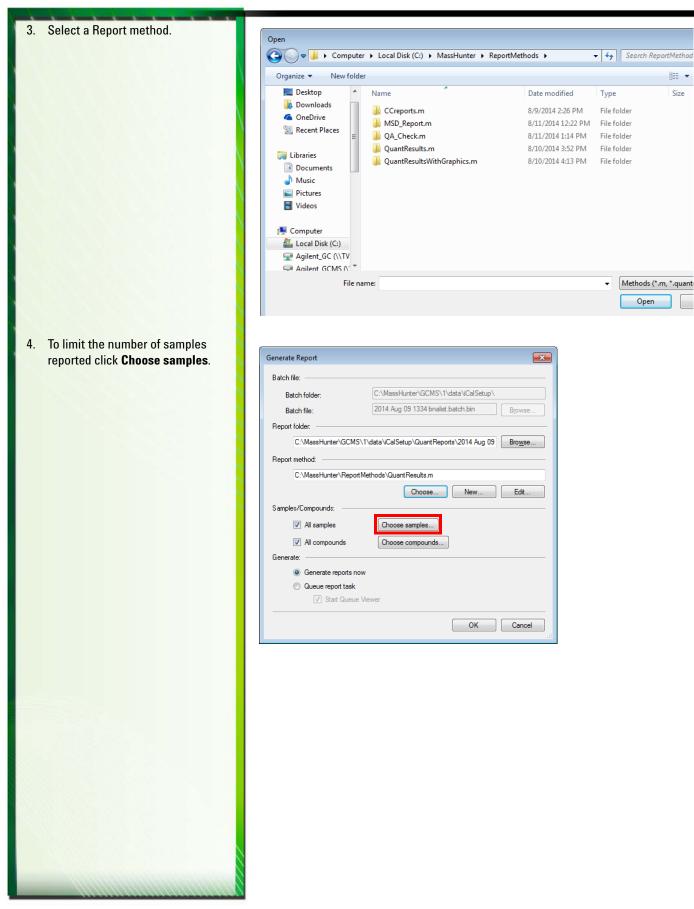
#### Introduction 68

Step 1: Generate an interactive report. 68
Step 2: Create an Initial Calibration Report Method. 72
Step 3: Create a Quant Report Method. 75
Step 4: Create a Continuing Calibration Report Method. 80
Step 5: Create a Matrix Spike Duplicate Report Method. 83
Step 6: Create a QA Check Report Method. 86
Step 7: Run samples. 88

Agilent Technologies

#### Introduction Reports can be generated in two ways: · Automatically, at the end of a run Interactively, after manual integration, for example Report methods enable you to save report parameters including multiple report templates, to a file than can be applied to a single sample in an automated sequence or interactively to a single sample or group of samples. When you create the sequence for a run you can enter the report method you want processed for an individual sample in the run. This can be done by saving the report method in the unified method for that sample or by specifying the report method for a sample in the sequence table report method column. When you are working interactively with a batch of data, after doing manual integration for example, you may select any saved report method, or create one on the spot, and generate a report interactively. This section describes how to generate reports both automatically, and interactively. **Step 1: Generate an** interactive report. From MassHunter's main menu 1. select Report > Generate. 2. Click **Choose** and navigate to × Generate Report where you saved your report Batch file: method templates. C:\MassHunter\GCMS\1\data\iCalSetup\ Batch folder: 2014 Aug 09 1334 bnalist.batch.bin Browse. Batch file: Report folder: C:\MassHunter\GCMS\1\data\iCalSetup\QuantReports\2014 Aug 09 Browse... Benort method: C:\MassHunter\Report Templates\Quant\PDF-Reporting\TuneCheck.m Choose... New... Edit.. Samples/Compounds: All samples Choose samples... Choose compounds.. All compounds Generate: Generate reports now Queue report task ✓ Start Queue Viewe OK Cancel

## Step 1: Generate an interactive report.



5. Select the samples to be included in the report and click **OK**.

	Name	Data File	Туре	Level	Acq. Date-Time
	Tune Evaluation	TuneChk.d	TuneCheck		8/9/2014 2:38 PN
	Calbration 20 ng/ul	20NG.d	Calibration		8/9/2014 2:39 PM
Þ	Calbration 50 ng/ul	50NG.d	Calibration	50	8/9/2014 2:42 PM
	Calbration 80 ng/ul	80NG.d	Calibration	80	8/9/2014 2:44 PM
	Calbration 120 ng	120NG.d	Calibration	120	8/9/2014 2:46 PM
	Calbration 160 ng	160NG.d	Calibration	160	8/9/2014 2:48 PM
	CC 50 ng/ul	CC50NG.d	CC	CC	8/9/2014 2:51 PM

6. To limit the number of compounds to include in the report, click **Choose compounds**.

 Select the compounds to be included in the report then click
 OK. (In this example we selected the compounds by target group.)

Batch folder:	C:\MassHunter\GCMS\1\data\iCalSetup\
Batch file:	2014 Aug 09 1334 bnalist.batch.bin Browse
Report folder:	
C:\MassHunter\GCMS	S\1\data\iCalSetup\QuantReports\2014 Aug 09 Browse
Report method:	
·	rtMethods\QuantResults.m
	Choose New Edit
	Crioose New Edit
amples/Compounds:	
All samples	Choose samples
All compounds	Choose compounds
aenerate:	214
enerate:	UW
	uw.

	Name	RT	Transition	Cmpd. Group	
	2-Fluorophenol	8.255		S	
	bis(2-Chloroethyl)	10.979		т	-
	Phenol-d5	11.019		S	
•	Phenol	11.040		М	
	2-Chlorophenol	11.080		М	
	1,3-Dichlorobenz	11.386		т	
	1,4-Dichlorobenz	11.548		М	<b>T</b>
	1,2-Dichlorobenz	12.077		т	
	Benzyl alcohol	12.179			
	bis(2-chloroisopro	12.565			

## Step 1: Generate an interactive report.

8.	Click <b>OK</b> to generate the report.	(							
		Generate Report				<b>—X</b> —			
		Batch file:							
		Batch folder:	C:\MassHunter\G0	MS\1\data\iCalSe	etup\				
		Batch file:	2014 Aug 09 1334		Brov				
			20117039001001						
		Report folder:							
		C:\MassHunter\GCM	S\1\data\iCalSetup\Qua	ntReports\2014 Au	ug 09 Bro <u>v</u>	<u>/</u> se			
		Report method:							
	N N	C:\MassHunter\Repo	ort Methods \Quant Results.	m					
			Choos	se New	Ed	it			
		Samples/Compounds:							
		All samples	Choose samples						
		All compounds	Choose compou	nus					
		Generate:							
		<ul> <li>Generate reports r</li> </ul>							
		Queue report task  Start Queu							
	S		e viewer						
				ОК	Car	ncel			
		The report is gene	erated.						
			0.00	titation Docu	lto Doport			Anile	ent Technologies
		Data File	20NG.d	ntitation Resu	its Report			¥ min	an nemorogreo
			HP Chemist bnalist						
		Acq. Date-Time	9/08/2014 2:39:01 p.m.						
			Calbration 20 ng/ul 11						
		Multiplier Sample Info	1						
		DA Method File							
		Tune File Tune Date							
			: 2014 Aug 09 1334 bnalist : 1/01/0001 12:00:00 a.m.	.batch.bin					
	-	Reference Library	C:\MassHunter\GCMS\1\2						- (
		Compound Internal Standards	RT	QIon	Resp.	Conc.	Units		Dev(Min)
		System Monitoring Compour	nds						
		Target Compounds							QValue
		bis(2-Chloroethyl)ether 1,3-Dichlorobenzene	10.966 11.393	93.0 146.0	39045 32062	22.9181 21.5260	ul/l ul/l		92 98
		1,2-Dichlorobenzene	12.084	146.0 108.0	33184 19421	22.3524	ul/I ul/I		98 97
		Benzyl alcohol bis(2-chloroisopropyl)ether	12.145 12.572	45.0	43980	19.4834 19.7452	ul/I	#	26
		2-Methylphenol Hexachloroethane	12.694 12.979	108.0 117.0	30431 11764	21.3121 20.7558	ul/I ul/I		98 95
		4-Methylphenol	13.141 13.284	108.0 77.0	31507 35818	22.2105 21.8600	ul/l ul/l		96 93
		Isophorone	14.056	82.0	76624	24.5706	ul/I		96
		2-Nitrophenol 2,4-Dimethylphenol	14.259 14.666	139.0 107.0	18231 30005	19.8725 20.6260	ul/l ul/l		96 98
		bis(2-Chloroethoxy)methane 2,4-Dichlorophenol		93.0 162.0	39225 25280	19.5988 21.4179	ul/I ul/I		99 95
		Naphthalene	15.398	128.0	90102	23.3065	ul/I		99
		4-Chloroaniline Hexachlorobutadiene	15.723 16.028	127.0 225.0	28843 14919	18.4459 23.6588	ul/I ul/I		100 96
		2-Methylnaphthalene Hexachlorocyclopentadiene	17.532 18.284	142.0 237.0	84781 9975	23.0990 18.8520	ul/I ul/I		84 97
		2,4,6-Trichlorophenol	18.629	196.0	18585	21.5830	ul/I		95
		2,4,5-Trichlorophenol 2-Chloronaphthalene	18.792 19.036	196.0 162.0	21037 59865	23.7508 23.9144	ul/I ul/I		100 98
		2-Nitroaniline Dimethylphthalate	19.564 20.316	65.0 163.0	22260 72234	20.4201 24.7798	ul/I ul/I		90 100
1.00		2,6-Dinitrotoluene	20.479	165.0	18911	22.1867	ul/I		93
		3-Nitroaniline Acenaphthene	20.886 20.926	138.0 153.0	15368 53897	21.2042 24.9469	ul/l ul/l		93 98
		2,4-Dinitrophenol Dibenzofuran	21.211 21.435	184.0 168.0	5966 85487	12.5218 24.1041	ul/I ul/I		88 94
100		Fluorene	22.512	166.0	67274	24.2113	ul/I		97
		4-Chlorophenyl-phenylether Diethylphthalate	22.614 22.553	204.0 149.0	34537 75043	28.1610 27.2175	ul/l ul/l		94 99
		4-Nitroaniline 4,6-Dinitro-2-methylphenol	22.817 22.959	138.0 198.0	12827 13282	16.7349 23.6831	ul/l ul/l		95 100
		n-Nitrosodiphenylamine	23.041	169.0	45138	25.8601	ul/I		96
	N	4-Bromophenyl-phenylether 20NG.d	24.098	248.0 Broo 1 of 4	21262	23.6682	ul/l	200.00	90
	N N	2010.0		Page 1 of 4		Gene	aved at 3:	2 p.m. on	10/09/2014

## Step 2: Create an Initial Calibration Report Method.

## Step 2: Create an Initial Calibration Report Method.

- 1. In the **Report Method Edit** dialog, click **Add Template** then navigate to the PDF-Reporting folder and select **Env\_InitialCal.report.xml**.
- 2. In the **Templates** tab, under **Report mode**, keep the **Batch** default. Leave the other parameters in this tab with their default settings for a PDF report.

 Click the **Results** tab and select GCMS for a single quad instrument.

4. Skip the **Generate report results** section since this is a PDF report.

An Initial Calibration Report is always generated interactively in Quant since it reports on all the calibration samples in the batch.

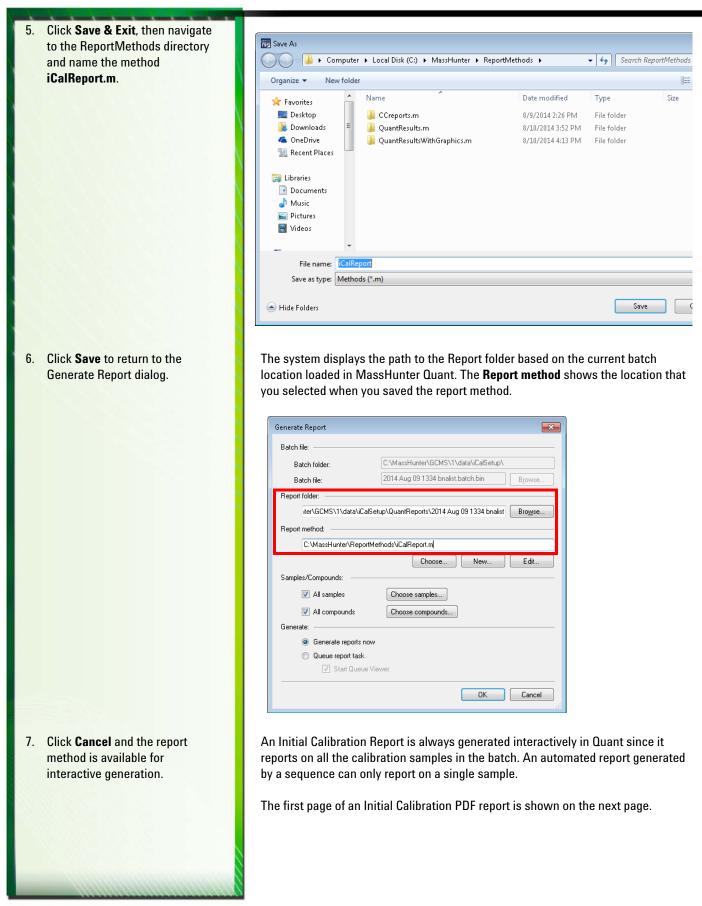
The specified template is added to the Report Method Edit dialog. If you wanted to add additional reports you could add more templates here.

When this method is run, the report is saved as Env\_InitCal.pdf. This report is located in a subfolder of QuantReports folder in the batch directory. The subfolder has the same name as the batch with a numbered prefix.

📅 Report Method Edit	
File Edit	
You (1) (1) (1) (1) (1) (1) (1) (1) (1) (1)	
Templates Results Graphics settings	
Template	Report mode
C:\MassHunter\Report Templates\Quant\PDF-Reporting\Env_InitialCal.report.xml	Batch 🔻 Env_InitialCal.pdf

📆 Report Method Edit	- • ×
File Edit	
Template Results raphics settings	
GCMS Generate report results (report results xml):	
Auto Generate results file only when Excel report templates are selected.	
Yes Always generate results file	
No Never generate results file	

A pdf report does not allow graphic customizations found in the **Graphic settings** tab. Custom settings found in the **Graphic Settings** tab are used with excel templates only.



#### Step 2: Create an Initial Calibration Report Method.

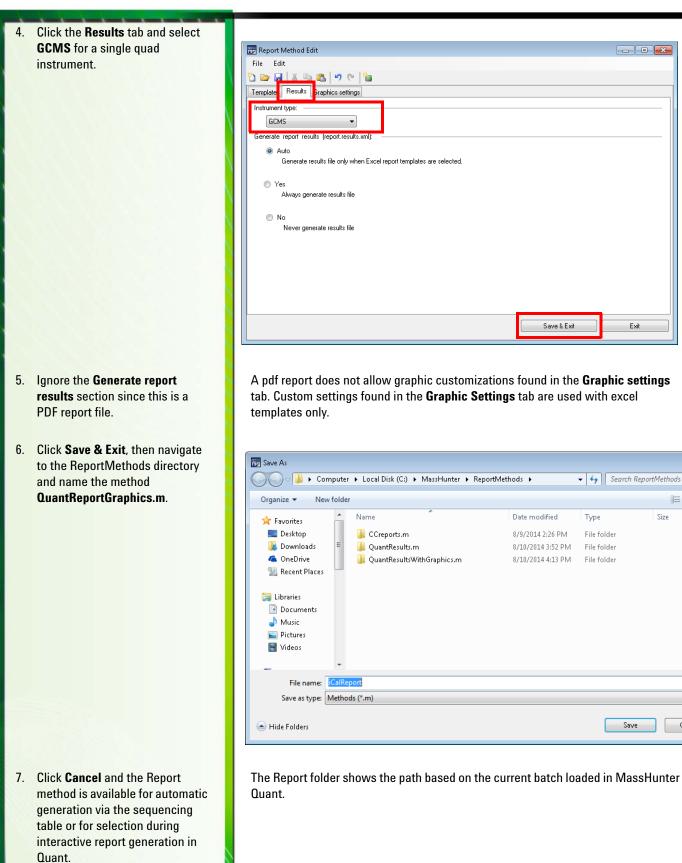
	I	nitial Cali	bration R	eport		- *	Agilent Technolo
Method Path							
Method File		and the state of the	or has to be				
	bnadata\QuantRe	esults\bhadata	_u1.batch.bin				
Last Calib Update 3/11/2014 3:2	.6:09 AM						
Level Name Calibration Files				Acq. Dat			st Update Time
20 C:\EnvDemo\bna					91 2:16:00 PM		4 3:26:09 AM
80 C:\EnvDemo\bna					91 3:11:00 PM		4 3:26:09 AM
120 C:\EnvDemo\bna					91 4:06:00 PM		4 3:26:09 AM
160 C:\EnvDemo\bna 50 C:\EnvDemo\bna					91 5:01:00 PM		4 3:26:09 AM
50 C:\EnvDemo\bna	.data\ciwb050.d			1/28/19	91 5:56:00 PM	3/11/201	4 3:26:09 AM
Compound	20	80	120	160	50	Avg RF	%RSD
I 1,4-Dichlorobenzene-d4				ISTD -			
S 2-Fluorophenol	1.2826	1.3675	1.3077	1.1766	1.3812	1.3031	6.268
T bis(2-Chloroethyl)ether	1.8237	1.6684	1.4883	1.3200	1.5792	1.5759	12.002
S Phenol-d5	1.9668	1.7185	1.5199	1.3675	1.8568	1.6859	14.472
M Phenol	2.0332	1.6681	1.4639	1.3112	1.7377	1.6428	16.782 #
M 2-Chlorophenol	1.4549	1.3096	1.1235	1.0279	1.3642	1.2560	14.003
T 1,3-Dichlorobenzene	1.4976	1.4352	1.2435	1.1775	1.5149	1.3737	11.189
M 1,4-Dichlorobenzene	1.5014	1.3018	1.2324	1.1325	1.5119	1.3360	12.503
T 1,2-Dichlorobenzene	1.5014	1.3018	1.2324	1.1325	1.4674	1.3681	11.542
T Benzyl alcohol	0.9071	0.9841	0.9651	0.8555	0.9008	0.9225	5.633
T bis(2-chloroisopropyl)ether	2.0542	2.2180	2.1602	1.9017	2.0764	2.0821	5.780
T 2-Methylphenol	1.4214	1.3229	1.2882	1.1782	1.3464	1.3114	6.792
T Hexachloroethane	0.5495	0.5455	0.4947	0.4413	0.5620	0.5186	9.695
M N-Nitroso-di-n-propylamine	1.2713	1.3040	1.5031	1.0896	1.2185	1.2773	11.771
T 4-Methylphenol	1.4716	1.3545	1.2259	1.1286	1.3737	1.3109	10.245
I Naphthalene-d8				ISTD -			
S Nitrobenzene-d5	0.4347	0.4441	0.4049	0.3919	0.4400	0.4231	5.502
T Nitrobenzene	0.4347	0.4001	0.4020	0.3476	0.3975	0.3964	7.880
T Isophorone	0.9300	0.9138	0.8740	0.7878	0.8533	0.8718	6.430
T 2-Nitrophenol	0.2213	0.2328	0.2337	0.2028	0.2126	0.2206	6.007
T 2,4-Dimethylphenol	0.3642	0.2328	0.2337	0.3295	0.3464	0.3535	5.181
T bis(2-Chloroethoxy)methane		0.3777			0.3464	0.3535	
	0.4761	0.4918	0.4710	0.4370	0.4864	0.4/25	4.539
	0.3068		0.2688	0.2368			9.824
M 1,2,4-Trichlorobenzene	0.3316	0.3257	0.2944	0.2706	0.3240	0.3093	8.401
T Naphthalene	1.0936	0.9722	0.8512	0.7610	0.9860	0.9328	13.816
T 4-Chloroaniline	0.3501	0.3905	0.3818	0.3664	0.3621	0.3701	4.336
T Hexachlorobutadiene	0.1811	0.1530	0.1499	0.1246	0.1660	0.1549	13.528
M 4-Chloro-3-methylphenol	0.3723	0.3711	0.3338	0.3049	0.3672	0.3499	8.498
T 2-Methylnaphthalene	1.0290	0.8461	0.7728	0.7284	0.9669	0.8686	14.647
I Acenaphthene-d10				ISTD -			
T Hexachlorocyclopentadiene	0.2080	0.2525	0.2191	0.1962	0.2283	0.2208	9.690
T 2,4,6-Trichlorophenol	0.3876	0.3549	0.3329	0.3031	0.3915	0.3540	10.538
T 2,4,5-Trichlorophenol	0.4387	0.3592	0.3061	0.2702	0.4282	0.3605	20.490
S 2-Fluorobiphenyl	1.3735	0.9759	0.9248	0.8498	1.2211	1.0690	20.450
T 2-Chloronaphthalene	1.2485	0.9759	0.9248	0.8500	1.1571	1.0690	16.025
T 2-Nitroaniline	0.4642	0.9535	0.9461	0.4138	0.4727	0.4511	5.018
T Dimethylphthalate	1.5065	1.1533	1.0743	1.0188	1.2722	1.2050	16.061
M Acenaphthylene T 2,6-Dinitrotoluene	1.9827	1.4204	1.2367	1.1352	1.5884	1.4727	22.669
	0.3944	0.3503	0.3381	0.2971	0.3602	0.3480	10.156
T 3-Nitroaniline	0.3205	0.2879	0.2738	0.2583	0.3415	0.2964	11.503
T Acenaphthene	1.1240	0.8258	0.7584	0.6908	1.0219	0.8842	20.630
T 2,4-Dinitrophenol	0.1244	0.2305	0.2319	0.2013	0.2065	0.1989	22.057
			age 1 of 3		Conor	ated at 9:26	AM on 3/13/
			agerois		Genera		

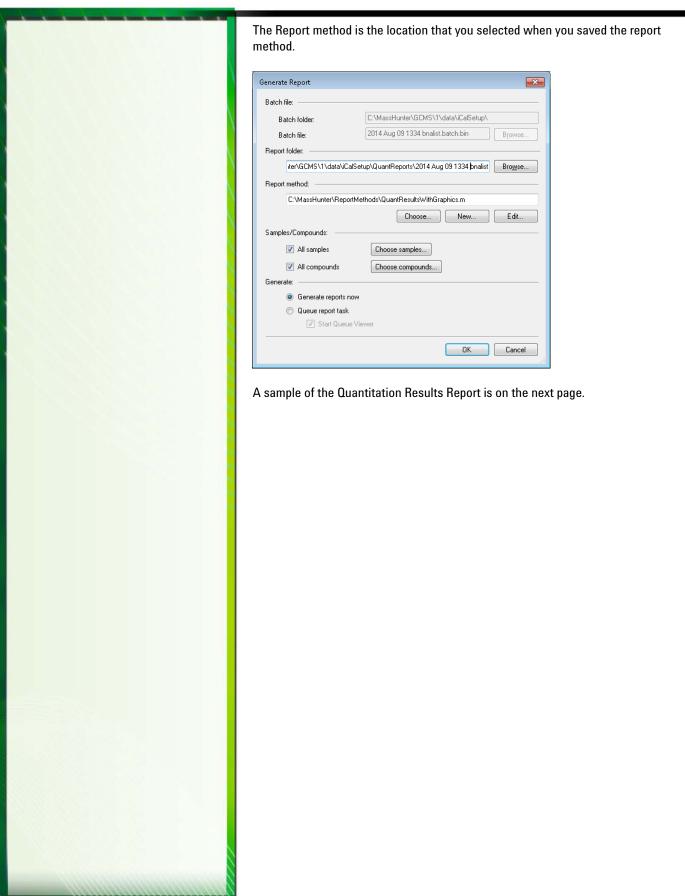
#### Step 3: Create a Quant Report Method.

- - -

A Quant report is an ideal candidate to run with every sample using this unified bnalist method. Save this report method to bnalist.m to have it automatically generate a Quant report each time a sample is run with this unified method.
to ting epo cs.
epo cs.
ay I
te 🕅 Report Method Edit
File Edit
Templates         Results         Graphics settings           Template         Report mode         Destination file
Add Template     Remove Template     Edit Post Processes
Save & Exit Exit
1

#### Step 3: Create a Quant Report Method.

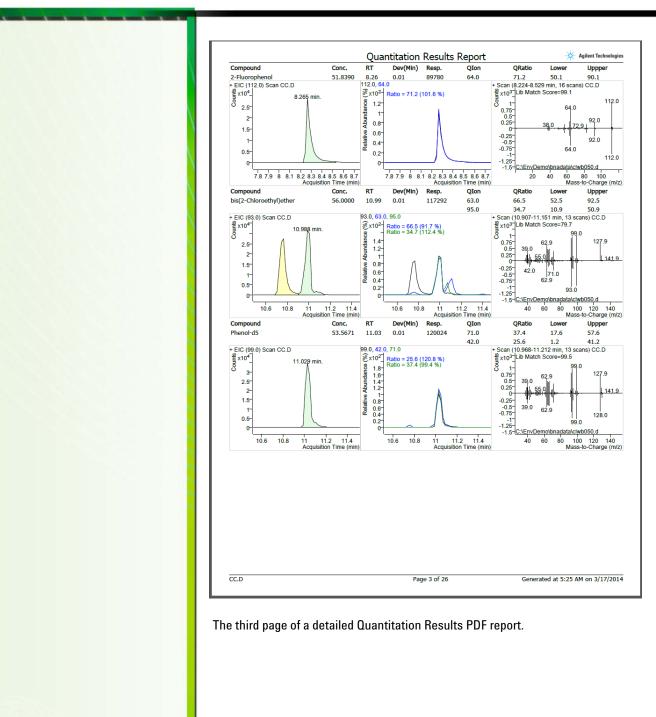




-

		Quanti	itation Res	ults Report			🔆 Agilent Technologi
Data File	: CC.D						
Operator	: HP Chemist						
Acq. Method	: 8260C						
Acq. Date-Time	: 3/26/2014 6:29:0	08 PM					
Sample Name:	: CC						
Vial	: 2						
Multiplier	: 1						
Sample Info	4						
DA Method File	: 8260C.M						
Tune File	1						
Tune Date	4						
Batch Name	: 2014 Mar 26 1741	1 8260C.ba	itch.bin				
Last Calib Update	: 3/26/2014 5:36:1	18 PM					
Compound	RT	т	QIon	Resp.	Conc.	Units	Dev(Min
Internal Standards							
Bromochloromethane	7 0	953	128.0	11753	50.0000	ug/l	# 0.00
1,4-Difluorobenzene		3.189	114.0	66432	50.0000	ug/l	0.00
Chlorobenzene-d5		2.959	117.0	56912	50.0000	ug/l	0.00
				50512	2010000	·	0.00
System Monitoring Compo							
1,2-Dichloroethane-d4		0.783	65.0	27951	49.0124	ug/l	0.00
Spiked Amount: 50.000	Ra	ange: 70.0 ·	- 130.0%		Recovery =	98.02%	
Toluene-d8	21	1.795	98.0	57736	46.9910	ug/l	0.00
Spiked Amount: 50.000	Ra	ange: 70.0 ·	- 130.0%		Recovery =	93.98%	
Bromofluorobenzene	26	5.720	95.0	60889	47.8139	ug/l	0.00
Spiked Amount: 50.000	Ra	ange: 70.0 ·	- 130.0%		Recovery =	95.63%	
Target Compounds							QValu
Chloromethane	0.9	935	50.0	22697	56.5783	ug/l	9
Bromomethane	1.5	595	94.0	20107	50.3441	ug/l	9
Vinyl Chloride	2.0	060	62.0	24364	52.9130	ug/l	10
Chloroethane	2.7	796	64.0	15845	55.8761	ug/l	9
Methylene Chloride	4.6	657	84.0	25338	52.1980	ug/l	9
Acetone	5.2	278	43.0	5973	62.2877	ug/l	9
Carbon Disulfide	6.0	053	76.0	67619	48.7868	ug/l	10
1,1-Dichloroethene		410	96.0	22503	52.3404	ug/l	9
1,1-Dichloroethane	8.7	728	63.0	53766	50.7923	ug/l	9
1,2-Dichloroethene (total)		542	96.0	49055	52.0435	ug/l	9
Chloroform		0.163	83.0	54361	51.6489	ug/l	9
2-Butanone		0.822	43.0	10586	48.1767	ug/l	9
1,2-Dichloroethane		0.900	62.0	34902	49.6957	ug/l	9
1,1,1-Trichloroethane		2.063	97.0	42530	48.1024	ug/l	9
Carbon Tetrachloride		2.451	117.0	34876	46.9982	ug/l	9
Vinyl Acetate		2.722	43.0	76597	49.2078	ug/l	10
Bromodichloromethane		3.148	83.0	50509	48.2418	ug/l	9
1,2-Dichloropropane		4.350	63.0	38472	48.2057	ug/l	9
cis-1,3-Dichloropropene		4.661	75.0	55677	49.2258	ug/l	9
Trichloroethene		5.242	130.0	27706	49.4570	ug/l	9
Benzene		5.630	78.0	76861	48.8134	ug/l	10
Dibromochloromethane		5.902	129.0	31823	47.9801	ug/l	9
trans-1,3-Dichloropropene		5.979	75.0	21542	44.7259	ug/l	7
1,1,2-Trichloroethane		5.979	97.0	24769	51.5477	ug/l	9
Bromoform		3.577	173.0	18220	45.8956	ug/l	9
4-Methyl-2-Pentanone		3.926	43.0	29316	47.7556	ug/l	9
2-Hexanone		0.438	43.0	18294	48.1704	ug/l	9
Z-Hexanone Tetrachloroethene		0.787	43.0	21623	46.3880	ug/l	9
CC.D							5:56 PM on 3/26/201
			Page 1 of	10	G	enerated at	5:56 PM on 3/26/201

The first page of a simple Quantitation Results PDF report.



# Step 4: Create a Continuing Calibration Report Method.

 In the Report Method Edit dialog, click Add template, navigate to the PDF-Reporting folder and select Env\_CC\_MidPoint.report.xml.

2. Click the **Results** tab and select **GCMS** for a single quad instrument.

3. Ignore the **Generate report results** section since this is a PDF report file. In the Templates tab leave the default settings for a PDF report.

	rt Method Edit						
	Edit						
	🚽 👗 🗈 🕰 🔊						
Template	Results Graphics s	ettings					
	Template				Report mode	Destination file	Publish format
•	C:\MassHunter\Report	Templates\Quant\Env_0	C_MidPoint.report.:	xml	Batch	▼ Env_CC_MidPoin	
•							
A	dd Template	Remove Template				E dit Po:	st Processes
					S	ave & Exit	Exit

📅 Report Method Edit	- • •
File Edit	
1 🗁 🕞 🛃 🛤 📽 🔊 (* 1	
Templates Results Graphics settings	
Instrument lype: GCMS Generate report results (report, results xm);	
Auto     Generate results file only when Excel report templates are selected.	
Yes Always generate results file	
No Never generate results file	
Save & Exit	Exit

A pdf report does not allow graphic customizations found in the **Graphic settings** tab. Custom settings found in the **Graphic Settings** tab are used with excel templates only.

<ol> <li>Click Save &amp; Exit, navigate to the ReportMethods directory and name the method iCalReport.m.</li> </ol>	
5. Click <b>Save</b> to return to the	
Generate Report dialog.	Generate Report
	Batch file:
	Batch folder: C:\MassHunter\GCMS\1\data\iCalSetup\
	Batch file: 2014 Aug 09 1334 bhalist.batch.bin Browse
	Report folder:
	iter\GCMS\1\data\iCalSetup\QuantReports\2014 Aug 09 1334 bnalist Browse
	Report method:
	C: \MassHunter\ReportMethods \iCalReport.m
	Choose New Edit
	Samples/Compounds:
	All samples     Choose samples
	All compounds Choose compounds
	Generate:
	Generate reports now
	O Queue report task ✓ Start Queue Viewer
	OK Cancel
	location loaded in MassHunter Quant. The <b>Report method</b> shows the location that you selected when saving the report method. When this method is run, the report is saved in Env_CC_MidPoint.pdf. This report is located in the batch directories' QuantReports folder in a time stamped folder of the
	same name as the quant method.
	If the results of this Continuing Calibration Report are acceptable the abundance data for each compound replaces the current value in the calibration table for the CC level.
	4

6.	To generate this report
	interactively, click Choose
	samples and Choose compounds
	then generate the report.

Batch Name	C:\MassHunter\GCMS	\1\data\Co	nCal8260C\Q	uantResults\20	L4 Mar 26 1729	8260C.bato	h.bin		
Method File	C:\MassHunter\GCMS								
Daily CC	C:\MassHunter\GCMS			C.D					
	njection Time	Calibrati							
	3/26/2014 6:09:01 AM			1\DATA\ICAL					
	3/26/2014 6:09:02 AM			1\DATA\ICAL					
	3/26/2014 6:09:03 AM		C:\MassHunter\GCMS\1\DATA\ICAL8260C\100PPB.D						
	3/26/2014 6:10:04 AM	C:\Mass	Hunter\GCMS	1\DATA\ICAL	3260C\150PPB.	D			
200 3	3/26/2014 6:10:05 AM	C:\Mass	Hunter\GCMS	1\DATA\ICAL	3260C\200PPB.	D			
CC 3	3/26/2014 6:29:08 PM	C:\Mass	Hunter\GCM9	\1\data\ConCa	8260C\CC.D	<=====			
ISTD Compound:		А	vg Resp	Mid Resp	CC Resp	Are	a%	A/M	
Bromochloromethane	9	1	2491	13419	11753	12.4	42	M	
1,4-Difluorobenzene			7469	70129	66432	5.2		M	
Chlorobenzene-d5		5	7456	59487	56912	4.3	3	М	
Target Compound Bromochloromethane		wgRF/R2	CC RF	Exp. Conc	Calc. Conc	%Dev	Area%	Curve Fit	
Chloromethane		.7066	1.9311	50.00	56.58	13.16	0.59	Avg RF	
Bromomethane	1	.6991	1.7108	50.00	50.34	0.69	11.61	Avg RF	
Vinyl Chloride	1	.9588	2.0730	50.00	52.91	5.83	8.30	Avg RF	
Chloroethane	1	.2063	1.3481	50.00	55.88	11.75	5.38	Avg RF	
Methylene Chloride	2	.0650	2.1558	50.00	52.20	4.40	8.32	Avg RF	
Acetone	0	.4080	0.5082	50.00	62.29	24.58 #	-10.93	Avg RF	
Carbon Disulfide		.8963	5.7533	50.00	48.79	2.43	12.39	Avg RF	
1.1-Dichloroethene		.8290	1.9146	50.00	52.34	4.68	4.22	Avg RF	
1,1-Dichloroethane		.5032	4.5746	50.00	50.79	1.58	8.22	Avg RF	
1,2-Dichloroethene (		.0099	4.1738	50.00	52.04	4.09	10.02	Avg RF	
Chloroform		.4776	4.6252	50.00	51.65	3.30	7.84	Avg RF	
1.2-Dichloroethane-d		.4261	2.3782	50.00	49.01	1.98	1.24	Avg RF	
1,2-Dichloroethane		.9877	2.9695	50.00	49.70	0.61	8.56	Avg RF	
1.4-Difluorobenzene	-			ISTD				2	
2-Butanone	0	.1654	0.1594	50.00	48.18	3.65	7.27	Avg RF	
1.1.1-Trichloroethane	e 0	.6655	0.6402	50.00	48.10	3.80	11.40	Avg RF	
Carbon Tetrachloride	0	.5585	0.5250	50.00	47.00	6.00	15.00	Avg RF	
Vinyl Acetate	1	.1716	1.1530	50.00	49.21	1.58	5.02	Avg RF	
Bromodichlorometha	ne 0	.7880	0.7603	50.00	48.24	3.52	9.23	Avg RF	
1,2-Dichloropropane	0	.6007	0.5791	50.00	48.21	3.59	8.17	Avg RF	
cis-1,3-Dichloroprope	ene 0	.8513	0.8381	50.00	49.23	1.55	9.69	Avg RF	
Trichloroethene	0	.4216	0.4171	50.00	49.46	1.09	10.62	Avg RF	
Benzene		.1851	1.1570	50.00	48.81	2.37	5.87	Avg RF	
Dibromochlorometha	ne 0	.4992	0.4790	50.00	47.98	4.04	9.65	Avg RF	
trans-1,3-Dichloropro	pene 0	.3625	0.3243	50.00	44.73	10.55	9.73	Avg RF	
1,1,2-Trichloroethan	e O	.3617	0.3729	50.00	51.55	3.10	2.24	Avg RF	
Bromoform	0	.2988	0.2743	50.00	45.90	8.21	15.39	Avg RF	
Chlorobenzene-d5				ISTD				-	
4-Methyl-2-Pentanon	e 0	.5393	0.5151	50.00	47.76	4.49	2.15	Avg RF	
2-Hexanone		.3337	0.3214	50.00	48.17	3.66	3.85	Avg RF	
Tetrachloroethene	0	.4095	0.3799	50.00	46.39	7.22	14.88	Avg RF	
1,1,2,2-Tetrachloroet	hane 0	.6888	0.6896	50.00	50.06	0.12	2.87	Avg RF	
Toluene-d8	1	.0794	1.0145	50.00	46.99	6.02	8.10	Avg RF	
Toluene		.8449	0.8535	50.00	50.51	1.02	4.52	Avg RF	
Chlorobenzene	1	.0752	1.0243	50.00	47.63	4.73	7.57	Avg RF	
Ethylbenzene		.5142	0.4930	50.00	47.94	4.13	6.78	Avg RF	
Bromofluorobenzene		.1188	1.0699	50.00	47.81	4.37	4.36	Avg RF	

The first page of a Continuing Calibration PDF report.

#### Step 5: Create a Matrix Spike Duplicate Report Method.

#### Step 5: Create a Matrix Spike Duplicate Report Method.

1. In the **Report Method Edit** dialog, click **Add template**, navigate to the PDF-Reporting folder and select **Env\_MSD.report.xml**. A Matrix Spike Duplicate Report is always generated interactively in Quant since it reports on multiple samples in the batch.

In the Templates tab leave the default settings for a PDF report.

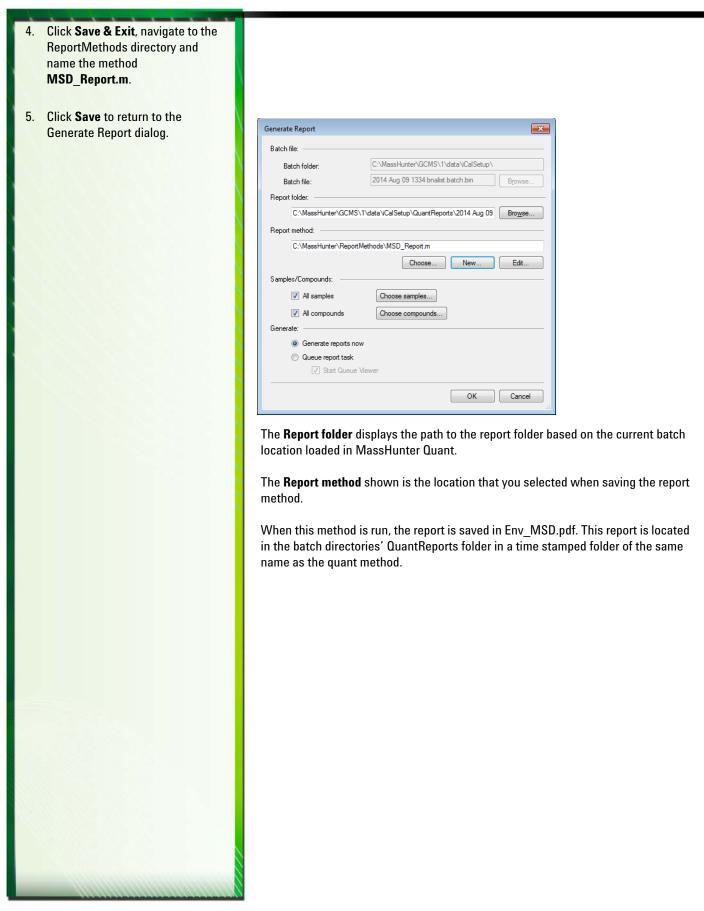
摺 Report Method Edit File Edit			
🛅 🗁 🛃 🖄 🛍 🖉 🕫 🛍			
Templates Results Graphics settings			
Template	Report mode	Destination file	Publish
C:\MassHunter\Report Templates\Quant\PDF-Reporting\Env_MSD.report.xml	Batch	<ul> <li>Env_MSD.pdf</li> </ul>	
4			
Add Template		Edit Post Proc	esses
		Edit Post Proc	resses
	Save & E		esses

1	📅 Report Method Edit
	File Edit
	Template Results Graphics settings
	Instrument type: GCMS
	Generate report results (report.results.xml):
	<ul> <li>Auto Generate results file only when Excel report templates are selected.</li> </ul>
	Yes Always generate results file
	No Never generate results file
	Save & Exit Exit

A pdf report does not allow graphic customizations found in the **Graphic settings** tab. Custom settings found in the **Graphic Settings** tab are used with excel templates only.

2. Click the **Results** tab and select **GCMS** for a single quad instrument.

3. Ignore the **Generate report results** section since this is a PDF report file.





This report must be generated interactively since it must include results from multiple samples in the batch.

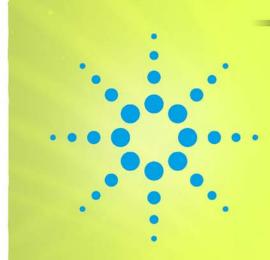
Batch Name	Matrix Spi C:\MassHunter\GCI								Agilent Technolog
Last Calib Update	3/26/2014 5:36:18		concalozoot	Quantitesu	103 (2014 148)	20 1/41 02	ouc.batch		
Method File	C:\MassHunter\GCI		ds\8260C.M						
Data Path	C:\MassHunter\GCI			c\					
						1			
Sample Name			Sample Typ	pe	Matrix Spike Group			Date Time	
Sample 10 MS Sample 10			Matrix Non Spiko		Soil Soil			6/2014 6:46 6/2014 6:46	
Sample 10 Sample 10 MSD			Non Spike Matrix Dup		Soil			6/2014 6:40 6/2014 6:47	
Sample 10 MSD			Matrix Dup		Water			6/2014 6:44	
Sample 1			Non Spike		Water			6/2014 6:43	
Sample 1 MSD			Matrix Dup		Water			6/2014 6:45	
	Soil, Type B Results:								
Compound	Sample Conc		Spike Res	Dup Res	Spike Rec	Dup Rec	RPD	QC RPD	Limits %Red
1,1-Dichloroethene	0.000	50.000	61.743	60.723	123.49	121.45	1.67	5	70 - 130
Trichloroethene	2,985	50.000	52.122	50.723	123.49	121.45	2.60	5	70 - 130
Benzene	0.094	50.000	52.122	53.709	104.24	101.41	2.87	5	70 - 130
Foluene	0.000	0.000	51.161	52.253	101.07	207.12	2.11 #	-	0-0
Chlorobenzene	0.000	0.000	49.061	51.952			5.72 #		0-0
Matrix Spike Group	Water, Type A Resul Sample Conc		Spike Res	Dup Res	Spike Rec	Dup Rec	RPD	QC RPD	Limits %Red
1,1-Dichloroethene	0.000	50.000	61.743	60.723	123.49	121.45	1.67	5	70 - 130
Trichloroethene	0.000	50.000	55.107	53.692	123.49	121.45	2.60	5	70 - 130 70 - 130
Benzene	0.000	50.000	52.281	53.803	104.56	107.61	2.87	5	70 - 130
Toluene	0.000	0.000	51.161	52.253	104.50	107.01	2.11 #	5	0-0
Chlorobenzene	0.000	0.000	49.061	51.952			5.72 #		0-0

A Matrix Spike Duplicate PDF report.

to be the to be to be to be to be	
Step 6: Create a QA Check Report Method.	This report is used to make sure all the data files in the batch were injected within the specified time range of the Tune Check data file. We used the global outlier CC Maximum Elapsed Time in Hours that was defined in the initial setup of the method.
	This report will also:
	<ul> <li>Check to make sure that the ISTD's areas are within the specified allowable limit compare to the Con Cal ISTDs areas.</li> </ul>
	<ul> <li>Flag any of the surrogates that do not meet the outlier limits.</li> </ul>
	This report is always generated interactively since it operates on all samples in the batch.
1. In the <b>Report Method Edit</b> dialog, click <b>Add template</b> , navigate to	In the <b>Templates</b> tab leave the default settings for a PDF report.
the PDF-Reporting folder and	🖾 Report Method Edit
select Env QA Check.report.xml.	File Edit
Env_UA_Check.report.xmi.	Templates         Results         Graphics settings           Template         Report mode         Destination file         P
	Template     Report mode     Destination file     Pl       C:\MassHunter\Report     Templates\Quant\PDF-Reporting\Env_QA_Check.report.xml     Batch     Env_QA_Check.pdf
	Add Template     Remove Template     Edit Post Processes
2. Click the <b>Results</b> tab and select	E Report Method Edit
<b>GCMS</b> for a single quad instrument.	File Edit File E
	Yes Always generate results file
	No Never generate results file
3. Ignore the <b>Generate report</b> <b>results</b> section since this is a PDF report file.	A pdf report does not allow graphic customizations found in the <b>Graphic settings</b> tab. Custom settings found in the <b>Graphic Settings</b> tab are used with excel templates only.

4.	Click <b>Save &amp; Exit</b> , navigate to the ReportMethods directory and name the method <b>QA_Check.m</b> .	
5.	Click <b>Save</b> to return to the	Generate Report
	Generate Report dialog.	
		Batch file:
		Batch folder: C:\MassHunter\GCMS\1\data\CalSetup\
		Batch file: 2014 Aug 09 1334 bnalist.batch.bin Browse
		Report folder:
		C:\MassHunter\GCMS\1\data\iCalSetup\QuantReports\2014 Aug 09 Browse
		Report method:
		C:\MassHunter\ReportMethods\QA_Check.m
		Choose New Edit
		Samples/Compounds:
		All samples     Choose samples
		✓ All compounds Choose compounds
		Generate:
		Generate reports now
		© Queue report task
		✓ Start Queue Viewer
		OK Cancel
		h
		The <b>Report folder</b> displays the path to the report folder based on the current batch location loaded in MassHunter Quant. The <b>Report method</b> shown is the location that you selected when saving the report Click <b>Cancel</b> and the Report method is available for automatic generation via the sequencing table. When this method is run, the report is saved in the Env_QA_Checkpdf. This report is located in the batch directories' QuantReports folder in a time stamped folder of the same name as the quant method.
-		

<ul> <li>To generate this report interactively, click Choose samples and Choose compounds</li> </ul>	This report must samples in the ba	-	tively since it must	t include results from all
then generate the report.		OA C	heck Report	🔆 Agilent Technologies
	Tune Check C: TuneCheck Time 3/ Time Limit 12	014 Mar 26 1741 8260C.batch.bin :\MassHunter\GCMS\1\DATA\ConCal82 (26/2014 6:29:07 PM 2 hr DAcq.Time =3/26/2014 6:29:08 PM	•	
	ISTD Name ISTD Resp.	Bromochloromethane 11753	1,4-Difluorobenzene 66432	Chlorobenzene-d5 56912
		me= 3/26/2014 6:42:09 PM	100432	50512
	ISTD Name	Bromochloromethane	1,4-Difluorobenzene	Chlorobenzene-d5
	ISTD Resp.	11104	62095	54021
	Surr Name Surr Rec.	1,2-Dichloroethane-d4 96.70	Toluene-d8 98.17	Bromofluorobenzene 99.24
	Data File: Sample1.D, Aco	1.Time= 3/26/2014 6:43:00 PM		
	ISTD Name	Bromochloromethane	1,4-Difluorobenzene	Chlorobenzene-d5
	ISTD Resp.	10801	61525	51810
	Surr Name	1,2-Dichloroethane-d4	Toluene-d8	Bromofluorobenzene
	Surr Rec.	96.57	103.20	100.68
	Data File: Sample1MS.D,	Acq.Time= 3/26/2014 6:44:01 PM		
	ISTD Name ISTD Resp.	Bromochloromethane 12605	1,4-Difluorobenzene 73033	Chlorobenzene-d5 64338
	Surr Name	1,2-Dichloroethane-d4	Toluene-d8	Bromofluorobenzene
	Surr Rec.	106.88	96.91	100.02
		, Acq.Time= 3/26/2014 6:45:02 PM		
	ISTD Name ISTD Resp.	Bromochloromethane 12817	1,4-Difluorobenzene 72344	Chlorobenzene-d5 61547
	Surr Name Surr Rec.	1,2-Dichloroethane-d4 106.76	Toluene-d8 98.64	Bromofluorobenzene 103.23
		cq.Time= 3/26/2014 6:46:03 PM	1	
	ISTD Name	Bromochloromethane	1,4-Difluorobenzene	Chlorobenzene-d5
	ISTD Resp.	12314	72834	61107
	Surr Name	1,2-Dichloroethane-d4	Toluene-d8	Bromofluorobenzene
	Surr Rec.	105.78	100.76	104.24
	Data File: Sample10MS.D,	, Acq.Time= 3/26/2014 6:46:04 PM		
	ISTD Name ISTD Resp.	Bromochloromethane 12605	1,4-Difluorobenzene 73033	Chlorobenzene-d5 64338
	Surr Name Surr Rec.	1,2-Dichloroethane-d4 106.88	Toluene-d8 96.91	Bromofluorobenzene 100.02
		D, Acq.Time= 3/26/2014 6:47:05 PM	10002	120002
	ISTD Name	Bromochloromethane	1,4-Difluorobenzene	Chlorobenzene-d5
	ISTD Resp.	12817	72344	61547
	Surr Name	1,2-Dichloroethane-d4	Toluene-d8	Bromofluorobenzene
	Surr Rec.	106.76	98.64	103.23
			Page 1 of 1	Generated at 6:07 PM on 3/26/2014
tep 7: Run samples.	Next we will look "Run Samples".	k at some common w	orkflows for runnir	ng samples in Chapter 7,



Introduction92Step 1: Run a calibration of the instrument.92Step 2: Run daily unknown samples.97Step 3: Perform Data Analysis Interactively.103

**Agilent Technologies** 

Introduction	Two basic workflows exist when processing samples:
	One for calibrating the instrument
	One for daily sample processing
	These workflows are reviewed below.
Step 1: Run a calibration of the instrument.	For EPA method 8270, the initial calibration must be run to begin the process, as well as when a continuing calibration indicates the instrument is out of calibration. Our example uses 5 calibration levels for each compound. The responses for these 5 new calibration samples replace the calibration curve responses in the 5 levels in the quant method.
	In this example, at the start of the automatic calibration sequence for the initial calibration, we include a Tune Evaluation sample to verify the instrument is within
	the tune specifications set for EPA method 8270.
	The tune evaluation is processed and:
	• If the instrument fails the evaluation, the sequence will pause for operator inter- vention.
	• If the instrument passes the evaluation, the 5 calibration samples are then run and analyzed and, as shown in this example, an Initial Calibration report can then be generated interactively in Quant.
1. Load the default Sequence.	In the Data Acquisition Instrument Control view, click the <b>Load Sequence</b> icon then select the <b>default.sequence.xm</b> l file from your instrument directory sequence folder.
	Sequence Method
2. Edit the Sequence Table.	Click the <b>Edit Sequence</b> icon to open the Sequence Table for editing.
	Sequence Method

Step 1: Run a calibration of the instrument.

- 3. From the **Tools** menu, select Add/Remove Columns and add columns so the table resembles the example below.
- 4. Add additional samples to the table, name the samples, specify the ALS vial containing the sample, and specify the sample type.
- 5. Fill in the level for the Cal sample types as shown.

- 6. Fill in the **Data File** names as shown.
- 7. Fill in the **Method** names as shown.
- For the Cal samples, set the Update Response Factor parameter to Replace, and click OK to close the sequence table.

9. Save the completed sequence as **iCal.sequence.xml** for future initial calibrations.

	New Sample(s) 🔻	×	J 🕢 Tool	s <del>.</del>				_		
	Name	Vial	Туре		Level	Data File	Method File		Update Response Factor	
1	Tune Evaluation 01	10	TuneCheck	-		TuneChk.d	bnalist.m			-
2	Calbration 20 ng/ul	11	Cal	-	20	20NG.d	bnalist.m		Replace	-
3	Calbration 50 ng/ul	12	Cal	-	50	50NG.d	bnalist.m		Replace	-
4	Calbration 80 ng/ul	13	Cal	-	80	80NG.d	bnalist.m		Replace	-
5	Calbration 120 ng/ul	14	Cal	-	120	120NG.d	bnalist.m		Replace	-
6	Calbration 160 ng/ul	15	Cal	-	160	160NG.d	bnalist.m		Replace	-

We previously specified that all batch directories will be in the root of the **Data** folder for instrument #1 (**Method > Set New Default Paths**).

We previously specified that all master methods are located in the root of the **Method** folder for instrument #1. Here we are using the same bnalist unified method containing both the data acquisition, data analysis, report, and the tune evaluation methods.

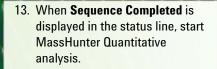
This automatically updates the calibration curves in the master method.

	New Sample(s)	X   I	Tvpe	-	Level	Data File	Method File	1	Update Response Factor		
1	Tune Evaluation 01		TuneCheck	-	Lever	TuneChk.d	hu aliat as		opulate mesponse ractor	-	
2	Calbration 20 ng/ul	11	Cal	•	20	20NG.d	bnalist.m		Replace	•	
3	Calbration 50 ng/ul	12	Cal	-	50	50NG.d	NG.d bnalist.m		Replace		
4	Calbration 80 ng/ul	13	Cal 🔻		80	80NG.d	bnalist.m		Replace	-	
5	Calbration 120 ng/ul	14	Cal	-	120	120NG.d	bnalist.m		Replace	-	
6	Calbration 160 ng/ul	15	Cal	-	160	160NG.d	bnalist.m		Replace	•	



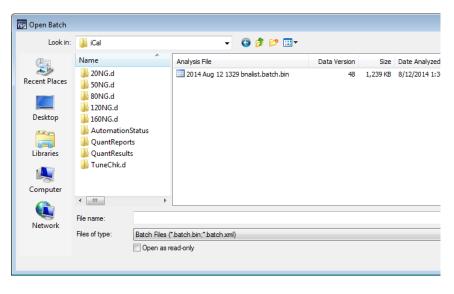
#### Step 1: Run a calibration of the instrument.

<ol> <li>Click the Run Sequence icon to start the automated acquisition of sample data.</li> <li>Change the Data File Directory name to iCal.</li> </ol>	Sequence       Method         Image: Sequence       Image: Sequence       Image: Sequence         Image: Sequence       Image: Sequence       Image: Sequence       Image: Sequence         Image: Sequence
S	start Sequence iCal.sequence.xml Last Modified: Tue Aug 12 10:46:48 2014
	Method Sections to Flun       Sequence Barcode Options <ul> <li>Full Method</li> <li>Disable barcode for this sequence.</li> <li>On mismatch, inject anyway.</li> <li>On mismatch, don't inject; continue the sequence.</li> <li>On mismatch, don't inject; stop the sequence.</li> </ul>
	☑ Overwrite Existing Data Files
	Sequence Comment:
	Post-Sequence Macros/Commands
	Acquistion: Browse Data Analysis: Browse
	Enter the name of the directory to put data files in
	Bun Sequence     OK     Cancel
12. Click <b>Run Sequence</b> to start the automated acquisition of sample data and generation of reports.	A Quant report is automatically generated for each sample since the report method was stored in the bnalist method. A Tune Evaluation report PDF is generated automatically by the tuneEvaluation method stored in the bnalist method. The Tune Evaluation sample is processed.
	If the tune evaluation passes, the 5 calibration samples are next processed. <b>If the Tune Evaluation fails</b> you are given the chance to pause the sequence or continue. EPA method 8270 does not accept quantitation results for samples run after a failed tune evaluation.
	Alert Evaluation Failed: 00101001.D Pause Sequence?



## 14. Select File > Open batch and navigate to the paused batch.

In this example we navigated to the iCal batch folder and selected the time stamped bnalist.batch.bin batch file.



The batch table opens.

📅 Agilent MassHunter Quantitative Analysis (Environmental Analysis for GCMS) - iCal - 2014 Aug 12 1329 bnalist.batch.bin File Edit View Analyze Method Update Report Tools Help 🎦 🗁 🛃 🐚 🛛 Quantitate Batch 🔹 🕢 📜 Layout: 🔜 🔛 🔛 🛄 🚺 🧭 Restore Default Layout Batch Table Sample: 👔 Tune Evaluation 01 ▼ ↓ Sample Type: <All> Compound: Image: 2-Fluorophenol ▼ ISTD: 1,4-Dichlorobenzene-d4 2-Fluorophenol Results bis(2-Chloroethyl)ether Resul... Phenol-d5 Results Sample Phenol Acq. Date-Time RT Final Conc. Accuracy  $(\mathbf{I})$ 8 Name Data File Туре Level RT Final Conc. Accuracy RT Final Conc. Accuracy RT Final C Tune Evaluation 01 TuneChk.d TuneCheck 8/12/2014 2:30 PM 1 Calbration 20 ng/ul 20NG.d 20 8/12/2014 2:30 PM 8.284 19.6847 98.4 10.966 23,1447 115.7 11.007 23.3320 116.7 11 047 24 Cal Calbration 50 ng/ul 50NG.d
 Calbration 80 ng/ul 80NG.d 50 8/12/2014 2:31 PM 80 8/12/2014 2:32 PM 8.285 52.9946 8.280 83.9553 106.0 11.008 104.9 11.044 52 Cal 50.1028 100.2 11.029 55.0696 110.1 11.069 84.6930 105.9 11.064 81.5465 101.9 11.105 81. Cal Calbration 120 ng/ul 120NG.d 120 8/12/2014 2:33 PM 120.421 100.4 11.058 113.3296 94.4 11.099 90.2 11.139 Cal 8.273 108.1841 106 Calbration 160 ng/ul 160NG.d Cal 160 8/12/2014 2:34 PM 8.267 90.3 11.052 134.0211 83.8 11.092 129 7824 81.1 11.133 127

15. To review the reports automatically generated by the sequence, select **Report > Open Report Folder**.

thod Update	Repo	ort Tools	Help							
ate Batch 👻 🚳 Generate										
	Open Report Folder									
Queue Viewer										
Sam	vr	Query		e						
Data File         Recent Report Methods           00101001.D         1: C:\MassHunter\Report Templates\Quant\PDF-Reporting\TuneCheck.m           CC.d         1: C:\MassHunter\Report Templates\Quant\PDF-Reporting\TuneCheck.m										
sample01.d	Samp		8/12/2014 11:58 AM 8.282 78.2591	4						

This opens the QuantReports directory that contains the report(s) for that sample. Here for example, the 20NG folder holds the QuantResults.pdf report for the level 20 compounds.

💽 🗢 🚺 « 1 → data → iCal → Qu	uantReports )	• • • •	Search QuantReports		
Organize 🔻 😝 Open 🛛 Include in	library 🔻	Share with 👻 New	folder	=	(
☆ Favorites	<b>^</b>	Name		Date modified	1
🌉 Desktop	=	퉬 20NG		8/12/2014 1:31	L PN
🝺 Downloads		]] 50NG		8/12/2014 1:31	L PN
🝊 OneDrive		퉬 80NG		8/12/2014 1:32	2 PN
🕮 Recent Places		퉬 120NG		8/12/2014 1:33	B PN
		퉬 160NG		8/12/2014 1:34	I PN
Documents					
👌 Music	- ₹				
20NG Date modified: 8/12 File folder	/2014 1:31 PM				

- 16. Open and review each sample's PDF report to see if the results are acceptable.
- 17. To review the **Tune Check** report, navigate to the batch directory, open the **TuneCheck.d** folder and then open the **TuneReport.pdf**.
- 18. Generate an Initial Calibration report interactively.

Select **Report > Generate**, choose the previous saved iCalReport.m method and click **OK** to generate the report.

Step 2: Run daily unknown samples.		Eva EP/ cor The	aluat A me ntinu ese a	ply with EPA ion sample ethod 8270, iing calibrat are the gene e detail on th	to ver follow ion, a ral sto	ify the inst ved by a co nd then by eps that oc	tru ont th	ment is wit inuing calil e unknowr r during da	thin th bration 1 samp	e tune sp 1 sample Iles to be	becificati to verify process	ons set fo the sed.	or
		1 The Tune Evaluation sample runs.											
				lf the instru runs.	ment	passes the	e e	valuation, t	he cor	ntinuing	calibratio	on sample	;
	A CONTRACTOR			If the instru intervention		fails the ev	/al	uation, the	seque	nce will	pause fo	r operato	r
		2		e continuing mpounds ar					t to ve	rify the c	alibratio	n curves t	for
		3	Af	ter the conti	inuing	calibratio	n s	ample run	s, the s	sequence	e pauses		
		4		e operator r acceptable.	eview	s the cont	in	uing calibra	bration report to verify the calibration	on			
		5		he continui dated with 1							od is ma	nually	
		6	Th	e paused se	quen	ce is then	res	started to p	rocess	s the rem	aining s	amples.	
1.	Open a default sequence, then from the <b>Tools</b> menu, select <b>Add/Remove Columns</b> and add columns so that the table resembles the example below.												
2.	Add additional sample rows to the table, name the samples,	Se	quence	Table							8	×	
	specify the ALS vial containing			New Sample(s) 🔻	×	🕢 Tools 🗸						-	
	the sample, and specify the			Name	Vial	Type Type	-	Keyword	Level	Data File	Method File		
	sample type.		1	Tune Evaluation 01 Continuing Cal		TuneCheck CC	•		СС	TuneChk.d CC.d	bnalist.m bnalist.m		
			3	containing Out		Keyword	•	Pause 🔻		00.0	or rande fit		
			4	Blank01		Blank	-			Blank.d	bnalist.m		
				Sample 1		MatrixBlank	-	•		S1.d	bnalist.m		
				Sample 1 MS		MatrixSpike	-			S1MS.d	bnalist.m		
			7	Sample 1 MSD	16	MatrixSpikeDup	•	-		S1MSD.d	bnalist.m		

- 3. Fill in the level for the CC sample type as shown in the red box in the step 2-2 graphic.
- 4. Fill in the **Data File** names as shown in the red box in the step 2-2 graphic.

We previously specified that all batch directories will be in the root of the **Data** folder for instrument #1 (**Method > Set New Default Paths**).

8 Sample 10

9 Sample 10 MS

10 Sample 10 MSD

Read Barcode

17 MatrixBlank

18 MatrixSpike

19 MatrixSpikeDup 💌

-

•

S10.d

ок

S10MS.d

S10MSD.d

bnalist.m

bnalist.m

bnalist.m

Cancel <u>H</u>elp

- 5. Fill in the **Method** names as shown in the red box in the step 2-2 graphic.
- 6. Click OK to close the Sequence table and save it as MSD.sequence.xml.
- 7. Click the **Run Sequence** icon.

8. Change the **Data File Directory** name to **MSD**. This becomes your Quant batch directory.

9. Click **Run Sequence** to start the automated acquisition of sample data.

We previously specified that all master methods are located in the root of the **Method** folder for instrument #1. Here we are using the same bnalist unified method containing both the data acquisition, data analysis, report, and the tune evaluation methods.



The Start Sequence dialog displays.

Method Sections to Run	Seque	ence Barcode Options	this sequence.		
Full Method		<ul> <li>On mismatch, inject</li> <li>On mismatch, don't</li> </ul>	anyway. inject; continue the		
✓ Overwrite Existing Data Files		On mismatch, don't	inject; stop the seq	uence.	
Sequence					
Opera	ator Name: jmt				
Data File	Directory: C:\MassHunte	er\GCMS\1\DATA\MSD			Browse
Pre-Sequence Macros/Commands					
A	cquisition:				Browse
Dat	a Analysis:				Browse
Post-Sequence Macros/Commands					
A	cquisition:				Browse
Dat	a Analysis:				Browse
ter the name of the directory to put data file	es in				
<u>R</u> un Sequence			ок	Cancel	Help

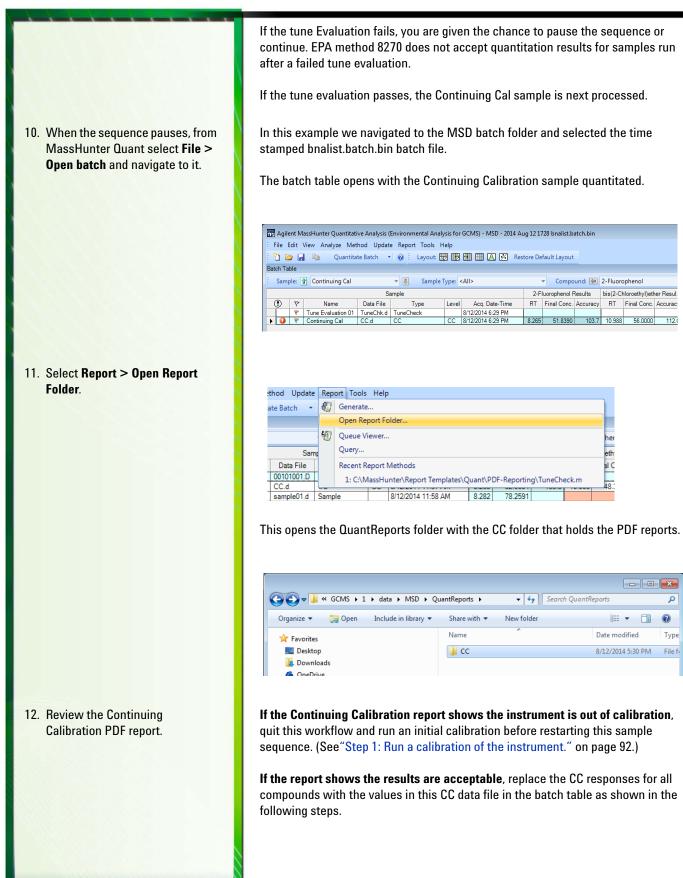
The Tune Evaluation sample is processed.

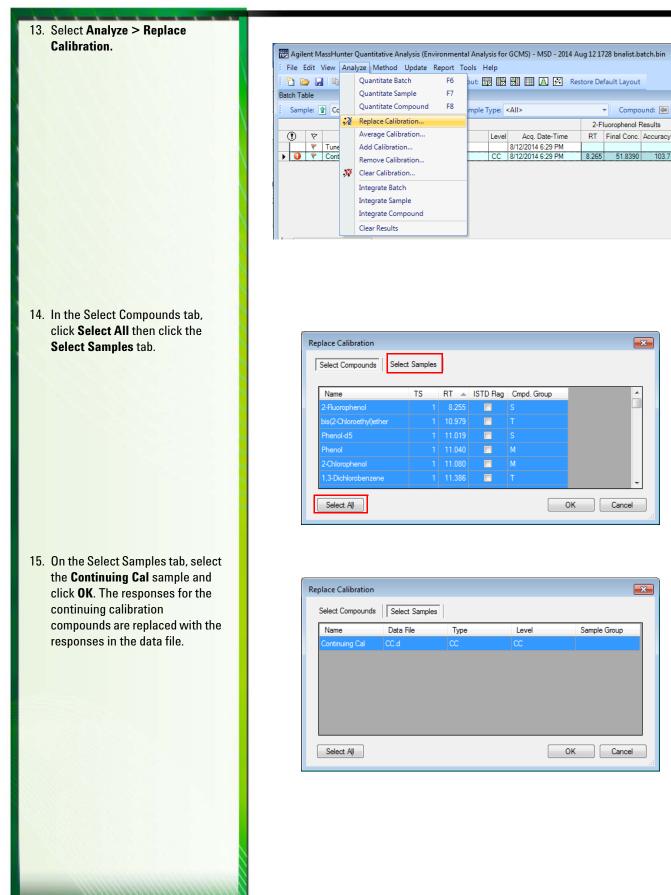
Q

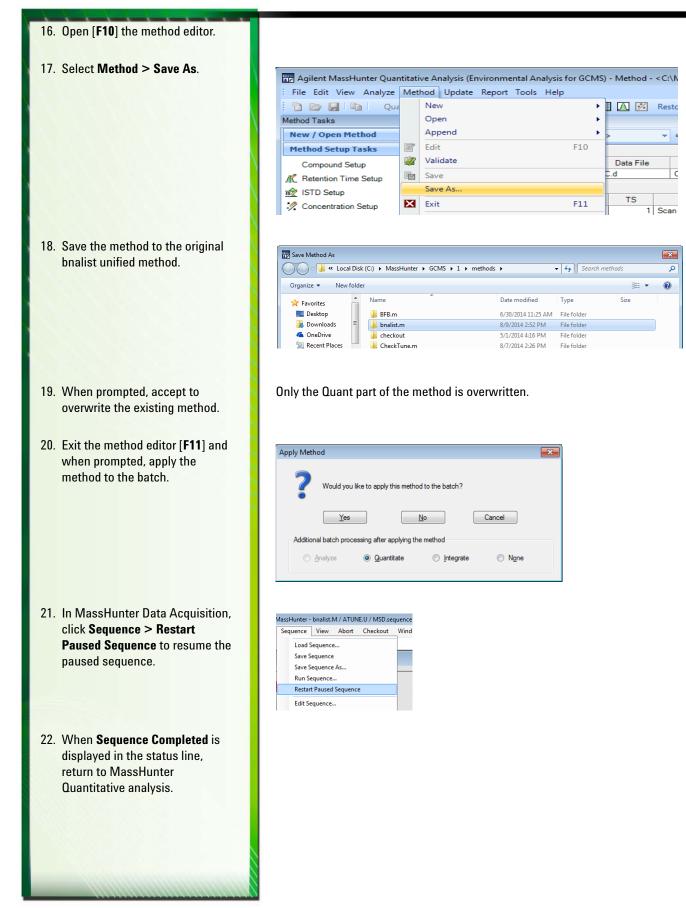
?

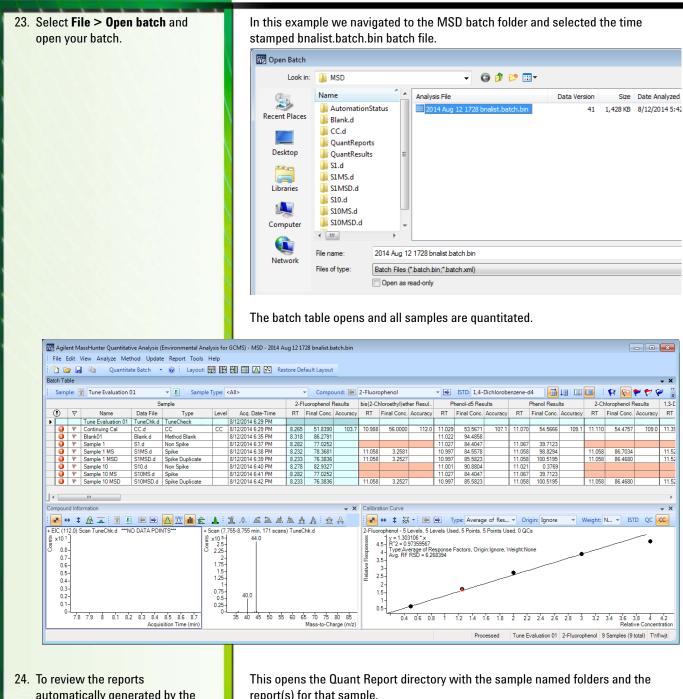
Туре

File f



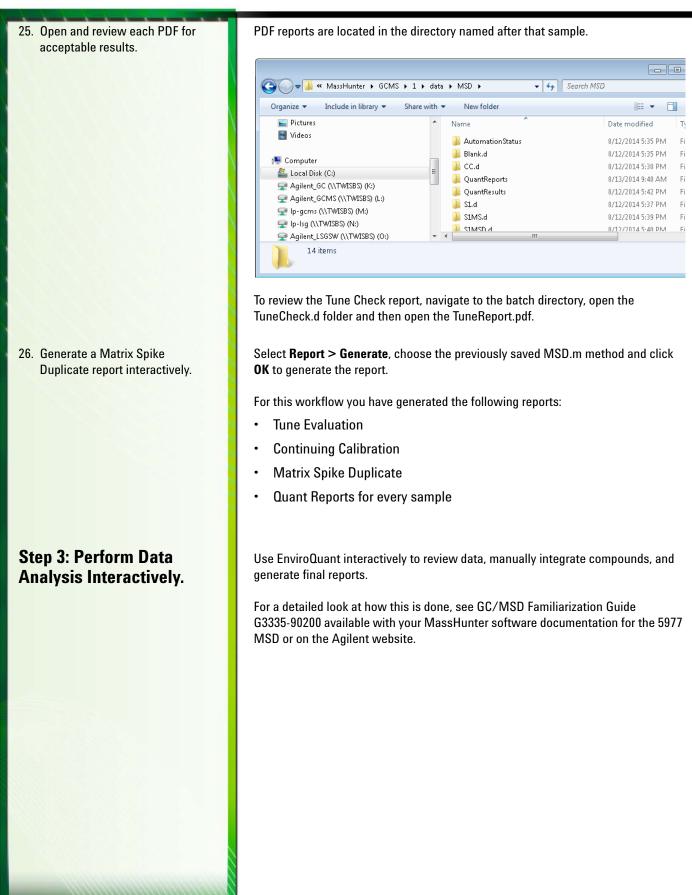






automatically generated by the sequence, select **Report > Open Report Folder**.

report(s) for that sample.





© Agilent Technologies, Inc. Printed in USA, August 2014