Agilent MassHunter EnviroQuant (EPA) Mode
Using Quantitative Analysis
Workflow Guide
Notices

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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 used 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).
Chapter 6 explains how to create report methods that enable you to save report parameters, including multiple report templates, to a file that 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.

Chapter 7 describes a workflow for running initial calibrations and a workflow for running daily field samples.

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

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**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.
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Before You Begin

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1. Before You Begin

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.

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

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.

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

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

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.

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.


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Create the Data Acquisition Method

Step 1: Load the data acquisition method.  
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Step 11: Create the basic quantitation method.
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.
2. Create the Data Acquisition Method

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.
2. Create the Data Acquisition Method

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.
2. Create the Data Acquisition Method

Step 6: Complete the GC Edit Parameters dialogs.

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.
2. Create the Data Acquisition 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.

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**Step 7: Skip the Real Time Plot displays.**

When you click **OK**, the Real Time Plot dialog 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.
2. Create the Data Acquisition Method

Step 9: Select the monitors.

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

![Monitors dialog](image)

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.

![Save Method dialog](image)

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”.
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Create a Quantitation Method

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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.

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.

Select Translation Task

Please choose a GC/MS Translator Option

MSD ChemStation

- Translate Data Files
- 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\bnaist.m` file that you converted in the last section and click **OK**.

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.
3. Create a Quantitation Method

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](image URL)
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.
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.
3. Create a Quantitation Method

Step 8: Set up the Integrator.

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

2. Review the integrator used.

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

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

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

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

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.


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”.

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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.

**Introduction**

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

Step 2: Complete the Tune Evaluation criteria.

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.

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.
4. Run Samples for Quant Method Creation

Step 2: Complete the Tune Evaluation criteria.

The compounds that will be included are:
- Pentachlorophenol
- DFTPP
- Benzidine
- DDT


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

3. Highlight the Tune Evaluation 01 data file.


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

The Tune Evaluation dialog opens.
4. Run Samples for Quant Method Creation

Step 2: Complete the Tune Evaluation criteria.

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.

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

   ![GC Performance Evaluation Table](image)

   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.

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

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

   ![Tailing Factor Table](image)

   Enter tailing factor parameters for Pentachlorophenol and Benzidine.

3. Apply the criteria.

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.
4. Run Samples for Quant Method Creation

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

**Tune Evaluation PDF Report**


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

5. Review the Trailing Factor.

On the next page you can see the tailing factor.
In the future, each time you run a tune check sample from a sequence with this bnaist 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 analysis methods.
4. Run Samples for Quant Method Creation

Step 6: Initialize the Continuing Calibration response.

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

6. Exit the method editor [F11].

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

You are returned to Batch table view.

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.

1. Select Analyze > Replace Calibration.

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

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**.

   ![Select Compounds and Select Samples](image)

   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**.

   ![Save As](image)
4. Run Samples for Quant Method Creation

Step 8: Complete the quantitation method.

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.

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.

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

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Introduction

Step 1: Open the batch.

1. In MassHunter EnviroQuant select File > Open Batch.

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

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.

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

The batch table opens with all samples quantitated.
5. Enter EnviroQuant Parameters in the Method

Step 2: Specify the surrogates and matrix spikes.

1. Open the method editor [F10].

2. Select Compound Setup.

3. Specify Surrogate as the Type for these compounds.

4. Compare your edits with this example.

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.

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

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.
5. Enter EnviroQuant Parameters in the Method

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.
5. Enter EnviroQuant Parameters in the Method

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.
5. Enter EnviroQuant Parameters in the Method

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

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

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

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

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

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.
5. Enter EnviroQuant Parameters in the Method

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

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.
5. **Enter EnviroQuant Parameters in the Method**

5. Select **Average Response Factor**.

   Fill in the shaded column as shown here.

   ![Outlier Setup Tasks](image)

   This will be used for ICAL Report minimum RF.

---

**Step 4: Set up outlier limits for the EPA method criteria.**
5. Enter EnviroQuant Parameters in the Method

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

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

This will be used for ICAL Report RSD.
5. Enter EnviroQuant Parameters in the Method

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

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.
5. Enter EnviroQuant Parameters in the Method

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

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.
5. Enter EnviroQuant Parameters in the Method

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


![Method Table Example](image-url)
5. Enter EnviroQuant Parameters in the Method

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

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

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

12. Select Surrogate Percent Recovery. Fill in the shaded columns as shown here.
5. Enter EnviroQuant Parameters in the Method

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

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

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<th>Name</th>
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5. Enter EnviroQuant Parameters in the Method

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.m` 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”.

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6
Create Report Methods

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Step 3: Create a Quant Report Method. 75
Step 4: Create a Continuing Calibration Report Method. 80
Step 5: Create a Matrix Spike Duplicate Report Method. 83
Step 6: Create a QA Check Report Method. 86
Step 7: Run samples. 88

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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.
6. Create Report Methods

Step 1: Generate an interactive report.


4. To limit the number of samples reported click **Choose samples**.
6. Create Report Methods

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.)
6. Create Report Methods

Step 1: Generate an interactive report.

8. Click OK to generate the report.

The report is generated.
6. Create Report Methods

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.
6. Create Report Methods

Step 2: Create an Initial Calibration Report Method.

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.
6. Create Report Methods

Step 2: Create an Initial Calibration Report Method.

The first page of an Initial Calibration PDF report.
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 bnafile method. Save this report method to bnafile.m to have it automatically generate a Quant report each time a sample is run with this unified method.

**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.
Step 3: Create a Quant Report 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.

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.

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.

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.
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.

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

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

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

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

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

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

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

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.

A Matrix Spike Duplicate PDF report.
6. Create Report Methods

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.

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

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

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

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

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_Check.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 all samples in the batch.

**Step 7: Run samples.**

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

8
Run Samples

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Step 2: Run daily unknown samples. 97
Step 3: Perform Data Analysis Interactively. 103
Two basic workflows exist when processing samples:

- One for calibrating the instrument
- One for daily sample processing

These workflows are reviewed below.

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.

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.

![Sequence and Method Icon]

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

![Sequence and Method Icon]
8. Run Samples

3. From the Tools menu, select Add/Remove Columns and add columns so the table resembles the example below.

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

5. Fill in the level for the Cal sample types as shown.

6. Fill in the Data File names as shown.

7. Fill in the Method names as shown.

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

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

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

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

This automatically updates the calibration curves in the master method.
8. Run Samples

Step 1: Run a calibration of the instrument.

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

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

The Start Sequence dialog displays.

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 binalist method. A Tune Evaluation report PDF is generated automatically by the tuneEvaluation method stored in the binalist 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.
8. Run Samples

Step 1: Run a calibration of the instrument.

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.

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

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

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 bnaist 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.
8. Run Samples

Step 2: Run daily unknown samples.

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

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

12. Review the Continuing Calibration PDF report.

---

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.

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.

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

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.
8. Run Samples

Step 2: Run daily unknown samples.

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.
8. Run Samples

Step 2: Run daily unknown samples.


17. Select Method > Save As.

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

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

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

21. In MassHunter Data Acquisition, click Sequence > RestartPaused 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 bnaist.batc.h.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.

26. Generate a Matrix Spike Duplicate report interactively.

Step 3: Perform Data Analysis Interactively.

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.

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

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.