Agilent MassHunter EnviroQuant (EPA) Mode Using Quantitative Analysis

Workflow Guide

Agilent Technologies

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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

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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

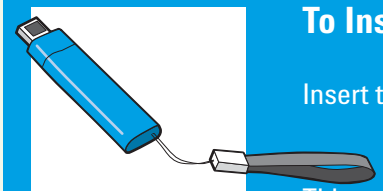
Accompanying your hardware and software is a comprehensive collection of manuals, videos, user applications, and method development tools. These are located on the:

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

To Install Your Hardware Library

Insert Disk 1 into your DVD drive and follow the prompts.

This can be installed by anyone who has authority to copy information onto the receiving computer.

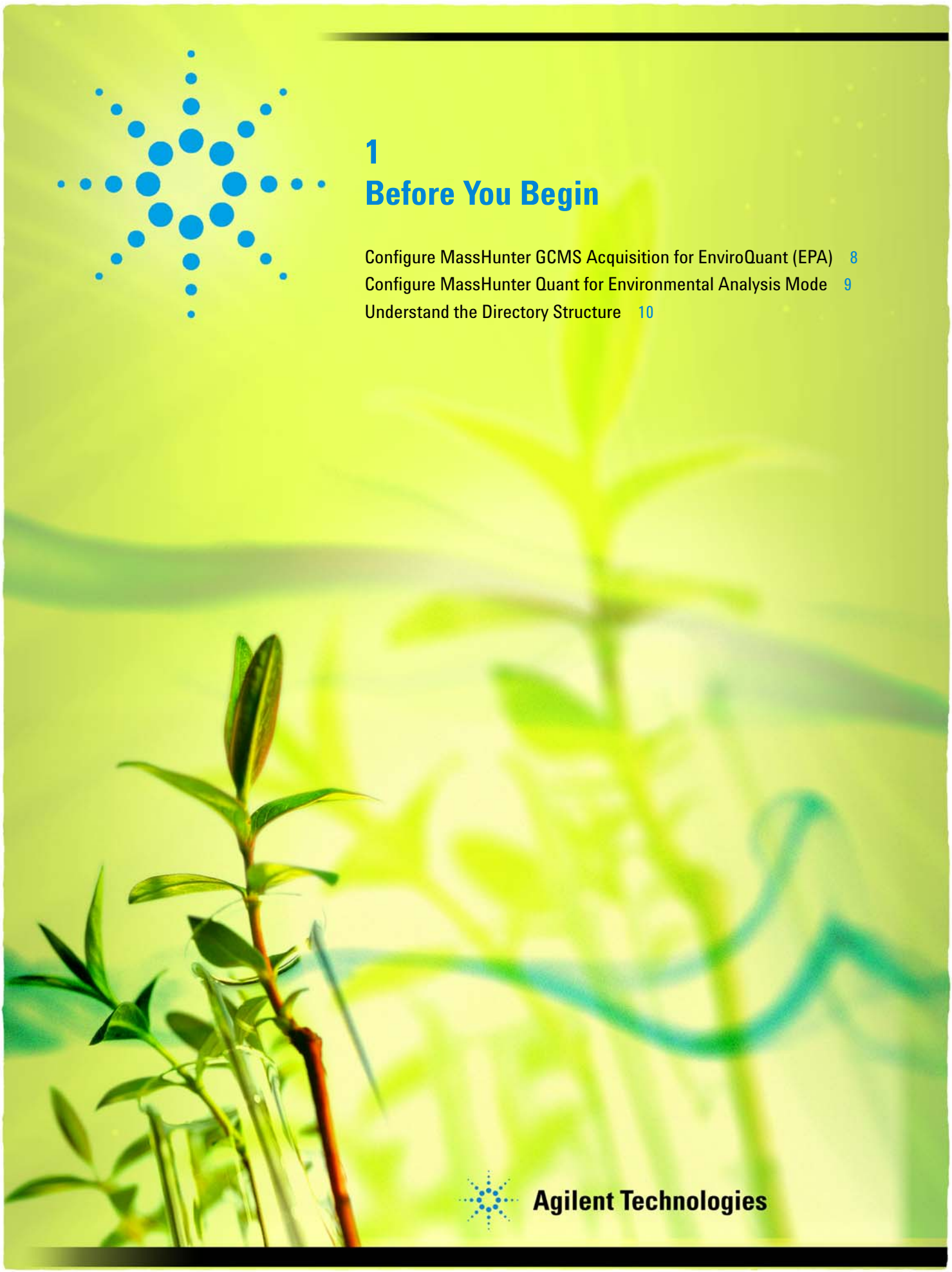


To Install Your Software Library

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

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Configure MassHunter GCMS Acquisition for EnviroQuant (EPA)

Depending on your instrument, MassHunter GCMS Acquisition and MassHunter Quantitative Analysis may be set up to run in several Workflow Modes, including:

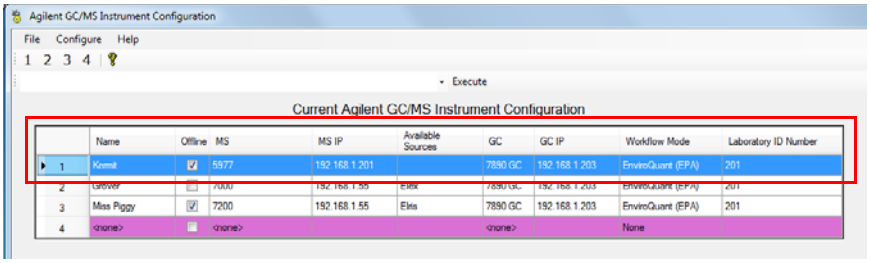
- Enhanced
- Drug Quant
- EnviroQuant (EPA)
- Aromatics in Gasoline

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.

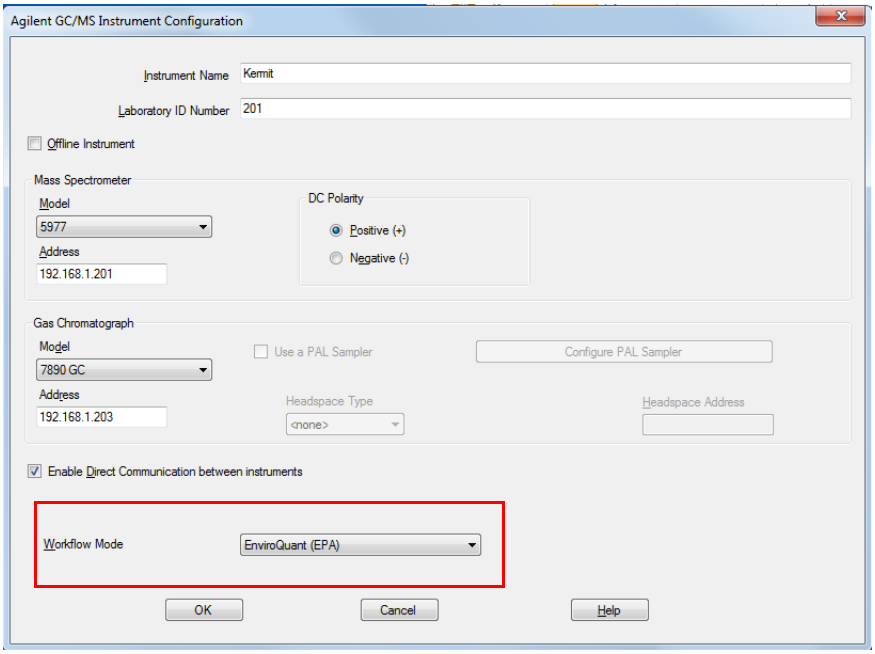
To reconfigure an existing GC/MSD instrument to work in the EnviroQuant Mode:

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.

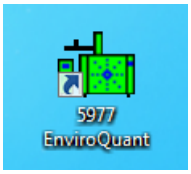


3. Select the **EnviroQuant (EPA) Workflow Mode** and click **OK** to close the dialog.



4. Click **Yes** to confirm the configuration and exit the Agilent GC/MS Configuration program.

5. Double-click the Instrument icon to launch MassHunter GCMS Acquisition.



Configure MassHunter Quant for Environmental Analysis Mode

Check for the Startup icon

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

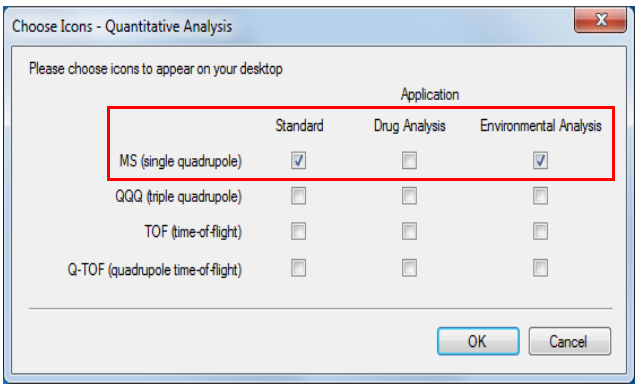
To begin MassHunter Quantitative Analysis, double-click the applicable icon.

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.

Add a startup icon

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

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.



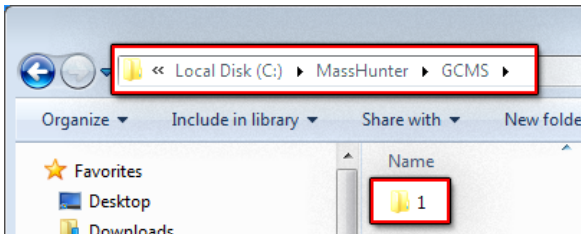
In this example, both the Standard and Environmental Analysis modes are selected for the MS, single quadrupole instrument.

Understand the Directory Structure

1. Locate the instrument directories.

You can configure and run up to four instruments with MassHunter GCMS Acquisition.

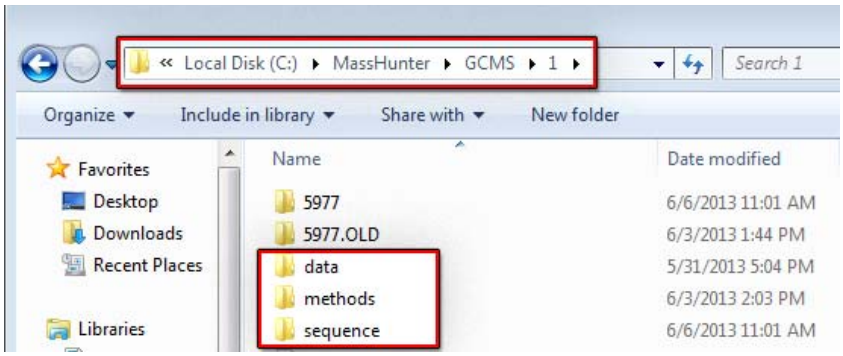
For each instrument you configure, MassHunter GCMS Acquisition will create a numbered directory corresponding to the instrument number; ***drive*:\MassHunter\GCMS\1** for example. Although drive C is shown here, Agilent supplied PCs with MassHunter factory installed store an instrument's data on the 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.

2. Review the default data, methods, and sequence directories.

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
Create the Data Acquisition Method

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Step 1: Load the data acquisition method.

1. Double-click the Instrument icon to launch MassHunter GCMS Acquisition.

2. From the Instrument Control view, select **Method > Load Method** then navigate to and select **c:\MassHunter\GCMS\1\Default.m**.

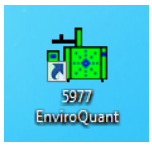
Step 2: Select the parts of the method to edit.

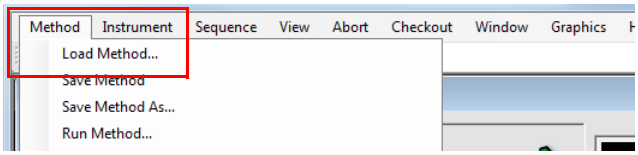
1. Select **Method > Edit Entire Method**.

2. Check each item listed.

3. Click **OK** to display the Method Information dialog.

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.

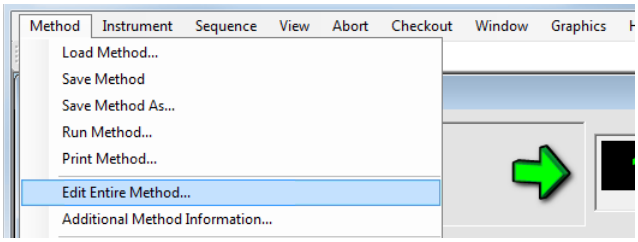


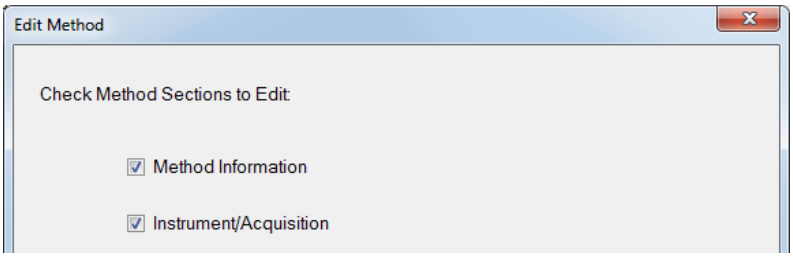


GC/MS Methods created in MSD Productivity ChemStation can be opened directly in MassHunter and used. It might be good practice to save as a new name to maintain compatibility with older systems if you are not moving every instrument to MassHunter.

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.

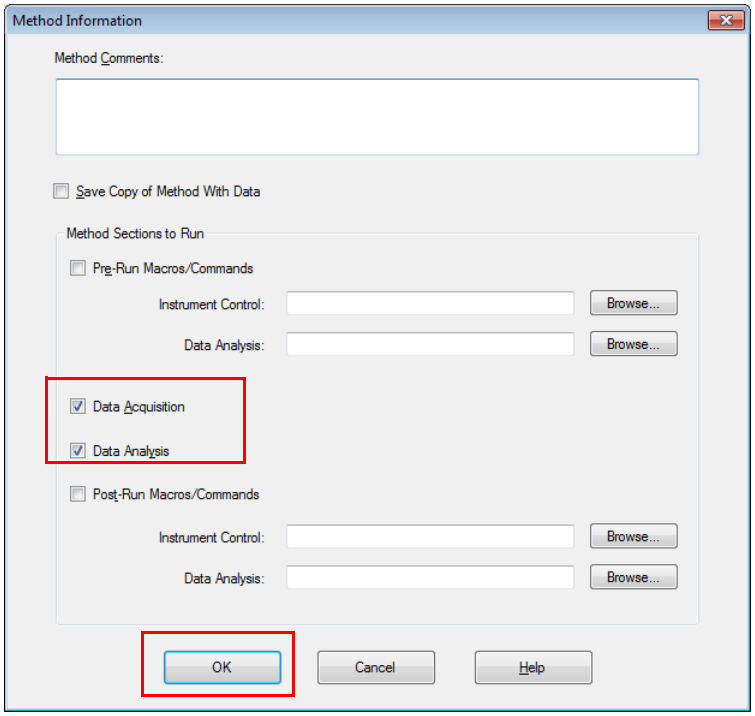
During this process we will cover the parts of a data acquisition method that are related to environmental analysis.





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.



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.

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.

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.

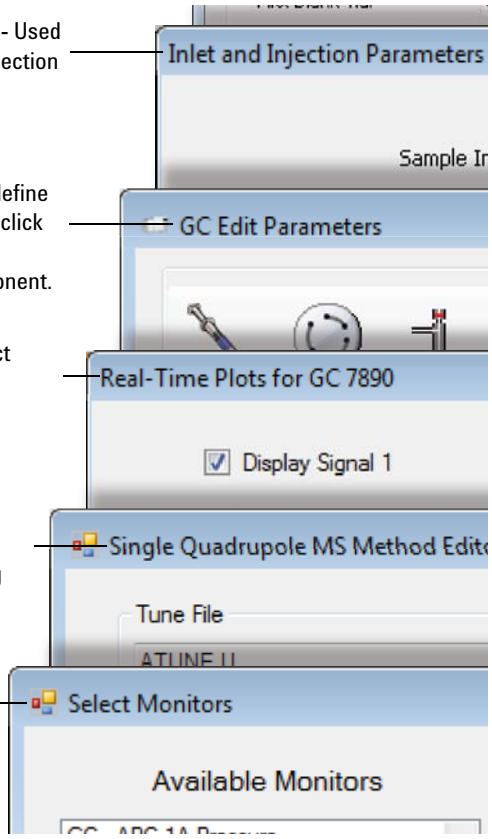
Inlet and Injection Parameters dialog - Used to select the sample type, inlet, and injection source.

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.

Real-Time Plots dialog - Used to select which signals you want displayed.

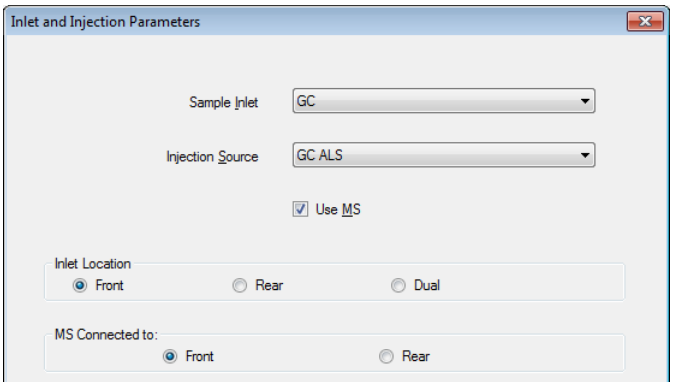
MS Method Editor dialog - Used to define the Tune File, SCAN, Real-Time Plot, and Timed Events, settings, using the single quadrupole or triple quadrupole method editor.

Monitors dialog - Used to define the MS monitors you wish to display.



Step 5: Complete the Inlet and Injection Parameters dialog.

Select the inlet, injection source, Use MS, inlet location, and MS Connected to.



Click **OK** when you are finished, and the **GC Edit Parameters** dialog is displayed.

Step 6: Complete the GC Edit Parameters dialogs.

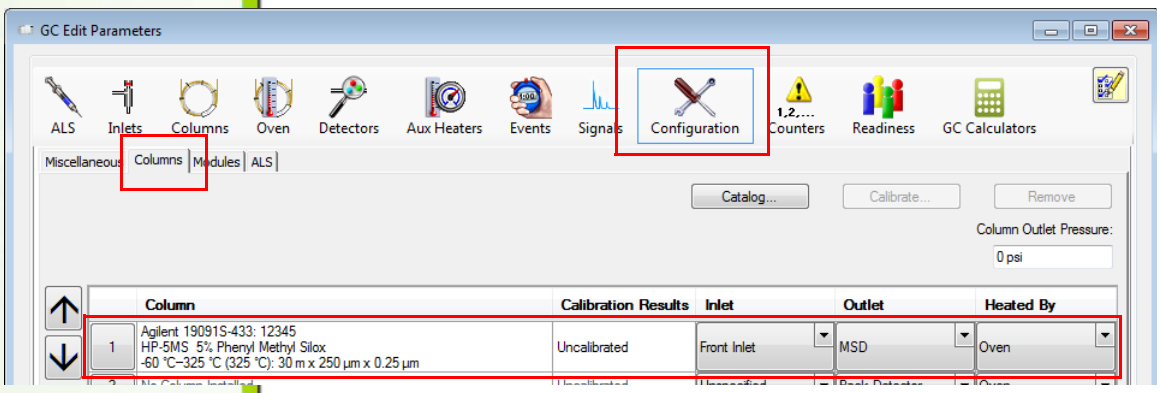
For this example we are going to complete five screens within the GC Edit Parameters dialog: **Configuration**, **Columns**, **Inlets**, **Oven**, and **Aux Heater.** The parameters entered are from the bnalist.m method previously noted.

Do NOT click OK until told to do so. Doing so will take you to the Real Time Plot dialog (shown in Step 7), and you do not want to do that until all the GC Parameters are set. Click OK only after completing all the GC Parameters; at the end of Step 6.

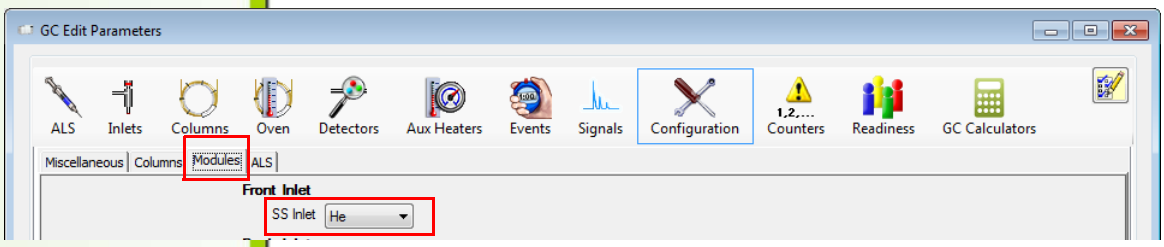
GC Configuration Settings

1. Click the **Configuration** icon, then go to the **Columns** tab and configure the column as shown here.

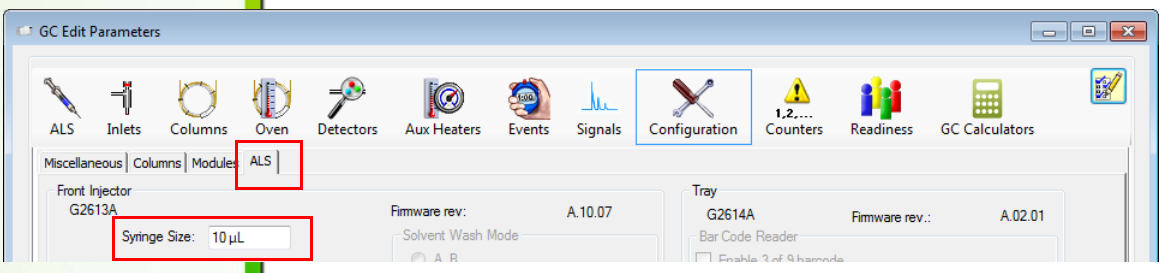
Under the **Configuration** icon, we will complete three tabs, the: **Columns**, **Modules**, and **ALS** tabs.



2. Select the **Modules** tab and set the Inlet to He.



3. Select the **ALS** tab and set the syringe size to 10 ML.

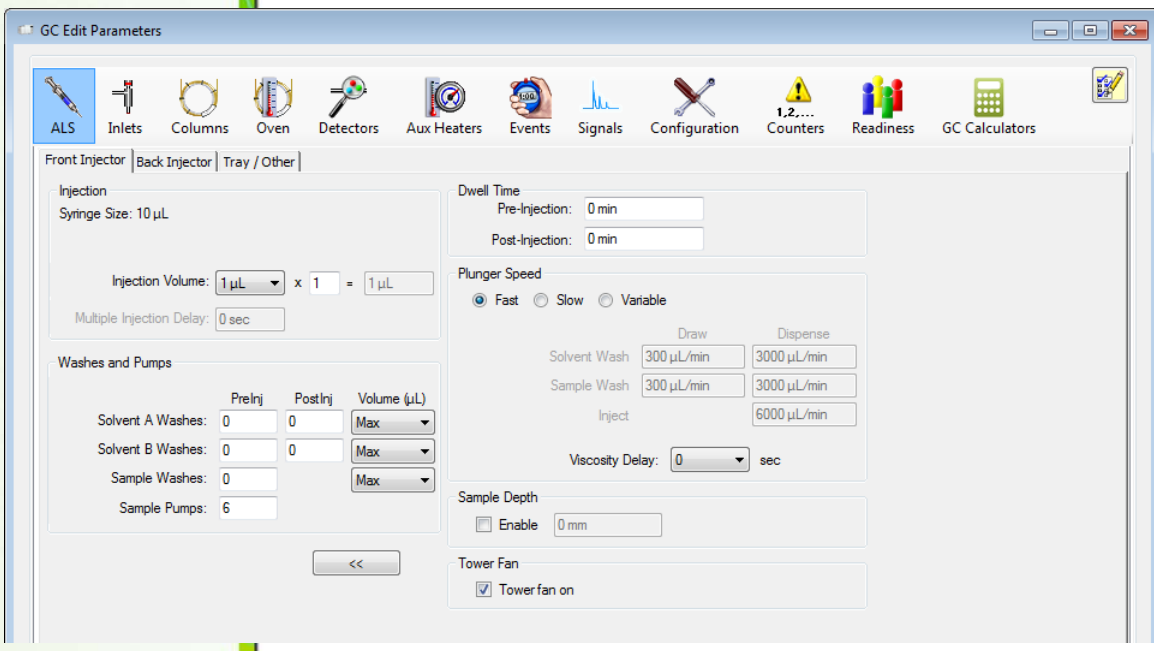


Do NOT click OK until you have finished all the GC Parameters; and you are told to do so, on page 18.

GC Method Parameters

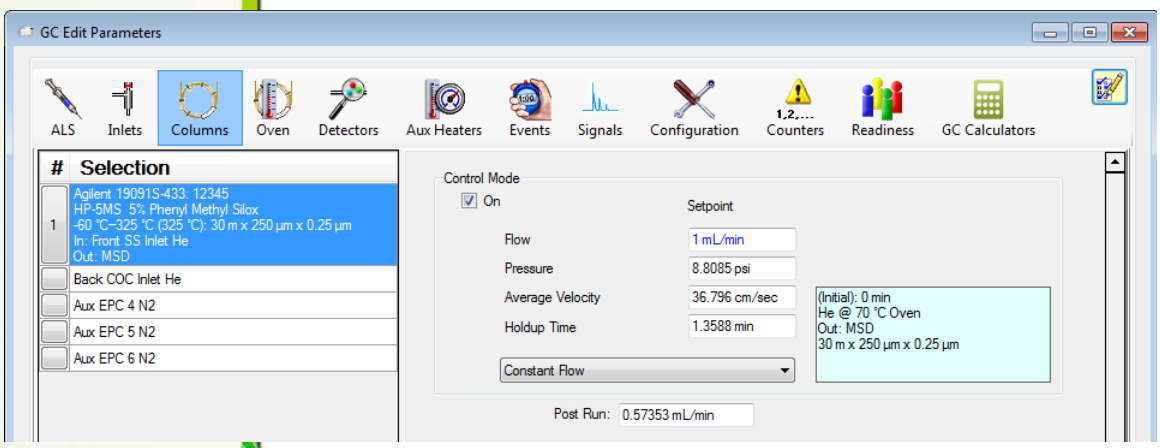
Next we will complete the settings for the **ALS, Columns**, **Inlets**, **Oven**, and **Aux Heater.**

1. Click the **ALS** icon and edit the ALS parameters appropriate to your method.

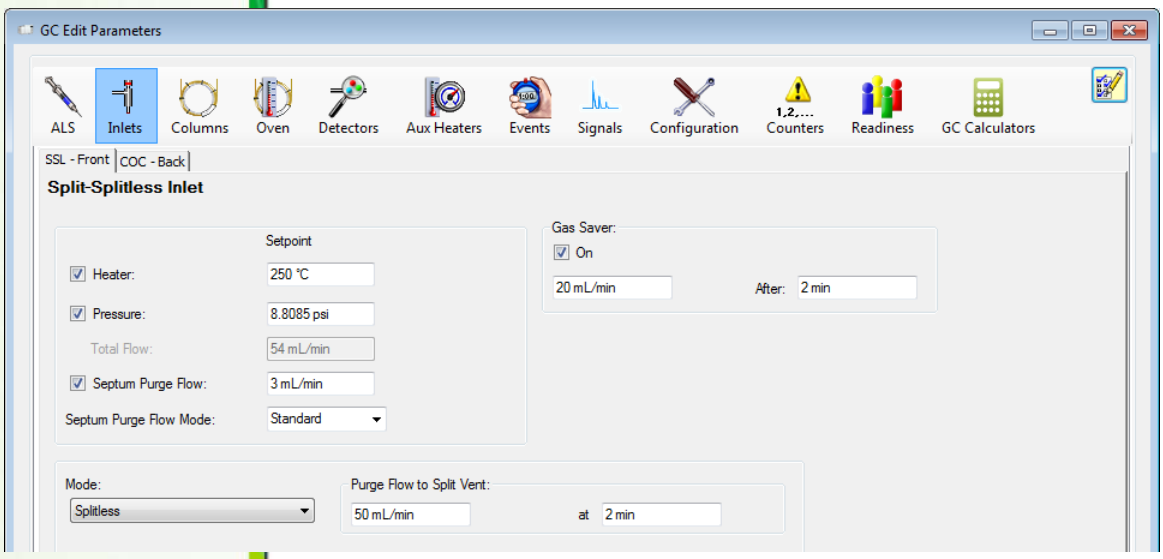


2. Click the **Columns** icon and edit the Column parameters appropriate to your method.

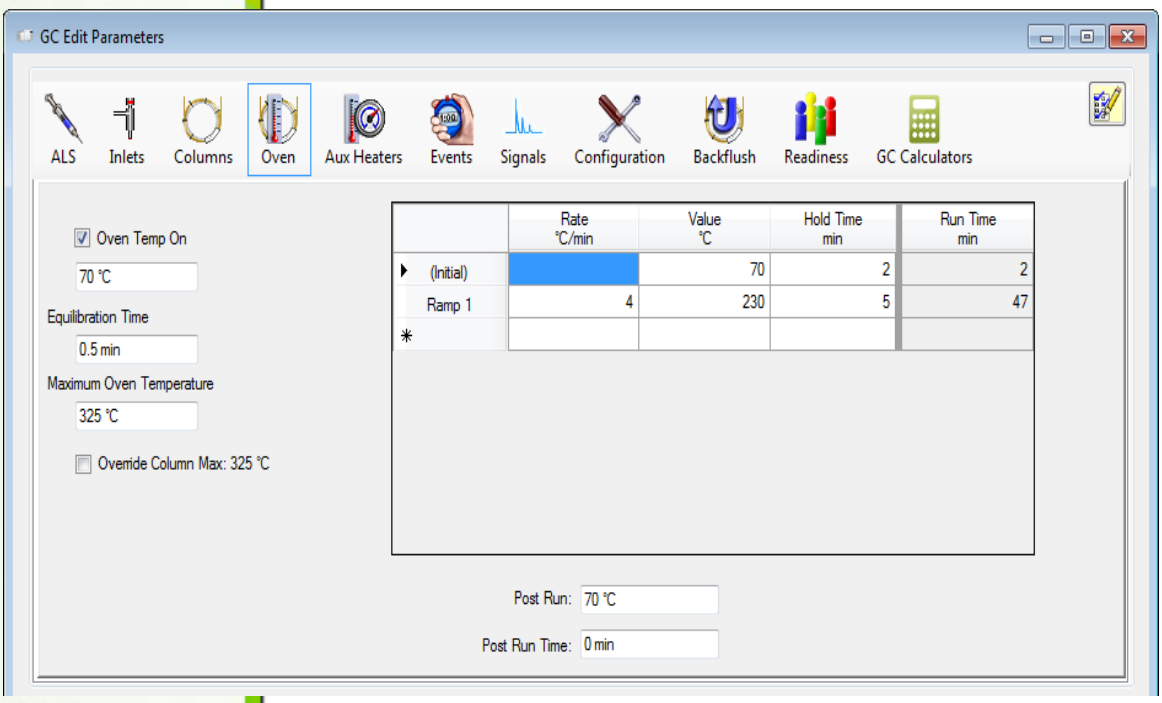
Because settings made in the **Columns** parameters dialog automatically modify Pressure and Flow parameters in the Inlet Parameters tab, and vice versa, it is a good idea to set the **Columns** settings before the **Inlets** settings. Therefore, we will enter the column settings first and the Inlet settings next.



3. Click the **Inlets** icon and edit the inlet parameters appropriate to your method.

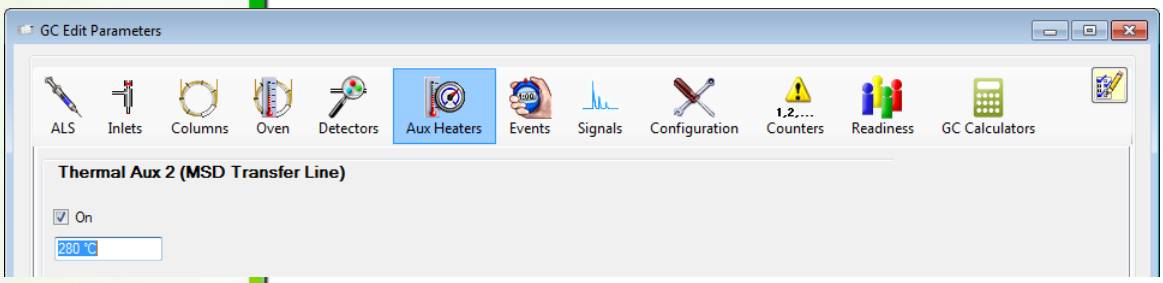


4. Click the **Oven** icon and edit the oven parameters appropriate to your method.



5. Click the **Aux Heaters** icon and edit the Aux Heaters parameters appropriate to your method, then click **OK**.

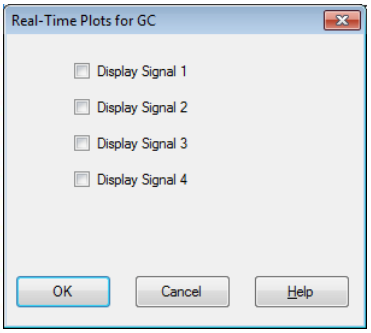
The MS Transfer line temperature is set via the GC.



When you click **OK**, the Real Time Plot dialog displays.

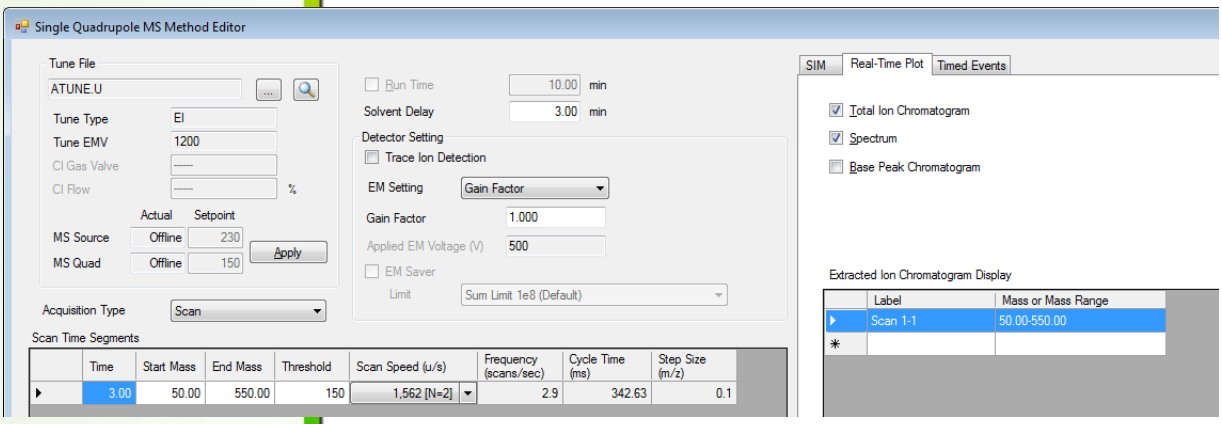
Step 7: Skip the Real Time Plot displays.

For this example, leave these entries blank, and click **OK** to continue.



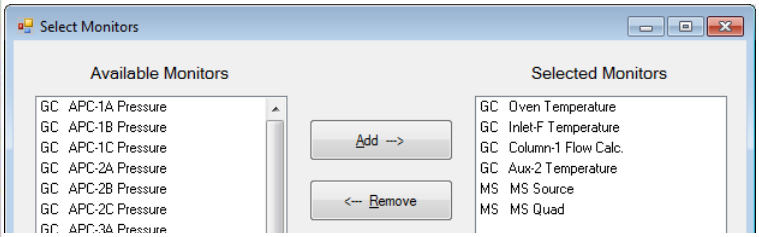
Step 8: Edit the MS Method parameters.

When done, click **OK** to continue.



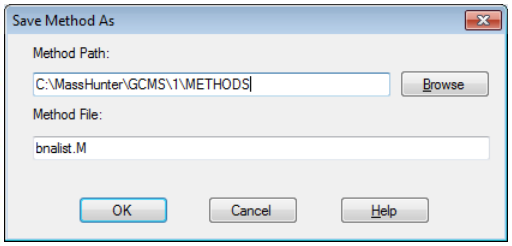
Step 9: Select the monitors.

In the Monitors dialog, select the monitors you want to see and click **OK** to continue.



Step 10: Save the method.

Save the method as C:\MassHunter\GCMS\1\METHODS\bnalist.m and click **OK** to continue. Although drive C is shown here, Agilent supplied PCs with MassHunter factory installed store an instrument's data on the D drive.



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

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Introduction

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.

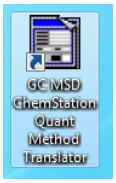
Step 1: Convert an MSD ChemStation method.

This step describes how to convert an existing MSD ChemStation method to a MassHunter Quantitative Analysis method using the **GC MSD Translator** tool.

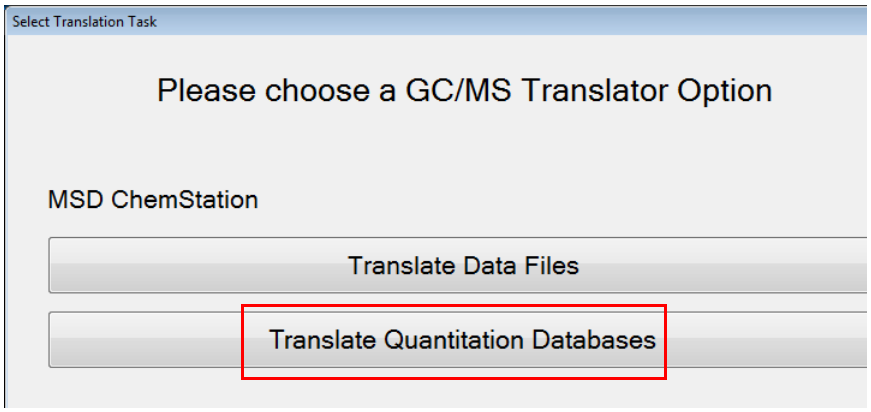
For this example we are using a sample SCAN method bnalist.m. This is an environmental demonstration method installed in **C:\envdemo\bnalist.m**. during a ChemStation installation.

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.

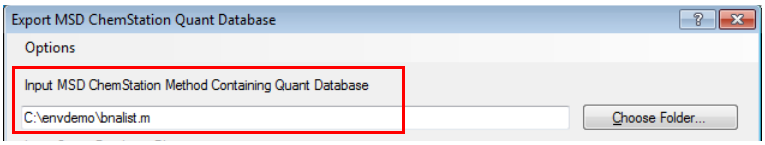
1. Start the GC MSD ChemStation Translator tool.



2. Select Translate Quantitation Databases.

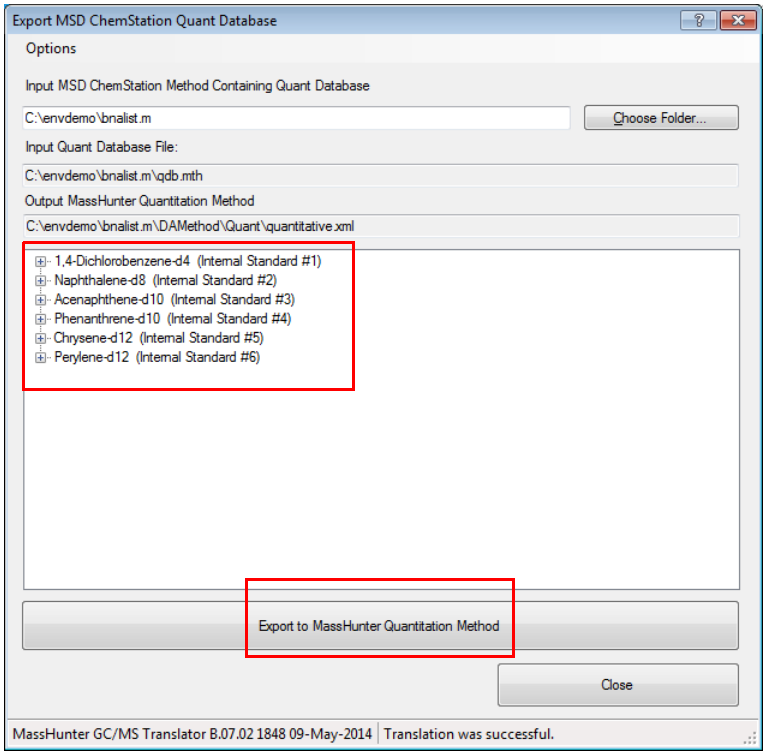


3. Select the **bnalist.m** method.



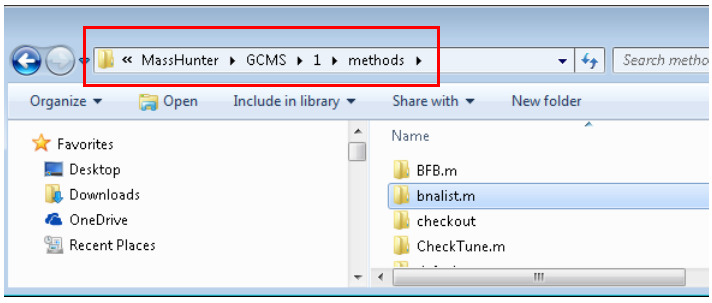
4. Click **Export to MassHunter Quantitation Method**.

The method is converted in place. When the process is complete, you will see **Translation was successful** at the bottom of the screen. The tool shows the assigned ISTDs which can be expanded to see the list of compounds assigned to an ISTD.



5. Copy the converted method to your master method directory.

Here we are using instrument 1's method directory as our master method directory.



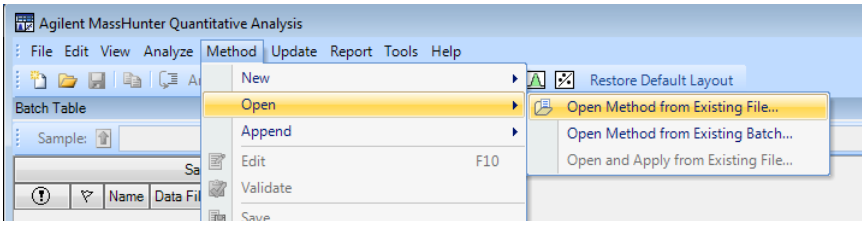
Step 2: Examine the method.

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

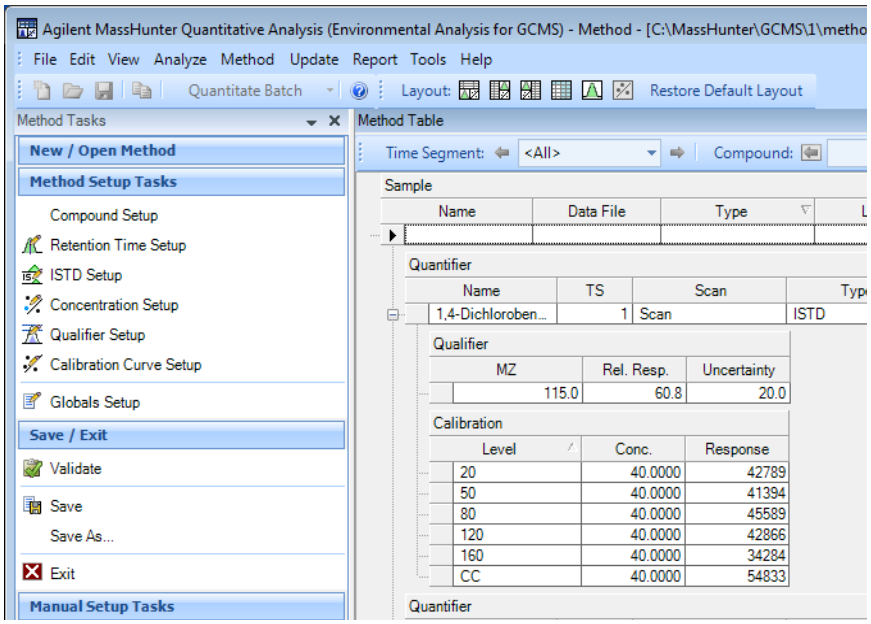
2. Select the **C:\MassHunter\GCMS\1\METHODS\bnalist.m** file that you converted in the last section and click **OK.**

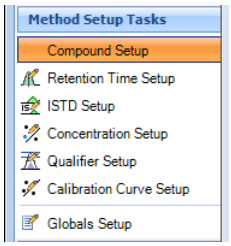
3. Select **Compound Setup**.

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.



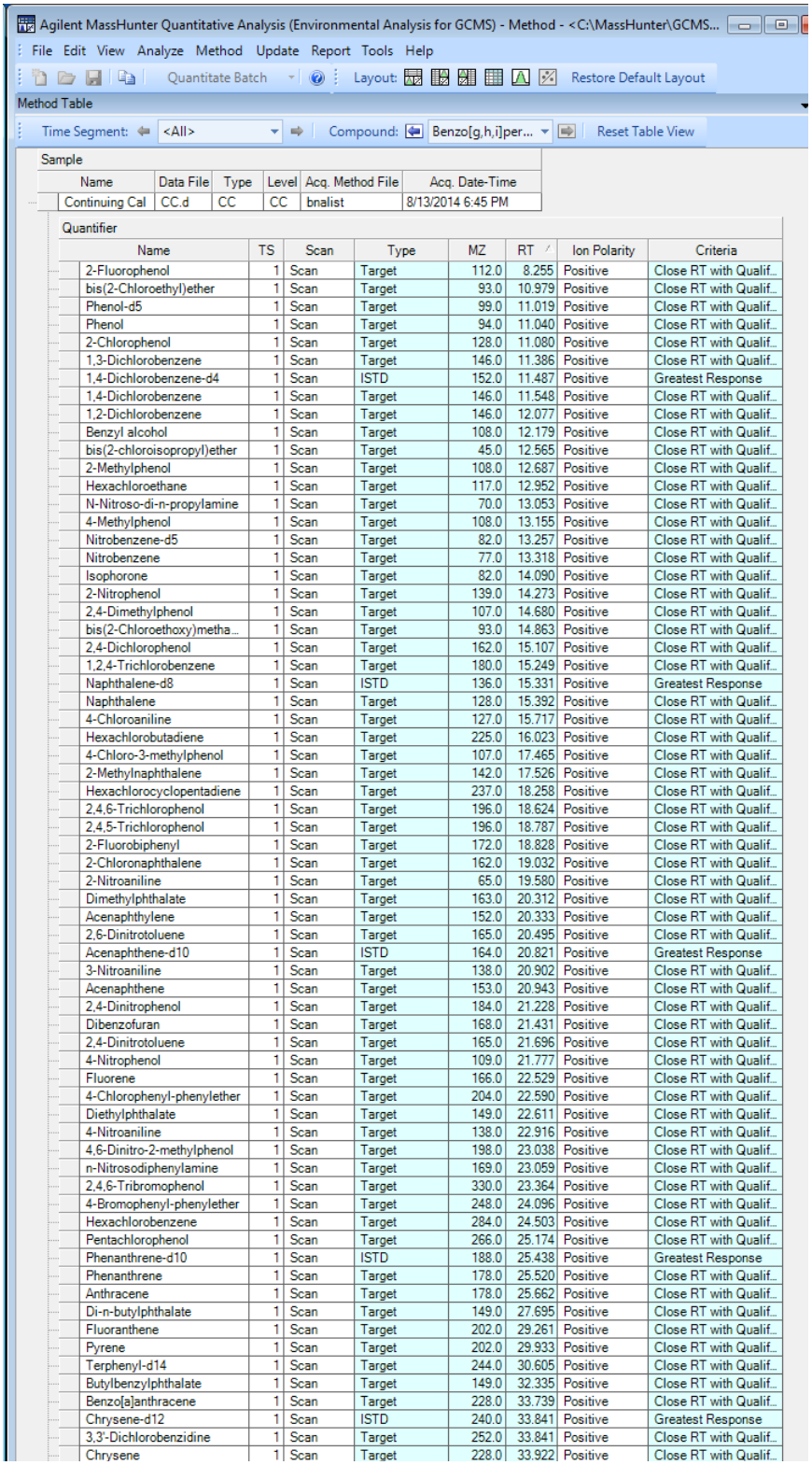
The EnviroQuant Method Editor opens with the converted method loaded. Although drive C is shown here, Agilent supplied PCs with MassHunter factory installed store an instrument's data on the D drive.





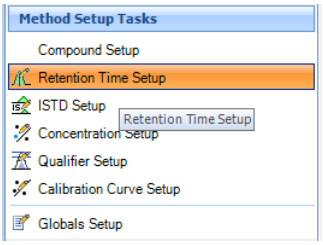
4. Review the newly imported list of compounds.

The compound parameters are displayed and may be edited. When first opened, the list is sorted by retention time. Notice that the converted method's compound **Type**, **mz**, **RT**, and identity **Criteria** are correctly converted.



Step 3: Review the Retention Times.

1. Select **Retention Time Setup**.



2. Review the converted retention times.

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.

Method Table

Time Segment: <All> Compound: Reset Table View

Sample

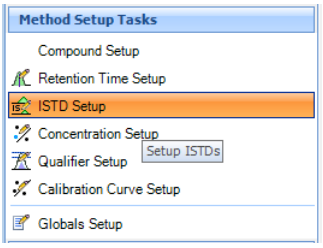
Name	Data File	Type	Level	Acq. Method File	Acq. Date-Time

Quantifier

Name	TS	Scan	Type	RT	Left RT Delta	Right RT Delta	RT Delta Units
1,4-Dichlorobenzene-d4	1	Scan	ISTD	11.487	0.500	0.500	Minutes
Naphthalene-d8	1	Scan	ISTD	15.331	0.500	0.500	Minutes
Acenaphthene-d10	1	Scan	ISTD	20.821	0.500	0.500	Minutes
Phenanthrene-d10	1	Scan	ISTD	25.438	0.500	0.500	Minutes
Chrysene-d12	1	Scan	ISTD	33.841	0.500	0.500	Minutes
Perylene-d12	1	Scan	ISTD	37.983	0.500	0.500	Minutes
2-Fluorophenol	1	Scan	Target	8.255	0.500	0.500	Minutes
bis(2-Chloroethyl)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-Chlorophenol	1	Scan	Target	11.080	0.500	0.500	Minutes
1,3-Dichlorobenzene	1	Scan	Target	11.386	0.500	0.500	Minutes
1,4-Dichlorobenzene	1	Scan	Target	11.548	0.500	0.500	Minutes
1,2-Dichlorobenzene	1	Scan	Target	12.077	0.500	0.500	Minutes
Benzyl alcohol	1	Scan	Target	12.179	0.500	0.500	Minutes
bis(2-chloroisopropyl)ether	1	Scan	Target	12.565	0.500	0.500	Minutes
2-Methylphenol	1	Scan	Target	12.687	0.500	0.500	Minutes
Hexachloroethane	1	Scan	Target	12.952	0.500	0.500	Minutes
N-Nitroso-di-n-propylamine	1	Scan	Target	13.053	0.500	0.500	Minutes
4-Methylphenol	1	Scan	Target	13.155	0.500	0.500	Minutes
Nitrobenzene-d5	1	Scan	Target	13.257	0.500	0.500	Minutes
Nitrobenzene	1	Scan	Target	13.318	0.500	0.500	Minutes
Isophorone	1	Scan	Target	14.090	0.500	0.500	Minutes
2-Nitrophenol	1	Scan	Target	14.273	0.500	0.500	Minutes
2,4-Dimethylphenol	1	Scan	Target	14.680	0.500	0.500	Minutes
bis(2-Chloroethoxy)methane	1	Scan	Target	14.863	0.500	0.500	Minutes
2,4-Dichlorophenol	1	Scan	Target	15.107	0.500	0.500	Minutes
1,2,4-Trichlorobenzene	1	Scan	Target	15.249	0.500	0.500	Minutes
Naphthalene	1	Scan	Target	15.392	0.500	0.500	Minutes
4-Chloroaniline	1	Scan	Target	15.717	0.500	0.500	Minutes
Hexachlorobutadiene	1	Scan	Target	16.023	0.500	0.500	Minutes
4-Chloro-3-methylphenol	1	Scan	Target	17.465	0.500	0.500	Minutes
2-Methylnaphthalene	1	Scan	Target	17.526	0.500	0.500	Minutes
Hexachlorocyclopentadiene	1	Scan	Target	18.258	0.500	0.500	Minutes
2,4,6-Trichlorophenol	1	Scan	Target	18.624	0.500	0.500	Minutes
2,4,5-Trichlorophenol	1	Scan	Target	18.787	0.500	0.500	Minutes
2-Fluorobiphenyl	1	Scan	Target	18.828	0.500	0.500	Minutes
2-Chloronaphthalene	1	Scan	Target	19.032	0.500	0.500	Minutes
2-Nitroaniline	1	Scan	Target	19.580	0.500	0.500	Minutes
Acenaphthylene	1	Scan	Target	20.333	0.500	0.500	Minutes
Dimethylphthalate	1	Scan	Target	20.312	0.500	0.500	Minutes

Step 4: Review the ISTDs.

1. Select **ISTD Setup**.



2. Review the converted ISTDs.

The compound parameters are displayed and may be edited. Notice that the conversion correctly identified the ISTD, the **ISTD concentration**, the **Time Reference Flag**, and the ISTD internal assignment to all target compounds.

The original ChemStation method assigned Surrogates and Matrix Spike compounds as subcategories of Target compounds. MassHunter assigns these as compound Types. This Type subcategory can't be directly converted so we will manually assign these EPA compound Types in Chapter 5, "Enter EnviroQuant Parameters in the Method".

Method Table

Time Segment: <All> Compound: Reset Table View

Sample

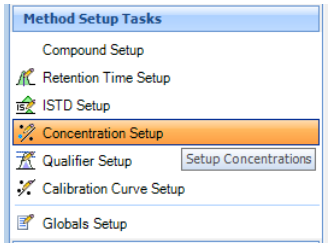
Name	Data File	Type	Level	Acq. Method File	Acq. Date-Time

Quantifier

Name	TS	Scan	Type	ISTD Compound Name	ISTD Flag	ISTD Conc.	Time Reference Fla
1,4-Dichlorobenzene-d4	1	Scan	ISTD	<None>	☑	40.0000	☑
Naphthalene-d8	1	Scan	ISTD	<None>	☑	40.0000	☑
Acenaphthene-d10	1	Scan	ISTD	<None>	☑	40.0000	☑
Phenanthrene-d10	1	Scan	ISTD	<None>	☑	40.0000	☑
Chrysene-d12	1	Scan	ISTD	<None>	☑	40.0000	☑
Perylene-d12	1	Scan	ISTD	<None>	☑	40.0000	☑
2-Fluorophenol	1	Scan	Target	1,4-Dichlorobenzene-d4	☐	-1.0000	☐
bis(2-Chloroethyl)ether	1	Scan	Target	1,4-Dichlorobenzene-d4	☐	-1.0000	☐
Phenol-d5	1	Scan	Target	1,4-Dichlorobenzene-d4	☐	-1.0000	☐
Phenol	1	Scan	Target	1,4-Dichlorobenzene-d4	☐	-1.0000	☐
2-Chlorophenol	1	Scan	Target	1,4-Dichlorobenzene-d4	☐	-1.0000	☐
1,3-Dichlorobenzene	1	Scan	Target	1,4-Dichlorobenzene-d4	☐	-1.0000	☐
1,4-Dichlorobenzene	1	Scan	Target	1,4-Dichlorobenzene-d4	☐	-1.0000	☐
1,2-Dichlorobenzene	1	Scan	Target	1,4-Dichlorobenzene-d4	☐	-1.0000	☐
Benzyl alcohol	1	Scan	Target	1,4-Dichlorobenzene-d4	☐	-1.0000	☐
bis(2-chloroisopropyl)ether	1	Scan	Target	1,4-Dichlorobenzene-d4	☐	-1.0000	☐
2-Methylphenol	1	Scan	Target	1,4-Dichlorobenzene-d4	☐	-1.0000	☐
Hexachloroethane	1	Scan	Target	1,4-Dichlorobenzene-d4	☐	-1.0000	☐
N-Nitroso-di-n-propylamine	1	Scan	Target	1,4-Dichlorobenzene-d4	☐	-1.0000	☐
4-Methylphenol	1	Scan	Target	1,4-Dichlorobenzene-d4	☐	-1.0000	☐
Nitrobenzene-d5	1	Scan	Target	Naphthalene-d8	☐	-1.0000	☐
Nitrobenzene	1	Scan	Target	Naphthalene-d8	☐	-1.0000	☐
Isophorone	1	Scan	Target	Naphthalene-d8	☐	-1.0000	☐
2-Nitrophenol	1	Scan	Target	Naphthalene-d8	☐	-1.0000	☐
2,4-Dimethylphenol	1	Scan	Target	Naphthalene-d8	☐	-1.0000	☐
bis(2-Chloroethoxy)methane	1	Scan	Target	Naphthalene-d8	☐	-1.0000	☐
2,4-Dichlorophenol	1	Scan	Target	Naphthalene-d8	☐	-1.0000	☐
1,2,4-Trichlorobenzene	1	Scan	Target	Naphthalene-d8	☐	-1.0000	☐
Naphthalene	1	Scan	Target	Naphthalene-d8	☐	-1.0000	☐
4-Chloroaniline	1	Scan	Target	Naphthalene-d8	☐	-1.0000	☐
Hexachlorobutadiene	1	Scan	Target	Naphthalene-d8	☐	-1.0000	☐
4-Chloro-3-methylphenol	1	Scan	Target	Naphthalene-d8	☐	-1.0000	☐
2-Methylnaphthalene	1	Scan	Target	Naphthalene-d8	☐	-1.0000	☐
Hexachlorocyclopentadiene	1	Scan	Target	Acenaphthene-d10	☐	-1.0000	☐
2,4,6-Trichlorophenol	1	Scan	Target	Acenaphthene-d10	☐	-1.0000	☐
2,4,5-Trichlorophenol	1	Scan	Target	Acenaphthene-d10	☐	-1.0000	☐
2-Fluorobiphenyl	1	Scan	Target	Acenaphthene-d10	☐	-1.0000	☐
2-Chloronaphthalene	1	Scan	Target	Acenaphthene-d10	☐	-1.0000	☐
2-Nitroaniline	1	Scan	Target	Acenaphthene-d10	☐	-1.0000	☐
Acenaphthylene	1	Scan	Target	Acenaphthene-d10	☐	-1.0000	☐
Dimethylphthalate	1	Scan	Target	Acenaphthene-d10	☐	-1.0000	☐

Step 5: Review the Concentrations.

1. Select **Concentration Setup.**



2. Review the converted concentrations and levels.

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 be updating these responses with new sample data in the next chapter.

Method Table

Time Segment: <All> Compound: Reset

Sample

Name	Data File	Type	Level	Acq. Method File	Acq. Date-Time

Quantifier

Name	TS	Scan	Type
1,4-Dichlorobenzene-d4	1	Scan	ISTD

Qualifier

MZ	Rel. Resp.	Uncertainty
115.0	60.8	20.0

Calibration

Level	Conc.	Response
20	40.0000	42789
50	40.0000	41394
80	40.0000	45589
120	40.0000	42866
160	40.0000	34284
CC	40.0000	54833

Quantifier

Name	TS	Scan	Type
Naphthalene-d8	1	Scan	ISTD

Qualifier

MZ	Rel. Resp.	Uncertainty
68.0	7.7	20.0

Calibration

Level	Conc.	Response
20	40.0000	164712
50	40.0000	160913
80	40.0000	177486
120	40.0000	165448
160	40.0000	132660
CC	40.0000	210879

Quantifier

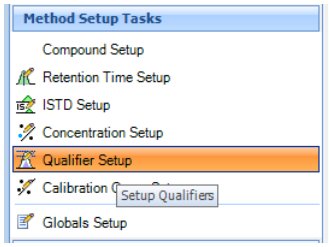
Name	TS	Scan	Type
Acenaphthene-d10	1	Scan	ISTD

Qualifier

MZ	Rel. Resp.	Uncertainty
162.0	105.4	20.0
160.0	44.0	20.0

Step 6: Review the Qualifiers.

1. Select **Qualifier Setup**.

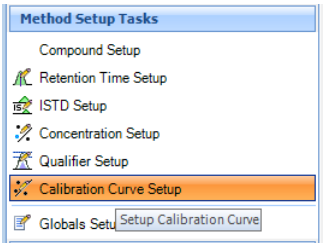


2. Review the converted qualifiers.

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.

Step 7: Review the Calibration Curve Settings.

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.

Method Table

Time Segment: <All> Compound: Reset Table View

Sample

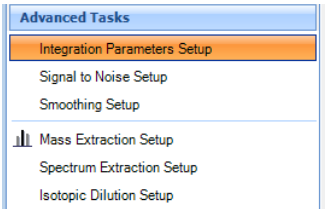
Name	Data File	Type	Level	Acq. Method File	Acq. Date-Time

Quantifier

Name	TS	Scan	Type	CF	CF Origin	CF Weight
1,4-Dichlorobenzene-d4	1	Scan	ISTD	Average of Response Factors	Ignore	None
Naphthalene-d8	1	Scan	ISTD	Average of Response Factors	Ignore	None
Acenaphthene-d10	1	Scan	ISTD	Average of Response Factors	Ignore	None
Phenanthrene-d10	1	Scan	ISTD	Average of Response Factors	Ignore	None
Chrysene-d12	1	Scan	ISTD	Average of Response Factors	Ignore	None
Perylene-d12	1	Scan	ISTD	Average of Response Factors	Ignore	None
2-Fluorophenol	1	Scan	Target	Average of Response Factors	Ignore	None
bis(2-Chloroethyl)ether	1	Scan	Target	Average of Response Factors	Ignore	None
Phenol-d5	1	Scan	Target	Average of Response Factors	Ignore	None
Phenol	1	Scan	Target	Average of Response Factors	Ignore	None
2-Chlorophenol	1	Scan	Target	Average of Response Factors	Ignore	None
1,3-Dichlorobenzene	1	Scan	Target	Average of Response Factors	Ignore	None
1,4-Dichlorobenzene	1	Scan	Target	Average of Response Factors	Ignore	None
1,2-Dichlorobenzene	1	Scan	Target	Average of Response Factors	Ignore	None
Benzyl alcohol	1	Scan	Target	Average of Response Factors	Ignore	None
bis(2-chloroisopropyl)ether	1	Scan	Target	Average of Response Factors	Ignore	None
2-Methylphenol	1	Scan	Target	Average of Response Factors	Ignore	None
Hexachloroethane	1	Scan	Target	Average of Response Factors	Ignore	None
N-Nitroso-di-n-propylamine	1	Scan	Target	Average of Response Factors	Ignore	None
4-Methylphenol	1	Scan	Target	Average of Response Factors	Ignore	None
Nitrobenzene-d5	1	Scan	Target	Average of Response Factors	Ignore	None
Nitrobenzene	1	Scan	Target	Average of Response Factors	Ignore	None
Isophorone	1	Scan	Target	Average of Response Factors	Ignore	None
2-Nitrophenol	1	Scan	Target	Average of Response Factors	Ignore	None
2,4-Dimethylphenol	1	Scan	Target	Average of Response Factors	Ignore	None
bis(2-Chloroethoxy)methane	1	Scan	Target	Average of Response Factors	Ignore	None
2,4-Dichlorophenol	1	Scan	Target	Average of Response Factors	Ignore	None
1,2,4-Trichlorobenzene	1	Scan	Target	Average of Response Factors	Ignore	None
Naphthalene	1	Scan	Target	Average of Response Factors	Ignore	None
4-Chloroaniline	1	Scan	Target	Average of Response Factors	Ignore	None
Hexachlorobutadiene	1	Scan	Target	Average of Response Factors	Ignore	None
4-Chloro-3-methylphenol	1	Scan	Target	Average of Response Factors	Ignore	None
2-Methylnaphthalene	1	Scan	Target	Average of Response Factors	Ignore	None
Hexachlorocyclopentadiene	1	Scan	Target	Average of Response Factors	Ignore	None
2,4,6-Trichlorophenol	1	Scan	Target	Average of Response Factors	Ignore	None
2,4,5-Trichlorophenol	1	Scan	Target	Average of Response Factors	Ignore	None
2-Fluorobiphenyl	1	Scan	Target	Average of Response Factors	Ignore	None
2-Chloronaphthalene	1	Scan	Target	Average of Response Factors	Ignore	None
2-Nitroaniline	1	Scan	Target	Average of Response Factors	Ignore	None
Acenaphthylene	1	Scan	Target	Average of Response Factors	Ignore	None
Dimethylphthalate	1	Scan	Target	Average of Response Factors	Ignore	None
2,6-Dinitrotoluene	1	Scan	Target	Average of Response Factors	Ignore	None

Step 8: Set up the Integrator.

1. In the **Advanced Tasks** area, select **Integration Parameters Setup**.

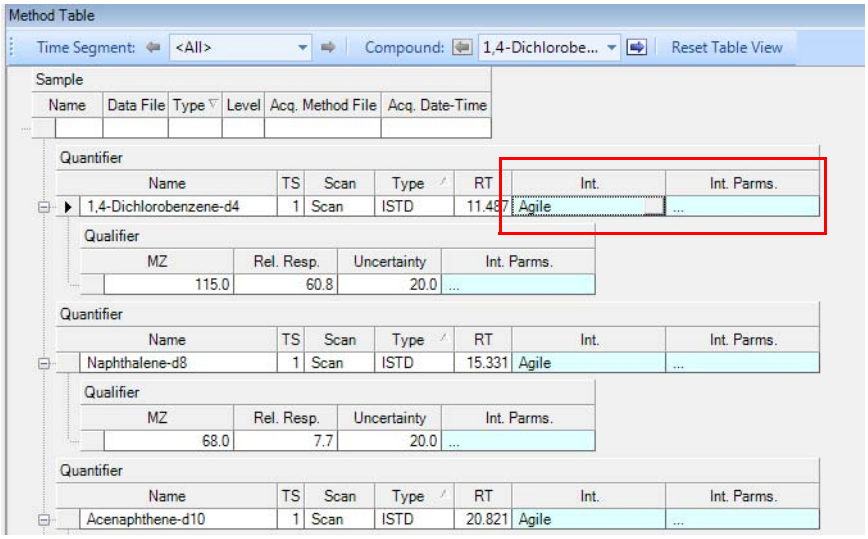


2. Review the integrator used.

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

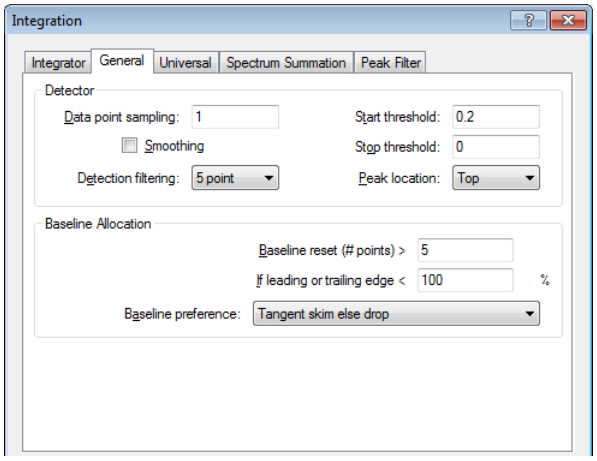
3. To change to the type of integrator used in the ChemStation method, select **General** for the first quantifier then select **Fill Down** from the context menu.

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



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.

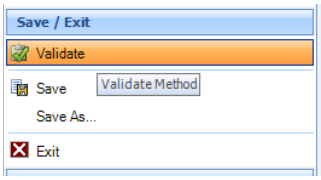
By default, the qualifiers are assigned the same integration parameters as the quantifier but this can be overridden by selecting the **Int Params** for the qualifiers.

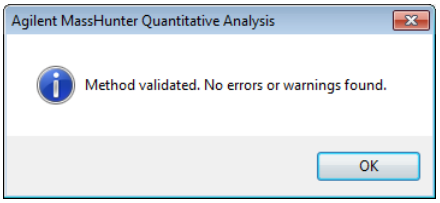


Step 9: Save the method.

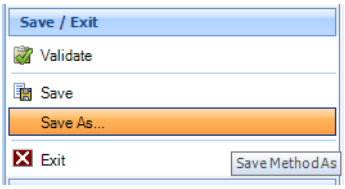
1. In the **Save/Exit** area, select **Validate.**

There should be no errors. If there is an error, click on the error and you will be directed to where you can change the settings.



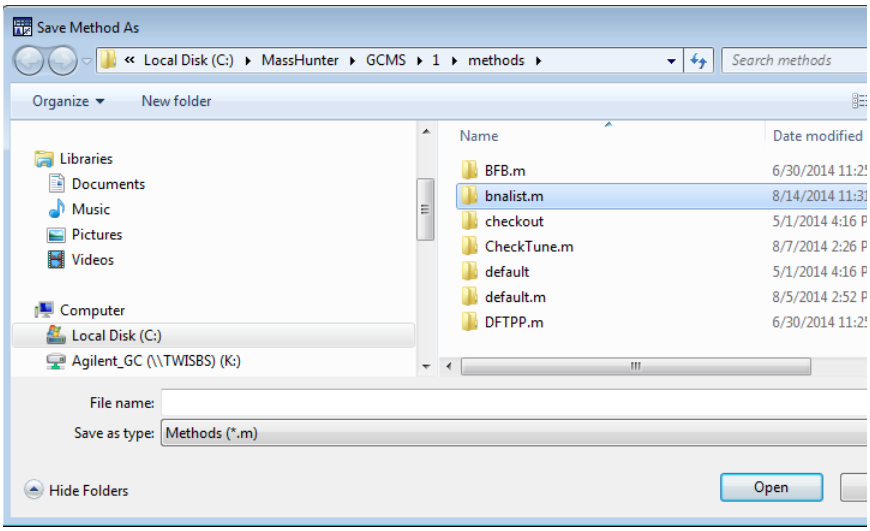


2. Select **Save As**.



3. Navigate to the MassHunter\GCMS\1\methods \ directory and double-click the **bnalist.m**. This is then added to the bnalist unified method where the data acquisition method was saved.

Although drive C is shown here, Agilent supplied PCs with MassHunter factory installed store an instrument's data on the D drive.



4. Exit **[F11]** the method editor.

You are returned to Batch table view where the batch table is empty.

This completes the creation of the basic quantitation method portion of the workflow.

Step 10: Run Samples.

Before you can complete the EPA portion of the Quantitation method you must run required samples as described in Chapter 4, "Run Samples for Quant Method Creation".

4
Run Samples for Quant Method Creation

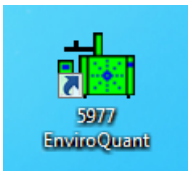
Agilent Technologies

Introduction

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.

Step 1: Create a batch.

1. Double-click the Instrument icon to launch MassHunter GCMS Acquisition.



2. Load a default sequence.

3. Select **Sequence > Edit Sequence,** complete the entries similar to those shown here, then click **OK**.

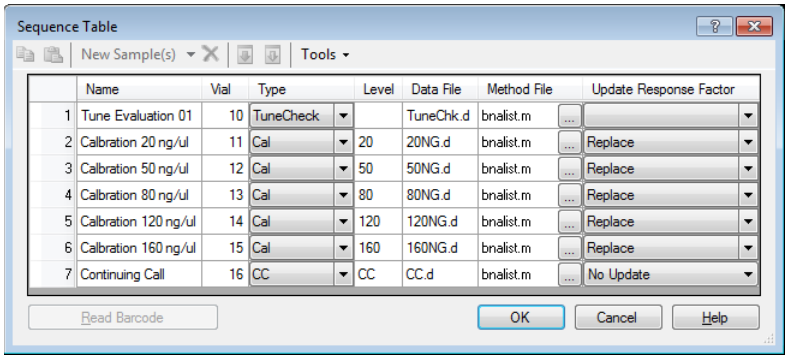
The first sample in this sequence should contain compounds that are representative of what will be analyzed (e.g., Pentachlorophenol, DFTPP, Benzidine, and DDT for EPA method 8270).

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.

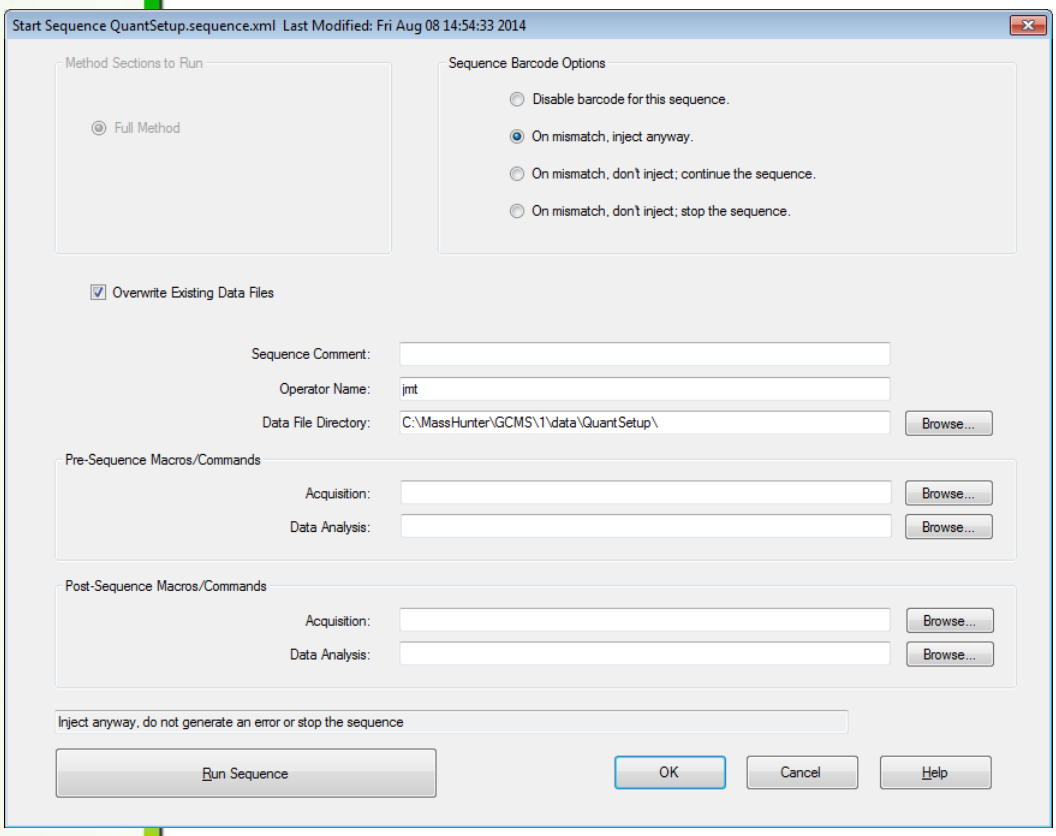
The Continuing Cal sample's compound responses will be manually entered into the method to initialize future CC's.



4. Select **Sequence > Save Sequence As**... and save the sequence as **QuantSetup.**

5. Select **Sequence > Run Sequence**, and complete the dialog as shown here.

.



6. Click **Run Sequence** when finished.

MassHunter Data Acquisition will automatically create a batch containing these data files and save it in the MassHunter folder specified in the Sequence table. In this case: **C:\MassHunter\GCMS\1\data\QuantSetup**.

The method's response factors for the 5 CAL samples are automatically updated.

Step 2: Complete the Tune Evaluation criteria.

The Tune Evaluation Tool in MassHunter EnviroQuant makes it easy to enter EPA required analyzer tune and GC performance criteria. Once the criteria are entered and saved (as *tunevaluation.xml*), they become part of the unified method.

In practice, the tune evaluation sample is processed as the first sample in the batch. During processing, if the tune evaluation sample fails to comply with the criteria specified in the Tune Evaluation method (which is one part of the unified method), the sequence will automatically stop to prevent the remaining samples from running on an instrument that requires tuning.

The following describes how to build the tune evaluation method (*tunevaluation.xml*). The example shown here includes the criteria for **EPA method 8270**. Entries for other EPA methods are entered in a similar manner. The last step in the process describes how to set up a Reference Library.

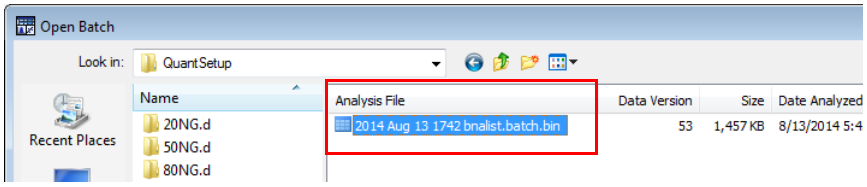
The compounds that will be included are:

- Pentachlorophenol
- DFTPP
- Benzidine
- DDT

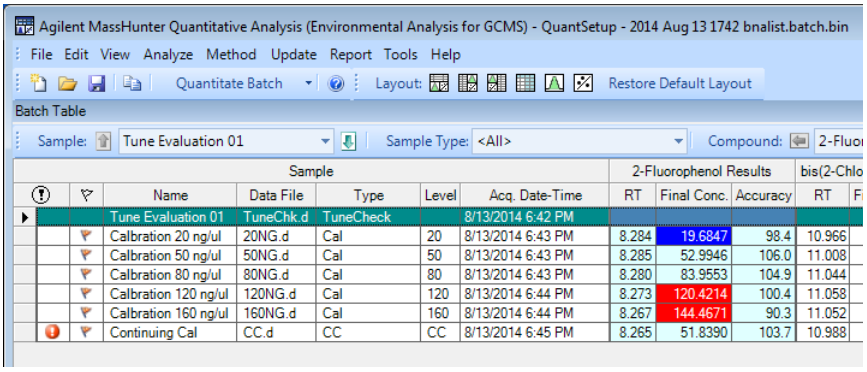
1. Start MassHunter EnviroQuant.

2. Select **File > Open Batch**, and open the timestamped bnalist.bin batch that was just created.

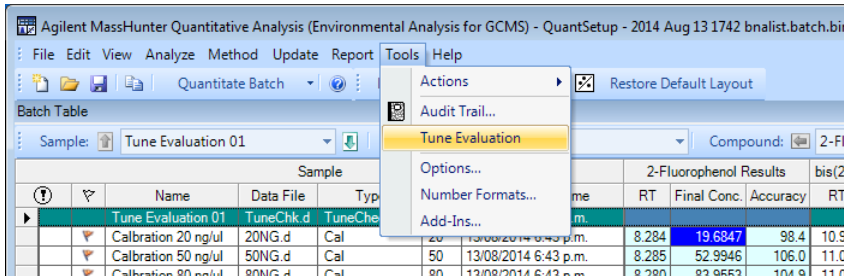
Navigate to the **C:\MassHunter\GCMS\1\data\QuantSetup folder.**



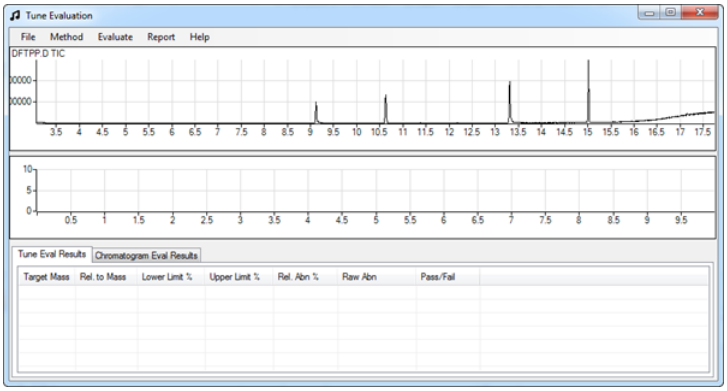
3. Highlight the **Tune Evaluation 01** data file.



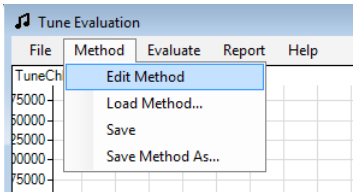
4. Select **Tools > Tune Evaluation**.



The Tune Evaluation dialog opens.

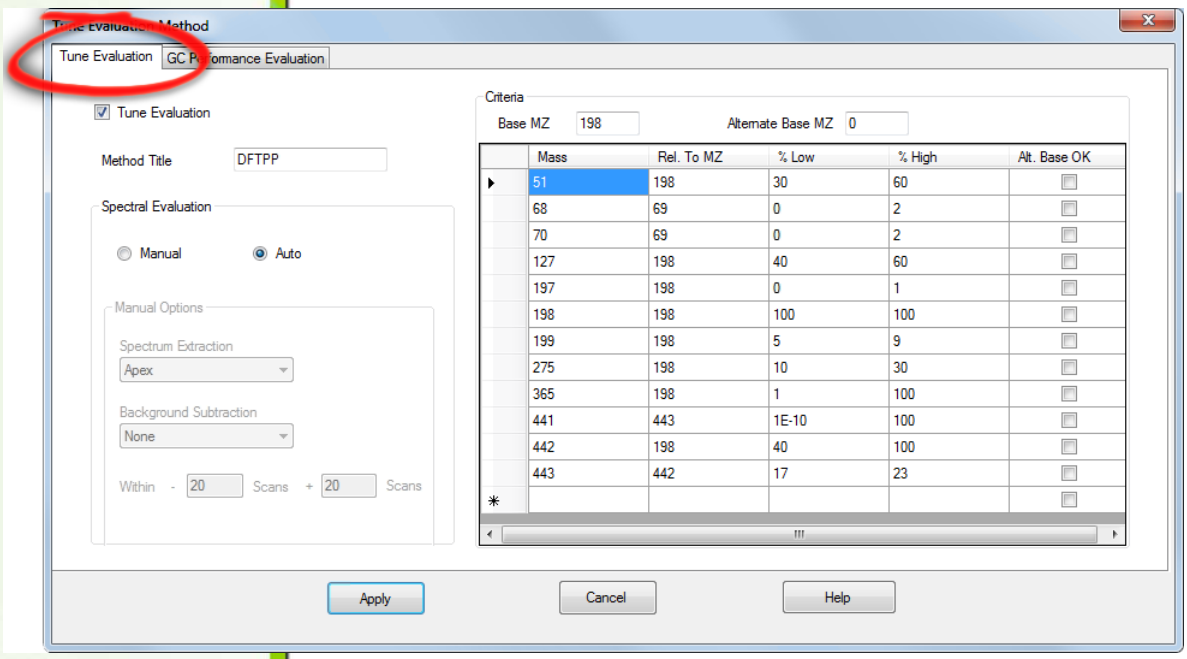


5. Select **Method > Edit Method**.



6. Complete the Tune Evaluation.

For EPA method 8270 you would complete this screen similar to the one shown here.



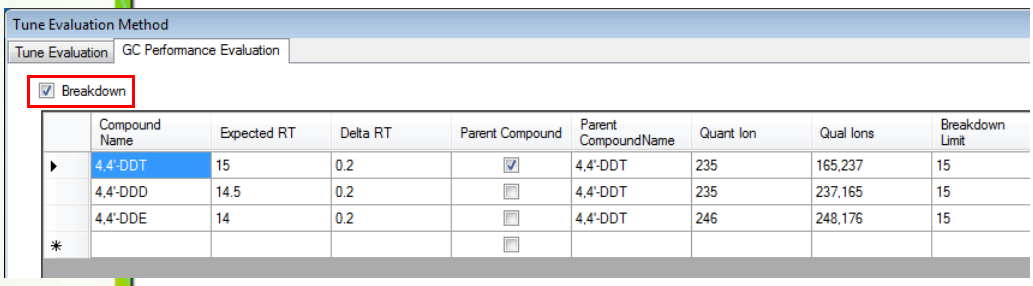
When you select Auto, as shown in this example, the system will use all of the criteria specified here to try and find the best fit.

Step 3: Complete the GC Performance Evaluation criteria.

For EPA method 8270, we will enter degradation of DDT, DDD, and DDE, and tailing for Pentachlorophenol and Benzidine. Notice that here we are finding the compounds by mass, however, the evaluation is done on the total ion chromatogram for the method.

1. Click the **GC Performance Evaluation** tab, select **Breakdown** to enable the test and enter the Breakdown parameters.

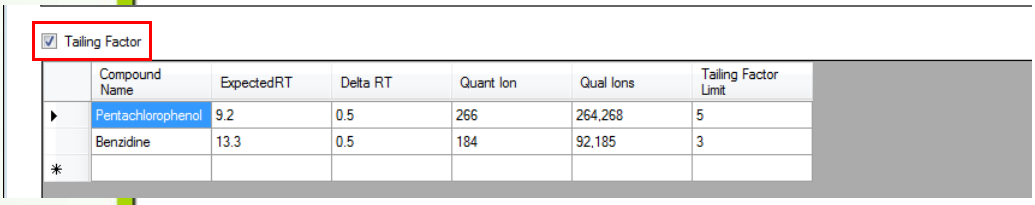
Enter the parameters for the degradation of DDT, DDD, and DDE as shown here.



Compound Name	Expected RT	Delta RT	Parent Compound	Parent CompoundName	Quant Ion	Qual Ions	Breakdown Limit
4,4'-DDT	15	0.2	☑	4,4'-DDT	235	165,237	15
4,4'-DDD	14.5	0.2	☐	4,4'-DDT	235	237,165	15
4,4'-DDE	14	0.2	☐	4,4'-DDT	246	248,176	15
			☐				

2. Select **Tailing Factor** to enable the test and enter the Tailing Factor parameters.

Enter tailing factor parameters for Pentachlorophenol and Benzidine.



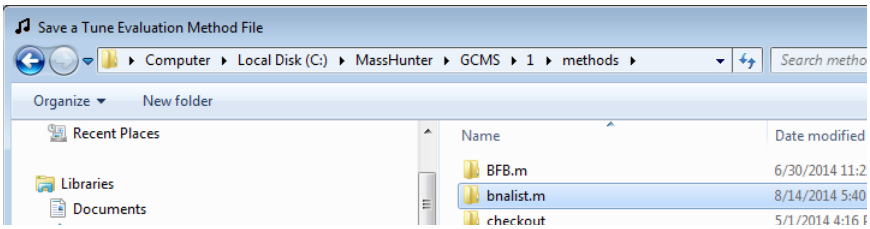
Compound Name	ExpectedRT	Delta RT	Quant Ion	Qual Ions	Tailing Factor Limit
Pentachlorophenol	9.2	0.5	266	264,268	5
Benzidine	13.3	0.5	184	92,185	3

3. **Apply** the criteria.

Click **Apply**, when ready, and the results are displayed online. See "Step 4: Review the tune evaluation results." on page 39.

4. Select **Method > Save Method As**, and save this to: **MassHunter\GCMS\1\Methods\bnalist.m.**

MassHunter saves this as the **tunevaluation.xml** method in the DAMethod\Quant\ sub-directory of the bnalist.m method.



5. Reply **Yes** when asked to overwrite the existing method.

Once the criteria are entered and saved, they become part of the bnalist method which now contains method parameters for data acquisition, quantitative analysis, and Tune Evaluation.

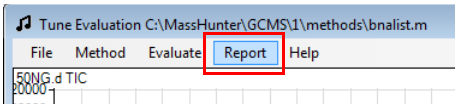
Step 4: Review the tune evaluation results.

Tune evaluation results can be viewed interactively in the Tune Evaluation Tool, shown below, or they can be generated as one of the printed reports for the batch.

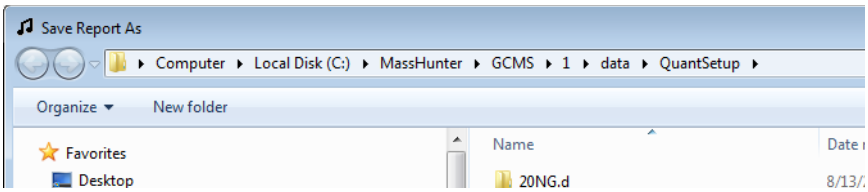
Online Results

Tune Evaluation PDF Report

1. Click **Report** in Tune Evaluation.

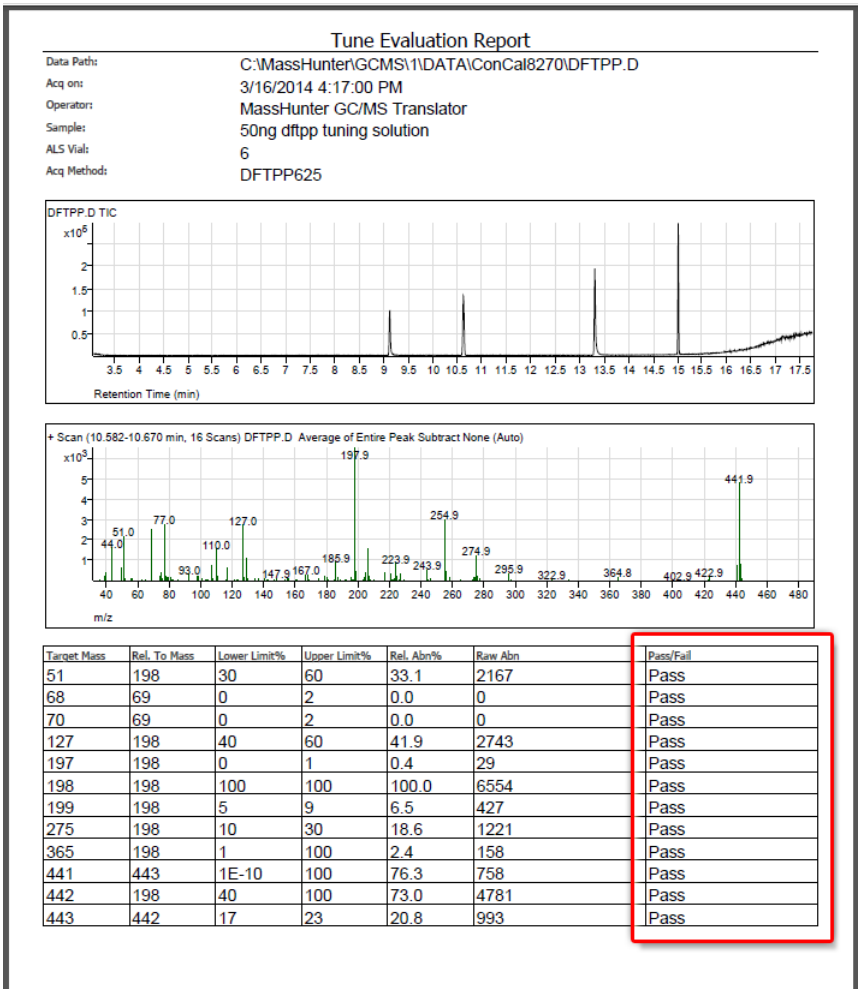


2. Accept the default location and name for the PDF report.



3. Review the Pass/Fail condition for the first compound.

The PDF is generated and opened in Acrobat.



Tune Evaluation Report

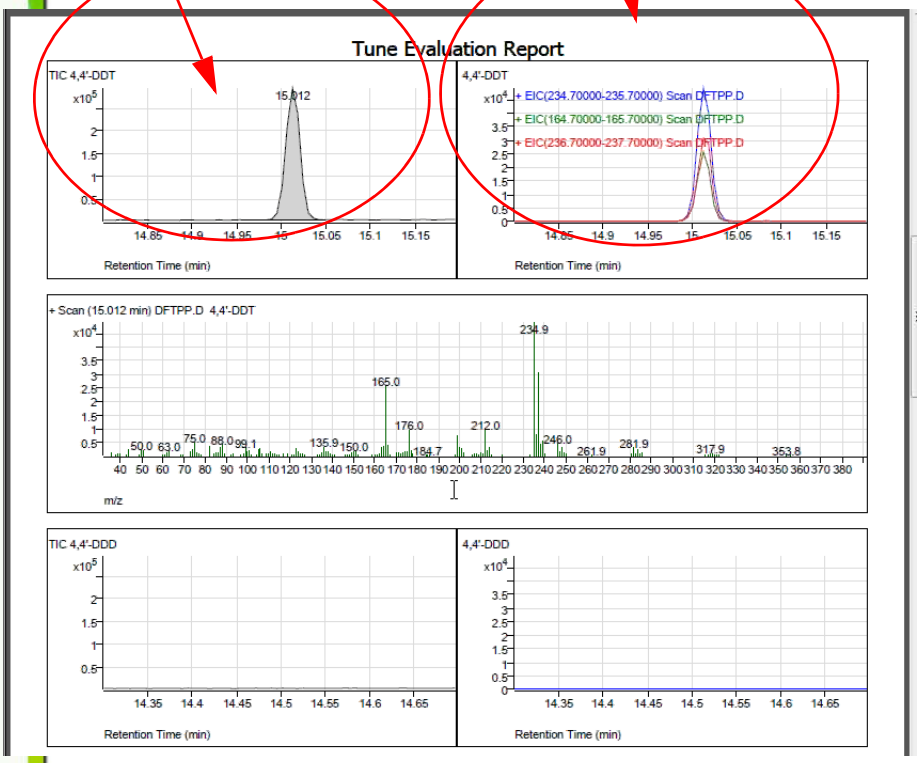
Data Path:	C:\MassHunter\GCMS\1\DATA\ConCal8270\DFTPP.D
Acq on:	3/16/2014 4:17:00 PM
Operator:	MassHunter GC/MS Translator
Sample:	50ng dftpp tuning solution
ALS Vial:	6
Acq Method:	DFTPP625

Target Mass	Rel. To Mass	Lower Limit%	Upper Limit%	Rel. Abn%	Raw Abn	Pass/Fail
51	198	30	60	33.1	2167	Pass
68	69	0	2	0.0	0	Pass
70	69	0	2	0.0	0	Pass
127	198	40	60	41.9	2743	Pass
197	198	0	1	0.4	29	Pass
198	198	100	100	100.0	6554	Pass
199	198	5	9	6.5	427	Pass
275	198	10	30	18.6	1221	Pass
365	198	1	100	2.4	158	Pass
441	443	1E-10	100	76.3	758	Pass
442	198	40	100	73.0	4781	Pass
443	442	17	23	20.8	993	Pass

4. Notice MassHunter locates the compound by mass, and also displays the TIC.

Compound TIC

Located compound by Mass

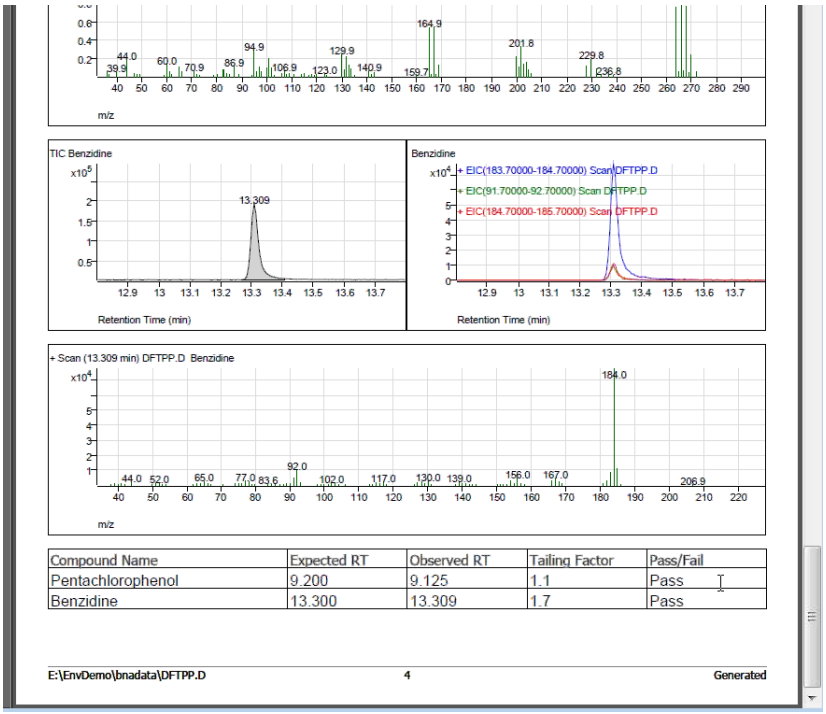


m/z

Compound Name	Expected RT	Observed RT	TIC Area	Breakdown %	Pass/Fail
4,4'-DDT	15.000	15.012	325703	0.0	Pass
4,4'-DDD	14.500	0.000	0		
4,4'-DDE	14.000	0.000	0		

5. Review the Trailing Factor.

On the next page you can see the tailing factor.



Compound Name	Expected RT	Observed RT	Tailing Factor	Pass/Fail
Pentachlorophenol	9.200	9.125	1.1	Pass
Benzidine	13.300	13.309	1.7	Pass

E:\EnvDemo\bnadata\DFTPP.D 4 Generated

In the future, each time you run a tune check sample from a sequence with this bnalist method this evaluation will be performed in MassHunter EnviroQuant. A tune evaluation report will be saved as TuneReport.pdf in the data file directory (here TuneChk.d). If the analyzed results do not pass the criteria listed here, the sequenced will be stopped.

Step 5: Create a Reference library.

1. In the Batch table select the **Calibration 80 ng** sample.

2. Enter the method editor **[F10]**, and select **Method > Setup Reference Library**.

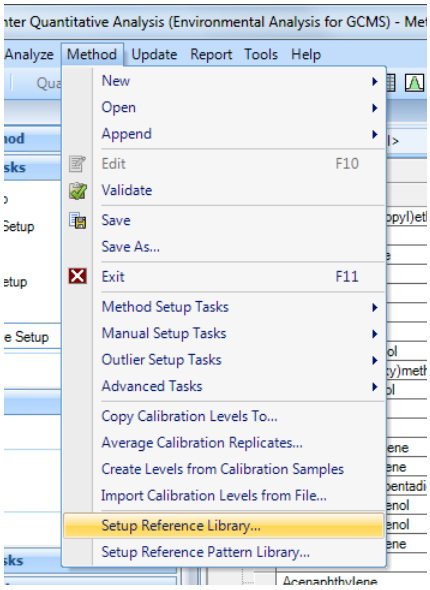
3. Select **Obtain reference spectra from sample**.

4. Click **OK** to save the library to the selected folder.

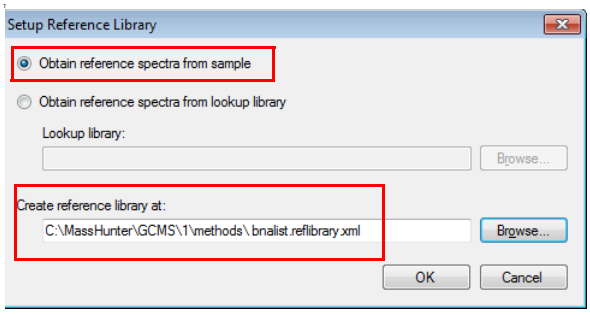
Using MassHunter's Reference Library allows you to easily compare your acquired sample's spectral data to the spectral data stored in a reference library.

The library match score is clearly displayed in the compound information window, showing the degree to which the sample compound data matches the library entries.

A representative clean sample containing all the compounds in the method is required to create the library.

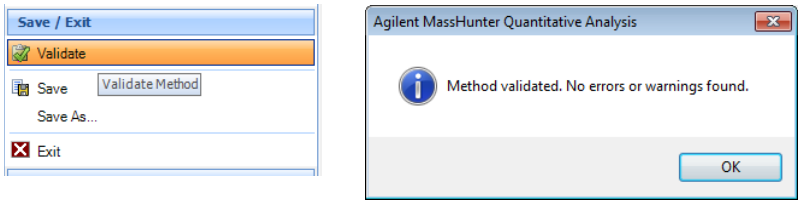


This is the Calibration 80 ng sample that we selected in the batch table before entering the method editor.



Save the library in a location accessible to future bnalist methods.

5. Validate the method. There should be no errors.

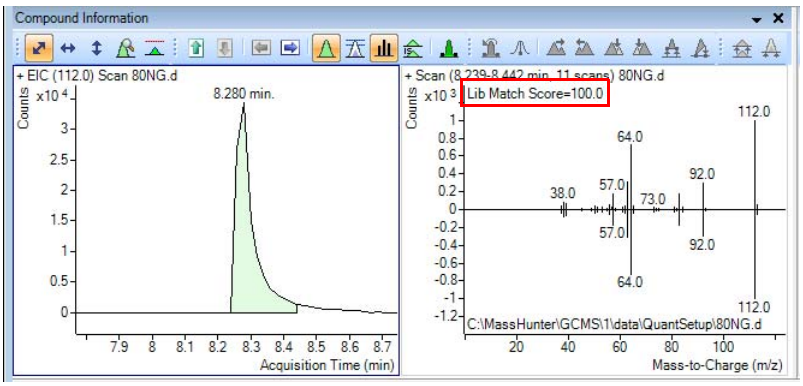


6. Exit the method editor **[F11]**.

You are returned to Batch table view.

7. Examine the scan data in the Compound Information window for various compounds.

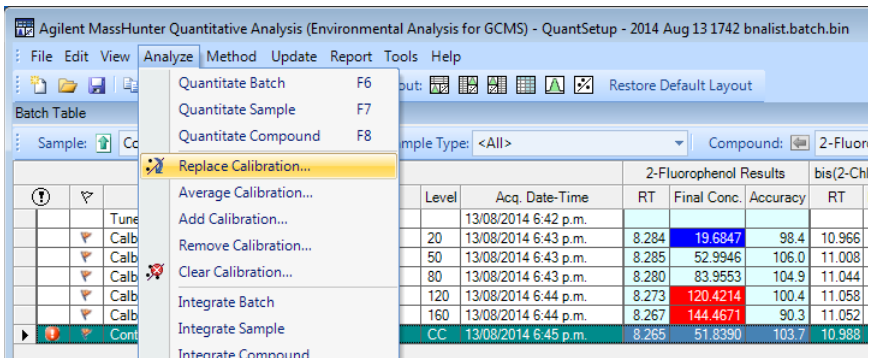
The Compound Information now shows the actual data file comparison to the library in the spectral data window. The library match score is displayed and its outlier can now be enabled.



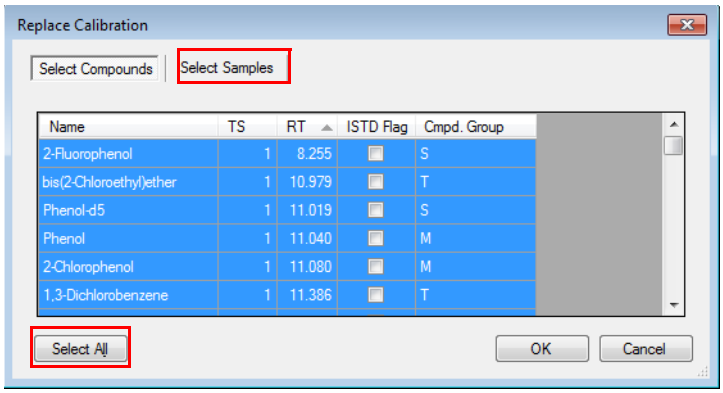
Step 6: Initialize the Continuing Calibration response.

The converted ChemStation method contains a CC level with a response, however, the Calibration STD Acquisition has an invalid acquisition time and date. This would generate an error if we tried to generate a QA Check Report. This step adds the newly acquired CC sample data and time stamp to the CC level so a valid report can be generated.

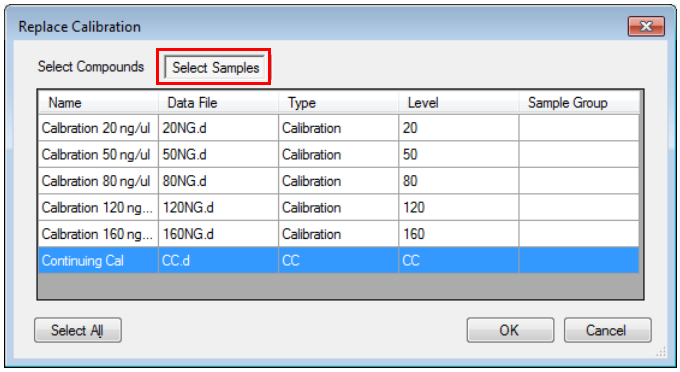
1. Select **Analyze > Replace Calibration.**



2. In the Select Compounds tab, click **Select All** then click **Select Samples** tab.



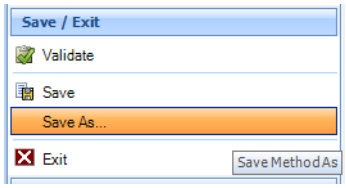
3. On the Select Samples tab, select the **Continuing Cal** sample and click **OK**.



The responses for the continuing calibration compounds are replaced with the responses in the data file.

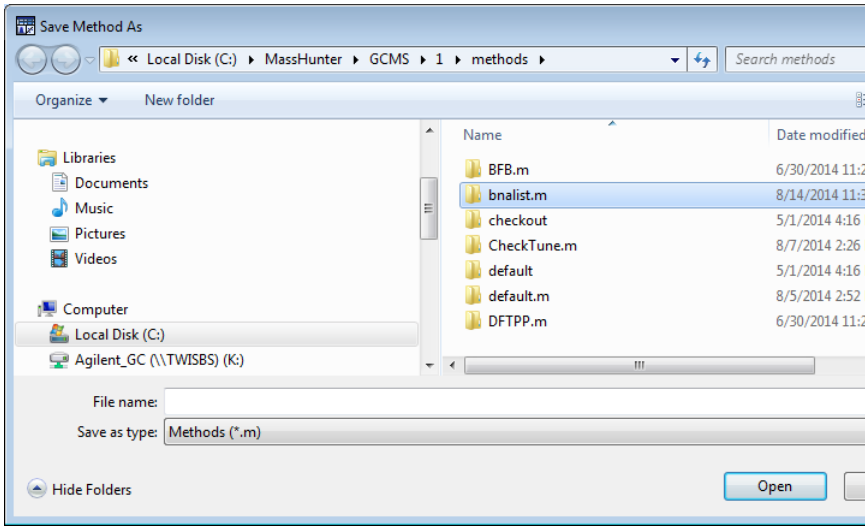
Step 7: Save the Method.

1. Select **Save As**.



2. Navigate to the MassHunter\GCMS\1\methods \ directory and select the **bnalist.m** unified method where the data acquisition was saved.

The unified bnalist method is used for the data acquisition, quantitative analysis, and Tune Evaluation methods.



3. Exit **[F11]** the method editor.

You are returned to the Batch table view.

Up to this point you have created the quantitation method, added calibration curve responses to all compounds in the method, and created a Tune Check method and a reference library.

Step 8: Complete the quantitation method.

Continue the workflow by adding EPA monitoring to the quantitation method Chapter 5, "Enter EnviroQuant Parameters in the Method".

5
Enter EnviroQuant Parameters in the Method

Agilent Technologies

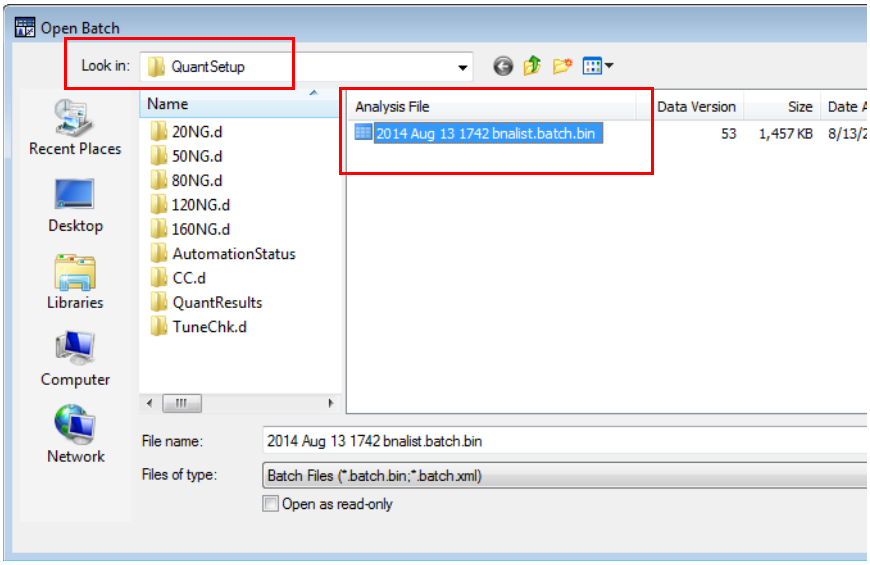
Introduction

In this chapter you will learn how to add outliers to a quantitative method that monitor compound properties and instrument performance as specified by EPA Method 8270.

Step 1: Open the batch.

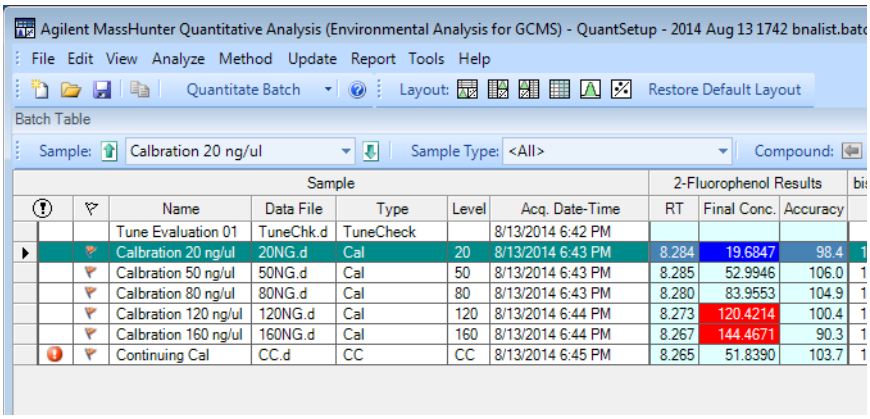
If the bnalist batch saved in the in the QuantSetup folder in the previous chapter is already open, skip this step.

1. In MassHunter EnviroQuant select **File > Open Batch**.



2. Navigate to the QuantSetup folder, select the bnalist batch, and click **Open**.

The batch table opens with all samples quantitated.

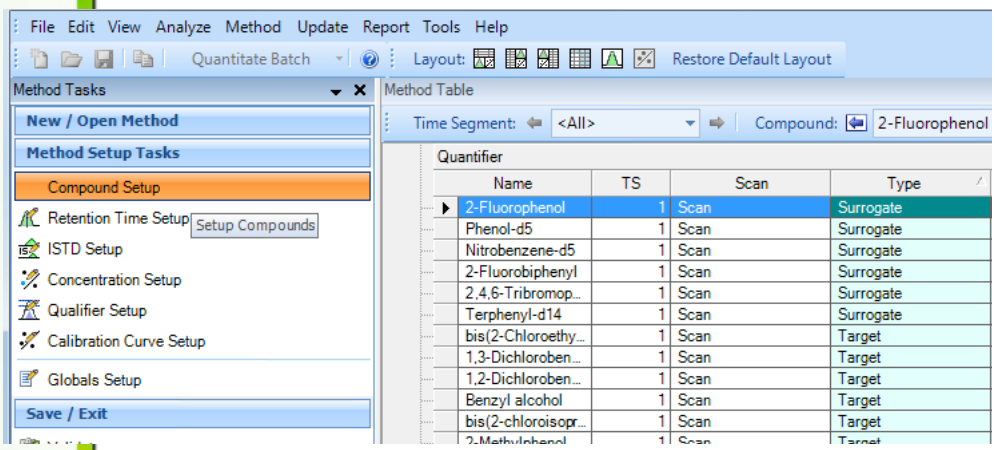


Step 2: Specify the surrogates and matrix spikes.

Surrogates and matrix spikes were identified as a subcategory of target compounds in ChemStation, here in MassHunter they need to be identified as a compound type.

1. Open the method editor **[F10]**.

2. Select **Compound Setup**.



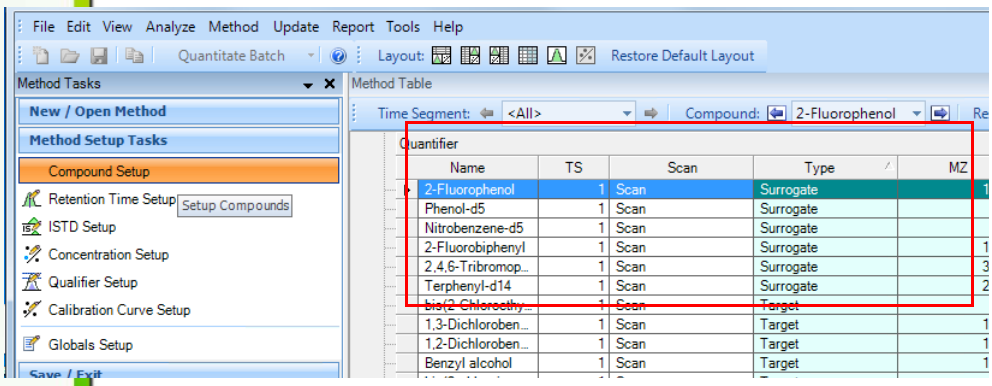
3. Specify **Surrogate** as the **Type** for these compounds.

In the Quantifier table set the compound **Type** for each of these 6 compounds to **Surrogate**.

2-Fluorophenol
Phenol-d5
Nitrobenzene-d5
2-Fluorobiphenyl
2,4,6-Tribromophenol
Terphenyl-d14

4. Compare your edits with this example.

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



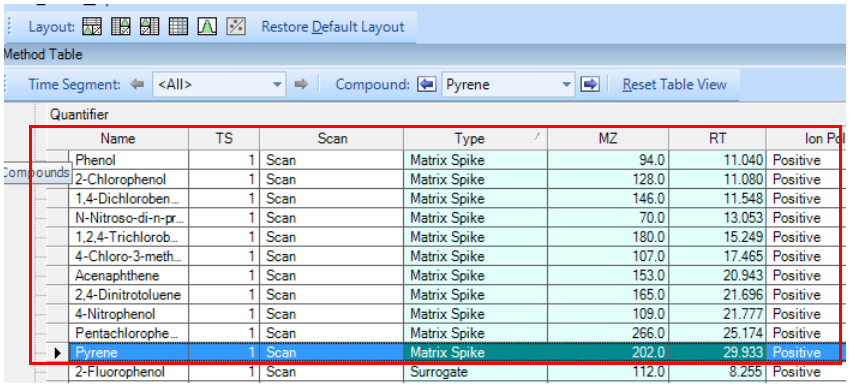
5. Specify **Matrix Spike** as the **Type** for these compounds.

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.



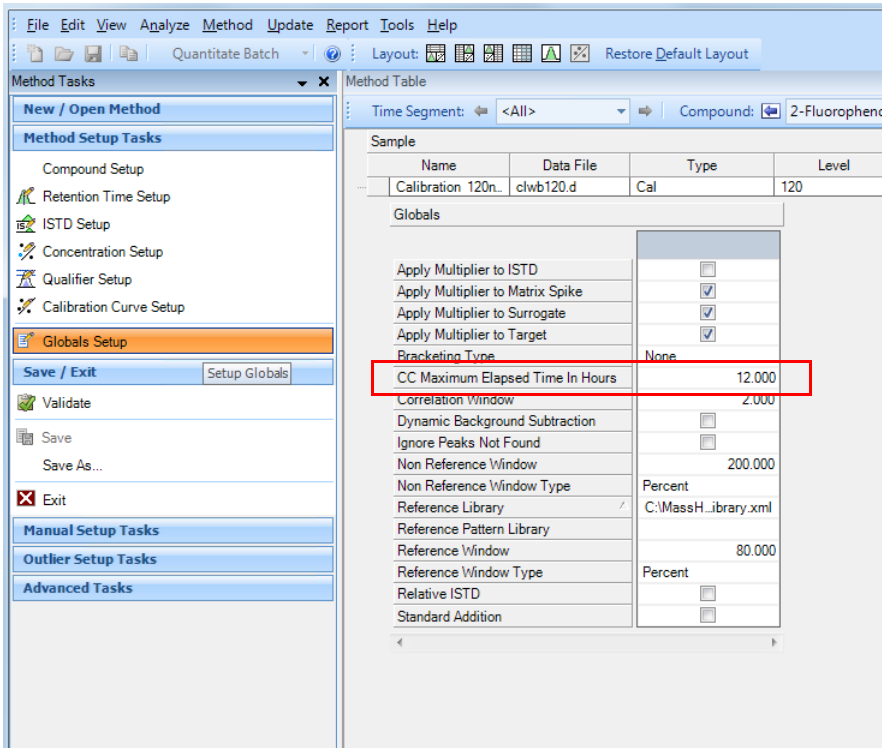
Name	TS	Scan	Type	MZ	RT	Ion Pol
Phenol	1	Scan	Matrix Spike	94.0	11.040	Positive
2-Chlorophenol	1	Scan	Matrix Spike	128.0	11.080	Positive
1,4-Dichloroben...	1	Scan	Matrix Spike	146.0	11.548	Positive
N-Nitroso-di-n-pr...	1	Scan	Matrix Spike	70.0	13.053	Positive
1,2,4-Trichlorob...	1	Scan	Matrix Spike	180.0	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

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.



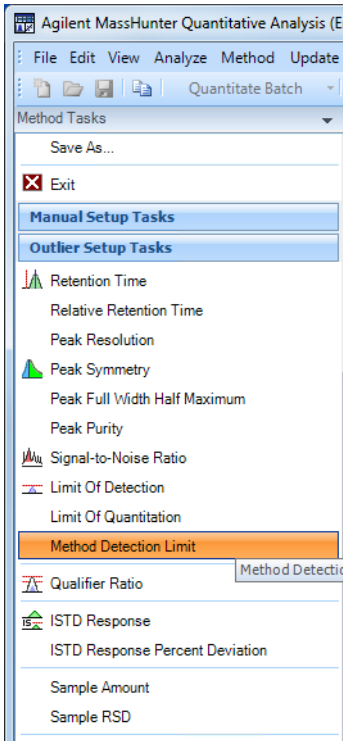
Step 4: Set up outlier limits for the EPA method criteria.

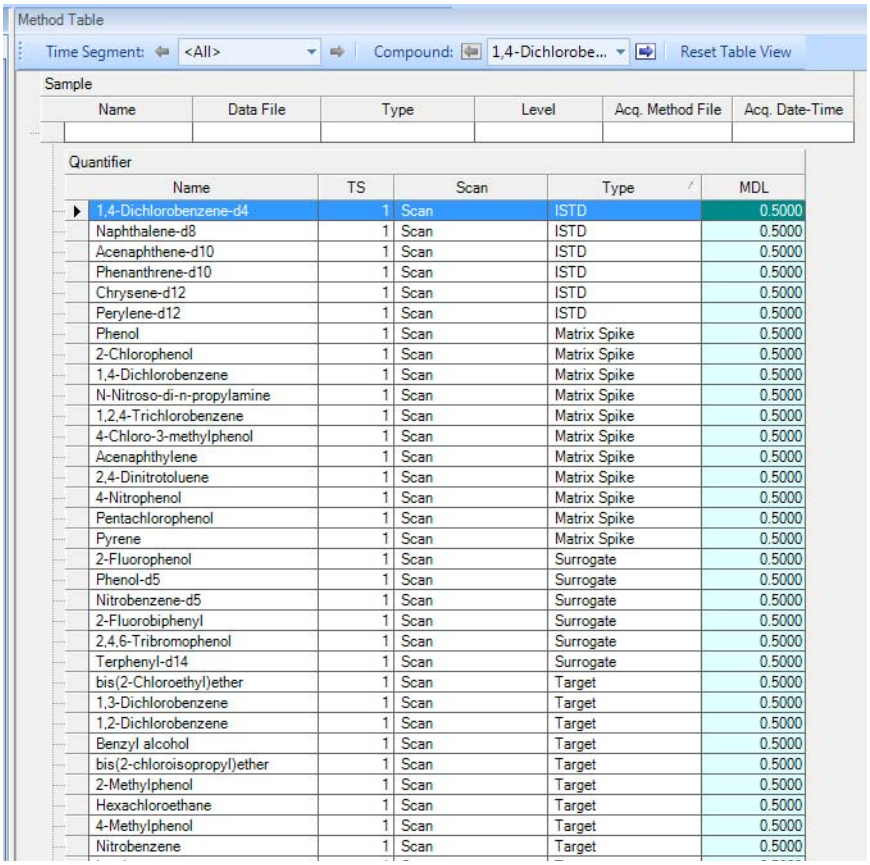
In this section you will set outlier criteria for monitoring compounds and instrument performance as required by EPA Method 8270, including the:

- Method Detection Limit
- Surrogate Concentration, Percent recovery min and max
- ISTD Response Min and Max Percent Deviation - to compare the Con Cal ISTD response to the Mid-point calibration levels ISTD responses.
- Accuracy max percent deviation for Con Cal if the curve fit is not average response
- 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
- CC Average Response Factor - Con Cal report if the curve fit is average response factor
- Matrix Spike Percent Difference
- Matrix Spike Percent Recovery
- Matrix Spike Group Recovery
- Surrogate Percent Recovery
- Library Match Score

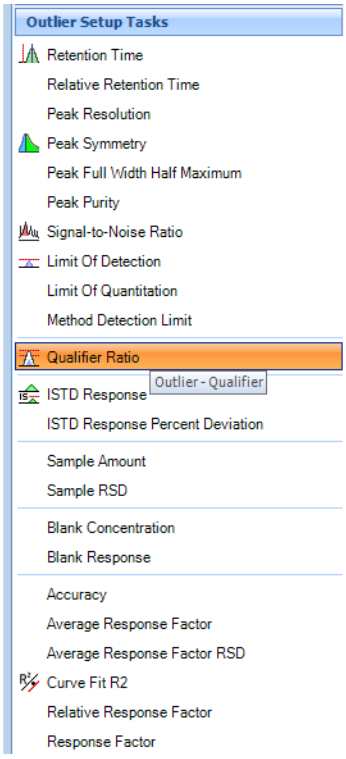
Once these outliers are set they can be displayed as color coded cells in the Batch Table and Compounds-at-a-Glance.

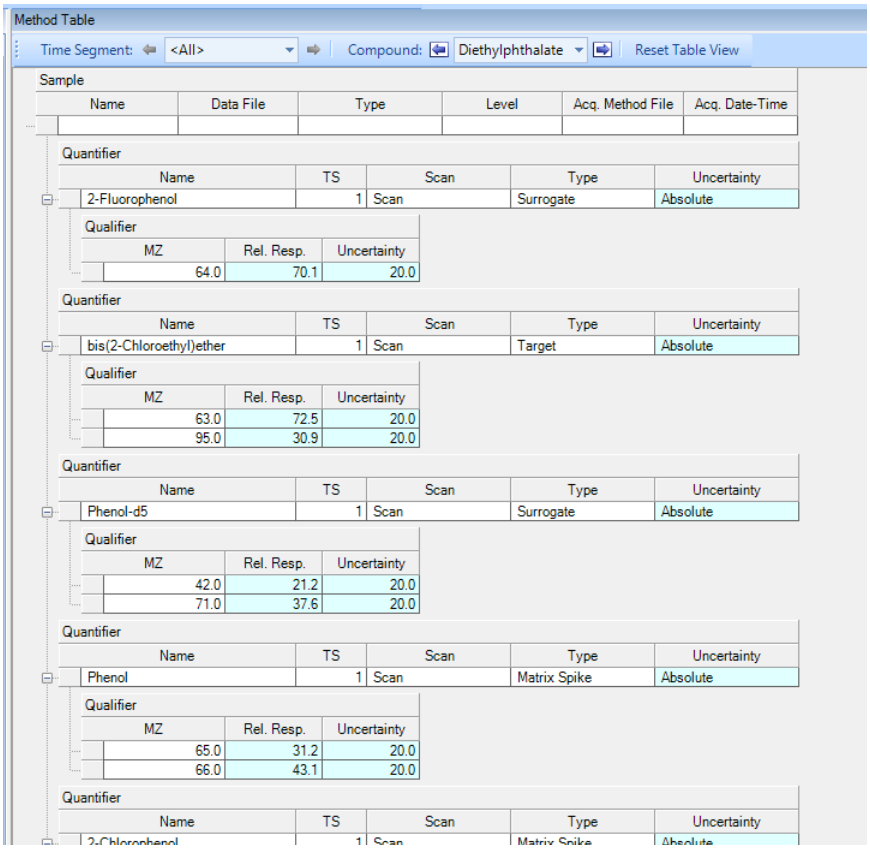
1. In the Method Editor view, from the **Outlier Setup Tasks**. area select **Method Detection Limit**. Fill in the shaded column as shown here.



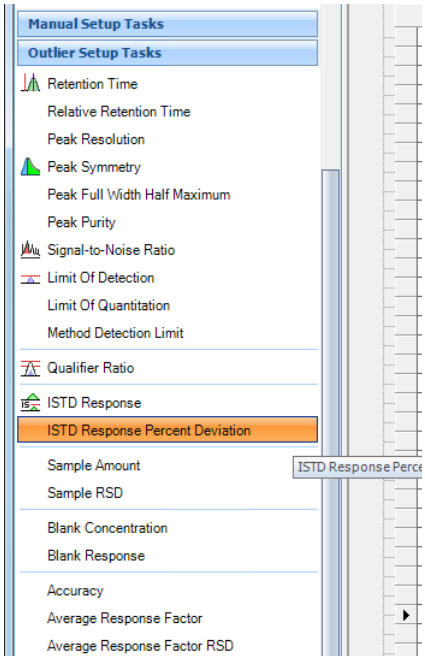


2. Scroll down the list of Outliers and select **Qualifier Ratio**. Fill in the shaded columns as shown here.





3. Select **ISTD Response Percent Deviation**. Fill in the shaded columns as shown here.



This will be used to compare Con Cal ISTD response to mid-point calibration levels ISTD responses.

Time Segment: <All> Compound: Diethylphthalate Reset Table View

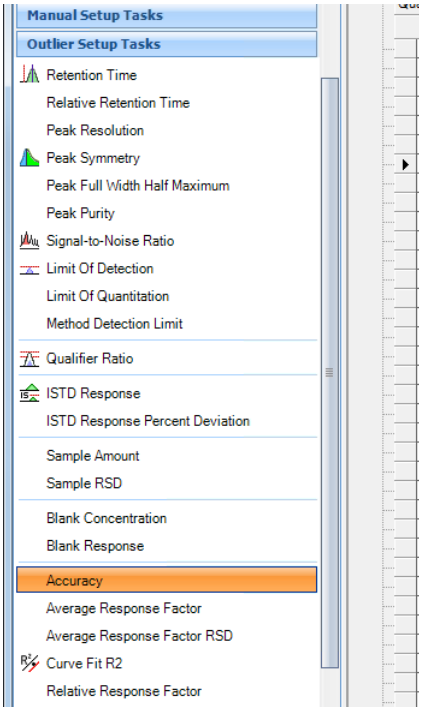
Sample

Name	Data File	Type	Level	Acq. Method File	Acq. Date-Time

Quantifier

Name	TS	Scan	Type	ISTD Resp. Min. % Dev.	ISTD Resp. Max. % Dev.
2-Fluorophenol	1	Scan	Surrogate	50.0	200.0
bis(2-Chloroethyl)ether	1	Scan	Target	50.0	200.0
Phenol-d5	1	Scan	Surrogate	50.0	200.0
Phenol	1	Scan	Matrix Spike	50.0	200.0
2-Chlorophenol	1	Scan	Matrix Spike	50.0	200.0
1,3-Dichlorobenzene	1	Scan	Target	50.0	200.0
1,4-Dichlorobenzene-d4	1	Scan	ISTD	50.0	200.0
1,4-Dichlorobenzene	1	Scan	Matrix Spike	50.0	200.0
1,2-Dichlorobenzene	1	Scan	Target	50.0	200.0
Benzyl alcohol	1	Scan	Target	50.0	200.0
bis(2-chloroisopropyl)ether	1	Scan	Target	50.0	200.0
2-Methylphenol	1	Scan	Target	50.0	200.0
Hexachloroethane	1	Scan	Target	50.0	200.0
N-Nitroso-di-n-propylamine	1	Scan	Matrix Spike	50.0	200.0
4-Methylphenol	1	Scan	Target	50.0	200.0
Nitrobenzene-d5	1	Scan	Surrogate	50.0	200.0
Nitrobenzene	1	Scan	Target	50.0	200.0
Isophorone	1	Scan	Target	50.0	200.0
2-Nitrophenol	1	Scan	Target	50.0	200.0
2,4-Dimethylphenol	1	Scan	Target	50.0	200.0
bis(2-Chloroethoxy)methane	1	Scan	Target	50.0	200.0
2,4-Dichlorophenol	1	Scan	Target	50.0	200.0
1,2,4-Trichlorobenzene	1	Scan	Matrix Spike	50.0	200.0
Naphthalene-d8	1	Scan	ISTD	50.0	200.0
Naphthalene	1	Scan	Target	50.0	200.0
4-Chloroaniline	1	Scan	Target	50.0	200.0
Hexachlorobutadiene	1	Scan	Target	50.0	200.0
4-Chloro-3-methylphenol	1	Scan	Matrix Spike	50.0	200.0
2-Methylnaphthalene	1	Scan	Target	50.0	200.0
Hexachlorocyclopentadiene	1	Scan	Target	50.0	200.0
2,4,6-Trichlorophenol	1	Scan	Target	50.0	200.0
2,4,5-Trichlorophenol	1	Scan	Target	50.0	200.0
2-Fluorobiphenyl	1	Scan	Surrogate	50.0	200.0

4. Under **Outlier Setup Tasks**, select **Accuracy**. Fill in the shaded columns as shown here.



This will be used for Con Cal *if the curve fit is not average response*.

Time Segment: <All> Compound: Diethylphthalate Reset Table View

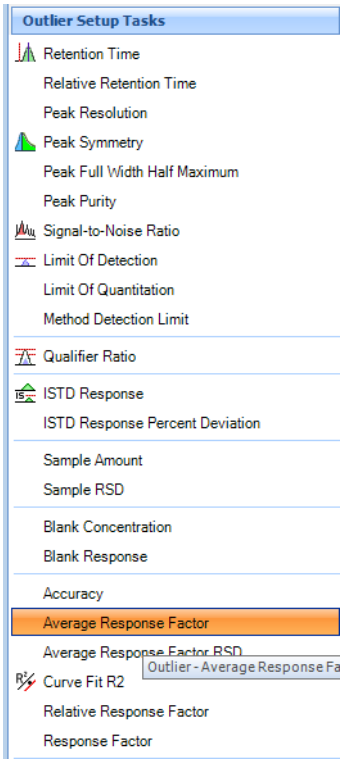
Sample

Name	Data File	Type	Level	Acq. Method File	Acq. Date-Time

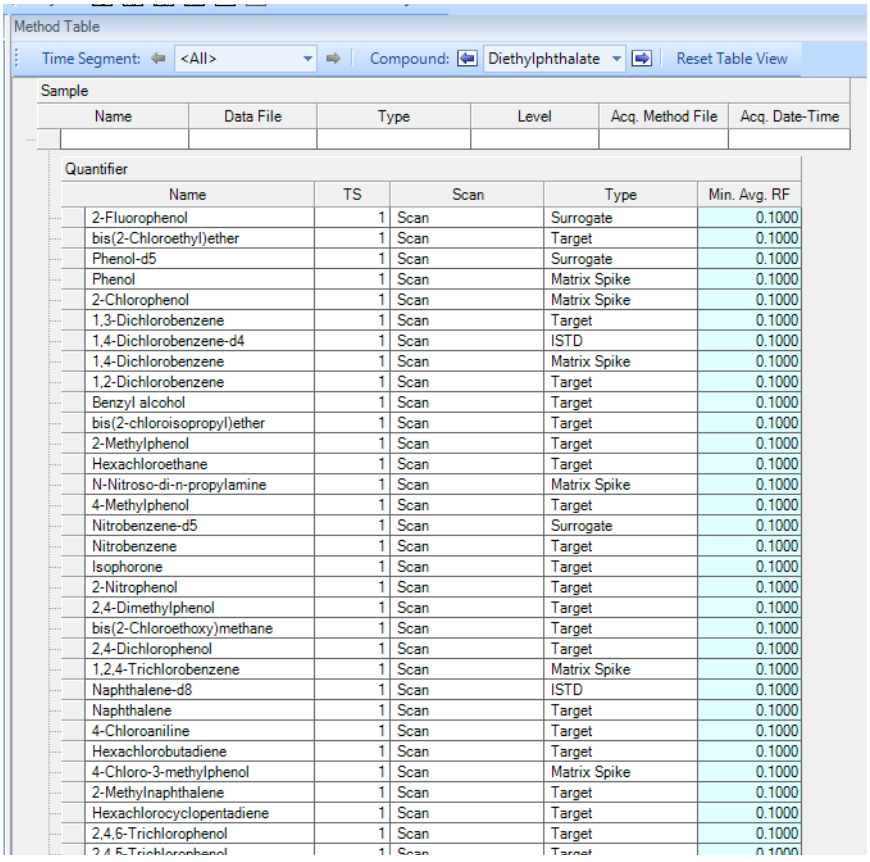
Quantifier

Name	TS	Scan	Type	Accuracy Max. % Dev.	LOQ Accuracy Multiplier
2-Fluorophenol	1	Scan	Surrogate	20.0	1.0
bis(2-Chloroethyl)ether	1	Scan	Target	20.0	1.0
Phenol-d5	1	Scan	Surrogate	20.0	1.0
Phenol	1	Scan	Matrix Spike	20.0	1.0
2-Chlorophenol	1	Scan	Matrix Spike	20.0	1.0
1,3-Dichlorobenzene	1	Scan	Target	20.0	1.0
1,4-Dichlorobenzene-d4	1	Scan	ISTD	20.0	1.0
1,4-Dichlorobenzene	1	Scan	Matrix Spike	20.0	1.0
1,2-Dichlorobenzene	1	Scan	Target	20.0	1.0
Benzyl alcohol	1	Scan	Target	20.0	1.0
bis(2-chloroisopropyl)ether	1	Scan	Target	20.0	1.0
2-Methylphenol	1	Scan	Target	20.0	1.0
Hexachloroethane	1	Scan	Target	20.0	1.0
N-Nitroso-di-n-propylamine	1	Scan	Matrix Spike	20.0	1.0
4-Methylphenol	1	Scan	Target	20.0	1.0
Nitrobenzene-d5	1	Scan	Surrogate	20.0	1.0
Nitrobenzene	1	Scan	Target	20.0	1.0
Isophorone	1	Scan	Target	20.0	1.0
2-Nitrophenol	1	Scan	Target	20.0	1.0
2,4-Dimethylphenol	1	Scan	Target	20.0	1.0
bis(2-Chloroethoxy)methane	1	Scan	Target	20.0	1.0
2,4-Dichlorophenol	1	Scan	Target	20.0	1.0
1,2,4-Trichlorobenzene	1	Scan	Matrix Spike	20.0	1.0
Naphthalene-d8	1	Scan	ISTD	20.0	1.0
Naphthalene	1	Scan	Target	20.0	1.0
4-Chloroaniline	1	Scan	Target	20.0	1.0
Hexachlorobutadiene	1	Scan	Target	20.0	1.0
4-Chloro-3-methylphenol	1	Scan	Matrix Spike	20.0	1.0
2-Methylnaphthalene	1	Scan	Target	20.0	1.0
Hexachlorocyclopentadiene	1	Scan	Target	20.0	1.0
2,4,6-Trichlorophenol	1	Scan	Target	20.0	1.0
2,4,5-Trichlorophenol	1	Scan	Target	20.0	1.0
2-Fluorobiphenyl	1	Scan	Surrogate	20.0	1.0
2-Chloronaphthalene	1	Scan	Target	20.0	1.0

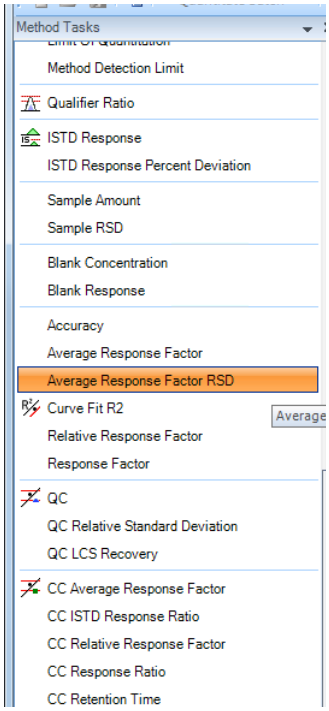
5. Select **Average Response Factor**. Fill in the shaded column as shown here.



This will be used for ICAL Report minimum RF.



6. Select **Average Response Factor RSD.** Fill in the column as shown here.



This will be used for ICAL Report RSD.

Method Table

Time Segment: <All> Compound: Diethylphthalate Reset Table View

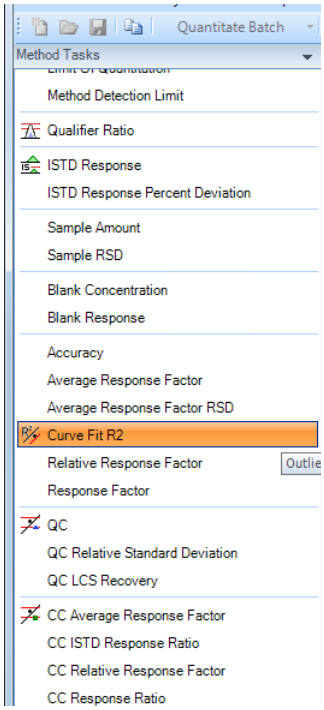
Sample

Name	Data File	Type	Level	Acq. Method File	Acq. Date-Time

Quantifier

Name	TS	Scan	Type	Max. Avg. RF RSD
2-Fluorophenol	1	Scan	Surrogate	30.000000
bis(2-Chloroethyl)ether	1	Scan	Target	30.000000
Phenol-d5	1	Scan	Surrogate	30.000000
Phenol	1	Scan	Matrix Spike	10.000000
2-Chlorophenol	1	Scan	Matrix Spike	30.000000
1,3-Dichlorobenzene	1	Scan	Target	30.000000
1,4-Dichlorobenzene-d4	1	Scan	ISTD	
1,4-Dichlorobenzene	1	Scan	Matrix Spike	30.000000
1,2-Dichlorobenzene	1	Scan	Target	30.000000
Benzyl alcohol	1	Scan	Target	30.000000
bis(2-chloroisopropyl)ether	1	Scan	Target	30.000000
2-Methylphenol	1	Scan	Target	30.000000
Hexachloroethane	1	Scan	Target	30.000000
N-Nitroso-di-n-propylamine	1	Scan	Matrix Spike	30.000000
4-Methylphenol	1	Scan	Target	30.000000
Nitrobenzene-d5	1	Scan	Surrogate	30.000000
Nitrobenzene	1	Scan	Target	30.000000
Isophorone	1	Scan	Target	30.000000
2-Nitrophenol	1	Scan	Target	30.000000
2,4-Dimethylphenol	1	Scan	Target	30.000000
bis(2-Chloroethoxy)methane	1	Scan	Target	30.000000
2,4-Dichlorophenol	1	Scan	Target	30.000000
1,2,4-Trichlorobenzene	1	Scan	Matrix Spike	30.000000
Naphthalene-d8	1	Scan	ISTD	
Naphthalene	1	Scan	Target	30.000000
4-Chloroaniline	1	Scan	Target	30.000000
Hexachlorobutadiene	1	Scan	Target	30.000000
4-Chloro-3-methylphenol	1	Scan	Matrix Spike	30.000000
2-Methylnaphthalene	1	Scan	Target	30.000000
Hexachlorocyclopentadiene	1	Scan	Target	30.000000
2,4,6-Trichlorophenol	1	Scan	Target	30.000000
2,4,5-Trichlorophenol	1	Scan	Target	30.000000
2-Fluorobiphenyl	1	Scan	Surrogate	30.000000
2-Chloronaphthalene	1	Scan	Target	30.000000
2-Nitroaniline	1	Scan	Target	30.000000
Dimethylphthalate	1	Scan	Target	30.000000

7. Select **Curve Fit R2**. Fill in the shaded column as shown here.



This will be used for ICAL Report curve fits other than Average Response Factor.

Method Table

Time Segment: <All> Compound: Diethylphthalate Reset Table View

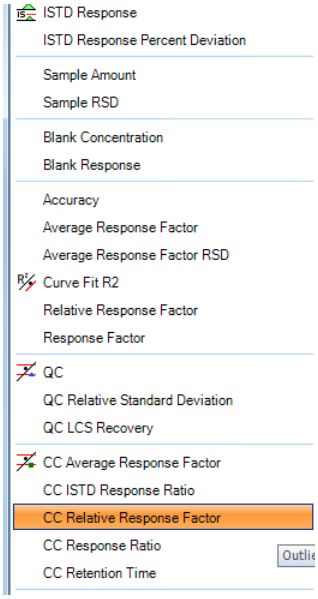
Sample

Name	Data File	Type	Level	Acq. Method File	Acq. Date-Time

Quantifier

Name	TS	Scan	Type	CF Min. R2
2-Fluorophenol	1	Scan	Surrogate	0.99000000
bis(2-Chloroethyl)ether	1	Scan	Target	0.99000000
Phenol-d5	1	Scan	Surrogate	0.99000000
Phenol	1	Scan	Matrix Spike	0.99000000
2-Chlorophenol	1	Scan	Matrix Spike	0.99000000
1,3-Dichlorobenzene	1	Scan	Target	0.99000000
1,4-Dichlorobenzene-d4	1	Scan	ISTD	0.99000000
1,4-Dichlorobenzene	1	Scan	Matrix Spike	0.99000000
1,2-Dichlorobenzene	1	Scan	Target	0.99000000
Benzyl alcohol	1	Scan	Target	0.99000000
bis(2-chloroisopropyl)ether	1	Scan	Target	0.99000000
2-Methylphenol	1	Scan	Target	0.99000000
Hexachloroethane	1	Scan	Target	0.99000000
N-Nitroso-di-n-propylamine	1	Scan	Matrix Spike	0.99000000
4-Methylphenol	1	Scan	Target	0.99000000
Nitrobenzene-d5	1	Scan	Surrogate	0.99000000
Nitrobenzene	1	Scan	Target	0.99000000
Isophorone	1	Scan	Target	0.99000000
2-Nitrophenol	1	Scan	Target	0.99000000
2,4-Dimethylphenol	1	Scan	Target	0.99000000
bis(2-Chloroethoxy)methane	1	Scan	Target	0.99000000
2,4-Dichlorophenol	1	Scan	Target	0.99000000
1,2,4-Trichlorobenzene	1	Scan	Matrix Spike	0.99000000
Naphthalene-d8	1	Scan	ISTD	0.99000000
Naphthalene	1	Scan	Target	0.99000000
4-Chloroaniline	1	Scan	Target	0.99000000
Hexachlorobutadiene	1	Scan	Target	0.99000000
4-Chloro-3-methylphenol	1	Scan	Matrix Spike	0.99000000
2-Methylnaphthalene	1	Scan	Target	0.99000000
Hexachlorocyclopentadiene	1	Scan	Target	0.99000000

8. Select **CC Relative Response Factor.** Fill in the shaded column as shown here.



This is the minimum RF for the continuing cal. It will be used for Minimum CC RF.

ethod Table

Time Segment: <All> Compound: Diethylphthalate Reset Table View

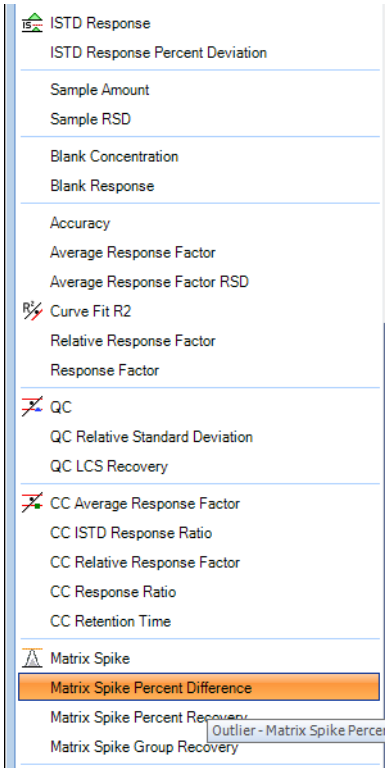
Sample

Name	Data File	Type	Level	Acq. Method File	Acq. Date-Time

Quantifier

Name	TS	Scan	Type	Min. CC Rel. Resp. Factor
2-Fluorophenol	1	Scan	Surrogate	0.1
bis(2-Chloroethyl)ether	1	Scan	Target	0.1
Phenol-d5	1	Scan	Surrogate	0.1
Phenol	1	Scan	Matrix Spike	0.1
2-Chlorophenol	1	Scan	Matrix Spike	0.1
1,3-Dichlorobenzene	1	Scan	Target	0.1
1,4-Dichlorobenzene-d4	1	Scan	ISTD	0.1
1,4-Dichlorobenzene	1	Scan	Matrix Spike	0.1
1,2-Dichlorobenzene	1	Scan	Target	0.1
Benzyl alcohol	1	Scan	Target	0.1
bis(2-chloroisopropyl)ether	1	Scan	Target	0.1
2-Methylphenol	1	Scan	Target	0.1
Hexachloroethane	1	Scan	Target	0.1
N-Nitroso-di-n-propylamine	1	Scan	Matrix Spike	0.1
4-Methylphenol	1	Scan	Target	0.1
Nitrobenzene-d5	1	Scan	Surrogate	0.1
Nitrobenzene	1	Scan	Target	0.1
Isophorone	1	Scan	Target	0.1
2-Nitrophenol	1	Scan	Target	0.1
2,4-Dimethylphenol	1	Scan	Target	0.1
bis(2-Chloroethoxy)methane	1	Scan	Target	0.1
2,4-Dichlorophenol	1	Scan	Target	0.1
1,2,4-Trichlorobenzene	1	Scan	Matrix Spike	0.1
Naphthalene-d8	1	Scan	ISTD	0.1
Naphthalene	1	Scan	Target	0.1
4-Chloroaniline	1	Scan	Target	0.1
Hexachlorobutadiene	1	Scan	Target	0.1
4-Chloro-3-methylphenol	1	Scan	Matrix Spike	0.1
2-Methylnaphthalene	1	Scan	Target	0.1

9. Still under **Outlier Setup tasks**, select **Matrix Spike Percent Difference.** Fill in the shaded columns as shown here.



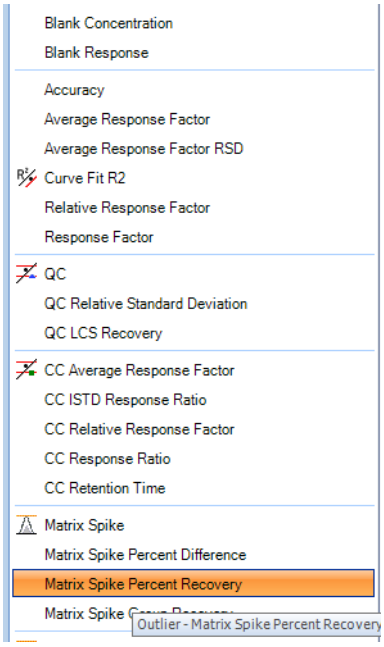
Method Table

Time Segment: <All> Compound: Benzo[g,h,i]per... Reset Table View

Quantifier

Name	TS	Scan	Type	Matrix Spike A Max. % Dev.	Matrix Spike B Max. % Dev.	Matrix Spike A Conc.	Matrix Spike B Conc.
2-Chlorophenol	1	Scan	Matrix Spike	40.0	50.0	200.0000	200.0000
1,4-Dichlorobenzene	1	Scan	Matrix Spike	28.0	27.0	100.0000	100.0000
N-Nitroso-di-n-propylamine	1	Scan	Matrix Spike	38.0	38.0	100.0000	100.0000
1,2,4-Trichlorobenzene	1	Scan	Matrix Spike	28.0	38.0	100.0000	100.0000
4-Chloro-3-methylphenol	1	Scan	Matrix Spike	42.0	33.0	200.0000	200.0000
Acenaphthene	1	Scan	Matrix Spike	31.0	19.0	100.0000	100.0000
2,4-Dinitrotoluene	1	Scan	Matrix Spike	0.0	0.0	100.0000	100.0000
4-Nitrophenol	1	Scan	Matrix Spike	50.0	50.0	200.0000	200.0000
Pentachlorophenol	1	Scan	Matrix Spike	50.0	47.0	200.0000	200.0000
Pyrene	1	Scan	Matrix Spike	31.0	36.0	100.0000	100.0000
2-Fluorophenol	1	Scan	Surrogate				

10. Still under **Outlier Setup tasks**, select **Matrix Spike Percent Recovery.** Fill in the shaded columns as shown here.



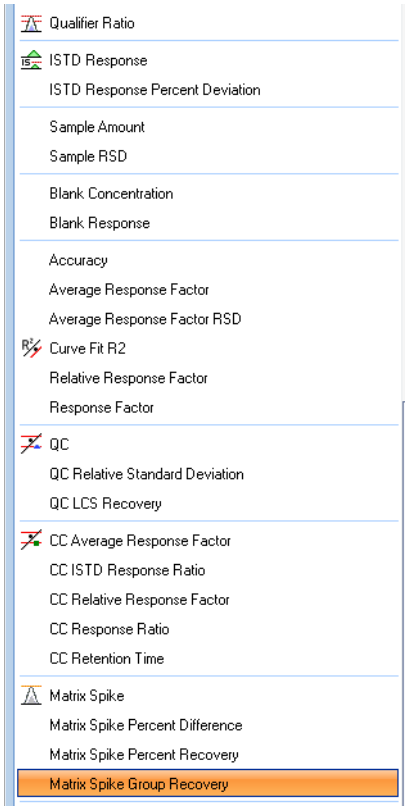
Method Table

Time Segment: <All> Compound: Benzo[g,h,i]per... Reset Table View

Quantifier

Name	TS	Scan	Type	Matrix Spike A % Recovery Min.	Matrix Spike A % Recovery Max.	Matrix Spike A Conc.
2-Chlorophenol	1	Scan	Matrix Spike	70.0	130.0	200.0000
1,4-Dichlorobenzene	1	Scan	Matrix Spike	70.0	130.0	100.0000
N-Nitroso-di-n-propylamine	1	Scan	Matrix Spike	70.0	130.0	100.0000
1,2,4-Trichlorobenzene	1	Scan	Matrix Spike	70.0	130.0	100.0000
4-Chloro-3-methylphenol	1	Scan	Matrix Spike	70.0	130.0	200.0000
Acenaphthene	1	Scan	Matrix Spike	70.0	130.0	100.0000
2,4-Dinitrotoluene	1	Scan	Matrix Spike	70.0	130.0	100.0000
4-Nitrophenol	1	Scan	Matrix Spike	70.0	130.0	200.0000
Pentachlorophenol	1	Scan	Matrix Spike	70.0	130.0	200.0000
Pyrene	1	Scan	Matrix Spike	70.0	130.0	100.0000

11. Still under **Outlier Setup tasks**, select **Matrix Spike Group Recovery.** Fill in the shaded columns as shown here.



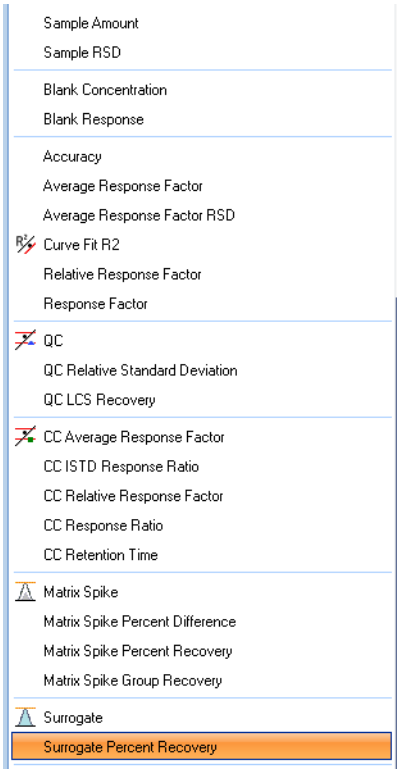
Method Table

Time Segment: <All> Compound: Benzo[g,h,i]per... Reset Table View

Quantifier

Name	TS	Scan	Type	Matrix Spike A % Recovery Min.	Matrix Spike A % Recovery Max.	Matrix Spike B % Recovery Min.	Matrix Spike B % Recovery Max.	Matrix Spike A Conc.	Matrix Spike B Conc.
2-Chlorophenol	1	Scan	Matrix Spike	70.0	130.0	70.0	130.0	200.0000	200.0000
1,4-Dichlorobenzene	1	Scan	Matrix Spike	70.0	130.0	70.0	130.0	100.0000	100.0000
N-Nitroso-di-n-propylamine	1	Scan	Matrix Spike	70.0	130.0	70.0	130.0	100.0000	100.0000
1,2,4-Trichlorobenzene	1	Scan	Matrix Spike	70.0	130.0	70.0	130.0	100.0000	100.0000
4-Chloro-3-methylphenol	1	Scan	Matrix Spike	70.0	130.0	70.0	130.0	200.0000	200.0000
Acenaphthene	1	Scan	Matrix Spike	70.0	130.0	70.0	130.0	100.0000	100.0000
2,4-Dinitrotoluene	1	Scan	Matrix Spike	70.0	130.0	70.0	130.0	100.0000	100.0000
4-Nitrophenol	1	Scan	Matrix Spike	70.0	130.0	70.0	130.0	200.0000	200.0000
Pentachlorophenol	1	Scan	Matrix Spike	70.0	130.0	70.0	130.0	200.0000	200.0000
Pyrene	1	Scan	Matrix Spike	70.0	130.0	70.0	130.0	100.0000	100.0000

12. Select **Surrogate Percent Recovery.** Fill in the shaded columns as shown here.



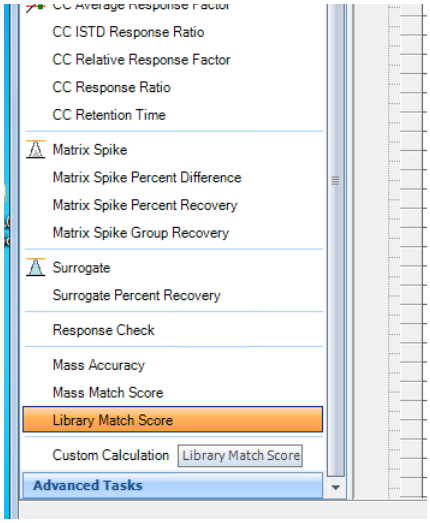
Method Table

Time Segment: <All> Compound: Benzo[g,h,i]per... Reset Table View

Quantifier

Name	TS	Scan	Type	Surrogate % Recovery Min.	Surrogate % Recovery Max.	Surrogate Conc.
2-Fluorophenol	1	Scan	Surrogate	70.0	130.0	200.0000
Phenol-d5	1	Scan	Surrogate	70.0	130.0	200.0000
Nitrobenzene-d5	1	Scan	Surrogate	70.0	130.0	100.0000
2-Fluorobiphenyl	1	Scan	Surrogate	70.0	130.0	100.0000
2,4,6-Tribromophenol	1	Scan	Surrogate	70.0	130.0	200.0000
Terphenyl-d14	1	Scan	Surrogate	70.0	130.0	100.0000

13. Select **Library Match Score.** Fill in the shaded column as shown here.



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thod Update Report Tools Help

te Batch Layout: Restore Default Layout

Method Table

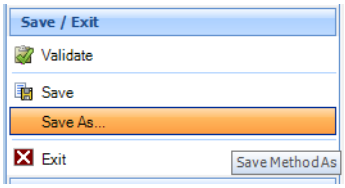
Time Segment: <All> Compound: 2-Fluorophenol

Quantifier

Name	TS	Scan	Type	Library Match Score Minimum
2-Fluorophenol	1	Scan	Surrogate	0.7
Phenol-d5	1	Scan	Surrogate	0.7
Nitrobenzene-d5	1	Scan	Surrogate	0.7
2-Fluorobiphenyl	1	Scan	Surrogate	0.7
2,4,6-Tribromophenol	1	Scan	Surrogate	0.7
Terphenyl-d14	1	Scan	Surrogate	0.7
bis(2-Chloroethyl)ether	1	Scan	Target	0.7
1,3-Dichlorobenzene	1	Scan	Target	0.7
1,2-Dichlorobenzene	1	Scan	Target	0.7
Benzyl alcohol	1	Scan	Target	0.7
bis(2-chloroisopropyl)ether	1	Scan	Target	0.7
2-Methylphenol	1	Scan	Target	0.7
Hexachloroethane	1	Scan	Target	0.7
4-Methylphenol	1	Scan	Target	0.7
Nitrobenzene	1	Scan	Target	0.7
Isophorone	1	Scan	Target	0.7
2-Nitrophenol	1	Scan	Target	0.7
2,4-Dimethylphenol	1	Scan	Target	0.7
bis(2-Chloroethoxy)methane	1	Scan	Target	0.7
2,4-Dichlorophenol	1	Scan	Target	0.7
Naphthalene	1	Scan	Target	0.7
4-Chloroaniline	1	Scan	Target	0.7
Hexachlorobutadiene	1	Scan	Target	0.7
2-Methylnaphthalene	1	Scan	Target	0.7
Hexachlorocyclopentadiene	1	Scan	Target	0.7
2,4,6-Trichlorophenol	1	Scan	Target	0.7
2,4,5-Trichlorophenol	1	Scan	Target	0.7
2-Chloronaphthalene	1	Scan	Target	0.7
2-Nitroaniline	1	Scan	Target	0.7
Acenaphthylene	1	Scan	Target	0.7
Dimethylphthalate	1	Scan	Target	0.7
2,6-Dinitrotoluene	1	Scan	Target	0.7
3-Nitroaniline	1	Scan	Target	0.7
2,4-Dinitrophenol	1	Scan	Target	0.7
Dibenzofuran	1	Scan	Target	0.7
Fluorene	1	Scan	Target	0.7
4-Chlorophenyl-phenylether	1	Scan	Target	0.7
Diethylphthalate	1	Scan	Target	0.7
4-Nitroaniline	1	Scan	Target	0.7
4,6-Dinitro-2-methylphenol	1	Scan	Target	0.7
n-Nitrosodiphenylamine	1	Scan	Target	0.7

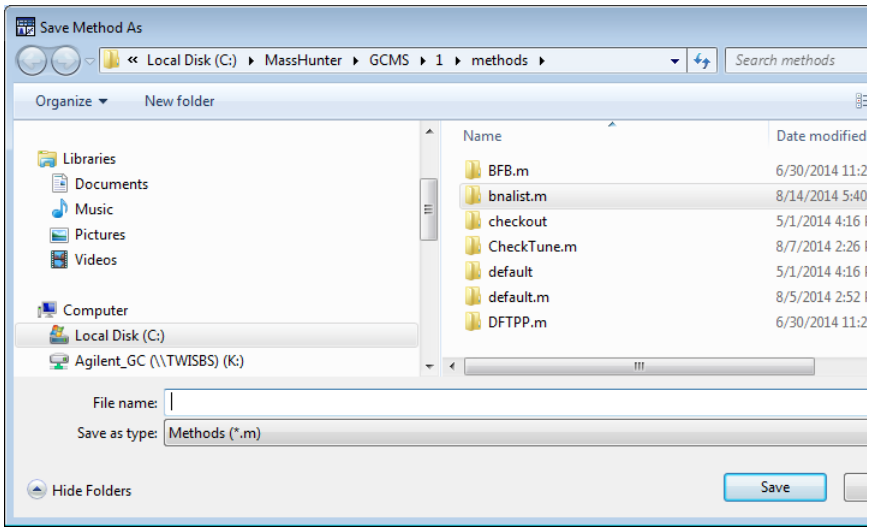
Step 5: Save the method.

1. Select **Save As**.



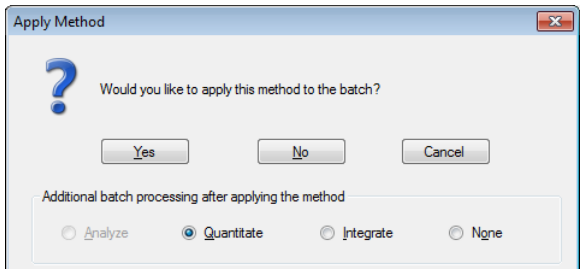
2. Navigate to the MassHunter\GCMS\1\methods \ directory and select the **bnalist.m** unified method where the data acquisition was saved, then click **Save**.

The unified bnalist method is used for the data acquisition, quantitative analysis, and Tune Evaluation analyses.



3. Reply **Yes** to the Overwrite prompt.

4. Exit **[F11]** the method editor. You are prompted to apply the method to the batch.



5. Click **Yes** to the Apply Method prompt.

You are returned to Batch table view.

Step 6: Create report methods.

Continue the workflow by creating report methods to automate report generation. See Chapter 6, "Create Report Methods".

6
Create Report Methods

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.

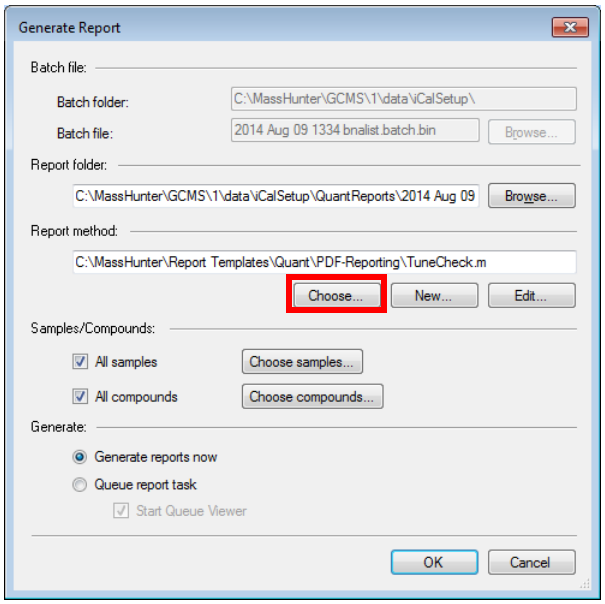
When you are working interactively with a batch of data, after doing manual integration for example, you may select any saved report method, or create one on the spot, and generate a report interactively.

This section describes how to generate reports both automatically, and interactively.

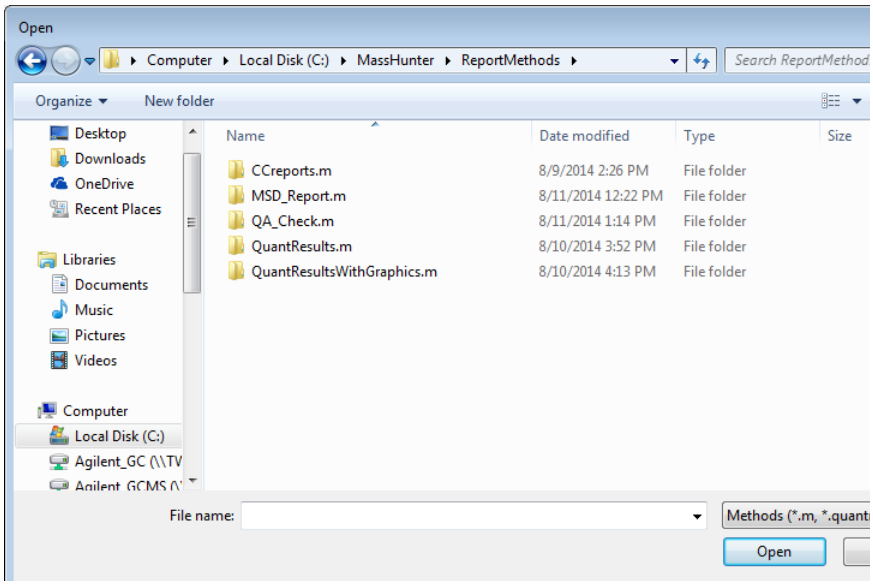
Step 1: Generate an interactive report.

1. From MassHunter's main menu select **Report > Generate**.

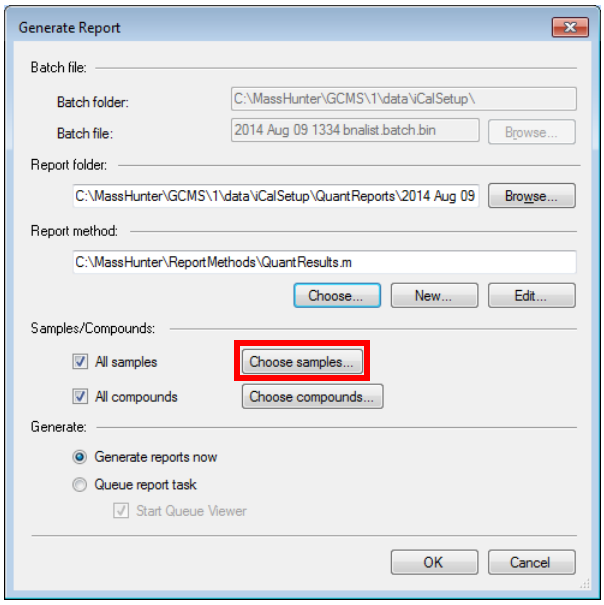
2. Click **Choose** and navigate to where you saved your report method templates.



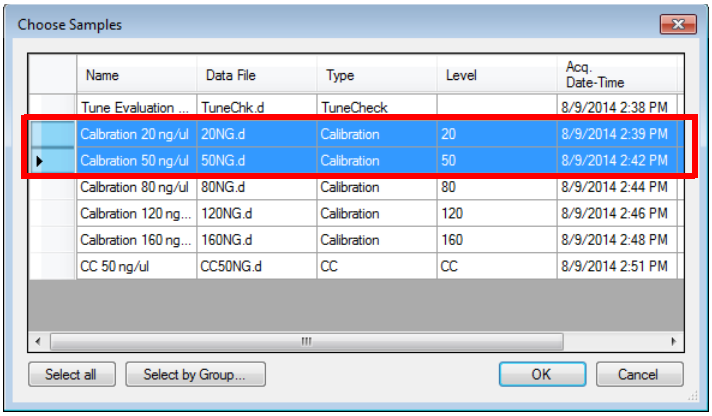
3. Select a Report method.



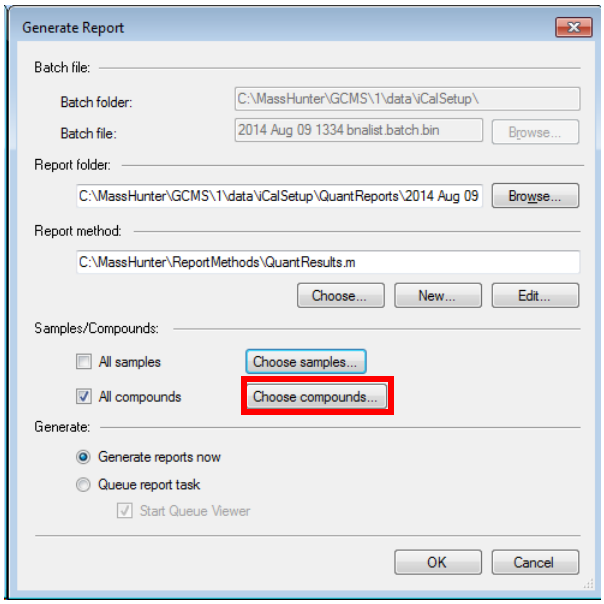
4. To limit the number of samples reported click **Choose samples**.



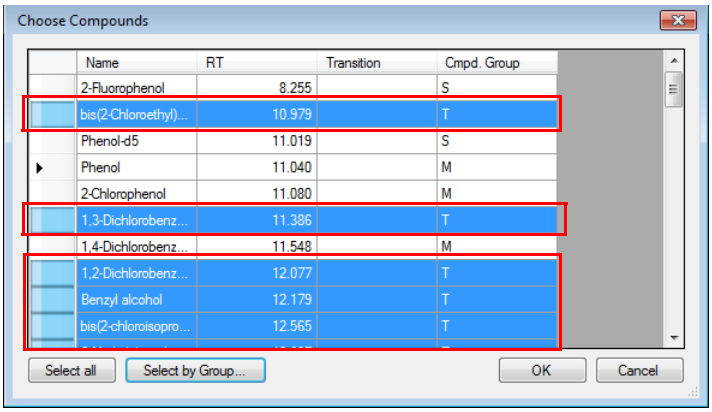
5. Select the samples to be included in the report and click **OK**.



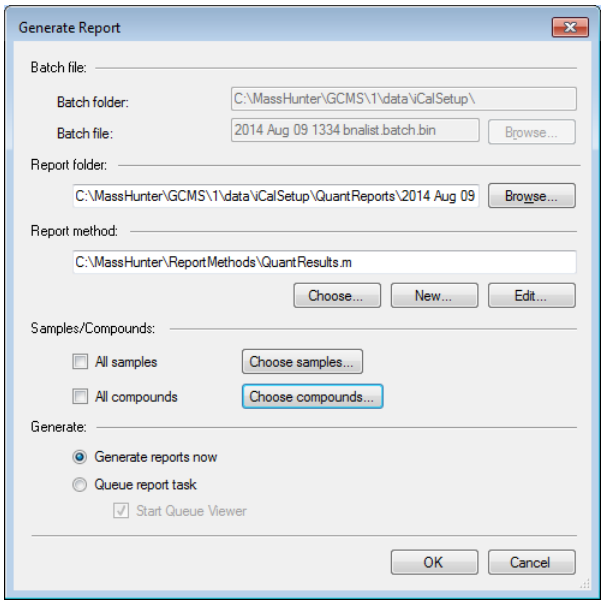
6. To limit the number of compounds to include in the report, click **Choose compounds**.



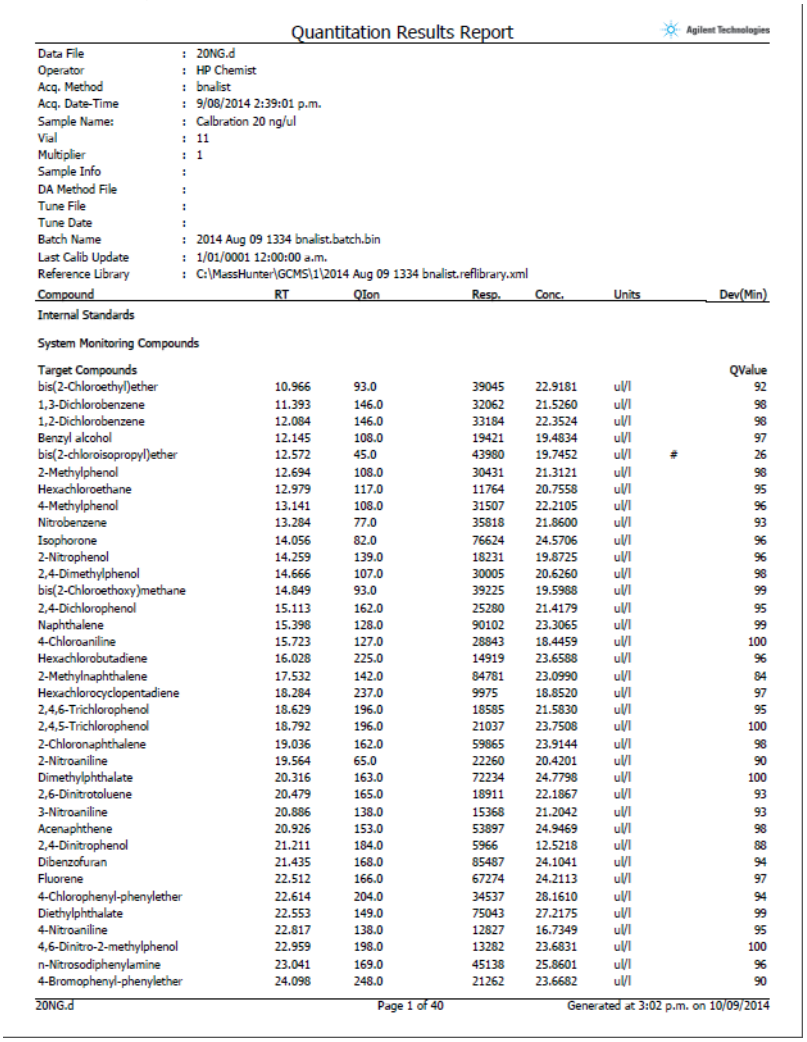
7. Select the compounds to be included in the report then click **OK**. (In this example we selected the compounds by target group.)



8. Click **OK** to generate the report.



The report is generated.



Quantitation Results Report

Agilent Technologies

Data File	:	20NG.d
Operator	:	HP Chemist
Acq. Method	:	bnalist
Acq. Date-Time	:	9/08/2014 2:39:01 p.m.
Sample Name:	:	Calbration 20 ng/ul
Vial	:	11
Multiplier	:	1
Sample Info	:	
DA Method File	:	
Tune File	:	
Tune Date	:	
Batch Name	:	2014 Aug 09 1334 bnalist.batch.bin
Last Calib Update	:	1/01/0001 12:00:00 a.m.
Reference Library	:	C:\MassHunter\GCMS\1\2014 Aug 09 1334 bnalist.reflibrary.xml

Compound	RT	QIon	Resp.	Conc.	Units		Dev(Min)
Internal Standards							
System Monitoring Compounds							
Target Compounds							QValue
bis(2-Chloroethyl)ether	10.966	93.0	39045	22.9181	ul/l		92
1,3-Dichlorobenzene	11.393	146.0	32062	21.5260	ul/l		98
1,2-Dichlorobenzene	12.084	146.0	33184	22.3524	ul/l		98
Benzyl alcohol	12.145	108.0	19421	19.4834	ul/l		97
bis(2-chloroisopropyl)ether	12.572	45.0	43980	19.7452	ul/l	#	26
2-Methylphenol	12.694	108.0	30431	21.3121	ul/l		98
Hexachloroethane	12.979	117.0	11764	20.7558	ul/l		95
4-Methylphenol	13.141	108.0	31507	22.2105	ul/l		96
Nitrobenzene	13.284	77.0	35818	21.8600	ul/l		93
Isophorone	14.056	82.0	76624	24.5706	ul/l		96
2-Nitrophenol	14.259	139.0	18231	19.8725	ul/l		96
2,4-Dimethylphenol	14.666	107.0	30005	20.6260	ul/l		98
bis(2-Chloroethoxy)methane	14.849	93.0	39225	19.5988	ul/l		99
2,4-Dichlorophenol	15.113	162.0	25280	21.4179	ul/l		95
Naphthalene	15.398	128.0	90102	23.3065	ul/l		99
4-Chloroaniline	15.723	127.0	28843	18.4459	ul/l		100
Hexachlorobutadiene	16.028	225.0	14919	23.6588	ul/l		96
2-Methylnaphthalene	17.532	142.0	84781	23.0990	ul/l		84
Hexachlorocyclopentadiene	18.284	237.0	9975	18.8520	ul/l		97
2,4,6-Trichlorophenol	18.629	196.0	18585	21.5830	ul/l		95
2,4,5-Trichlorophenol	18.792	196.0	21037	23.7508	ul/l		100
2-Chloronaphthalene	19.036	162.0	59865	23.9144	ul/l		98
2-Nitroaniline	19.564	65.0	22260	20.4201	ul/l		90
Dimethylphthalate	20.316	163.0	72234	24.7798	ul/l		100
2,6-Dinitrotoluene	20.479	165.0	18911	22.1867	ul/l		93
3-Nitroaniline	20.886	138.0	15368	21.2042	ul/l		93
Acenaphthene	20.926	153.0	53897	24.9469	ul/l		98
2,4-Dinitrophenol	21.211	184.0	5966	12.5218	ul/l		88
Dibenzofuran	21.435	168.0	85487	24.1041	ul/l		94
Fluorene	22.512	166.0	67274	24.2113	ul/l		97
4-Chlorophenyl-phenylether	22.614	204.0	34537	28.1610	ul/l		94
Diethylphthalate	22.553	149.0	75043	27.2175	ul/l		99
4-Nitroaniline	22.817	138.0	12827	16.7349	ul/l		95
4,6-Dinitro-2-methylphenol	22.959	198.0	13282	23.6831	ul/l		100
n-Nitrosodiphenylamine	23.041	169.0	45138	25.8601	ul/l		96
4-Bromophenyl-phenylether	24.098	248.0	21262	23.6682	ul/l		90

20NG.d Page 1 of 40 Generated at 3:02 p.m. on 10/09/2014

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.

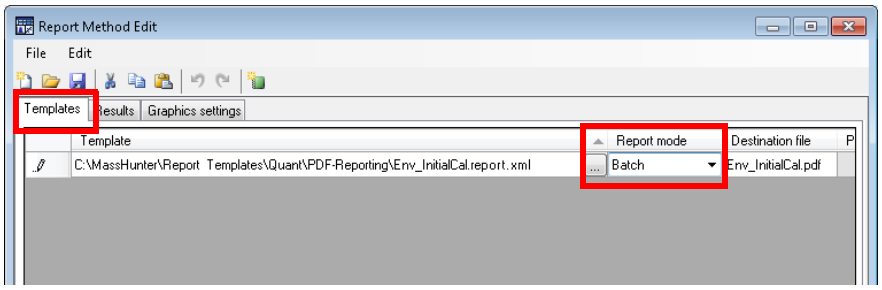
3. Click the **Results** tab and select **GCMS** for a single quad instrument.

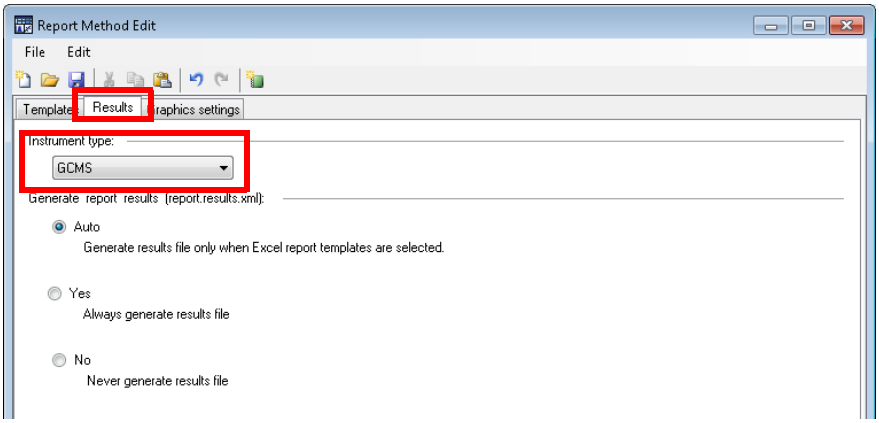
4. Skip the **Generate report results** section since this is a PDF report.

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.

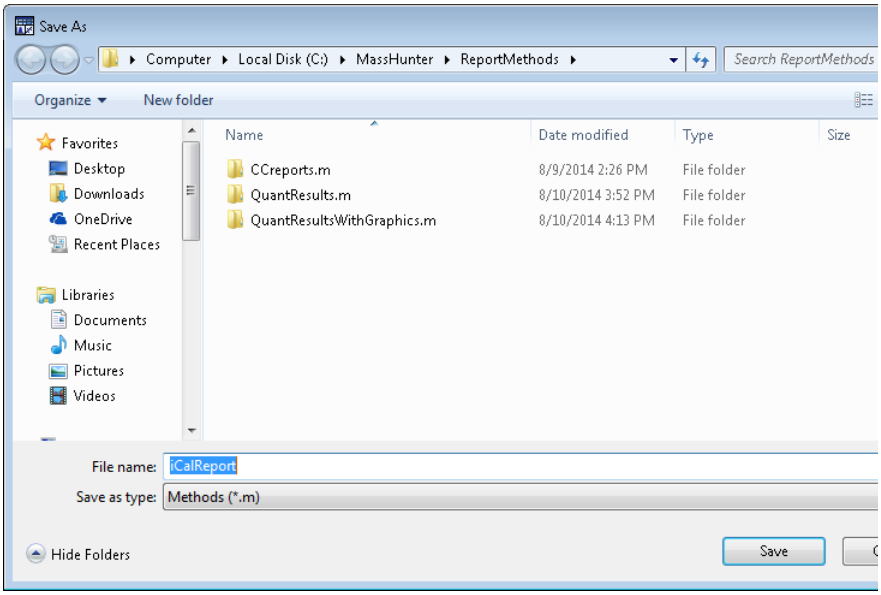
When this method is run, the report is saved as Env_InitCal.pdf. This report is located in a subfolder of QuantReports folder in the batch directory. The subfolder has the same name as the batch with a numbered prefix.





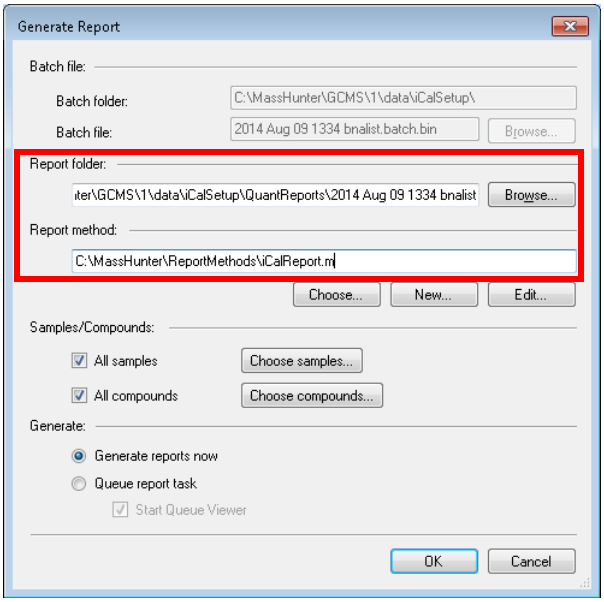
A pdf report does not allow graphic customizations found in the **Graphic settings** tab. Custom settings found in the **Graphic Settings** tab are used with excel templates only.

5. Click **Save & Exit**, then navigate to the ReportMethods directory and name the method **iCalReport.m**.



6. Click **Save** to return to the Generate Report dialog.

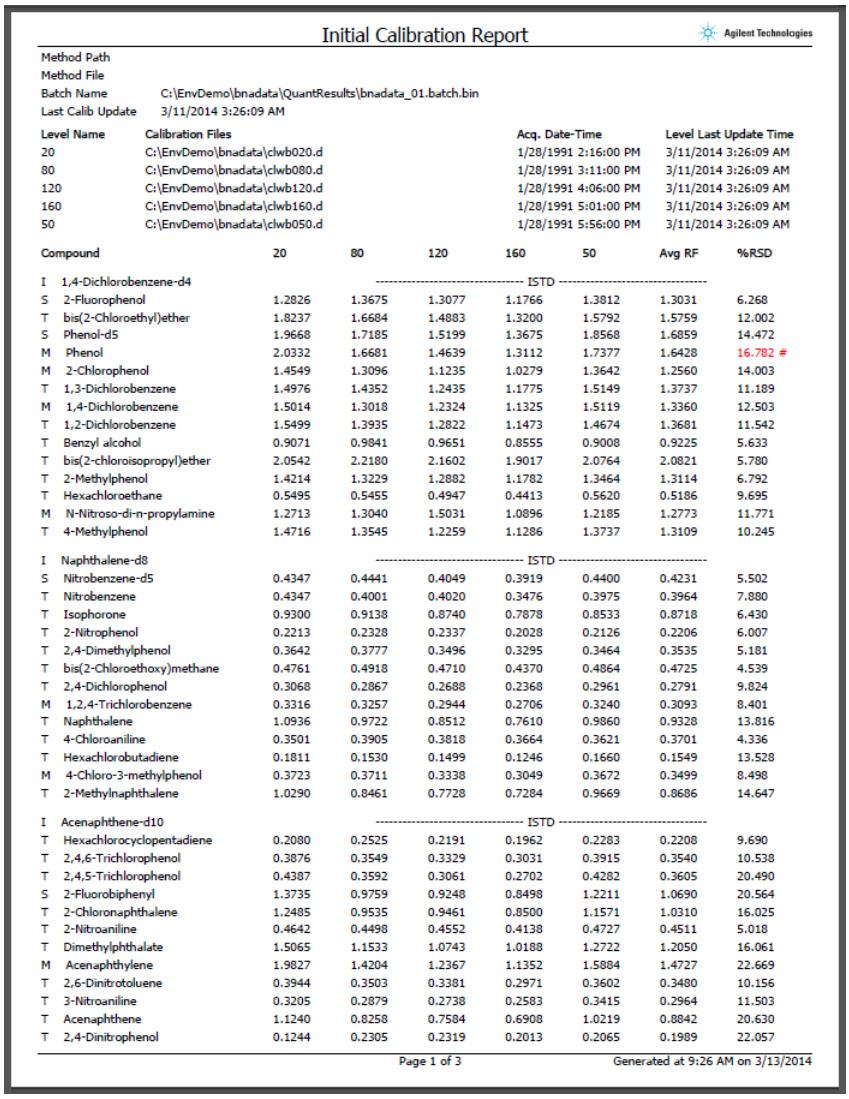
The system displays the path to the Report folder based on the current batch location loaded in MassHunter Quant. The **Report method** shows the location that you selected when you saved the report method.



7. Click **Cancel** and the report method is available for interactive generation.

An Initial Calibration Report is always generated interactively in Quant since it reports on all the calibration samples in the batch. An automated report generated by a sequence can only report on a single sample.

The first page of an Initial Calibration PDF report is shown on the next page.



Initial Calibration Report

Agilent Technologies

Method Path
Method File
Batch Name C:\EnvDemo\bnadata\QuantResults\bnadata_01.batch.bin
Last Calib Update 3/11/2014 3:26:09 AM

Level Name	Calibration Files	Acq. Date-Time	Level Last Update Time
20	C:\EnvDemo\bnadata\clwb020.d	1/28/1991 2:16:00 PM	3/11/2014 3:26:09 AM
80	C:\EnvDemo\bnadata\clwb080.d	1/28/1991 3:11:00 PM	3/11/2014 3:26:09 AM
120	C:\EnvDemo\bnadata\clwb120.d	1/28/1991 4:06:00 PM	3/11/2014 3:26:09 AM
160	C:\EnvDemo\bnadata\clwb160.d	1/28/1991 5:01:00 PM	3/11/2014 3:26:09 AM
50	C:\EnvDemo\bnadata\clwb050.d	1/28/1991 5:56:00 PM	3/11/2014 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	1.5499	1.3935	1.2822	1.1473	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	0.3777	0.3496	0.3295	0.3464	0.3535	5.181
T	bis(2-Chloroethoxy)methane	0.4761	0.4918	0.4710	0.4370	0.4864	0.4725	4.539
T	2,4-Dichlorophenol	0.3068	0.2867	0.2688	0.2368	0.2961	0.2791	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	20.564
T	2-Chloronaphthalene	1.2485	0.9535	0.9461	0.8500	1.1571	1.0310	16.025
T	2-Nitroaniline	0.4642	0.4498	0.4552	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	1.9827	1.4204	1.2367	1.1352	1.5884	1.4727	22.669
T	2,6-Dinitrotoluene	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

Page 1 of 3 Generated at 9:26 AM on 3/13/2014

The first page of an Initial Calibration PDF report.

Step 3: Create a Quant Report Method.

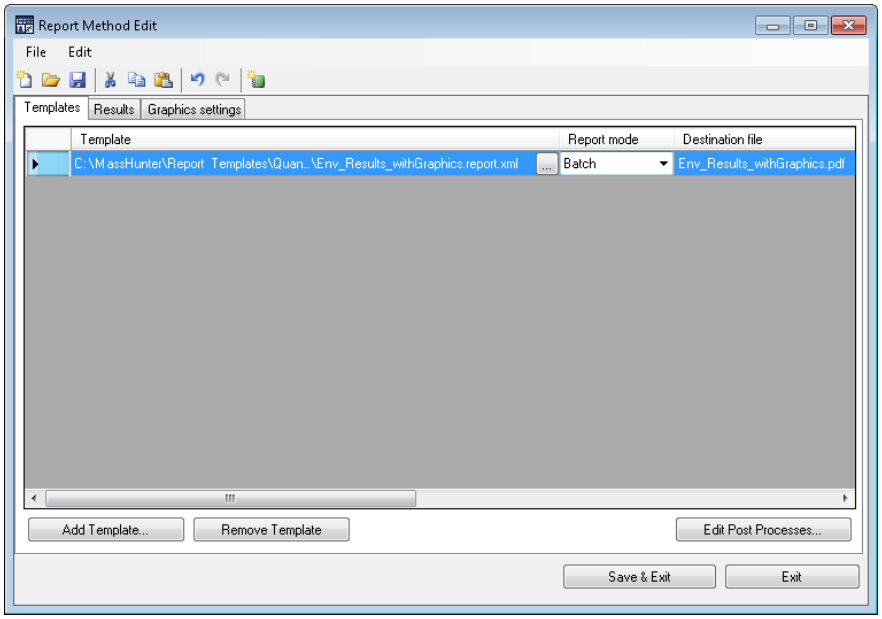
1. In the **Report Method Edit** dialog, click **Add template**, navigate to the PDF-Reporting folder.

2. For this example we are selecting **Env_Results_withGraphics.report.xml** for a report with graphics. However, alternatively, you may select **Env_Results.report.xml** for a simple report.

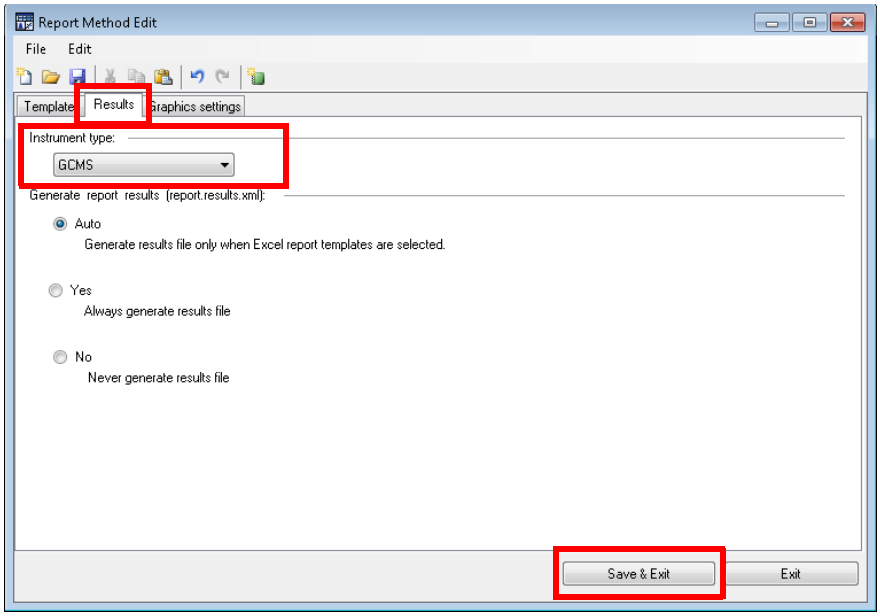
3. For this example, leave the default entries on the **Template** tab as they are.

You can create a simple Quant Report without graphics, or a detailed report containing graphics. This section explains creating both types.

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.



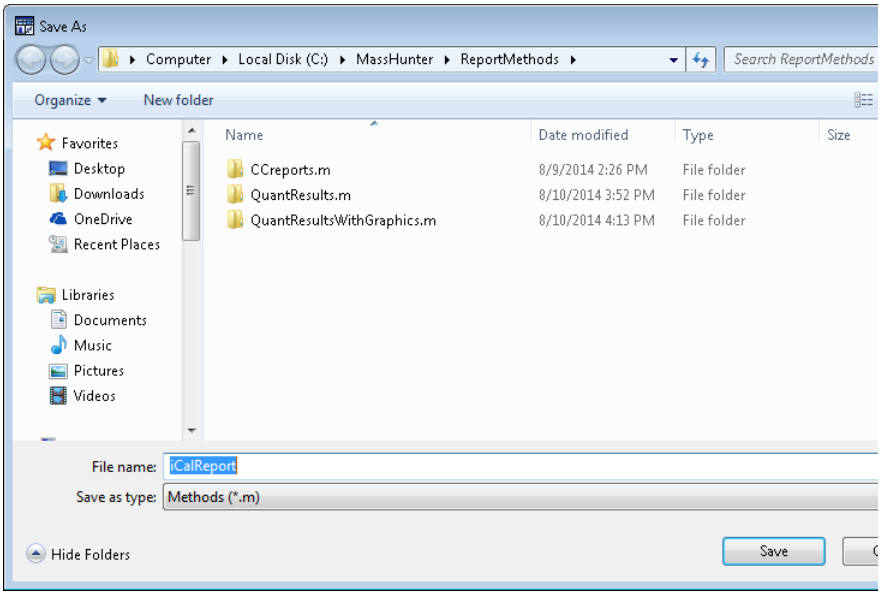
4. Click the **Results** tab and select **GCMS** for a single quad instrument.



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

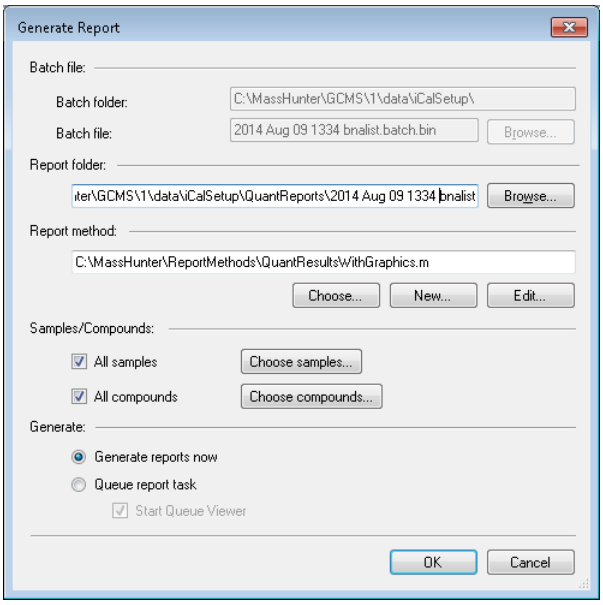
6. Click **Save & Exit**, then navigate to the ReportMethods directory and name the method **QuantReportGraphics.m**.



7. Click **Cancel** and the Report method is available for automatic generation via the sequencing table or for selection during interactive report generation in Quant.

The Report folder shows the path based on the current batch loaded in MassHunter Quant.

The Report method is the location that you selected when you saved the report method.



A sample of the Quantitation Results Report is on the next page.

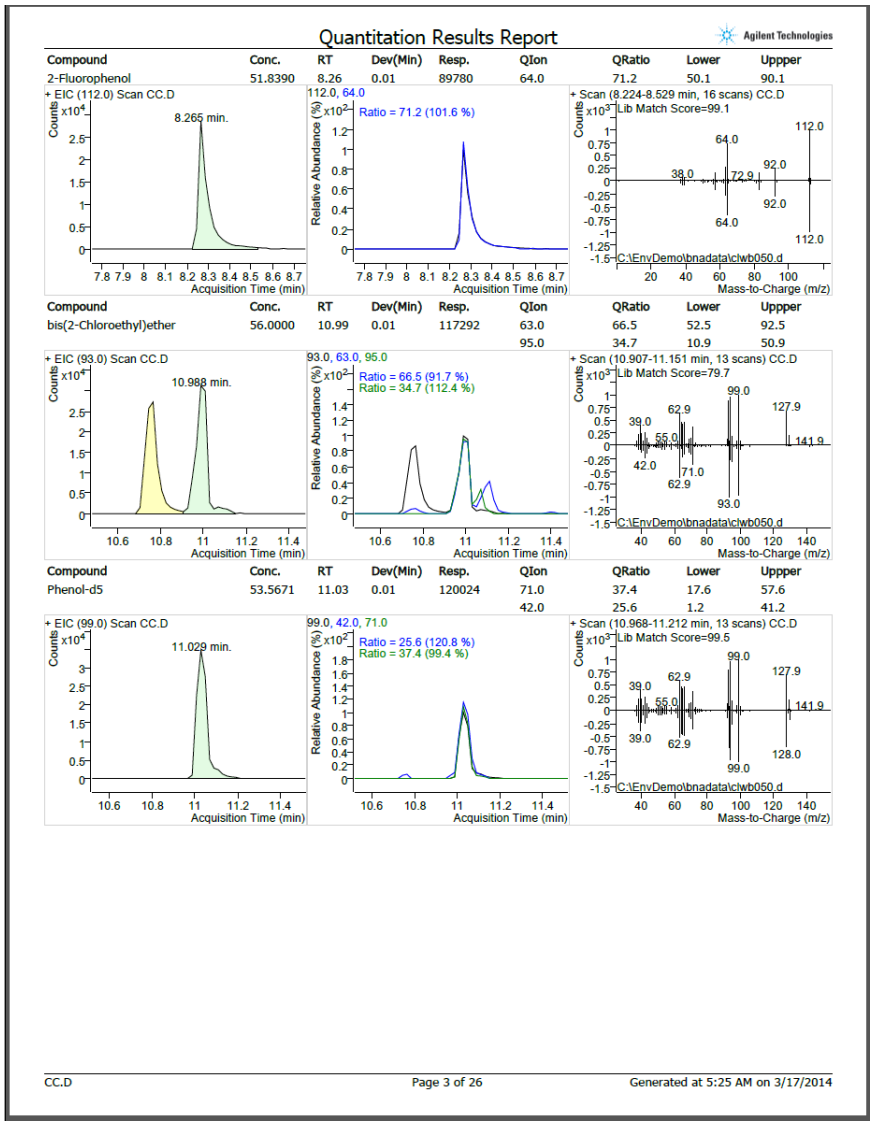
Quantitation Results Report

Agilent Technologies

Data File	:	CC.D
Operator	:	HP Chemist
Acq. Method	:	8260C
Acq. Date-Time	:	3/26/2014 6:29:08 PM
Sample Name:	:	CC
Vial	:	2
Multiplier	:	1
Sample Info	:	
DA Method File	:	8260C.M
Tune File	:	
Tune Date	:	
Batch Name	:	2014 Mar 26 1741 8260C.batch.bin
Last Calib Update	:	3/26/2014 5:36:18 PM

Compound	RT	QIon	Resp.	Conc.	Units		Dev(Min)
Internal Standards							
Bromochloromethane	7.953	128.0	11753	50.0000	ug/l	#	0.000
1,4-Difluorobenzene	18.189	114.0	66432	50.0000	ug/l		0.000
Chlorobenzene-d5	22.959	117.0	56912	50.0000	ug/l		0.000
System Monitoring Compounds							
1,2-Dichloroethane-d4	10.783	65.0	27951	49.0124	ug/l		0.000
Spiked Amount: 50.000	Range: 70.0 - 130.0%			Recovery = 98.02%			
Toluene-d8	21.795	98.0	57736	46.9910	ug/l		0.000
Spiked Amount: 50.000	Range: 70.0 - 130.0%			Recovery = 93.98%			
Bromofluorobenzene	26.720	95.0	60889	47.8139	ug/l		0.000
Spiked Amount: 50.000	Range: 70.0 - 130.0%			Recovery = 95.63%			
Target Compounds							QValue
Chloromethane	0.935	50.0	22697	56.5783	ug/l		96
Bromomethane	1.595	94.0	20107	50.3441	ug/l		94
Vinyl Chloride	2.060	62.0	24364	52.9130	ug/l		100
Chloroethane	2.796	64.0	15845	55.8761	ug/l		95
Methylene Chloride	4.657	84.0	25338	52.1980	ug/l		94
Acetone	5.278	43.0	5973	62.2877	ug/l		97
Carbon Disulfide	6.053	76.0	67619	48.7868	ug/l		100
1,1-Dichloroethene	7.410	96.0	22503	52.3404	ug/l		97
1,1-Dichloroethane	8.728	63.0	53766	50.7923	ug/l		95
1,2-Dichloroethene (total)	9.542	96.0	49055	52.0435	ug/l		96
Chloroform	10.163	83.0	54361	51.6489	ug/l		94
2-Butanone	10.822	43.0	10586	48.1767	ug/l		94
1,2-Dichloroethane	10.900	62.0	34902	49.6957	ug/l		96
1,1,1-Trichloroethane	12.063	97.0	42530	48.1024	ug/l		94
Carbon Tetrachloride	12.451	117.0	34876	46.9982	ug/l		98
Vinyl Acetate	12.722	43.0	76597	49.2078	ug/l		100
Bromodichloromethane	13.148	83.0	50509	48.2418	ug/l		94
1,2-Dichloropropane	14.350	63.0	38472	48.2057	ug/l		99
cis-1,3-Dichloropropene	14.661	75.0	55677	49.2258	ug/l		98
Trichloroethene	15.242	130.0	27706	49.4570	ug/l		98
Benzene	15.630	78.0	76861	48.8134	ug/l		100
Dibromochloromethane	15.902	129.0	31823	47.9801	ug/l		98
trans-1,3-Dichloropropene	15.979	75.0	21542	44.7259	ug/l		74
1,1,2-Trichloroethane	15.979	97.0	24769	51.5477	ug/l		99
Bromoform	18.577	173.0	18220	45.8956	ug/l		92
4-Methyl-2-Pentanone	18.926	43.0	29316	47.7556	ug/l		97
2-Hexanone	20.438	43.0	18294	48.1704	ug/l		95
Tetrachloroethene	20.787	164.0	21623	46.3880	ug/l		98

The first page of a simple Quantitation Results PDF report.

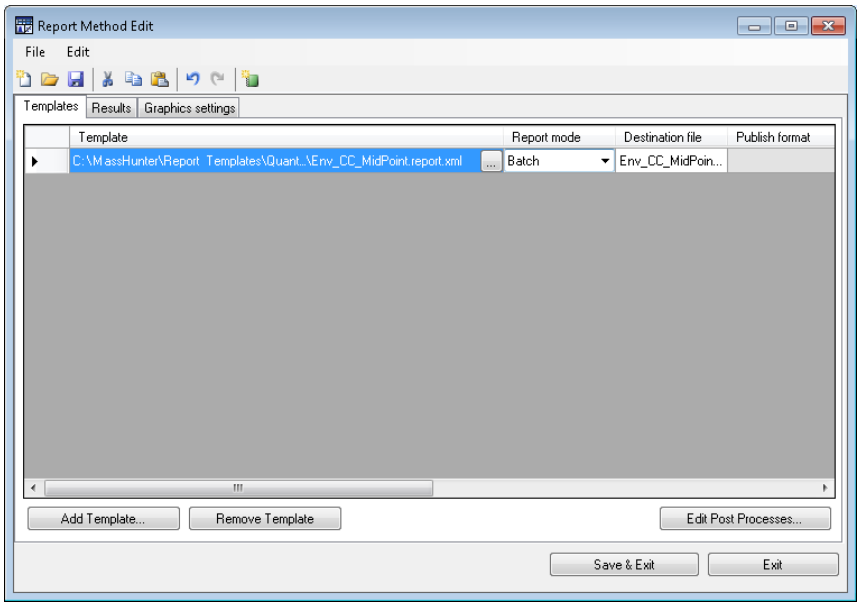


The third page of a detailed Quantitation Results PDF report.

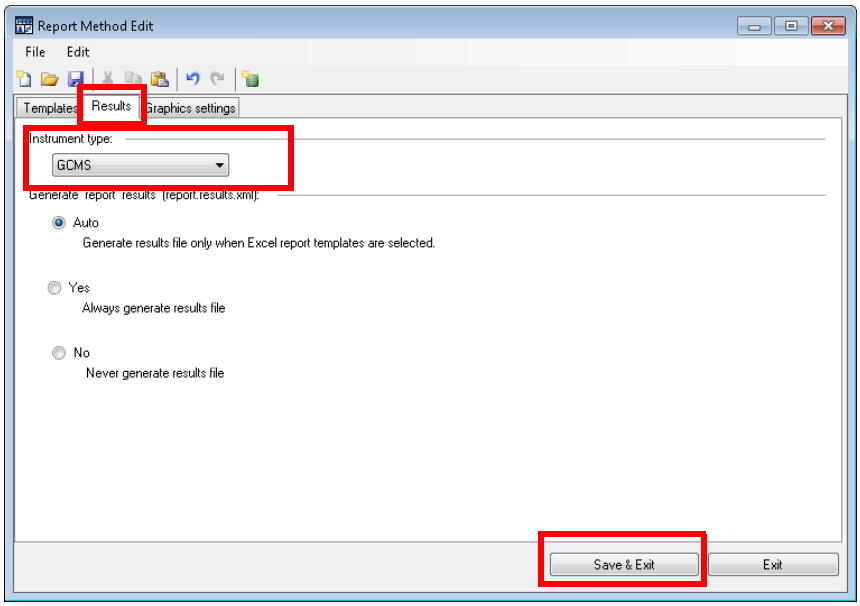
Step 4: Create a Continuing Calibration Report Method.

1. In the **Report Method Edit** dialog, click **Add template**, navigate to the PDF-Reporting folder and select **Env_CC_MidPoint.report.xml**.

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



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

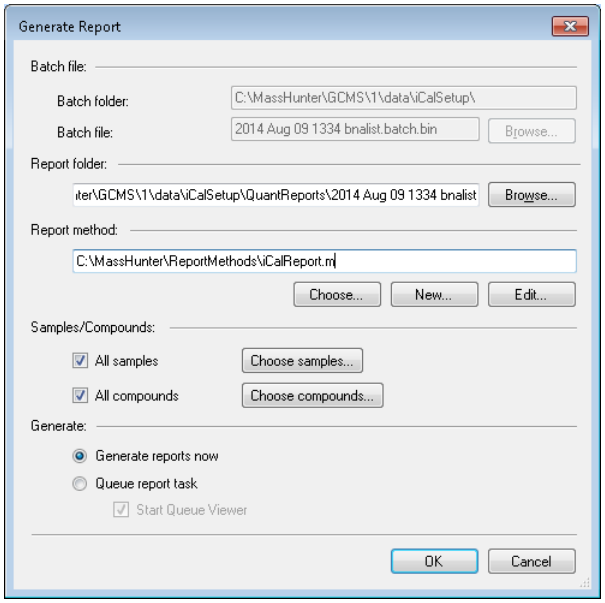


3. Ignore the **Generate report results** section since this is a PDF report file.

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.

4. Click **Save & Exit**, navigate to the ReportMethods directory and name the method **iCalReport.m**.

5. Click **Save** to return to the Generate Report dialog.



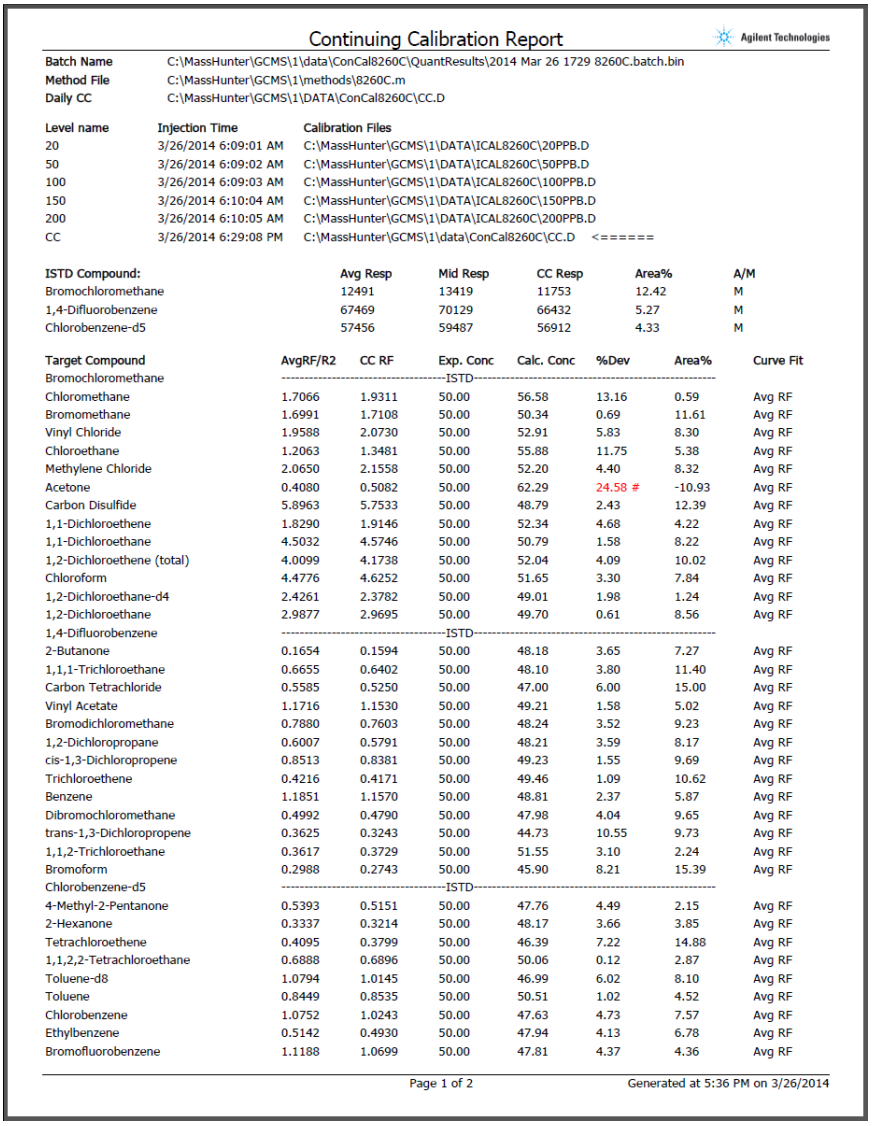
The **Report folder** displays the path to the report folder based on the current batch location loaded in MassHunter Quant.

The **Report method** 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.

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



Continuing Calibration Report

Agilent Technologies

Batch Name	C:\MassHunter\GCMS\1\data\ConCal8260C\QuantResults\2014 Mar 26 1729 8260C.batch.bin
Method File	C:\MassHunter\GCMS\1\methods\8260C.m
Daily CC	C:\MassHunter\GCMS\1\DATA\ConCal8260C\CC.D

Level name	Injection Time	Calibration Files
20	3/26/2014 6:09:01 AM	C:\MassHunter\GCMS\1\DATA\ICAL8260C\20PPB.D
50	3/26/2014 6:09:02 AM	C:\MassHunter\GCMS\1\DATA\ICAL8260C\50PPB.D
100	3/26/2014 6:09:03 AM	C:\MassHunter\GCMS\1\DATA\ICAL8260C\100PPB.D
150	3/26/2014 6:10:04 AM	C:\MassHunter\GCMS\1\DATA\ICAL8260C\150PPB.D
200	3/26/2014 6:10:05 AM	C:\MassHunter\GCMS\1\DATA\ICAL8260C\200PPB.D
CC	3/26/2014 6:29:08 PM	C:\MassHunter\GCMS\1\data\ConCal8260C\CC.D <======

ISTD Compound:	Avg Resp	Mid Resp	CC Resp	Area%	A/M
Bromochloromethane	12491	13419	11753	12.42	M
1,4-Difluorobenzene	67469	70129	66432	5.27	M
Chlorobenzene-d5	57456	59487	56912	4.33	M

Target Compound	AvgRF/R2	CC RF	Exp. Conc	Calc. Conc	%Dev	Area%	Curve Fit
Bromochloromethane	----------ISTD----------						
Chloromethane	1.7066	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	5.8963	5.7533	50.00	48.79	2.43	12.39	Avg RF
1,1-Dichloroethene	1.8290	1.9146	50.00	52.34	4.68	4.22	Avg RF
1,1-Dichloroethane	4.5032	4.5746	50.00	50.79	1.58	8.22	Avg RF
1,2-Dichloroethene (total)	4.0099	4.1738	50.00	52.04	4.09	10.02	Avg RF
Chloroform	4.4776	4.6252	50.00	51.65	3.30	7.84	Avg RF
1,2-Dichloroethane-d4	2.4261	2.3782	50.00	49.01	1.98	1.24	Avg RF
1,2-Dichloroethane	2.9877	2.9695	50.00	49.70	0.61	8.56	Avg RF
1,4-Difluorobenzene	----------ISTD----------						
2-Butanone	0.1654	0.1594	50.00	48.18	3.65	7.27	Avg RF
1,1,1-Trichloroethane	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
Bromodichloromethane	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-Dichloropropene	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	1.1851	1.1570	50.00	48.81	2.37	5.87	Avg RF
Dibromochloromethane	0.4992	0.4790	50.00	47.98	4.04	9.65	Avg RF
trans-1,3-Dichloropropene	0.3625	0.3243	50.00	44.73	10.55	9.73	Avg RF
1,1,2-Trichloroethane	0.3617	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-Pentanone	0.5393	0.5151	50.00	47.76	4.49	2.15	Avg RF
2-Hexanone	0.3337	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-Tetrachloroethane	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	0.8449	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	0.5142	0.4930	50.00	47.94	4.13	6.78	Avg RF
Bromofluorobenzene	1.1188	1.0699	50.00	47.81	4.37	4.36	Avg RF

Page 1 of 2 Generated at 5:36 PM on 3/26/2014

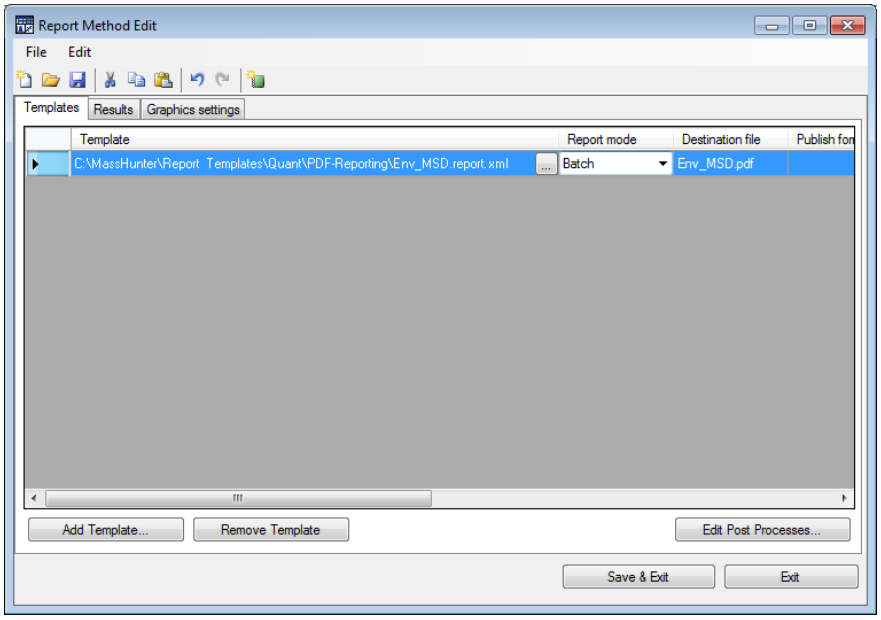
The first page of a Continuing Calibration PDF report.

Step 5: Create a Matrix Spike Duplicate Report Method.

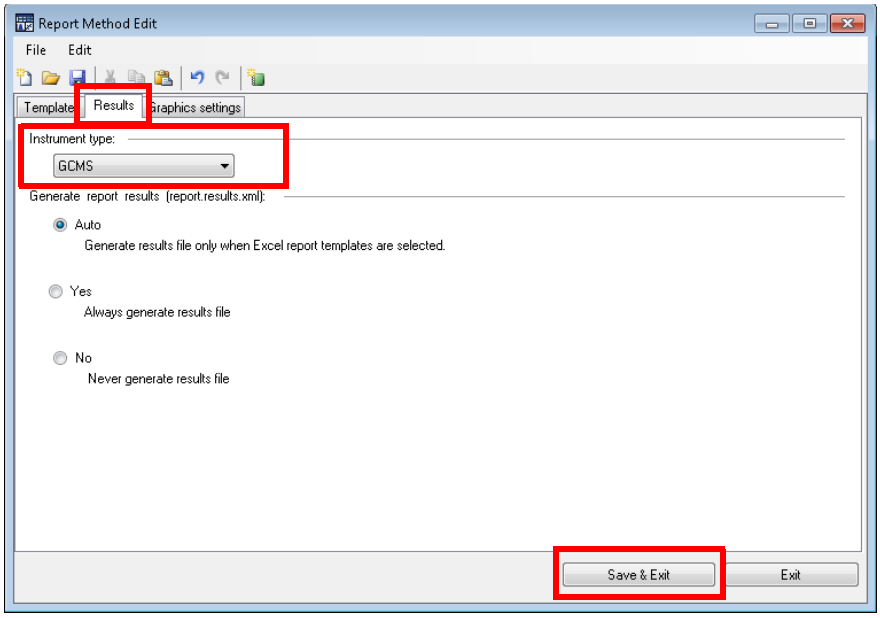
A Matrix Spike Duplicate Report is always generated interactively in Quant since it reports on multiple samples in the batch.

1. In the **Report Method Edit** dialog, click **Add template**, navigate to the PDF-Reporting folder and select **Env_MSD.report.xml**.

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



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

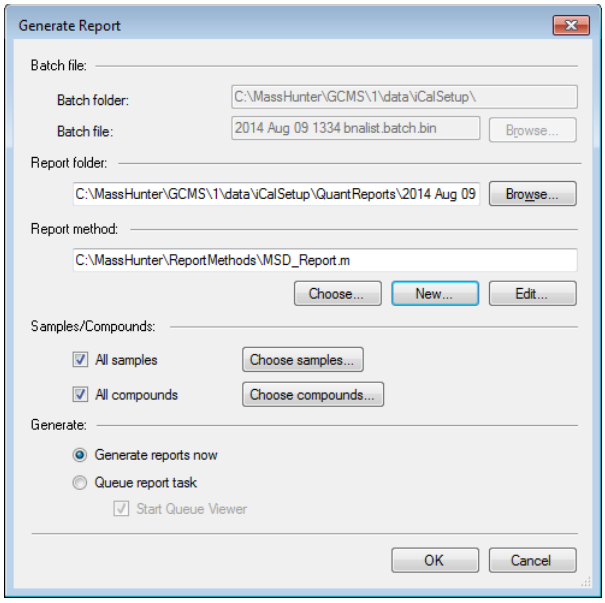


3. Ignore the **Generate report results** section since this is a PDF report file.

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.

4. Click **Save & Exit**, navigate to the ReportMethods directory and name the method **MSD_Report.m**.

5. Click **Save** to return to the Generate Report dialog.



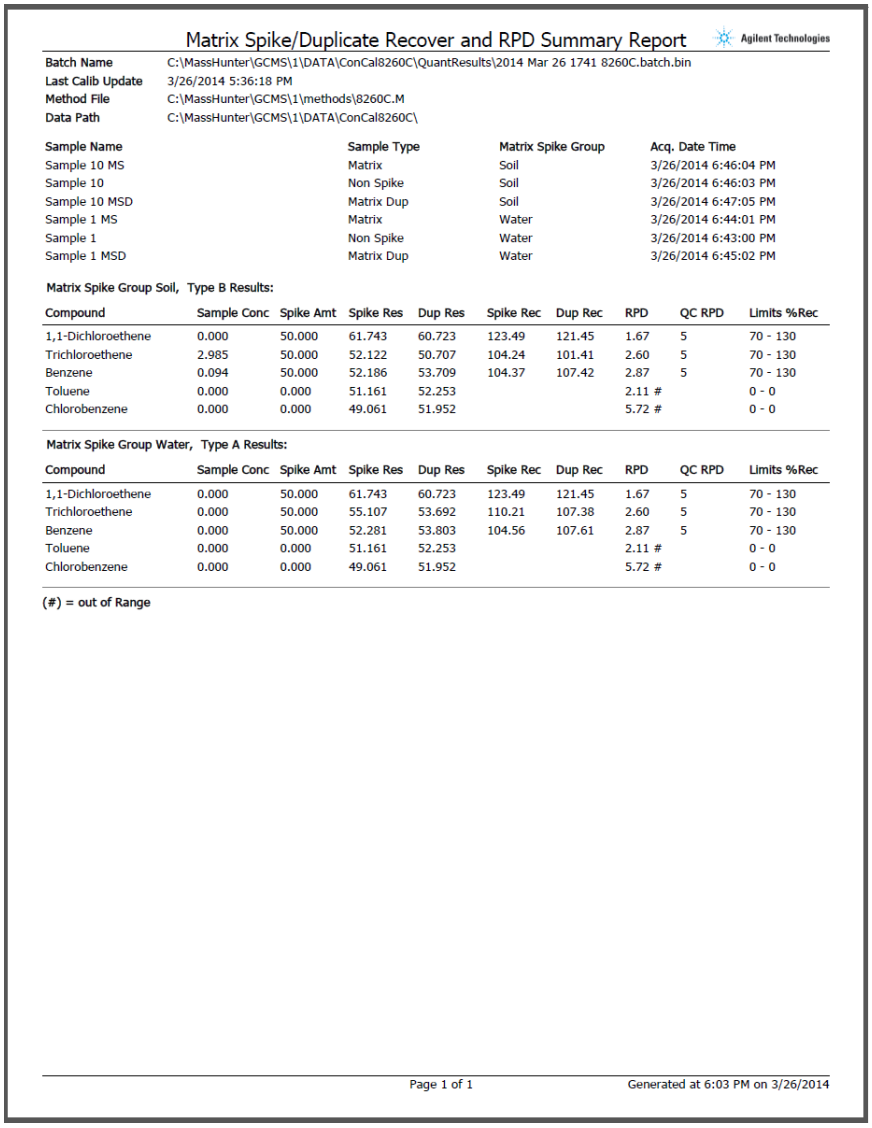
The **Report folder** displays the path to the report folder based on the current batch location loaded in MassHunter Quant.

The **Report method** shown is the location that you selected when saving the report method.

When this method is run, the report is saved in Env_MSD.pdf. This report is located in the batch directories' QuantReports folder in a time stamped folder of the same name as the quant method.

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

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



Matrix Spike/Duplicate Recover and RPD Summary Report

Agilent Technologies

Batch Name	C:\MassHunter\GCMS\1\DATA\ConCal8260C\QuantResults\2014 Mar 26 1741 8260C.batch.bin
Last Calib Update	3/26/2014 5:36:18 PM
Method File	C:\MassHunter\GCMS\1\methods\8260C.M
Data Path	C:\MassHunter\GCMS\1\DATA\ConCal8260C\

Sample Name	Sample Type	Matrix Spike Group	Acq. Date Time
Sample 10 MS	Matrix	Soil	3/26/2014 6:46:04 PM
Sample 10	Non Spike	Soil	3/26/2014 6:46:03 PM
Sample 10 MSD	Matrix Dup	Soil	3/26/2014 6:47:05 PM
Sample 1 MS	Matrix	Water	3/26/2014 6:44:01 PM
Sample 1	Non Spike	Water	3/26/2014 6:43:00 PM
Sample 1 MSD	Matrix Dup	Water	3/26/2014 6:45:02 PM

Matrix Spike Group Soil, Type B Results:

Compound	Sample Conc	Spike Amt	Spike Res	Dup Res	Spike Rec	Dup Rec	RPD	QC RPD	Limits %Rec
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	50.707	104.24	101.41	2.60	5	70 - 130
Benzene	0.094	50.000	52.186	53.709	104.37	107.42	2.87	5	70 - 130
Toluene	0.000	0.000	51.161	52.253			2.11 #		0 - 0
Chlorobenzene	0.000	0.000	49.061	51.952			5.72 #		0 - 0

Matrix Spike Group Water, Type A Results:

Compound	Sample Conc	Spike Amt	Spike Res	Dup Res	Spike Rec	Dup Rec	RPD	QC RPD	Limits %Rec
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	110.21	107.38	2.60	5	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			2.11 #		0 - 0
Chlorobenzene	0.000	0.000	49.061	51.952			5.72 #		0 - 0

(#) = out of Range

Page 1 of 1 Generated at 6:03 PM on 3/26/2014

A Matrix Spike Duplicate PDF report.

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.

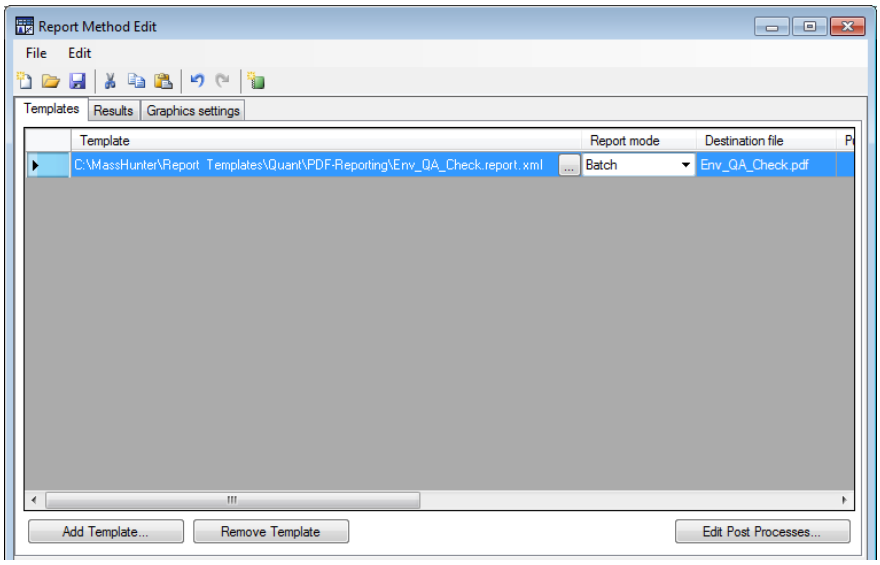
This report will also:

- Check to make sure that the ISTD's areas are within the specified allowable limit compare to the Con Cal ISTDs areas.
- Flag any of the surrogates that do not meet the outlier limits.

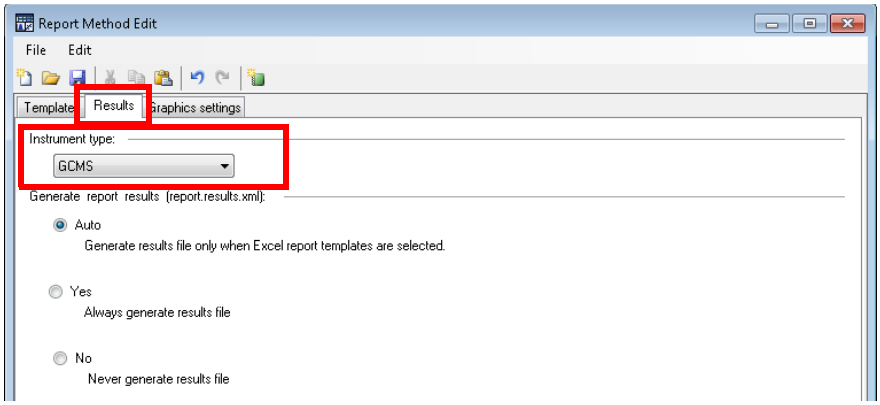
This report is always generated interactively since it operates on all samples in the batch.

1. In the **Report Method Edit** dialog, click **Add template**, navigate to the PDF-Reporting folder and select **Env_QA_Check.report.xml**.

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



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

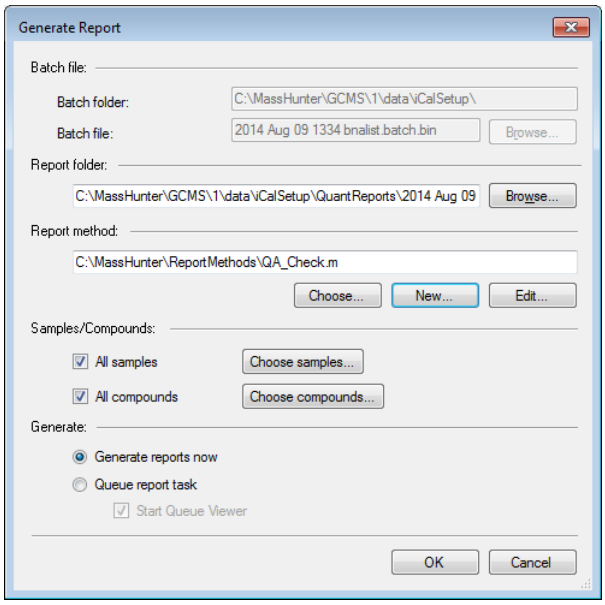


3. Ignore the **Generate report results** section since this is a PDF report file.

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.

4. Click **Save & Exit**, navigate to the ReportMethods directory and name the method **QA_Check.m**.

5. Click **Save** to return to the Generate Report dialog.



The **Report folder** displays the path to the report folder based on the current batch location loaded in MassHunter Quant.

The **Report method** shown is the location that you selected when saving the report Click **Cancel** 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.

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

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

QA Check Report

Agilent Technologies

Batch Name	2014 Mar 26 1741 8260C.batch.bin
Tune Check	C:\MassHunter\GCMS\1\DATA\ConCal8260C\BFB.D
TuneCheck Time	3/26/2014 6:29:07 PM
Time Limit	12 hr

Daily Calibration File: CC.DAcq.Time =3/26/2014 6:29:08 PM

ISTD Name	Bromochloromethane	1,4-Difluorobenzene	Chlorobenzene-d5
ISTD Resp.	11753	66432	56912

Data File: Blank.D, Acq.Time= 3/26/2014 6:42:09 PM

ISTD Name	Bromochloromethane	1,4-Difluorobenzene	Chlorobenzene-d5
ISTD Resp.	11104	62095	54021

Surr Name	1,2-Dichloroethane-d4	Toluene-d8	Bromofluorobenzene
Surr Rec.	96.70	98.17	99.24

Data File: Sample1.D, Acq.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	Bromochloromethane	1,4-Difluorobenzene	Chlorobenzene-d5
ISTD Resp.	12605	73033	64338

Surr Name	1,2-Dichloroethane-d4	Toluene-d8	Bromofluorobenzene
Surr Rec.	106.88	96.91	100.02

Data File: Sample1MSD.D, Acq.Time= 3/26/2014 6:45:02 PM

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

Data File: Sample10.D, Acq.Time= 3/26/2014 6:46:03 PM

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	Bromochloromethane	1,4-Difluorobenzene	Chlorobenzene-d5
ISTD Resp.	12605	73033	64338

Surr Name	1,2-Dichloroethane-d4	Toluene-d8	Bromofluorobenzene
Surr Rec.	106.88	96.91	100.02

Data File: Sample10MSD.D, Acq.Time= 3/26/2014 6:47:05 PM

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

Step 7: Run samples.

Next we will look at some common workflows for running samples in Chapter 7, "Run Samples".

8
Run Samples

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.

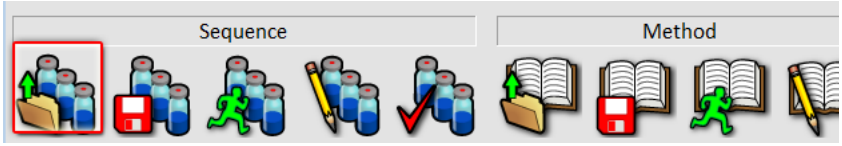
In this example, at the start of the automatic calibration sequence for the initial calibration, we include a Tune Evaluation sample to verify the instrument is within the tune specifications set for EPA method 8270.

The tune evaluation is processed and:

- **If the instrument fails the evaluation**, the sequence will pause for operator intervention.
- **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.

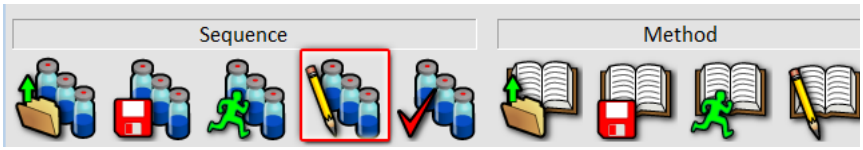
1. Load the default Sequence.

In the Data Acquisition Instrument Control view, click the **Load Sequence** icon then select the **default.sequence.xml** file from your instrument directory sequence folder.



2. Edit the Sequence Table.

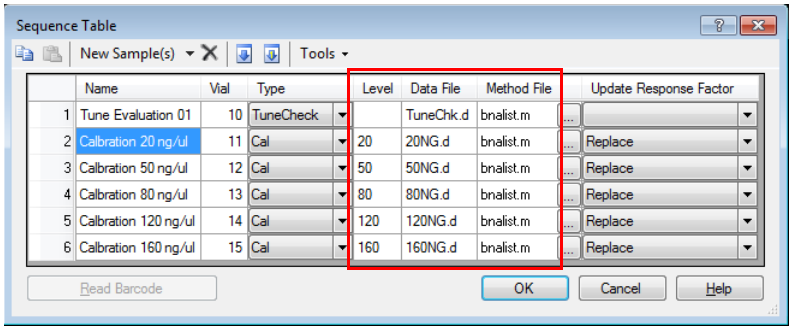
Click the **Edit Sequence** icon to open the Sequence Table for editing.



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.

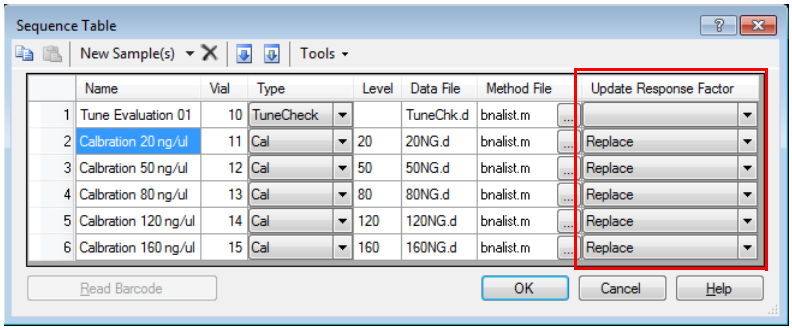
We previously specified that all batch directories will be in the root of the **Data** folder for instrument #1 (**Method > Set New Default Paths**).

7. Fill in the **Method** names as shown.

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.

8. For the Cal samples, set the **Update Response Factor** parameter to **Replace**, and click **OK** to close the sequence table.

This automatically updates the calibration curves in the master method.



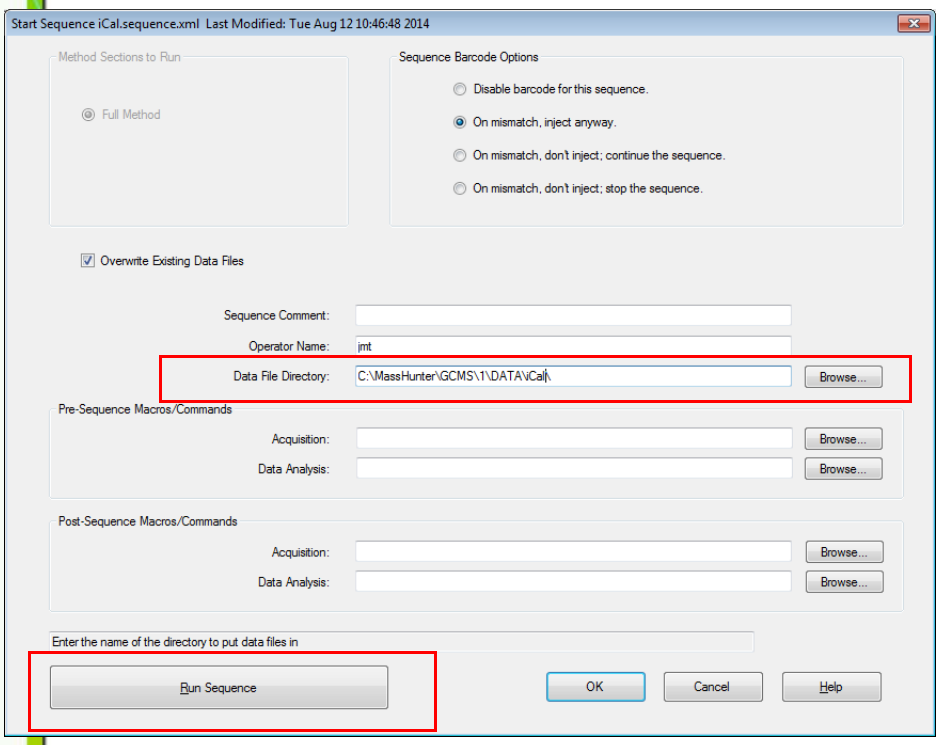
9. Save the completed sequence as **iCal.sequence.xml** for future initial calibrations.

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

The Start Sequence dialog displays.

11. Change the **Data File Directory** name to **iCal**.

This becomes your Quant batch directory.



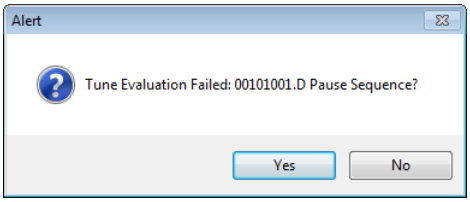
12. Click **Run Sequence** to start the automated acquisition of sample data and generation of reports.

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.

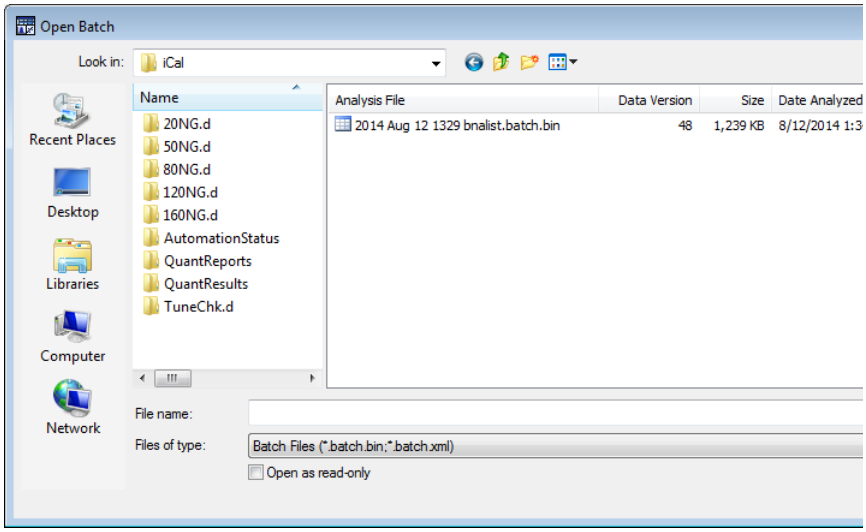
If the Tune Evaluation fails you are given the chance to pause the sequence or continue. EPA method 8270 does not accept quantitation results for samples run after a failed tune evaluation.



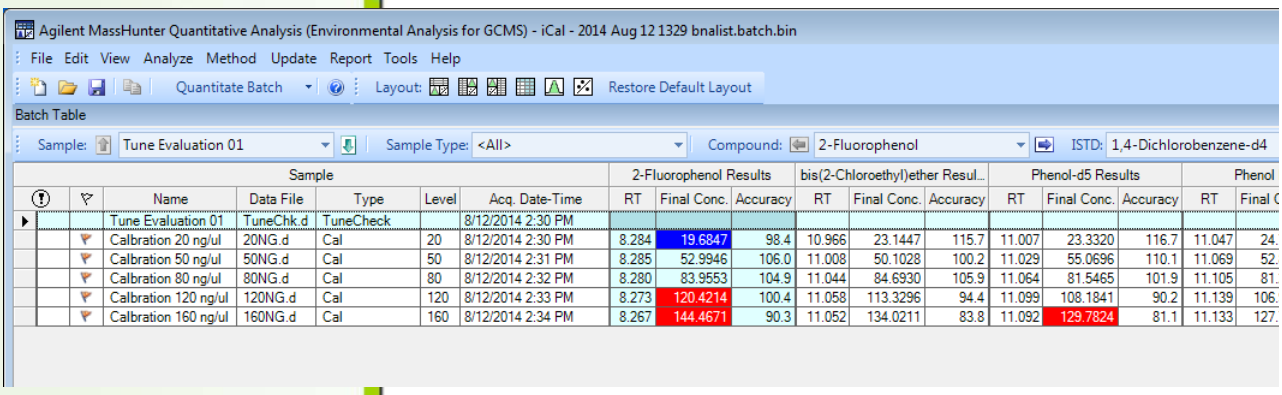
13. When **Sequence Completed** is displayed in the status line, start MassHunter Quantitative analysis.

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

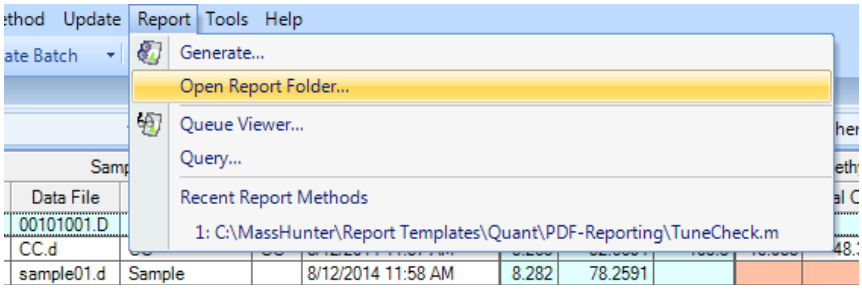
In this example we navigated to the iCal batch folder and selected the time stamped bnalist.batch.bin batch file.



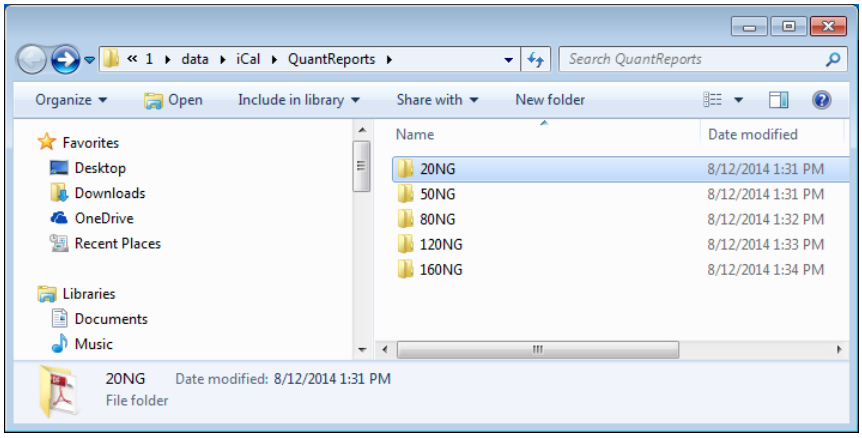
The batch table opens.



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



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.



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.

To comply with EPA method 8270, at the start of the sequence you include a Tune Evaluation sample to verify the instrument is within the tune specifications set for EPA method 8270, followed by a continuing calibration sample to verify the continuing calibration, and then by the unknown samples to be processed.

These are the general steps that occur during daily processing. These are discussed in more detail on the following pages.

1 The Tune Evaluation sample runs.

- If the instrument passes the evaluation, the continuing calibration sample runs.
- If the instrument fails the evaluation, the sequence will pause for operator intervention.

2 The continuing calibration sample runs next to verify the calibration curves for compounds are valid for this sample.

3 After the continuing calibration sample runs, the sequence pauses.

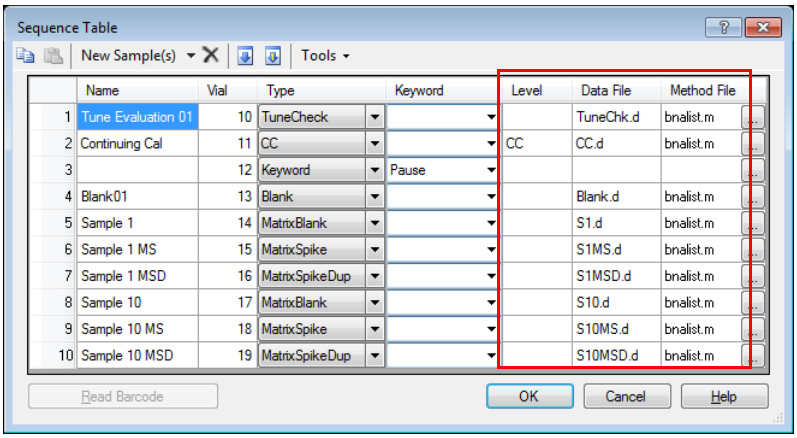
4 The operator reviews the continuing calibration report to verify the calibration is acceptable.

5 If the continuing calibration is acceptable, the Quant method is manually updated with these newly acquired CC responses.

6 The paused sequence is then restarted to process the remaining samples.

1. Open a default sequence, then from the **Tools** menu, select **Add/Remove Columns** and add columns so that the table resembles the example below.

2. Add additional sample rows to the table, name the samples, specify the ALS vial containing the sample, and specify the sample type.



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**).

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**.

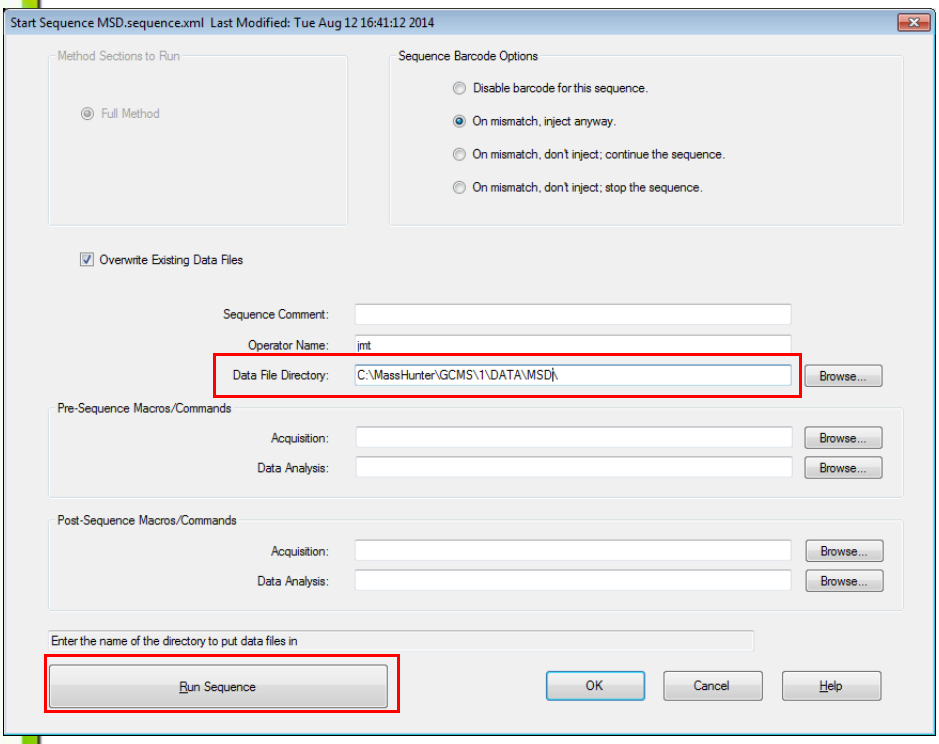
7. Click the **Run Sequence** icon.

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.



The Tune Evaluation sample is processed.

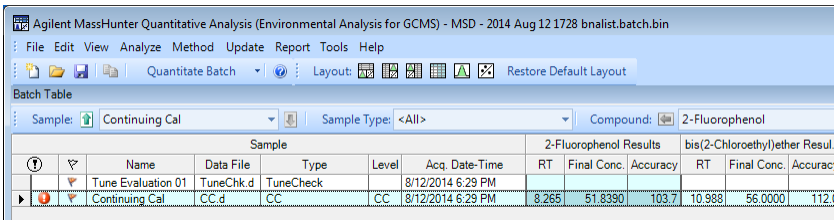
If the tune Evaluation fails, you are given the chance to pause the sequence or continue. EPA method 8270 does not accept quantitation results for samples run after a failed tune evaluation.

If the tune evaluation passes, the Continuing Cal sample is next processed.

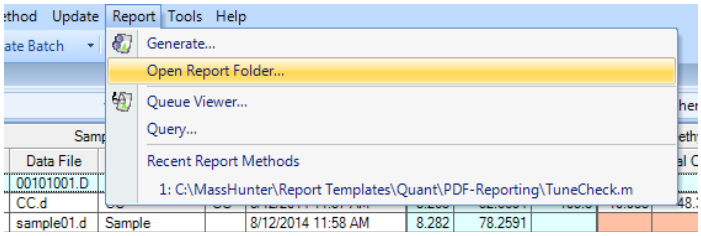
10. When the sequence pauses, from MassHunter Quant select **File > Open batch** and navigate to it.

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

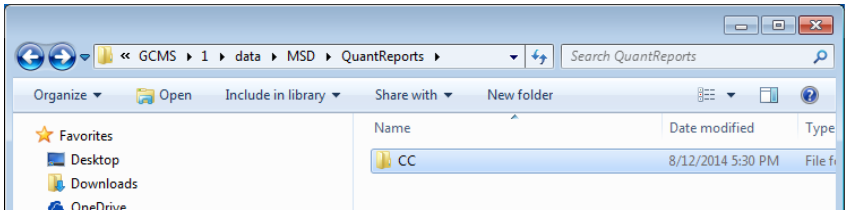
The batch table opens with the Continuing Calibration sample quantitated.



11. Select **Report > Open Report Folder**.



This opens the QuantReports folder with the CC folder that holds the PDF reports.

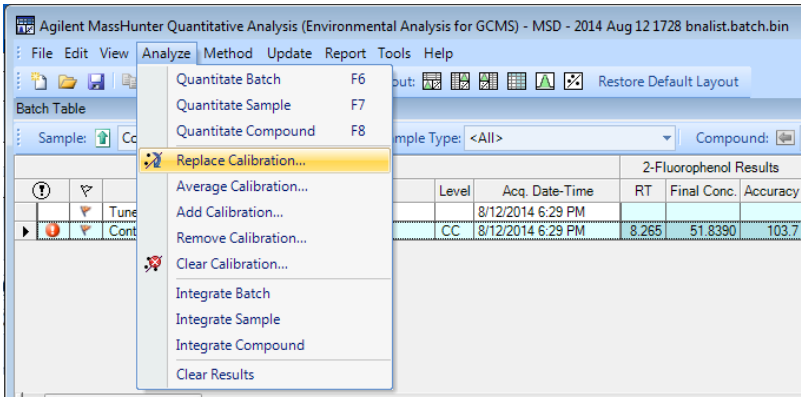


12. Review the Continuing Calibration PDF report.

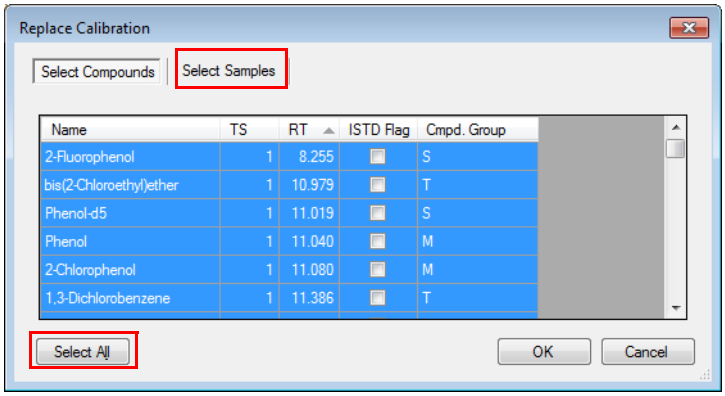
If the Continuing Calibration report shows the instrument is out of calibration, quit this workflow and run an initial calibration before restarting this sample sequence. (See"Step 1: Run a calibration of the instrument." on page 92.)

If the report shows the results are acceptable, replace the CC responses for all compounds with the values in this CC data file in the batch table as shown in the following steps.

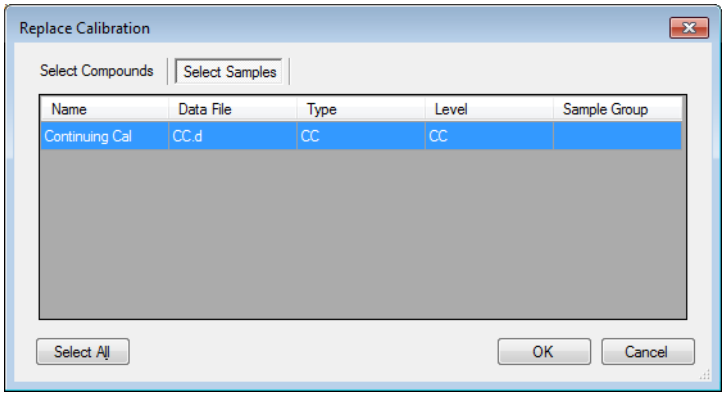
13. Select **Analyze > Replace Calibration.**



14. In the Select Compounds tab, click **Select All** then click the **Select Samples** tab.

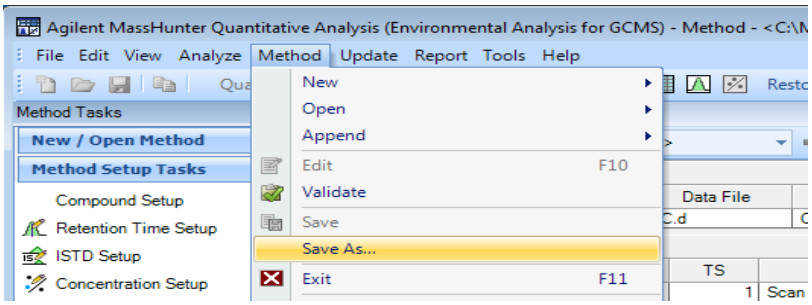


15. On the Select Samples tab, select the **Continuing Cal** sample and click **OK**. The responses for the continuing calibration compounds are replaced with the responses in the data file.

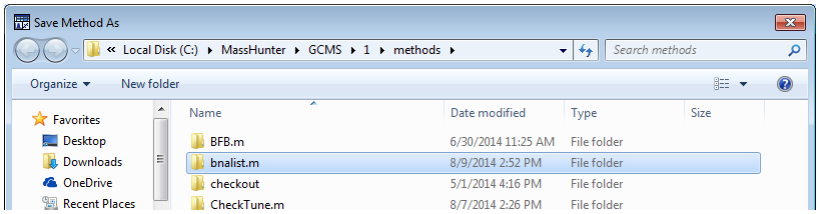


16. Open [**F10**] the method editor.

17. Select **Method > Save As**.



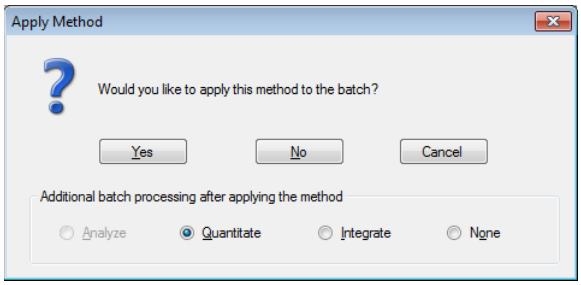
18. Save the method to the original bnalist unified method.



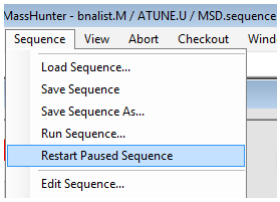
19. When prompted, accept to overwrite the existing method.

Only the Quant part of the method is overwritten.

20. Exit the method editor [**F11**] and when prompted, apply the method to the batch.



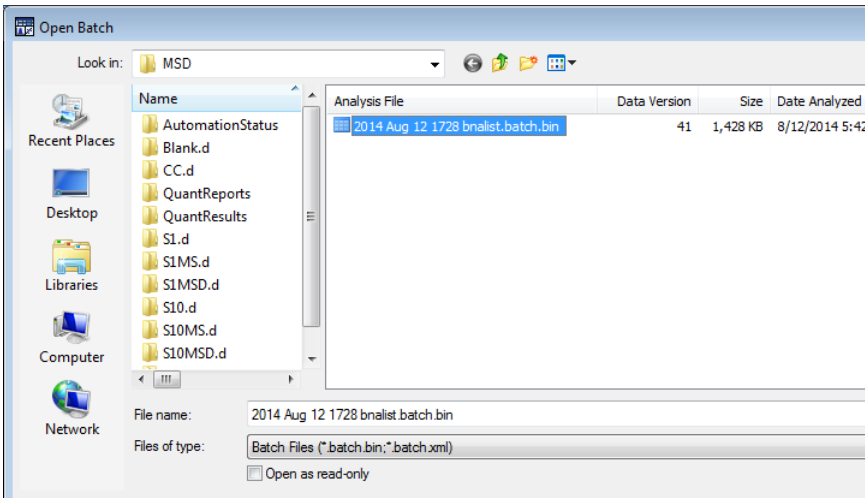
21. In MassHunter Data Acquisition, click **Sequence > Restart Paused Sequence** to resume the paused sequence.



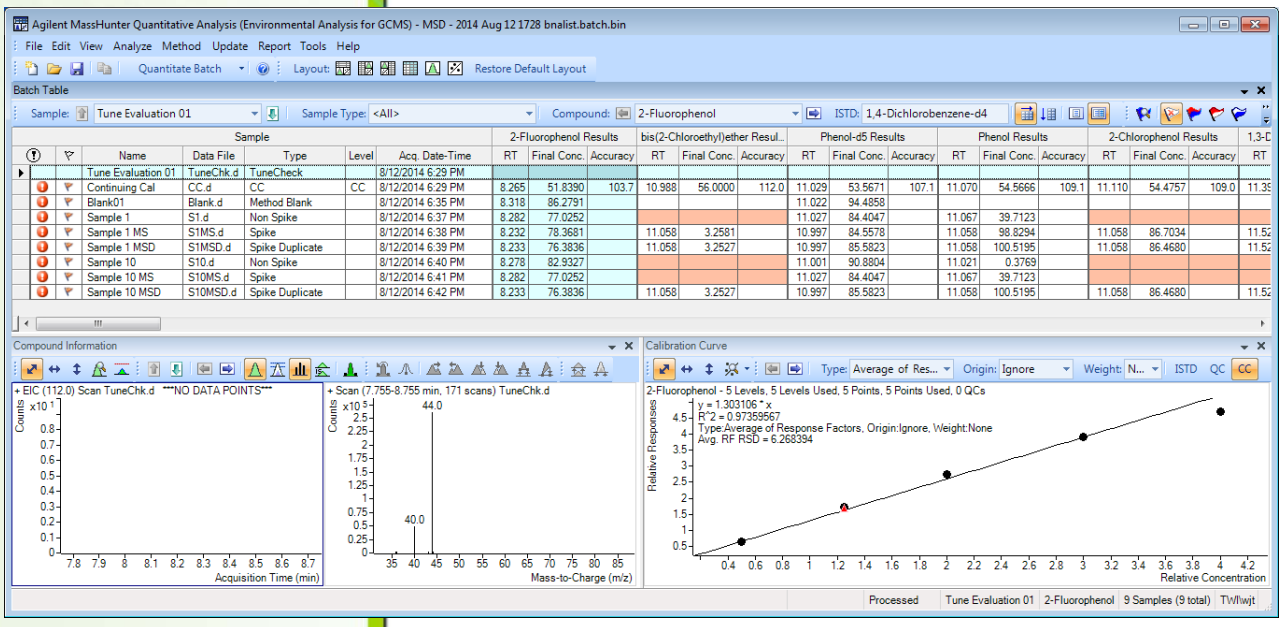
22. When **Sequence Completed** is displayed in the status line, return to MassHunter Quantitative analysis.

23. Select **File > Open batch** and open your batch.

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



The batch table opens and all samples are quantitated.

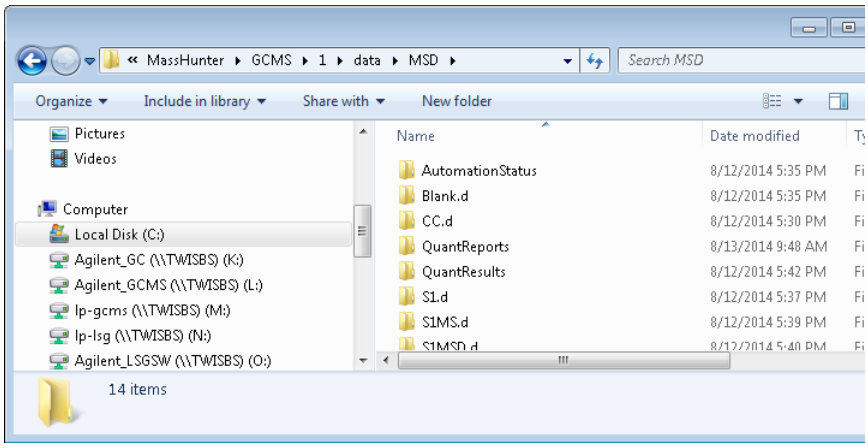


24. To review the reports automatically generated by the sequence, select **Report > Open Report Folder**.

This opens the Quant Report directory with the sample named folders and the report(s) for that sample.

25. Open and review each PDF for acceptable results.

PDF reports are located in the directory named after that sample.



To review the Tune Check report, navigate to the batch directory, open the TuneCheck.d folder and then open the TuneReport.pdf.

26. Generate a Matrix Spike Duplicate report interactively.

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

For this workflow you have generated the following reports:

- Tune Evaluation
- Continuing Calibration
- Matrix Spike Duplicate
- Quant Reports for every sample

Step 3: Perform Data Analysis Interactively.

Use EnviroQuant interactively to review data, manually integrate compounds, and generate final reports.

For a detailed look at how this is done, see GC/MSD Familiarization Guide G3335-90200 available with your MassHunter software documentation for the 5977 MSD or on the Agilent website.

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Printed in USA, August 2014