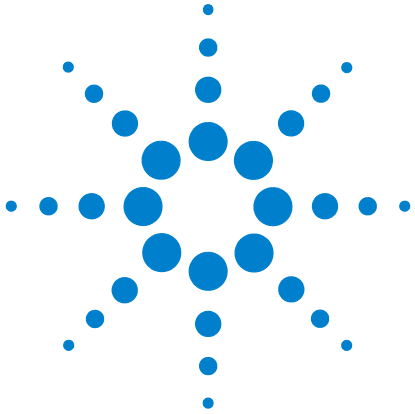

GC/MS Translator

Quick Start

Agilent Technologies

Notices

Manual Part Number

G3335-90089

Edition

Second edition, Feb. 2014
First edition, Aug. 2010

Printed in USA

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

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About this book...

This guide walks you through the process of collecting sample data with the GC/MS ChemStation, translating it into the MassHunter format, and analyzing it in MassHunter Quantitative Analysis. Also included is a procedure for converting a ChemStation data analysis method to the MassHunter format.

One of the primary difference between the GC/MS ChemStation and MassHunter Quantitative Analysis, is how data analysis is done.

- In the GC/MS ChemStation, each sample data file is analyzed individually.
- Conversely, in MassHunter, related data files are saved in a single folder, called a batch folder, then, each file in that batch is analyzed together using a single data analysis method.

  This allows for extremely flexible side-by-side comparison of chromatograms from the analyzed files.

  In this guide you will learn how to:

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

Contents

1 Translate an GC/MS ChemStation Quant Method into a MassHunter Method

Methods that were created by the GC/MS ChemStation can be automatically converted for use in MassHunter Quantitative Data Analysis using the MSD ChemStation File Translation software.

Quantitation methods that have been running successfully in the GC/MS ChemStation frequently import and are validated 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.

Some of the most common items that require resolution during the method validation process in MassHunter are:

- Qualifier ratios set to zero
- Calibration level labels that are not identical for all compounds

  This would happen if, for example, there were four compounds in a method, and:

  - Compounds A, B, and C each had calibration levels **100, 150**, and **200**
  - But, compound D had calibration levels **100**, **150**, and **175**.
- Missing calibration levels for a compound in the Method table

  This would happen if, for example, there were four compounds in a method and:

  - Compounds A, B, and C each had calibration levels **100, 150**, and **200**
  - But, compound D had only calibration levels **100**, and **150**

If your methods require changes, such as those listed above, the changes may be done in the MassHunter Quantitative Analysis software, or in the GC/MS ChemStation prior to translating the method, whichever you prefer.

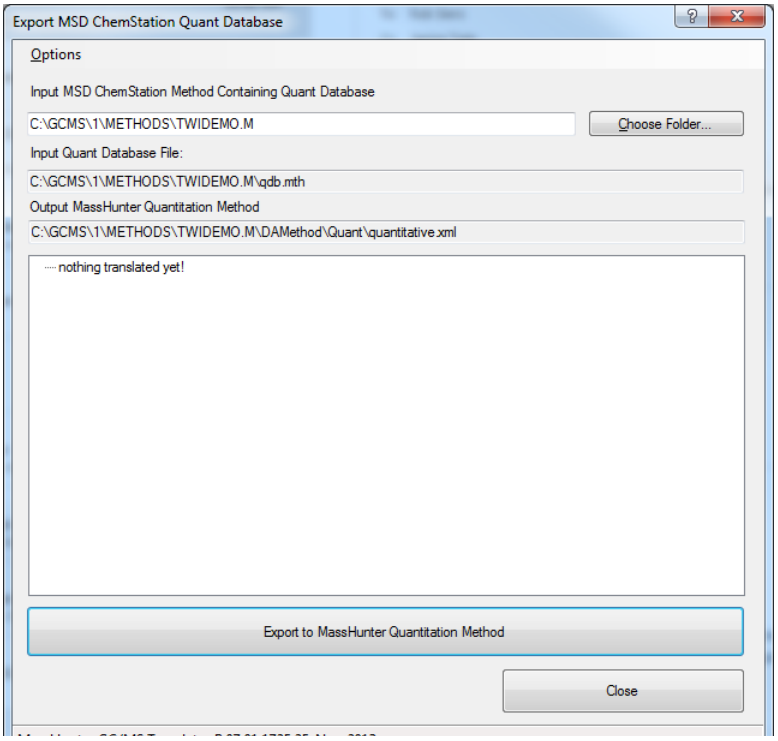
Once validated, this MassHunter quantitation method can be run without further modification. However, just like any method originally created in MassHunter, the newly imported method can be further customized to take advantage of the extensive features available in MassHunter Quantitative Analysis.

Translate the Method

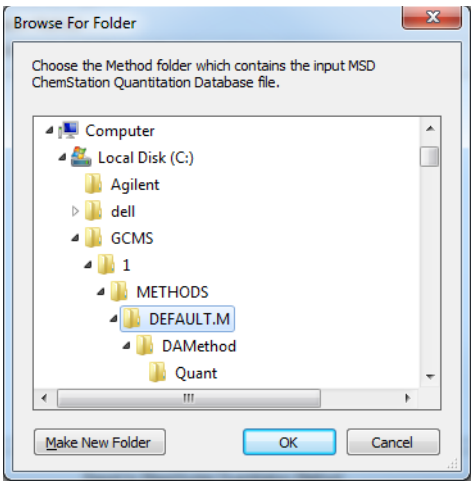
This procedure requires that the GC/MS ChemStation quantitation method is accessible from the PC where the MSD ChemStation File Translation software is installed.

1 Click **MSD ChemStation Translate Quantitation Databases** after opening the **GCMS Translator** desktop icon or the Windows **Start** menu.

2 The Export MSD ChemStation Quant Database dialog appears.



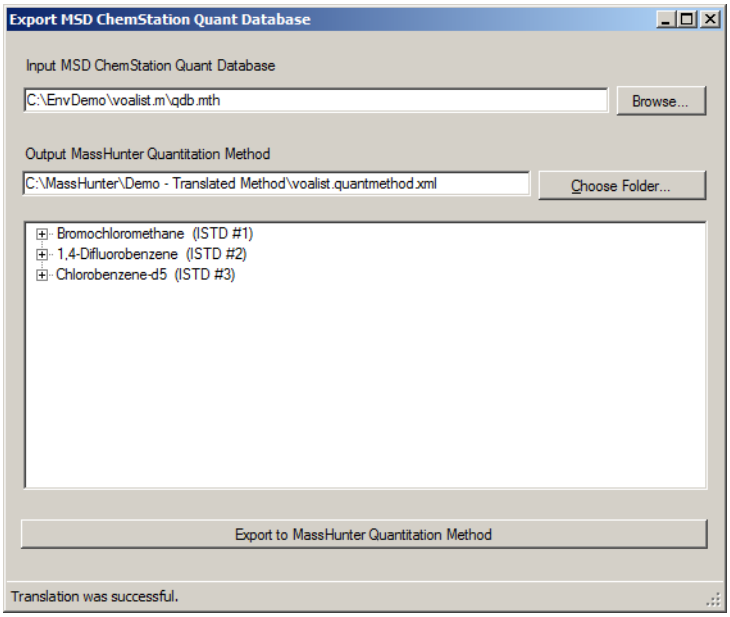
3 Click the **Choose Folder** button. The **Browse for Folder** dialog displays. Navigate to the folder containing the method to be translated.



4 The input quantitation database file (qdb.mth) and the output MassHunter Quantitation method file are selected automatically with unified method handling.

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 Close the **GCMS Translator** software.

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

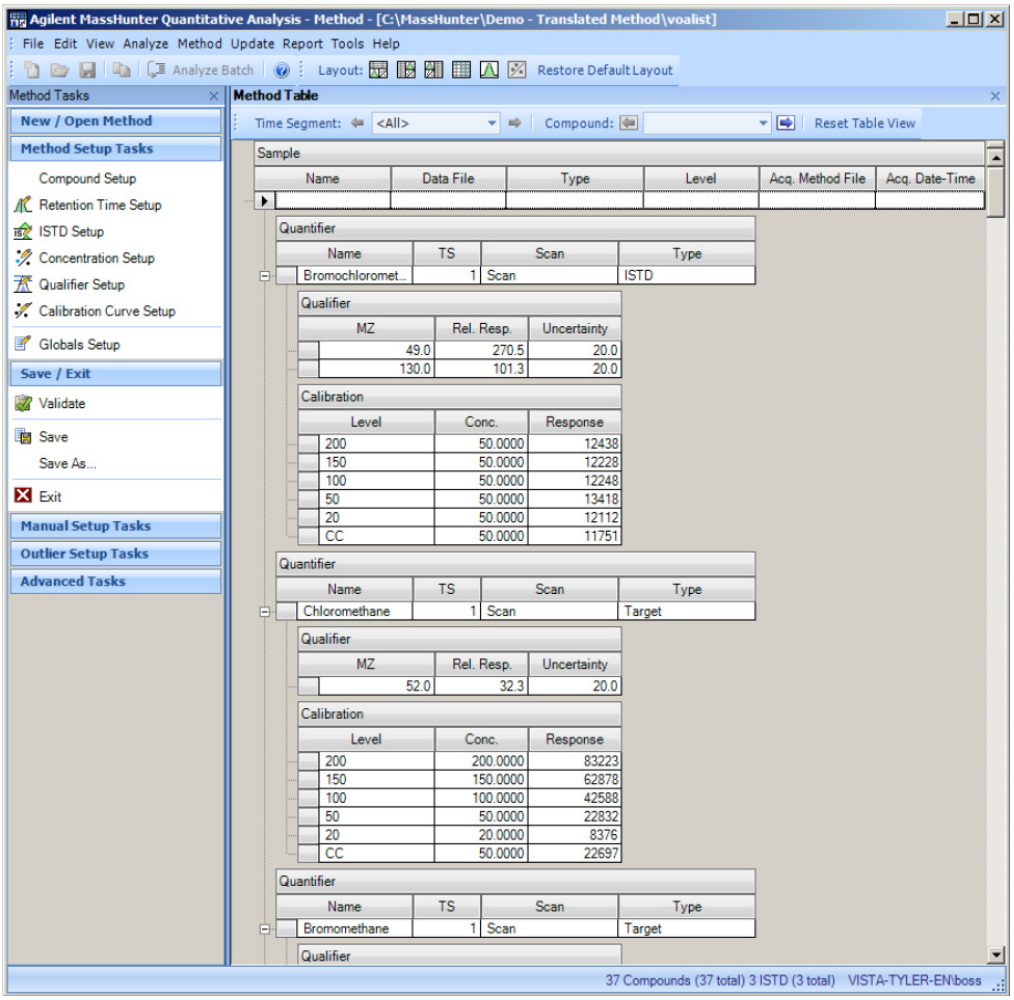
Validate the Converted GC/MS ChemStation Method in MassHunter

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.

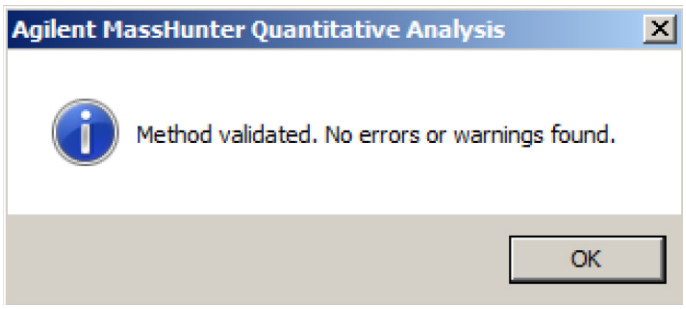
3 Navigate to the translated method that requires validation in MassHunter, then click **Open**. The **Method Table** is displayed in the MassHunter method editor (ME).



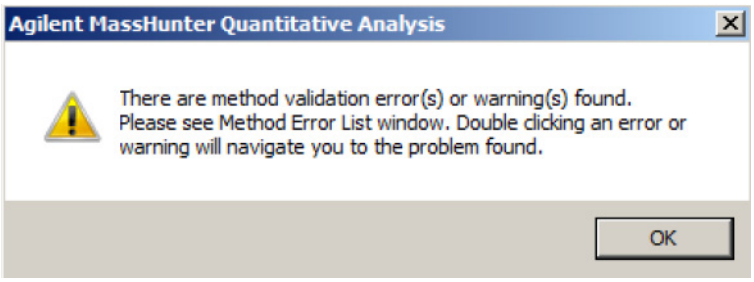
4 Scroll through the **Method Table** to see how a MassHunter quantitative analysis method is displayed.

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

From her you may use this method to analyze samples in MassHunter.



If errors are found in the method, they must be corrected and the method is validated again, until no errors are found.



Some of the most common causes of validation errors are:

- Qualifier ratios set to zero
- Calibration level labels that are not identical for all compounds
  This would happen if, for example, there were four compounds in a method, and:
  - Compounds A, B, and C each had calibration levels **100, 150**, and **200**
  - But, compound D had calibration levels **100**, **150**, and **175**.
- Missing calibration levels for a compound in the Method table? This would happen if, for example, there were four compounds in a method and:
  - Compounds A, B, and C each had calibration levels **100, 150**, and **200**
  - But, compound D had only calibration levels **100**, and **150**

6 Correct each error by first double-clicking on the error line in the **Method List Table,** located in the lower right corner of the ME. This action highlights the area in the ME where a problem exists. Fix the error as necessary, then select **Validate** again.

7 The entries for the error you fixed are removed from the **Method Error List**. Double-click on the next message in the **Method Error List**, fix the error in the ME, validate, 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.

1 Translate an GC/MS ChemStation Quant Method into a MassHunter Method

2 Translate Data Files

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

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

Manually

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

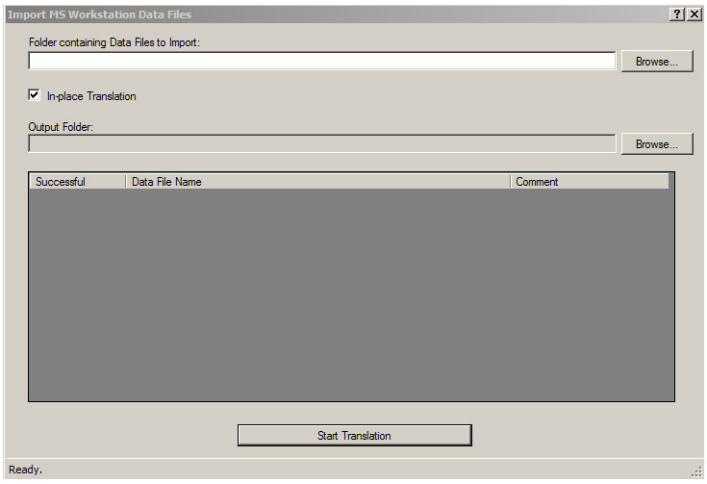
NOTE This process can be automated when the GC/MS ChemStation File Translation software is installed on the same PC as the GC/MS ChemStation that is collecting the raw data, as described in the next section.

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 GC/MS ChemStation raw data files are not altered in any way. They may continue to be accessed using GC/MS ChemStation for data analysis, if desired.

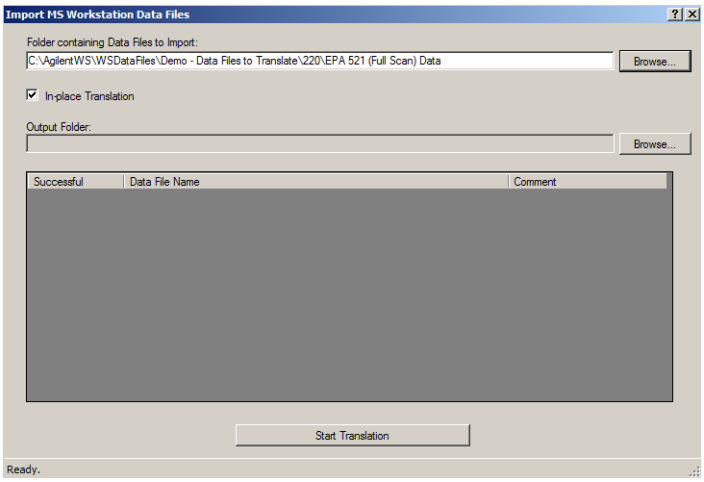
Procedure

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

2 Select **MSD ChemStation Translate Data Files** after opening the **GCMS Translator** desktop shortcut. The **Import MSD ChemStation 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.

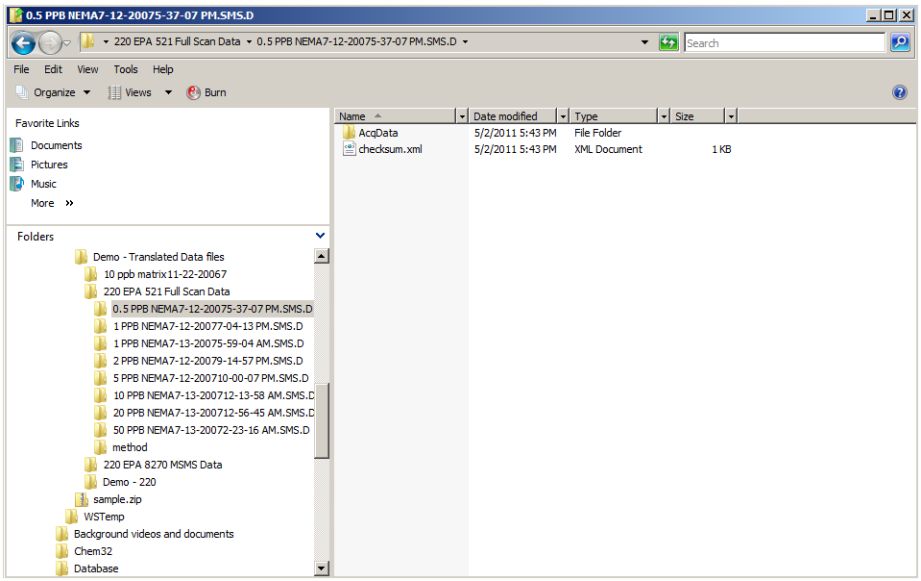
In either case, the original GC/MS ChemStation raw data files are not altered in any way by this conversion. You may continue to access them using the
GC/MS ChemStation at any time.

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. The **checksum.xml** file and an **AcqData** folder that were added during the conversion process. The original data files remain unchanged.



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 ChemStation data will remain untouched, and available to use in the GC/MS ChemStation if you desire.

Identify the Post-Run macro in the ChemStation method

1. Open the GC/MS ChemStation and load the method that will be used to acquire the data.
2. Click the edit method icon to display the **Edit Method** dialog box.
3. Because we only need to edit the **Method Information**, uncheck the **Instrument/Acquisition** and **Data Analysis** check boxes.
4. Then click **OK** to continue. That displays the **Method Information** screen which is where we will identify the post-run translator macro.
5. Check the **Post-Run Macros/Commands** checkbox.
6. In the **Instrument Control** field, navigate to the **MSDChem/MSexe** folder, and select the **MassHunterG17701DataTranslatorUtilityMacro.mac** file.

   This macro was copied to the ChemStation's **/Msexe** folder during installation of the Translator. (The default location is **MsdChem/Msexe**.)

   That is all that is necessary to define the MSD ChemStation File Translation software as the post-run macro for this method.

   However, one additional thing to think about at this point is the Data Analysis option. If you are planning to do all your data analysis in MassHunter, to save processing time, you may uncheck the **Data Analysis** checkbox on the **Method Information** screen, otherwise, you may keep it checked.
7. Click **OK** to continue. A **Save method** dialog box is displayed.
8. Click **OK** once again, to save the changes to the method.

   That is all the changes needed for the method.

   Now, each time this method is run, the sample data gathered by it will automatically be saved in both the ChemStation and MassHunter formats.

Prepare the sample log table

Once the conversion utility is assigned to your method, prepare the sample log table as described below.

1 Open the sample log table you will use to collect your data.

2 Consider the data analysis process.

When developing your sequence, one of the primary points to consider is how the data will be analyzed by MassHunter.

In MassHunter, unlike the GC/MS ChemStation, data analysis is done in batches. That is, all the files that can be processed using a single data analysis method are grouped into a single **batch** and processed together, using a single method. This allows for extremely flexible side-by-side comparison of chromatograms from the analyzed files.

As you will see when we bring the sample data files into MassHunter, the most efficient way to collect the data gathered by your GC/MS ChemStation is to create a sample log table that groups similar samples, so the resulting data folder will contain only those files that can be analyzed using a single data analysis method.

If all the data files collected from your sequence can be analyzed using the same data analysis method, processing will be significantly streamlined.

3 Complete the sample log table as usual, keeping in mind the fact that it would be most efficient to include only those samples that can be analyzed using the same data analysis method as all the others in the group.

For this tutorial, we are using the sample data files included with the GC/MS ChemStation.

This sequence includes 5 calibration samples, 1 daily calibration sample, a method blank, two normal samples, a matrix spike, and a matrix spike duplicate.

When the data files resulting from this sequence are translated into the MassHunter format, the **Type** and **Level** columns, are not included.

It is a good practice to provide information about the sample **Type** and concentration **Level** in the Sample Name. This allows easy identification when sample **Type** and concentration **Level** are entered in MassHunter.

If all of your data will be analyzed in MassHunter only, you may leave the **Type** and **Level** columns blank.

4 Click **OK** to continue.

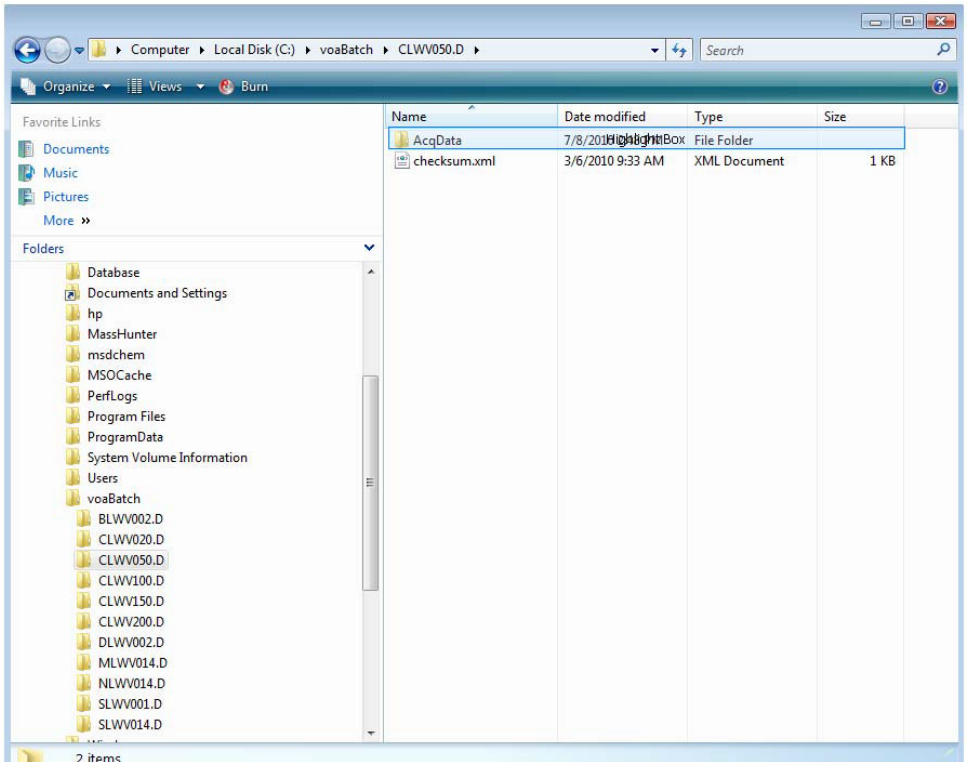
5 With the post-run macro defined in the method, and the sequence defined, click the run sequence icon to display the **Start Sequence** dialog box.

6 Enter the destination folder for the files that will be created when this sequence runs. (Ideally, that folder will become the batch folder when we create a batch in MassHunter.)

7 Click **Run Sequence** to process the samples.

Review the data files generated

Once the data is acquired, review the folder and data files created by the GC/MS ChemStation.



The .D folders contain all the standard GC/MS ChemStation sample data files. If you would like to use your GC/MS ChemStation to analyze this data, you may do so at any time. These data files are not altered in any way.

Under each data file folder, you will also see the **AcqData** folder and the **checksum.xml** file. These are created by the MSD ChemStation File Translation utility post-run macro and are needed in order for the data to be used in MassHunter

3 Create a Batch in MassHunter Using GC/MS ChemStation Generated Files

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

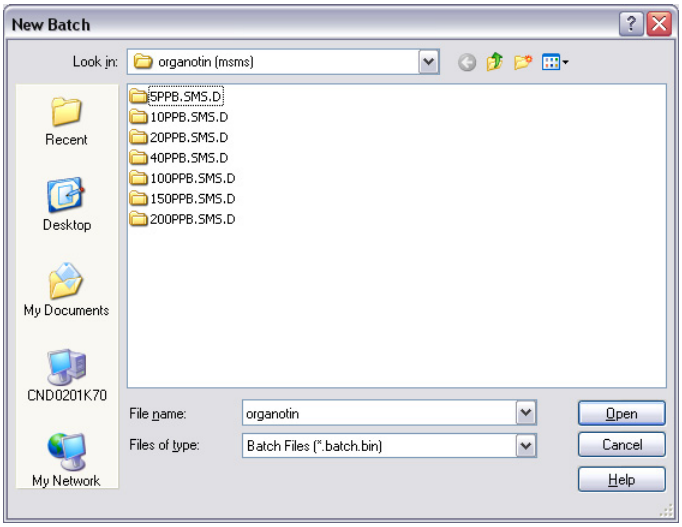
As you will see, it is most convenient if the batch folder is the same folder that contains the data files you will put into the batch. In this example, we are using the folder that contains the translated data files from the GC/MS ChemStation.

1 Open MassHunter Quantitative Data Analysis.

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 GC/MS ChemStation (those identified in the Sample log table).

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).

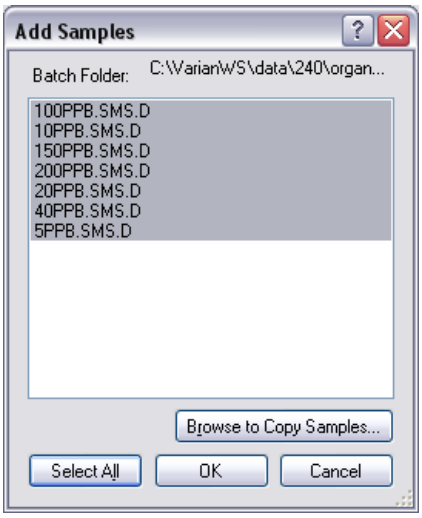


4 Enter a **File name** for this batch, then click **Open**. The system displays the **Batch** table, with the name you specified in the title bar. It will also:

- 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 GC/MS ChemStation 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.

8 To finalize the process, use the drop-down box and select the applicable **Type** for each sample.

- For Calibration samples select **Cal**.
- For Daily Calibrations **CC**
- **Blank** for Blanks
- **Matrix Spike**
- **Matrix Spike Duplicate**

9 Enter the appropriate calibration **Level** label for each calibration sample. Similar to ChemStation processing, these labels must be identical to the label names stored in the quantitative data analysis method.

For this batch enter: 50, 100, 150, 200, 20, and CC

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

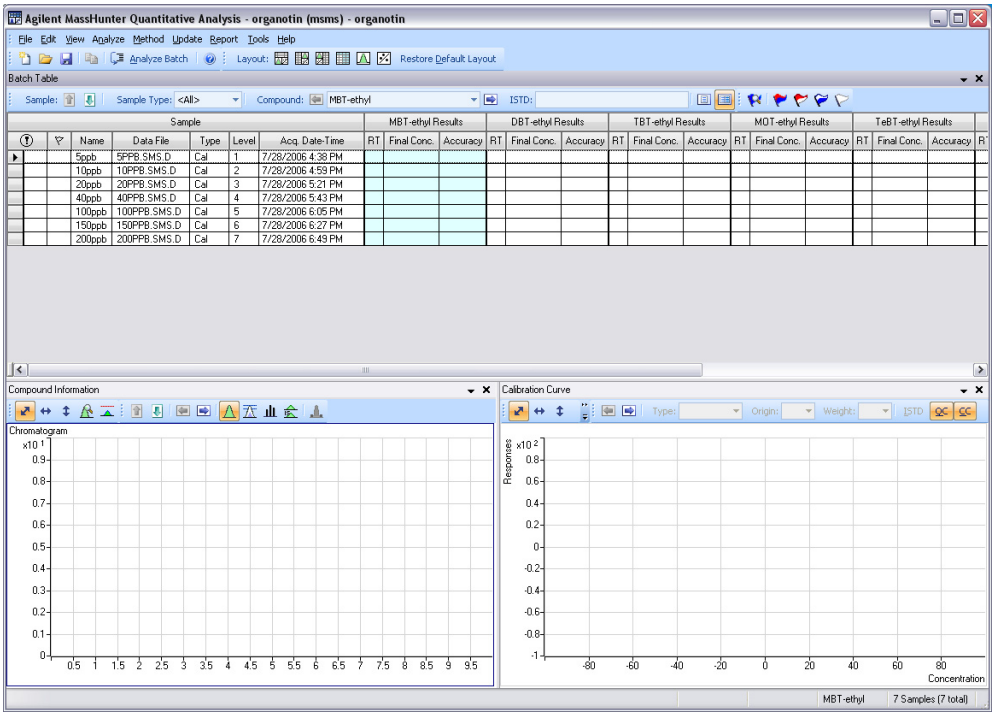
10 Select **Method>Open>Open and Apply from Existing File...**.

11 Navigate to the folder containing your validated MassHunter quantitative analysis methods and select the method to apply to this batch.

For this example, we are going to attach a method we translated from the GC/MS ChemStation, and previously validated in MassHunter.

12 Click **Open** to apply the selected method to the current batch.

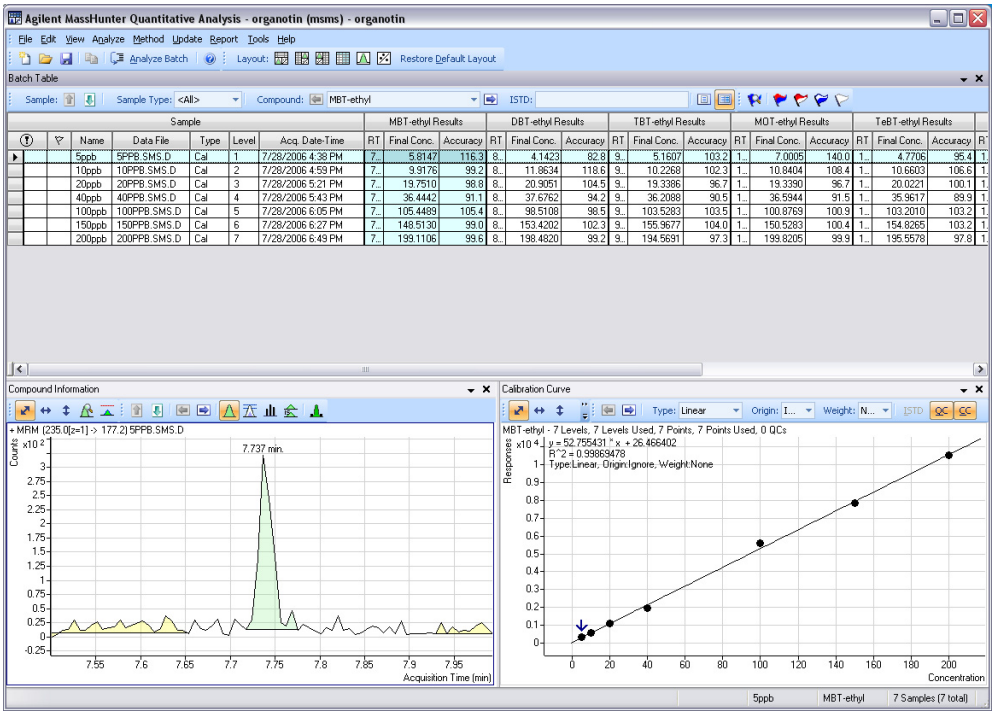
13 Select **File > Save Batch** from the main menu to save this method with this batch.



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.

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

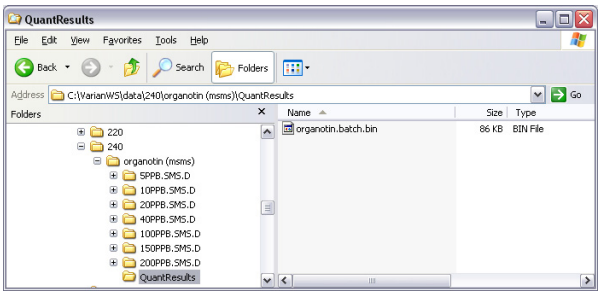
MassHunter displays the results in the **Batch Table**.



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

15 Click the **Next** compound button to view the results for each compound, one-at-a time.

16 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.

3 Create a Batch in MassHunter Using GC/MS ChemStation Generated Files

4 Installing the GC/MS ChemStation File Translation Software

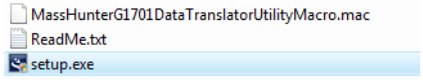
The following describes how to install the GCMS Translation software, which is used to convert GC/MS ChemStation data and methods to MassHunter Quantitative Analysis format.

The GCMS Translation software is delivered on the MassHunter Supplemental disk supplied with your GC/MS ChemStation.

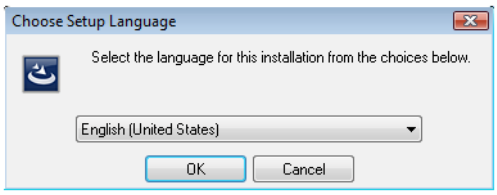
Installation

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 GC/MS ChemStation installation directory (for example: **C:\GCMS**).

b Identify this utility as the post-run AutoLink macro in the GC/MS ChemStation Sample List, as described in "Identify the Post-Run macro in the ChemStation method" on page 19.

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Printed in USA
Second edition, February 2014

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