

GC/MS Translator for the MS Workstation

Quick Start



Notices

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About this book...

This guide walks you through the process of collecting sample data with the MS Workstation, translating it into the MassHunter format, and analyzing it in MassHunter Quantitative Analysis.

Topics in this guide

In this guide you will learn how to:

- Translate a MS Workstation data analysis method into a MassHunter Data Analysis method.
- Define a post-run macro in the MS Workstation method that will automatically translate your sample data files into a MassHunter format.
- Prepare your MS Workstation Sample List and methods with a conversion to MassHunter in mind.
- Translate MS Workstation data files into MassHunter format.
- Create a batch in MassHunter with the translated MS Workstation sample data files and method.
- Analyze the data in MassHunter.

Primary MassHunter and MS Workstation differences

There are two primary differences between the MS Workstation and MassHunter regarding data analysis.

- 1 While all data analysis is done in a single MS Workstation software program, there are two customized versions of MassHunter for data analysis.
 - MassHunter Quantatitive Analysis (MS)—designed for single MS analyses
 - MassHunter Quantitative Analysis (QQQ)—designed for MS/MS analyses
- **2** For MS/MS analyses, product ions may be defined differently in the MS Workstation and MassHunter.
 - In the MS Workstation the product ion (quantifier ion) may be specified as a mass range, as a sum of single ions, or as a sum of mass ranges.
 - In MassHunter, the product ion is specified as a single mass, or as a single mass with qualifier ions.

To resolve this, the translator automatically converts any quantifier ion mass range from the MS Workstation method into product ions and qualifier ions in MassHunter.

See Table 1 on page 8 for more details on this conversion process.

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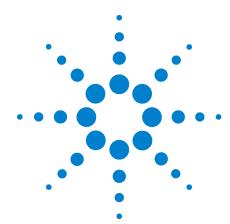
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Installation



Translate an MS Workstation Quant Method into a MassHunter Method

Methods that were created by the MS Workstation can be automatically converted for use in MassHunter Quantitative Data Analysis using the GC/MS Translator software. Quantitation methods that were running successfully in the MS Workstation frequently convert and validate with no errors in MassHunter Quantitative Analysis. When validation issues are found, they are automatically identified and are correctable using the MassHunter Quantitative Analysis software.

Once validated, the MassHunter quantitation method can be run without further modification. However, to be certain the translation was accomplished as you expected, review how mass ranges were translated and adjust any quan ion assignments if desired.

Remember, there are two primary differences between the MS Workstation and MassHunter programs:

- 1 While all data analysis is done in a single MS Workstation software program, there are two customized versions of MassHunter for data analysis.
 - MassHunter Quantatitive Analysis (MS)—designed for single MS analyses
 - MassHunter Quantative Analysis (QQQ)—designed for MS/MS analyses
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 - In the MS Workstation the product ion (quantifier ion) may be specified as a mass range, as a sum of single ions, or as a sum of mass ranges.
 - In MassHunter, the product ion is specified as a single mass, or as a single mass with qualifier ions.

To resolve this, the translator automatically converts any quantifier ion mass range from the MS Workstation method into product ions and qualifier ions in MassHunter.

Quan ion specifications that are currently made in the MS Workstation will not be translated exactly the same to MassHunter. Table 1 illustrates how a Quan ion defined in the MS Workstation will be defined in MassHunter.



Translate an MS Workstation Quant Method into a MassHunter Method

Table 1 Entries from the Quan lons tab of the Compound Table Setup in MS Workstation Method Builder as they are translated into MassHunter fields

Original MS Workstatio n Entries ¹	Translated into these fields in MassHunter									
Quan Ion (MSWS)	MZ/Product Ion	Product Ion Extract Left ²	Product Ion Extract Right ²	Calculated Qualifier Ion MZ	Relative Response based on the calculated qualifier ³	Qualifier Ion Extract Left ²	Qualifier Ion Extract Right ²	Use Area Sum (Qualifiers) ⁴		
M1	M1	Default	Default	N/A	N/A	N/A	N/A	No		
M1:M2	[M1+M2]/2 Average of the mass range.	MZ-M1 + Mass Width ⁵	M2-MZ+ Mass Width ⁵	N/A	N/A	N/A	N/A	No		
M1+M2+M3	M3 Highest mass. All other masses are translated as qualifier ions.	Default	Default	M1, M2	Default to 1% of calculated qualifiers	Default	Default	Yes		
M1:M2 + M3:M4	[M1+M2]/2 Average of M1:M2 range. M3:M4 are averaged and translated as a qualifier ion.	MZ-M1+ Mass Width ⁵	M2-MZ+ Mass Width ⁵	[M3+M4]/2	Default to 1% for calculated qualifiers	Qualifier Ion MZ-M3+ Mass Width ⁵	M4-Qualifier Ion MZ+Mass Width ⁵	Yes		
M1:M2 + M3 + M4	M4	Default	Default	[M1+M2]/2, M3	Default to 1% for calculated qualifiers	Mz-M1+ Mass Width ⁵ for first qualifier, Default for second qualifier (M3)	Mz-M1+ Mass Width ⁵ for first qualifier, Default for second qualifier (M3)	Yes		
M1:M2 + M3:M4 - M5:M6	[M1+M2]/2 Subtracted ions or ranges are not translated.	MZ-M1+ Mass Width ⁵	M2-MZ+Mass Width ⁵	[M3+M4]/2	Default to 1% for calculated qualifiers	Qualifier Ion MZ-M3+ Mass Width ⁵	M4-Qualifier Ion MZ + Mass Width ⁵	Yes		

- Represents entries from the Quan lons Tab of the Compound Table Setup in Method Builder
- In MassHunter you may enter a mass range in the Extract Left and Extract Right fields to further identify your target. Translator calculates these values from the Quan Ion entries you used in the MS Workstation method, as illustrated in the above table.
- Relative Response factors are entered into the MassHunter method table by the translator software. A qualifier ion that was specified as part of your MS Workstation method is translated directly into MassHunter with its relative response. Qualifier ions that were calculated as illustrated in the above table from the quan ions you entered in the MS Workstation method will have their relative response set to a default of 1% in MassHunter. Update the Qualifier Ratio in MassHunter to obtain a more accurate relative response factor.
- When you are calculating qualifier ions from quan ions, the translator will automatically turn on the Area Sum feature in MassHunter. Area summation adds together the areas of a group of adjacent peaks and reports the total as a single number.
- Mass Width is defined as +/- 0.50 m/z divided by the Charge State of the Quan Ion. It is ½ the nominal separation of adjacent mass peaks for the ions that are being quantitated. This parameter is enabled when a profile data file is associated with the MS Workstation method.
- The translation of an identification reference peak in the MSWS method will only occur if the compound is an internal standard. The time reference flag will be set if the identification reference peak is translated.

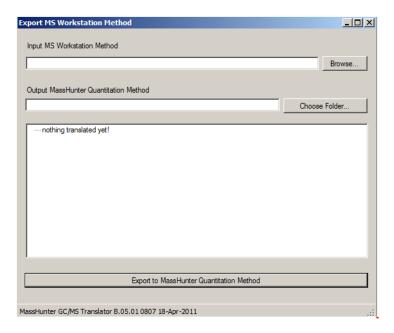
Translate the Method

This procedure requires that the MS Workstation method is accessible from the PC where the **GCMS Translator** software is installed.

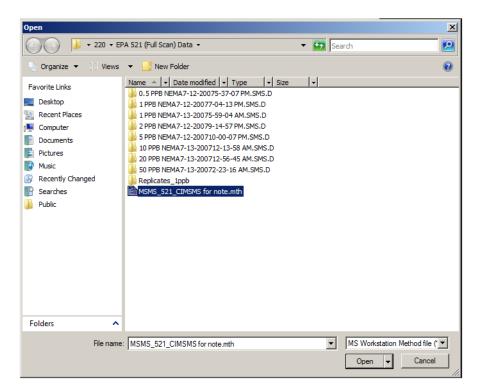
1 Click the **MS Workstation Translate Method Files** using the **GCMS Translator** desktop icon or the Windows **Start** menu.



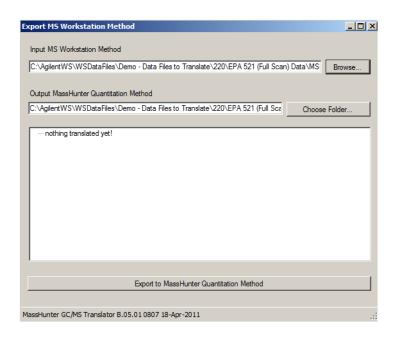
2 Click the **Browse** button. The **Open** dialog displays.



3 Navigate to the folder containing the method to be translated, select it and click **Open**. You are returned to the **Export MS Workstation Method** window.

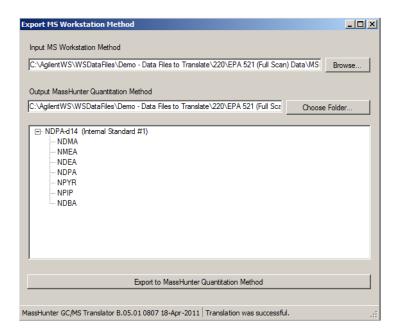


4 Click the **Choose Folder** button in the **Export MS Workstation Method** window and navigate to the location where this new MassHunter Quantitative Analysis method will be saved.



5 At the bottom of the window, click the Export to MassHunter Quantitation Method button. The conversion process begins.

When completed, a message is displayed on the bottom line of the window. The MassHunter quantitative method is saved in the specified location. The conversion result is also displayed in the window as a list of ISTDs from the quantitation method. Expand the listing under each ISTD to see the compounds grouped with this reference standard.

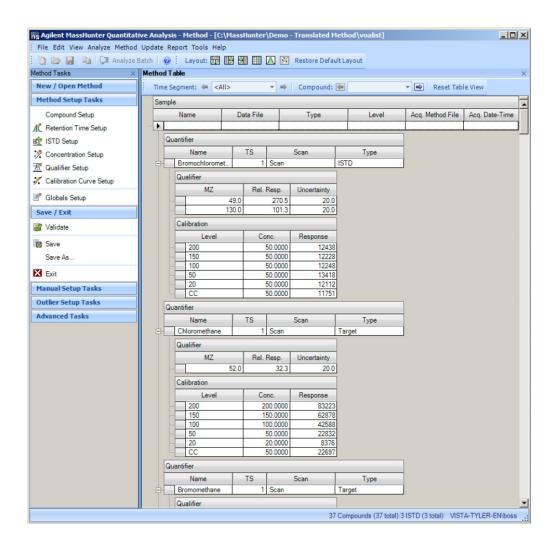


6 Exit the **MS Workstation File Translation** software.

The next step involves validation of this converted method using MassHunter Quantitative Analysis.

Validate the Converted MS Workstation Method in MassHunter

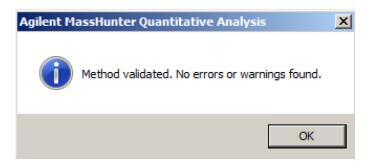
- 1 Open the applicable MassHunter Quantitative Analysis program:
 - MassHunter Quantatitive Analysis (MS) for single MS analyses
 - MassHunter Quantitative Analysis (QQQ) for MS/MS analyses
- 2 Select Method>Open>Open Method from Existing File. The Open Method dialog is displayed.
- 3 Navigate to the translated method that requires validation in MassHunter, then click **Open**. The **Method Table** is displayed in the MassHunter method editor (ME).



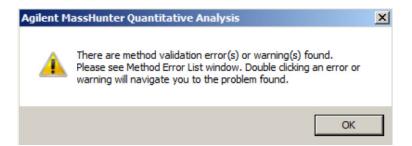
4 Scroll through the **Method Table** to see how a MassHunter quantitative analysis method is displayed.

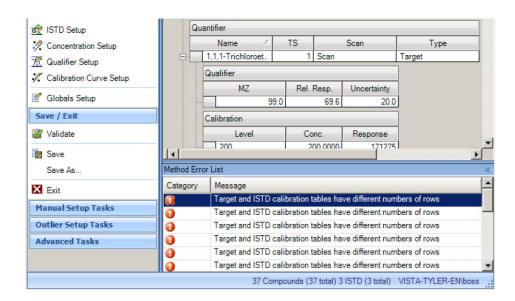
5 In the **Method Tasks** area, under **Save / Exit**, select **Validate**. The system displays a prompt with the validation results.

If no errors are found you will receive this message, and you may use this method to analyze samples in MassHunter.



If errors are found in the method, you will receive this message, and the errors will be listed in the lower section of the method editor. All errors must be corrected before the method can be used in MassHunter.





- 6 Correct each error by first double-clicking on the error line in the **Method**List Table. This action highlights the area in the **Method Editor** where a
 problem exists. Fix the error as necessary, then select **Validate** again.
- 7 Each time you fix an error, it is removed from the **Method Error List**.

 Double-click the next message in the list, fix the error, validate the method, and continue this process until the **Method Error List** is empty.
- 8 When no errors are found, in the **Method Tasks** area, under **Save / Exit,** select **Save As**.

The **Method Save As** dialog is displayed.

- **9** Navigate to the folder that you use to store your MassHunter validated methods. Enter a method name in the **File name** field and click **Save**. The file extension *.quantmethod.xml is added by the system.
- 10 In the **Method Tasks** area, under **Save / Exit** select **Exit** to leave MassHunter Quantitative Analysis.

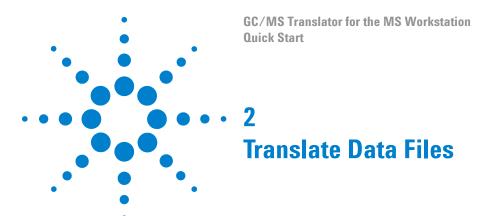
The validated method is now ready to use with MassHunter Quantitative Data Analysis.

Remember, for MS/MS analyses, product ions may be defined differently in the MS Workstation and MassHunter.

- In the MS Workstation the product ion (quantifier ion) may be specified as a mass range, as a sum of single ions, or as a sum of mass ranges.
- In MassHunter, the product ion is specified as a single mass, or as a single mass with qualifier ions.

To resolve this, the translator automatically converts any quantifier ion mass range from the MS Workstation method into product ions and qualifier ions in MassHunter. To be certain the translation was accomplished as you expected, review how mass ranges were translated, and adjust any quan assignments if desired.

See Table 1 on page 8 for details on the conversion is handled.



The following describes how to translate MS Workstation data, both automatically and manually, to a format that can be used by MassHunter Quantitative Analysis.

During this process, the original MS Workstation raw data files are not altered in any way. They may continue to be accessed using the MS Workstation for data analysis, if desired.

Manually

The following describes how to manually translate MS Workstation sample data files into a format that can be used by the MassHunter Quantitative Data Analysis program.

NOTE

This process can be automated when the MS Workstation File Translation software is installed on the same PC as the MS Workstation that is collecting the raw data, as described in the next section.

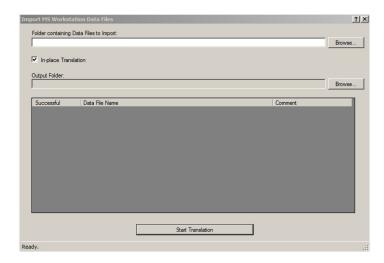
During the conversion process, the GC/MS Translator software will create a copy of the original data files and reformat them as necessary to conform to the MassHunter Quantitative data analysis format. The original MS Workstation raw data files are not altered in any way. They may continue to be accessed using MS Workstation for data analysis, if desired.

Procedure

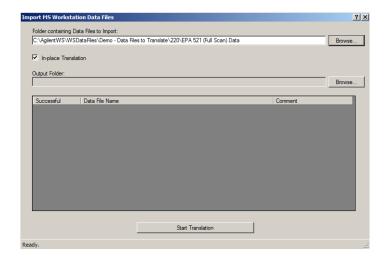
1 To begin, install the GC/MS Translator software as described in Chapter 4.



2 Click on the MS Workstation Translate Data Files after opening the GCMS Translator desktop shortcut to start the translator. The MS Workstation Data Files screen is displayed.



3 Type the path or click the **Browse** button and navigate to the folder containing the data files you wish to translate.



4 Next, identify where you would like the translated files stored.

If you select **In-place Translation**, the system will create a subdirectory for the translated data files, directly under the directory containing the original data files.

If you select **Output folder**, uncheck the **In-place Translation** checkbox, then type the path, or navigate to the directory you wish to use for the translated data files.

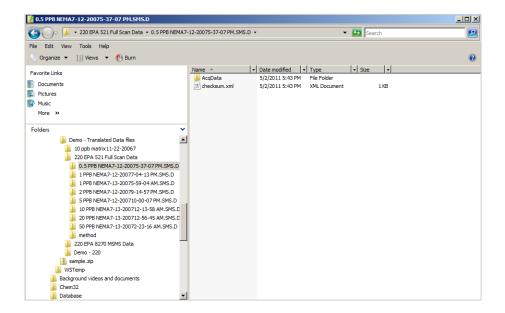
2 Translate Data Files

In either case, the original MS Workstation raw data files are not altered in any way by this conversion. You may continue to access them using the MS Workstation at any time.

- **5** Click **Start Translation** to continue.
- **6** Watch the progress. As each file is translated it will be listed in the display.
- 7 When all the files are translated, you can go back to the directory and see the translated files.

Here is what the saved folders look like. For each .SMS MS Workstation data file, a corresponding .D MassHunter data folder is created. The original data files remain unchanged.

The .D folder contains a **checksum.xml** file and an **AcqData** folder that holds the translated data file.



Now that the files have been translated, they can be analyzed using MassHunter Quantitative Data Analysis.

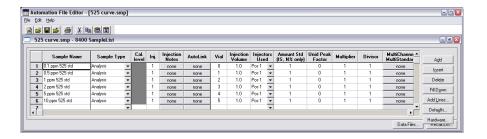
Automatically

Once the GC/MS Translator software is installed on the PC that will be collecting the data (Chapter 4), and you define it in your method, the Translator will automatically create a copy of each collected data file, and format it for use in MassHunter. The original MS Workstation data will remain untouched, and available to use in the MS Workstation if you desire.

Add a post-run command in MS Workstation to translate data files automatically

To define this command in your MS Workstation method:

- 1 Copy the **V2MassHunter.cmd** file from the GCMS installation directory (for example: C:\Program Files\Agilent\MassHunter\GCMS Translator\) to the MS Workstation installation directory (for example: c:\varianws\ or c:\agilentws\).
- 2 In System Control, open your SampleList.



- **3** Fill the **Command field**. Use the **Browse**... button to navigate to the capsule.exe program (for example: c:\varianws\capsule.exe or c:\agilentws\capsule.exe).
- 4 Fill the Other parameters field with the following string: c:\varianws\V2MassHunter.cmd, 11

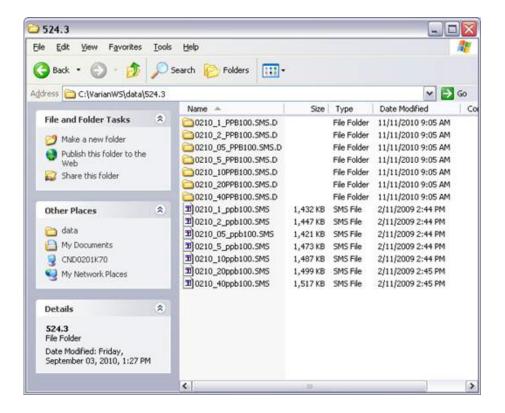
(or c:\agilentws\V2MassHunter.cmd, 11)



5 The data will now be saved in both the MS Workstation and MassHunter formats.

Review the data files generated

Once the data is acquired, review the folder and data files created by the MS Workstation.



The folder contains all the standard MS Workstation sample data files. If you would like to use your MS Workstation to analyze this data, you may do so at any time. These data files are not altered in any way.

For each .SMS Workstation data file, a corresponding .D MassHunter data file is created. These are created by the MS Workstation File Translation AutoLink utility post-run macro and are needed for the data to be used in MassHunter.



The following describes how to create a batch in MassHunter Quantitation Analysis with method and data files that were converted from MS Workstation files.

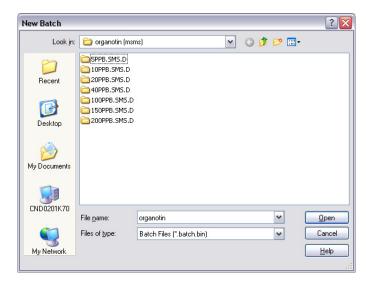
Creating a Batch

Creating a batch in MassHunter begins by defining the batch name and the folder in which it will be saved. This folder is often called the **batch folder**.

As you will see, it is most convenient if the batch folder is the same folder that contains the data files you will put into the batch. In this example, we are using the folder that contains the translated data files from the MS Workstation.

- 1 Open the applicable MassHunter Quantitative Analysis program:
 - MassHunter Quantatitive Analysis (MS) for single MS analyses
 - MassHunter Quantitative Analysis (QQQ)for MS/MS analyses
- 2 Select File>New Batch.
- 3 Navigate to the folder you want to use as the batch folder. In this case, it is the folder that contains the translated data files from the MS Workstation (those identified in the Sample List).

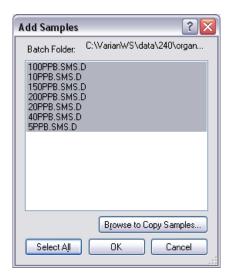
Notice the data folders (folders with the .D extension) are already in this folder. That will make it very easy to load them into the batch, when we do that (step 6).



- 4 Enter a File name for this batch, then click **Open**. The system displays the **Batch** table, with the name you specified in the title bar. It will also:
 - Create a folder named QuantResults in the batch directory.
 - Create a batch file with the name you specified and the extension .batch.bin.
 - Save the *batchname*.batch.bin file to the **QuantResults** folder.

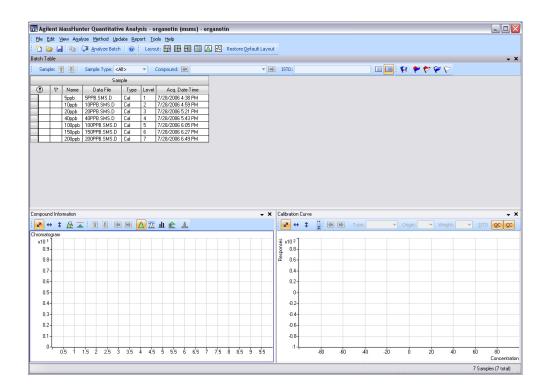
Next we will identify the samples that will be included in this batch.

5 Select File>Add Samples.



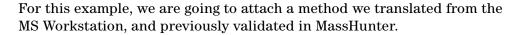
The system displays all the sample data files in this folder. In this case, these are the samples that were collected by the MS Workstation automatically translated by the MassHunter Translator macro.

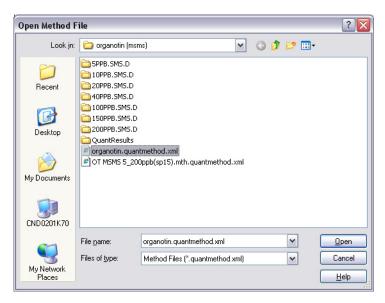
- 6 Click **Select All** to have all the samples in this folder included in the new batch.
- 7 Click **OK** to continue. Now each translated file is included in the new batch.



The final step in the process is to attach a quantitation method to the batch. For this example we will use the previously translated MS Workstation method.

- 8 Select Method>Open>Open and Apply from Existing File....
- **9** Navigate to the folder containing your validated MassHunter quantitative analysis methods and select the method to apply to this batch.

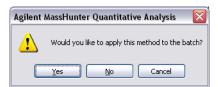




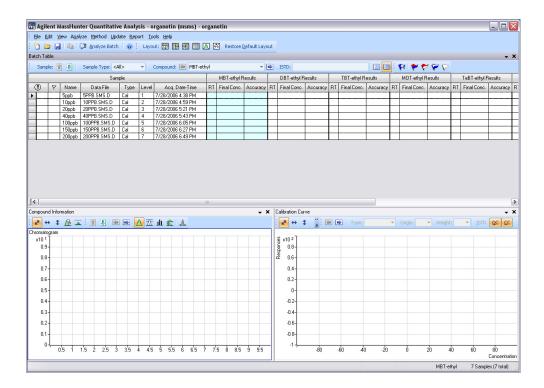
10 Click Open then Exit to go back to the batch screen.



11 A pop-up dialog opens. Click **Yes** to apply the selected method to the current batch.



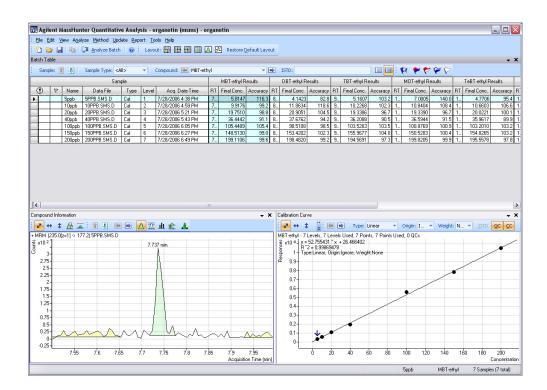
12 Select File > Save Batch from the main menu to save this method with this batch.



The batch directory now contains all the sample data files you selected, plus a folder created by **Quantitative Analysis** program, named **QuantResults**, with the *batchname*.batch.bin file.

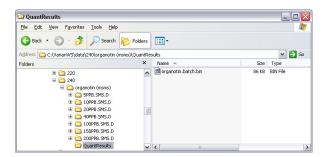
13 Now that the method is attached, click **Analyze Batch** to process the sample data and display the results.

MassHunter displays the results in the Batch Table.



Red and blue highlights indicate results that were either higher or lower than specified in the method.

- **14** Click the **Next** compound button to view the results for each compound, one-at-a time.
- **15** When a batch is analyzed, MassHunter creates a **QuantResults** folder inside the **Batch** folder.



The QuantResults folder will include a copy of the batch file.

Create a Batch in MassHunter Using MS Workstation Generated Files

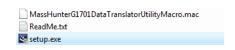


The following describes how to install the GCMS Translator software, which is used to convert MS Workstation data and methods to MassHunter Quantitative Analysis format.

The GCMS Translator software is delivered on the MassHunter Supplemental disk supplied with your MS Workstation.

Installation

- 1 To begin, insert the **Supplemental** disk into your disk drive.
- 2 Navigate to the GCMS Translator folder, and double-click on the Setup.exe.



3 Select the Language you want to use, and click **OK** to continue.



4 The Installation Wizard will complete the installation, and prompt you when it is completed.

Once installed, the GCMS Translator icon will appear on your desktop.



- **5** To allow automatic data file translation:
 - a Copy the V2MassHunter.cmd file from the GCMS installation directory (for example,: C\Program Files\Agilent\MassHunter\GCMS Translator\) to the MS Workstation installation directory (for example: C:\MSWS).
 - Identify this utility as the post-run AutoLink macro in the MS
 Workstation Sample List, as described in "Add a post-run command in MS Workstation to translate data files automatically" on page 19.

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