Agilent

Agilent GC/MS MassHunter Software Migration

User Guide

Guidelines on moving methods and data sets from Agilent MSD ChemStation to Agilent MassHunter.

Notices

© Agilent Technologies, Inc. 2026

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

Manual Part Number

5994-9072EN

Edition

First edition, April 2026

Printed in USA

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



Manufactured by:
Agilent Technologies, Inc.
In der Dalheimer Wiese 5
55120 Mainz
Germany

Warranty

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

Technology Licenses

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

Restricted Rights Legend

U.S. Government Restricted Rights. Software and technical data rights granted to the federal government include only those rights customarily provided to end user customers. Agilent provides this customary commercial license in Software and technical data pursuant to FAR 12.211 (Technical Data) and 12.212 (Computer Software) and, for the Department of Defense, DFARS 252.227-7015 (Technical Data -Commercial Items) and DFARS 227.7202-3 (Rights in Commercial Computer Software or Computer Software Documentation).

Safety Notices

CAUTION

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

WARNING

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

Contents

Introduction 5

Creation of GC/MS MassHunter Project Folder for Migration 7

Migration of Acquisition Parameters 8

Migration of Data Files 9

GC/MS MassHunter Quantitative Analysis 10

- Accessing the Quant program 10
- Creating a batch 16
- Applying the method to the batch 18
- Clearing and rebuilding the calibration curve 21
- Customizing Quant method with outliers 24

Reporting 28

Comparison of Results 33

Generating an iCal Report 35

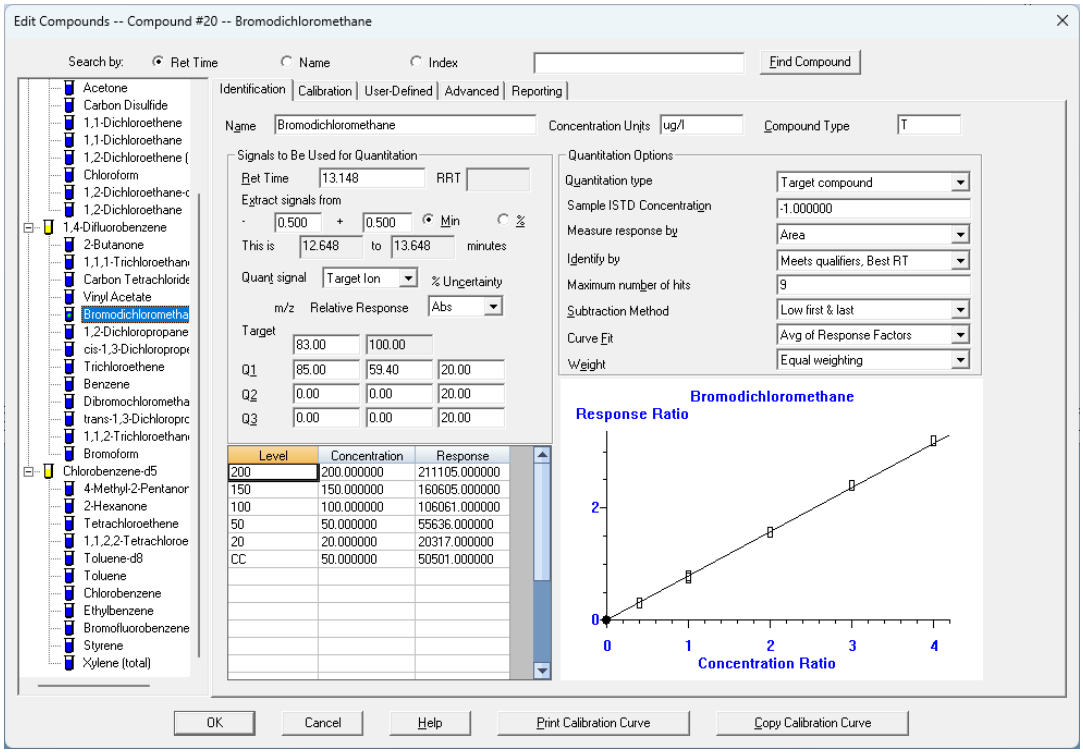
Conclusion 37

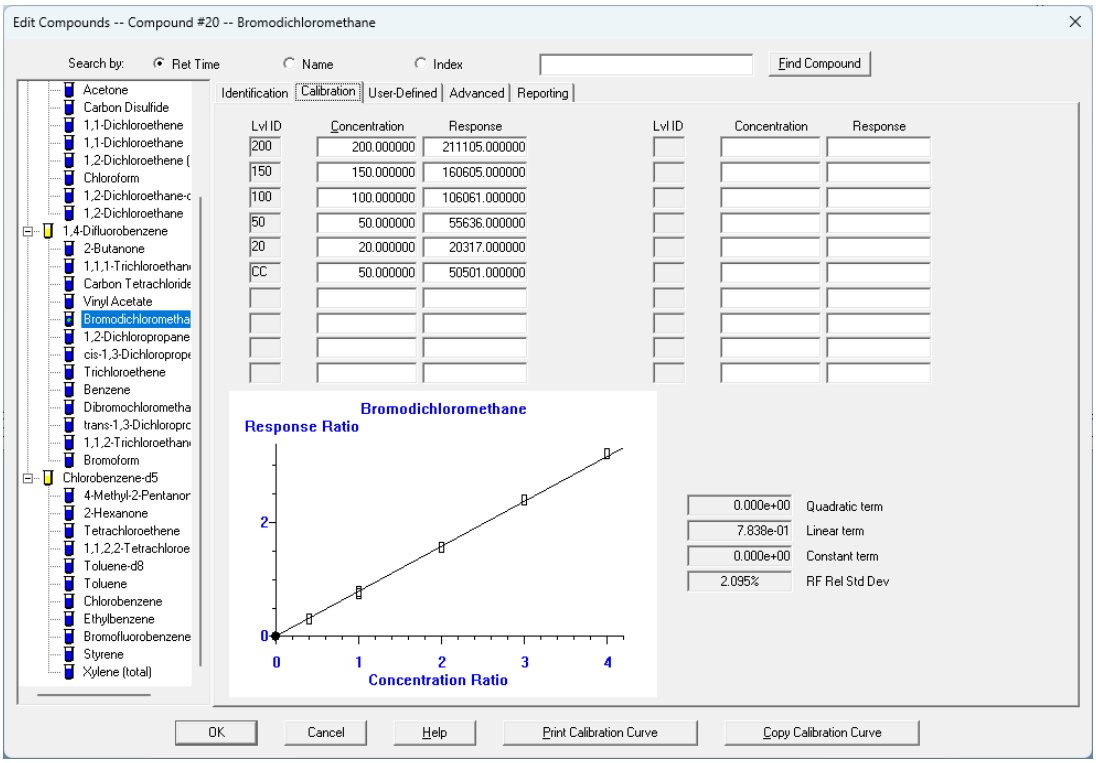
Introduction

This user guide demonstrates how to migrate an existing method and data set from Agilent MSD ChemStation into Agilent MassHunter Acquisition (version 13 or later) and Quantitative Analysis (version 12.1 or later).

The example data set for this workflow is located in the C:\EnvDemo\VOAdata directory of a typical MSD ChemStation installation. The method used is VOAList.M, which has been duplicated and renamed VOAList_demo.M to preserve the original parameters. The data set includes a method blank, an internal-standard-based calibration curve, continuing calibration checks, sample analyses, and tune evaluations.

The demo VOA data has already been processed in MSD ChemStation to generate an internal-standard-referenced calibration curve using the Average of Response Factors curve-fit option. However, the migration steps described in this guide apply to any supported calibration approach.





To begin, copy all methods and data files that require migration onto the computer running the newer software version. This guide uses MassHunter Acquisition 13.1 to illustrate the latest workflow for migrating existing data within the OpenLab Shared Services environment. The OpenLab integration is new with this version of MassHunter and will be present in versions moving forward.

Starting with version 13, MassHunter Acquisition uses a project-based file structure to improve data organization and management. For more information on working with projects, refer to the MassHunter Acquisition Help system and search for **Project**.

Creation of GC/MS MassHunter Project Folder for Migration

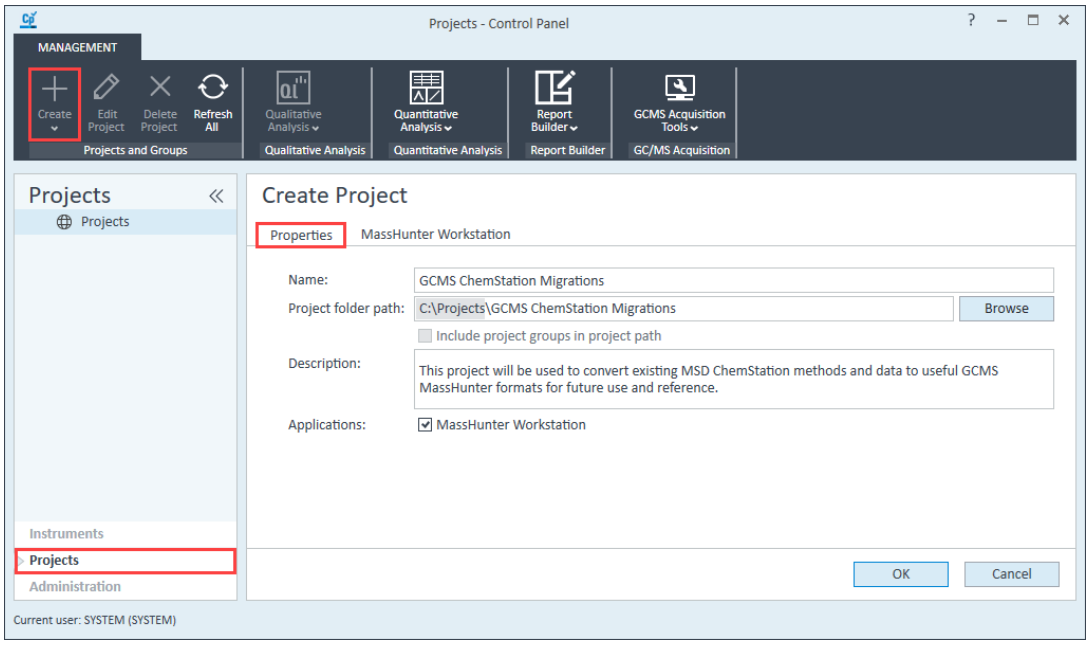
1 Launch the OpenLab Control Panel by clicking the desktop icon.



2 Select the **Projects** tab at the bottom of the window.

3 Click **Create** a new project using the ribbon tool.

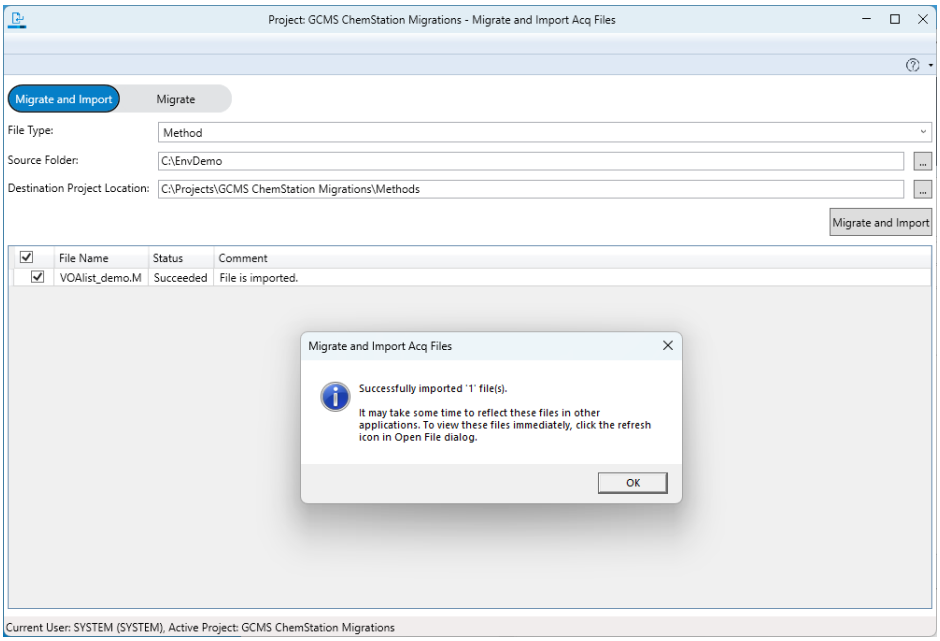
4 On the **Properties** tab, specify a name and note the path. To adjust path settings, select the **MassHunter Workstation** tab.



Migration of Acquisition Parameters

1 In the top ribbon of the Control Panel window, select **GCMS Acquisition Tools**.

2 Launch the migration tool. For this demo, the MSD ChemStation method and data files were copied to a local folder of the PC, but any accessible file path may be used.



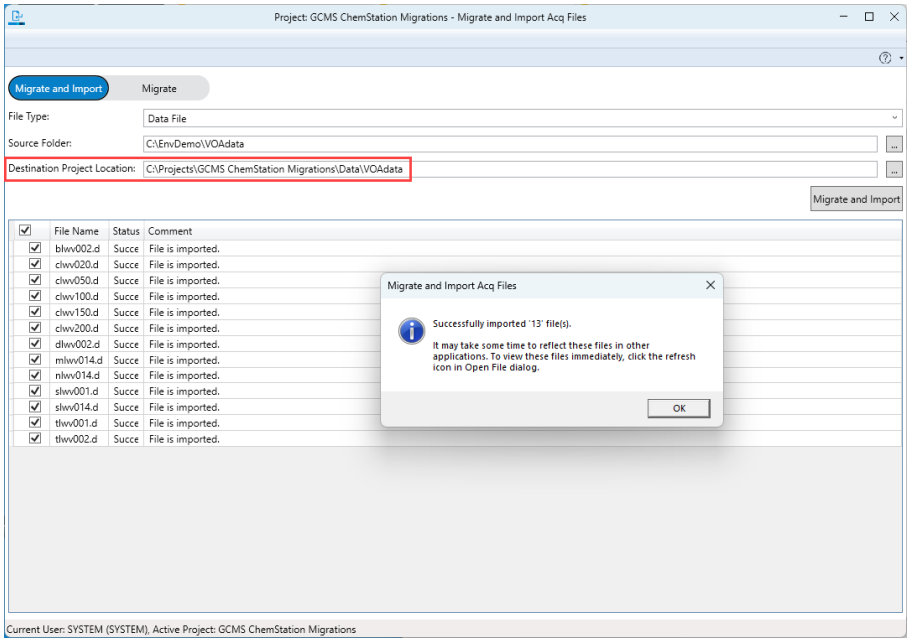
3 Click **Migrate and Import**. A success or failure message will indicate the status of the migration.

4 Verify results by navigating to the **Destination Project Location** in Windows Explorer and confirming that the migrated method appears in the **Method** folder.

Migration of Data Files

Using the aforementioned steps, data can be migrated in the same manner.

1. Select **Data File** as the file type.
2. Select the appropriate source folder. In this case, a **VOAdata** folder was created inside the local storage folder used for the method.
3. Browse to the desired output location within the project, then click **Migrate and Import**. A status window will confirm when the migration is successful.



Following these steps will ensure that data and methods are stored in a known location that can be easily found.

NOTE **The files have not yet been translated into the GC/MS MassHunter format. They have only been moved into the MassHunter folder structure.**

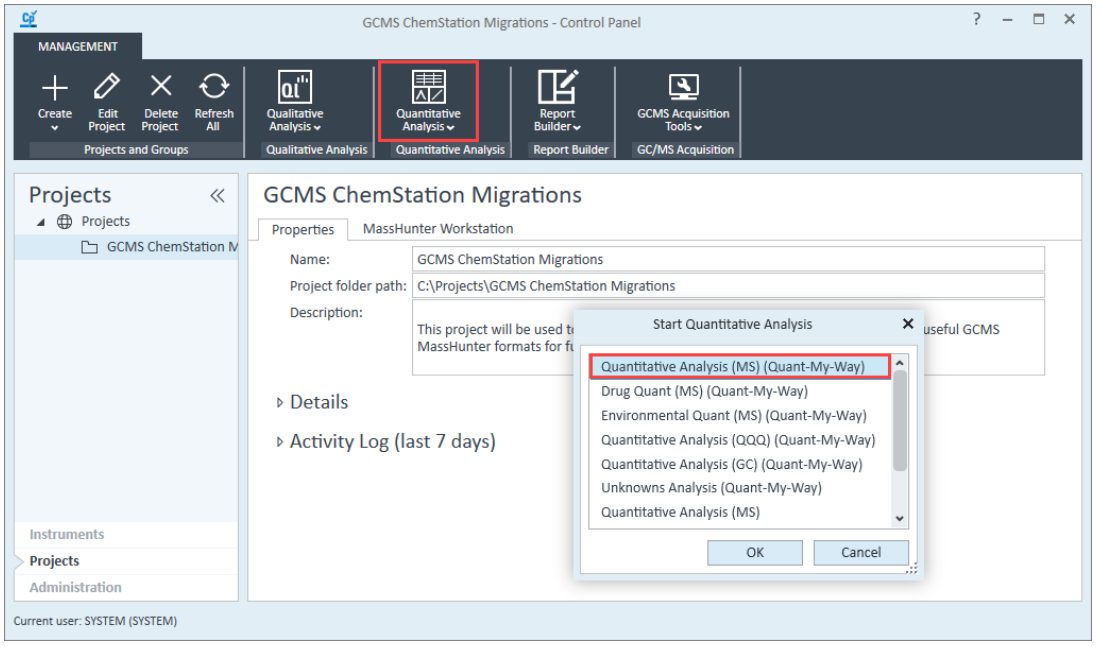
GC/MS MassHunter Quantitative Analysis

Targeted analysis using calibration workflows in the MassHunter software suite is performed in MassHunter Quantitative Analysis (Quant). Quant is available in several specialized configurations—such as EnviroQuant, DrugQuant, and Quant-My-Way—and can be tailored for a range of detection platforms, including GC, GC/MS single quadrupole, GC/MS triple quadrupole, and GC/Q-TOF systems.

Accessing the Quant program

After Quant has been installed on the PC, it must be launched from the OpenLab Control Panel by selecting the appropriate project and choosing **Quantitative Analysis** from the menu. Once selected, all available Quant configurations are displayed, and desktop shortcuts may be created for easy access.

For this demonstration, Quant-My-Way (MS) is used. In some sections of this guide, screen captures from Environmental Quant (MS) (Quant-My-Way) are shown to illustrate tasks commonly performed by those working under EPA guidance.



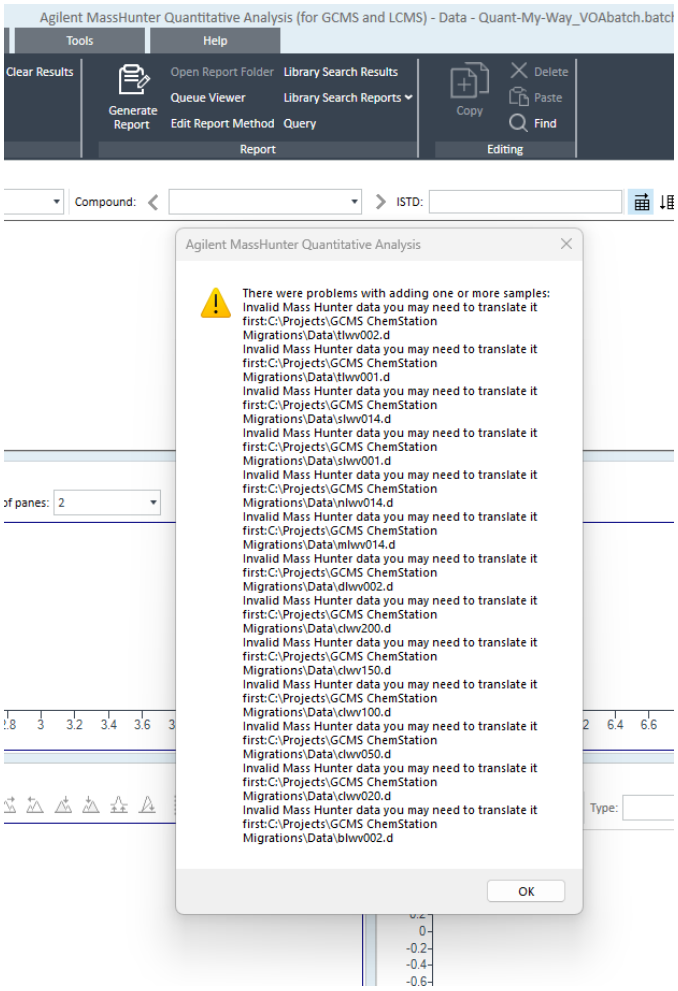
NOTE **Quantitative Analysis must be initially launched from the Control Panel. Desktop icons can also be created from this option.**

Translating MSD ChemStation data into GC/MS MassHunter Quant data

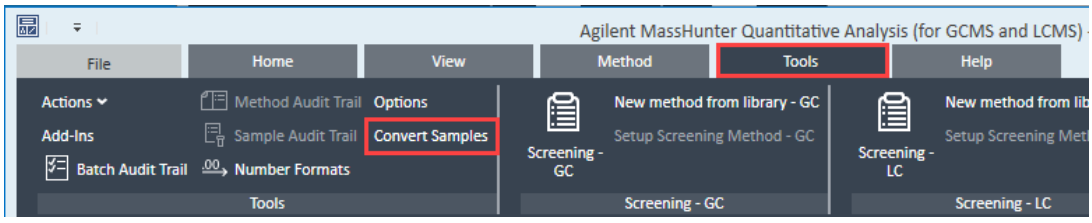
Quant uses batch files for grouping processed data, so the first step in checking the performance of the data analysis (DA) method is to create a batch.

1 In Quant, click **New Batch** on the **Home** tab and browse into the project/data folder to locate the migrated MSD ChemStation data.

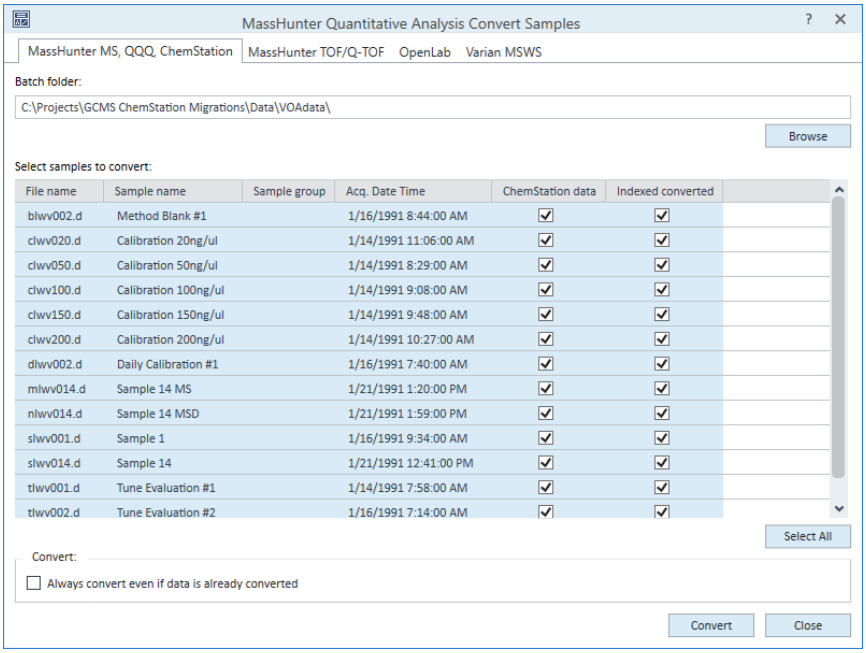
NOTE **If the steps to create a batch with this data are started and the following error message is shown, the data has not yet been translated.**

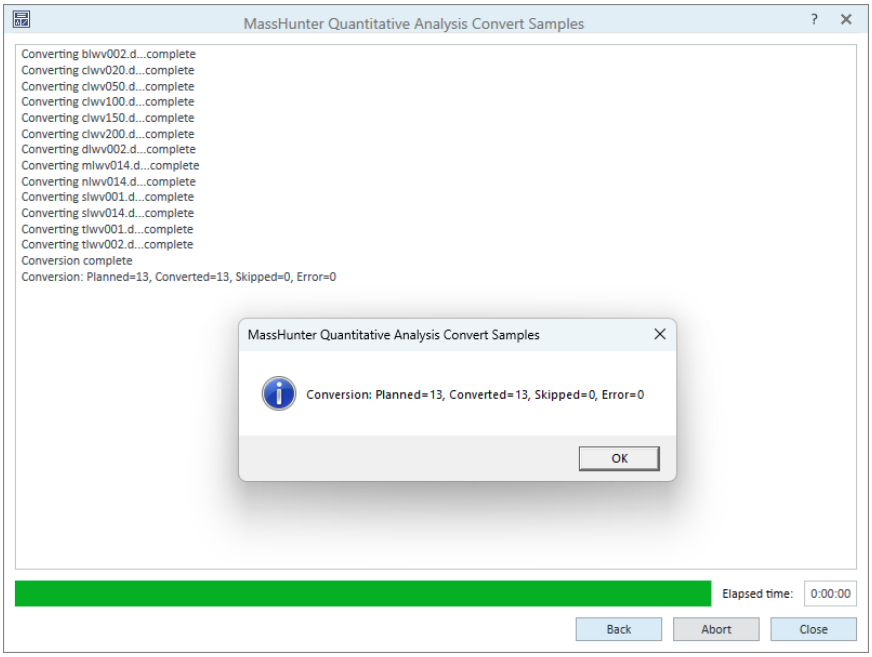


2 To translate the data into a readable format, select **Convert Samples** in the first section of the **Tools** tab. This step will launch the translator.



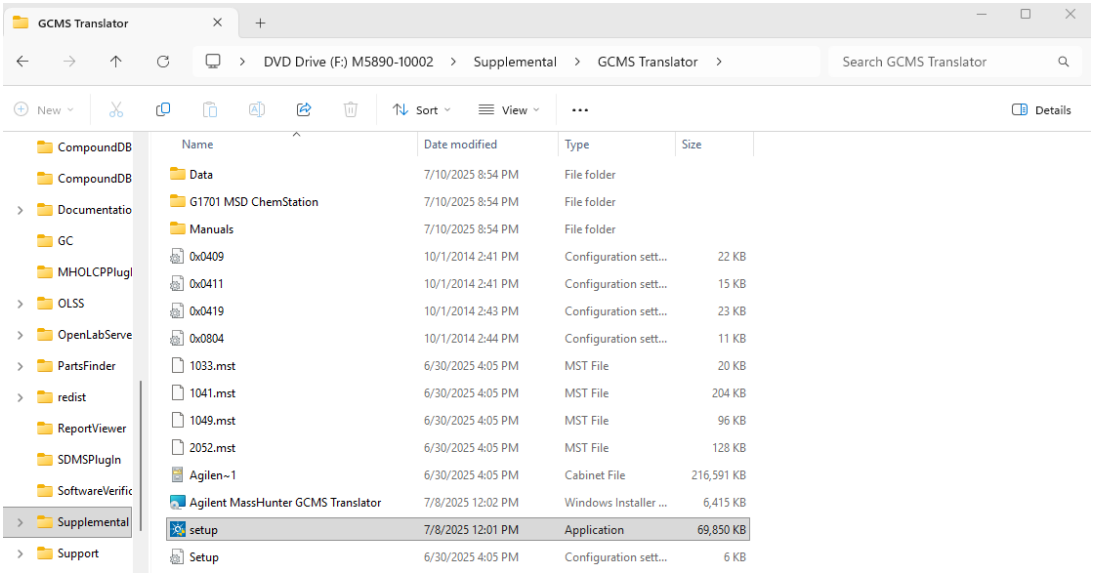
3 Select the files to translate and click **Convert**. The conversion will be confirmed by a pop-up window.



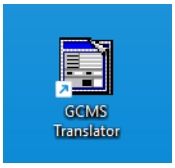


Installing and using the GCMS Translator program

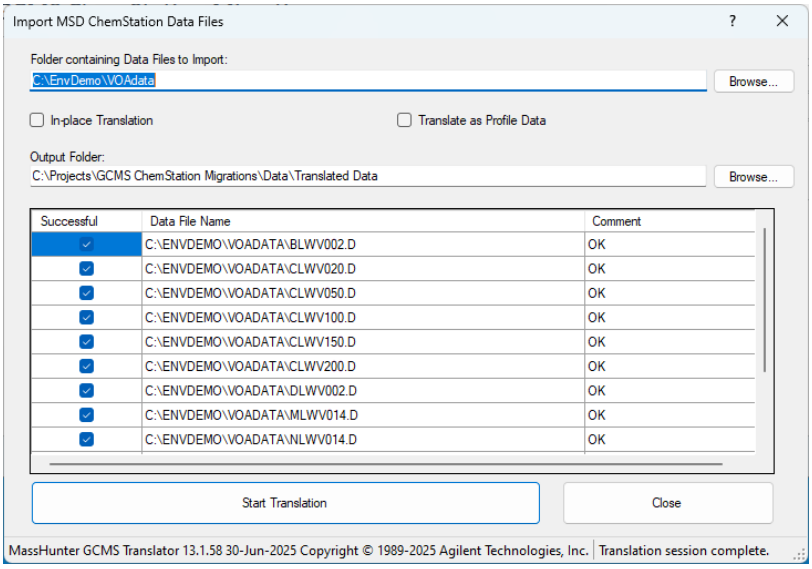
In some cases, the GC/MS ChemStation data may be too old for the embedded conversion feature in Quant, or the installed Quant version may predate this capability. If this occurs, a standalone translator tool is available. This translator can be found on the GC/MS Acquisition software media, located in the Supplemental folder.



Once installed, an icon should be present on the desktop for easy access.

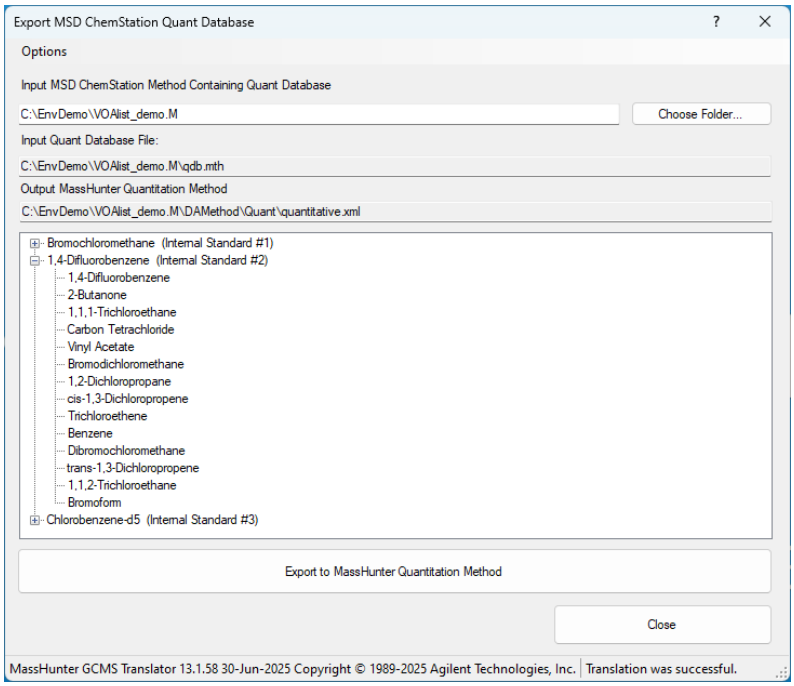


1 To use the translator, browse to the appropriate input and output locations, and click **Start Translation**. Each file will be marked with a check mark once the conversion is complete.



In addition to translating data files, the standalone translator can also convert the MSD ChemStation quant database including the compound list, internal standard assignments, and calibration details into a MassHunter compatible format. This greatly minimizes the time required to rebuild the Quant method from a new file.

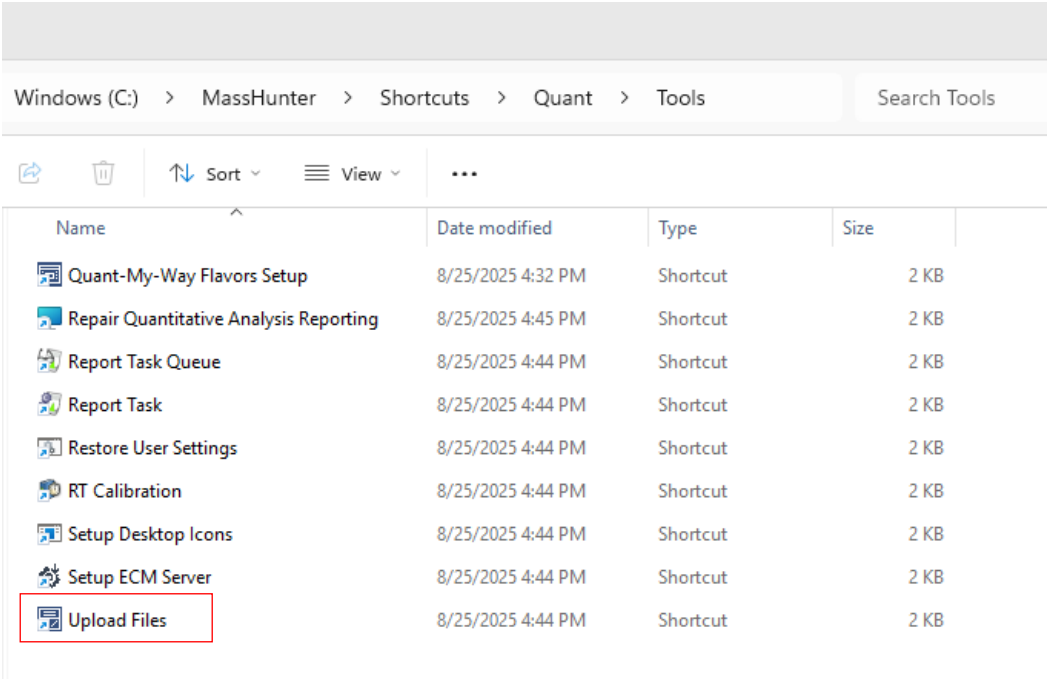
2 Browse in the method file that contains the MSD ChemStation calibration information and note the output location.



Upload Files tool

WARNING **For MassHunter Quant 12.1 Update 2 and newer, an extra step is required to create a method that can be successfully applied to the batch. If this step is skipped, applying the translated method will generate a hash checksum error.**

1 Launch the **Upload Files** tool located in the MassHunter\Shortcuts\Quant\Tools folder. Depending on how Quant was installed, this folder may be located on either the C: or D: drive.

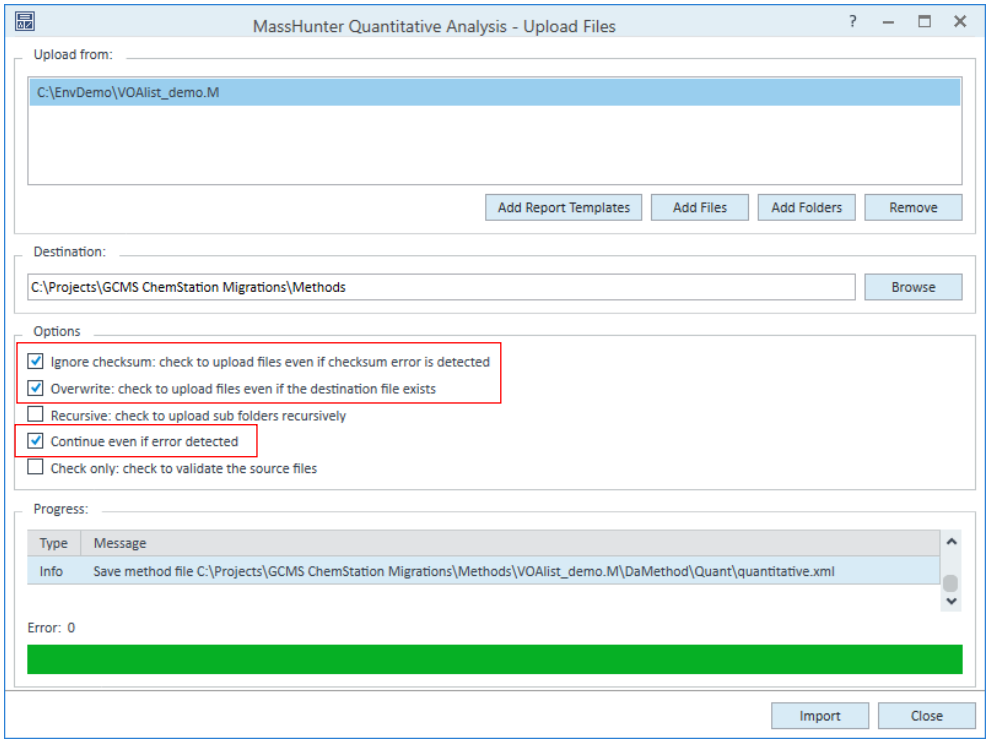


2 Select the project used in the migration process.

3 Click **Add Folders** and select the appropriate method folder.

4 Click **Browse** to specify where the translated method should be stored. Using the Project/Project Name/Methods folder is recommended.

5 Enable check boxes for: **Ignore checksum**, **Overwrite**, and **Continue even if error detected**.

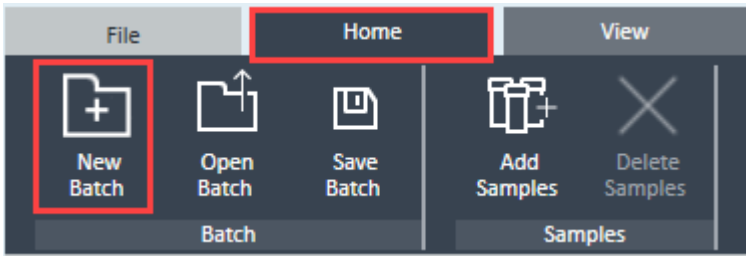


6 Verify a successful translation, by checking the folder specified in the destination and looking for the method file.

At this point, all the data and methods are in a format to be processed in GC/MS MassHunter.

Creating a batch

1 In Quantitative Analysis, select the **Home** tab, and **New Batch**.



2 Navigate to the folder containing the translated data files, provide a name for the batch and select **Create Batch**.

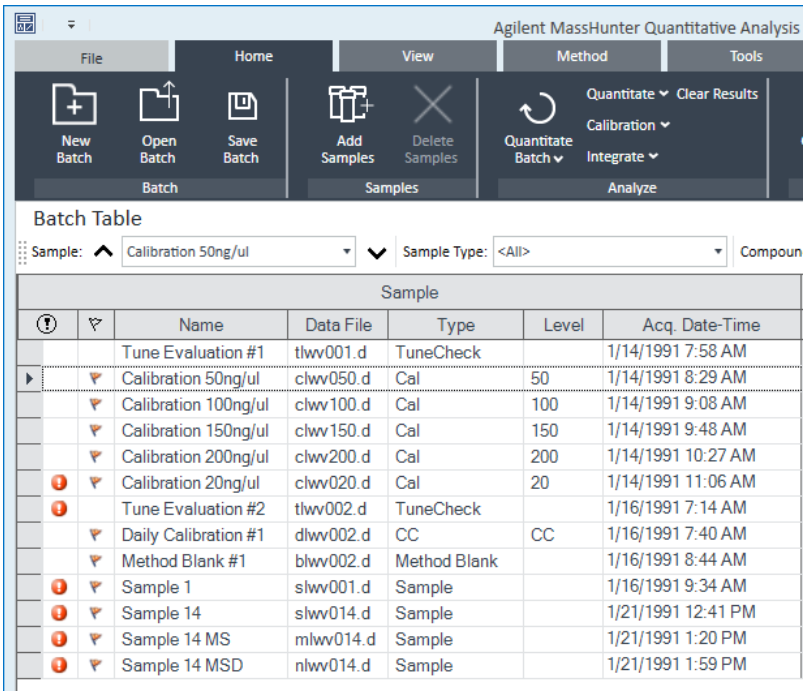
3 In the Add Samples window, choose the files required for batch processing.

At this point, the sample table will be viewable, but no method has been applied.

4 Verify the sample type is selected for **Calibration**, **QC**, **Blank**, and **Sample injections**.

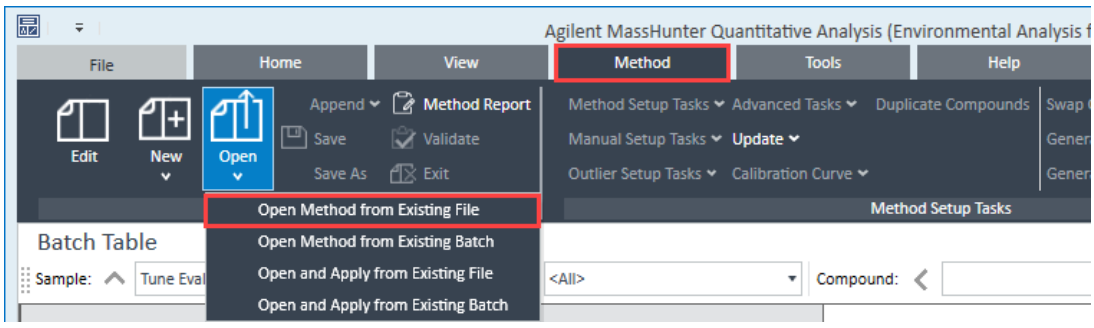
5 For sample types with known amounts (such as Cal, QC, CC, etc.), enter the values in the **Level** column.

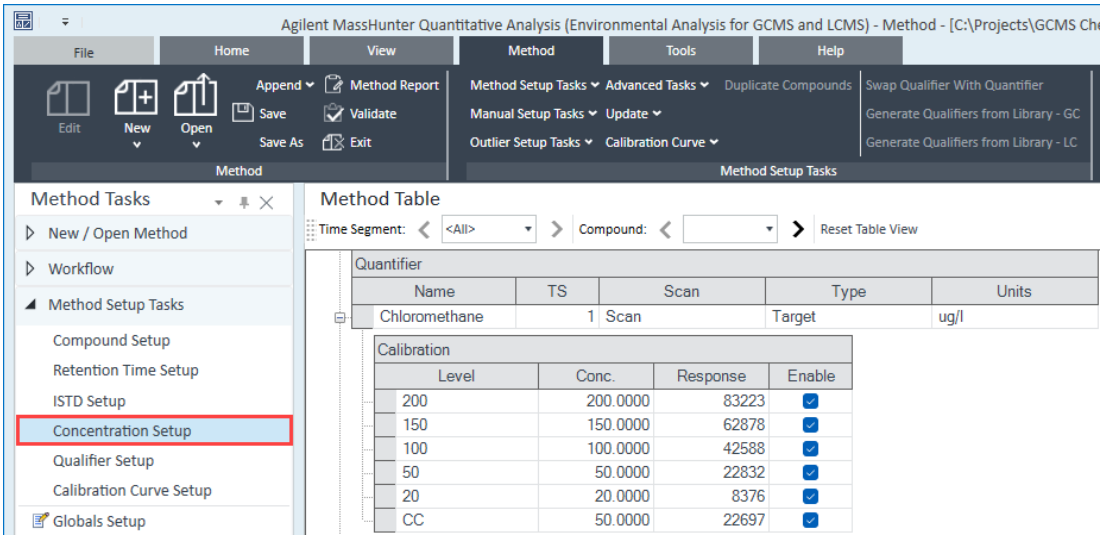
NOTE **In the Environmental configuration of Quant, additional sample types such as Method Blank and Spike Duplicate are available for EPA compliance.**



NOTE **The Level identifier in the method must match the batch table to avoid errors.**

If the Level value is unknown, click the **Method** tab at the top of the screen and select **Open > Open Method from Existing File**. Select the **VOAlist_demo** method. This will open the parameter section of the method. Selecting **Concentration Setup** will show the method levels that migrated in from the MSD ChemStation method.





Applying the method to the batch

The method editor has a **Validate** option that checks for errors before processing a batch. Error context is displayed at the bottom of the screen.

Once the errors are addressed, the method can be applied to the batch by clicking **Exit** and choosing the type of processing. For general Quant-My-Way users, either **Analyze** or **Quantitate** is recommended. For Environmental Quant-My-Way users, the Analyze option is disabled, so for calibration cannot be achieved using the Quantitate option in Environmental Quant. Since the Analyze option is disabled, as a result, calibration updates cannot be performed during batch processing. Calibration must be updated using the menu highlighted in the first image on **page 21**and by running integration first. Once the calibration has been replaced or updated, the batch should be processed using the Quantitate option.

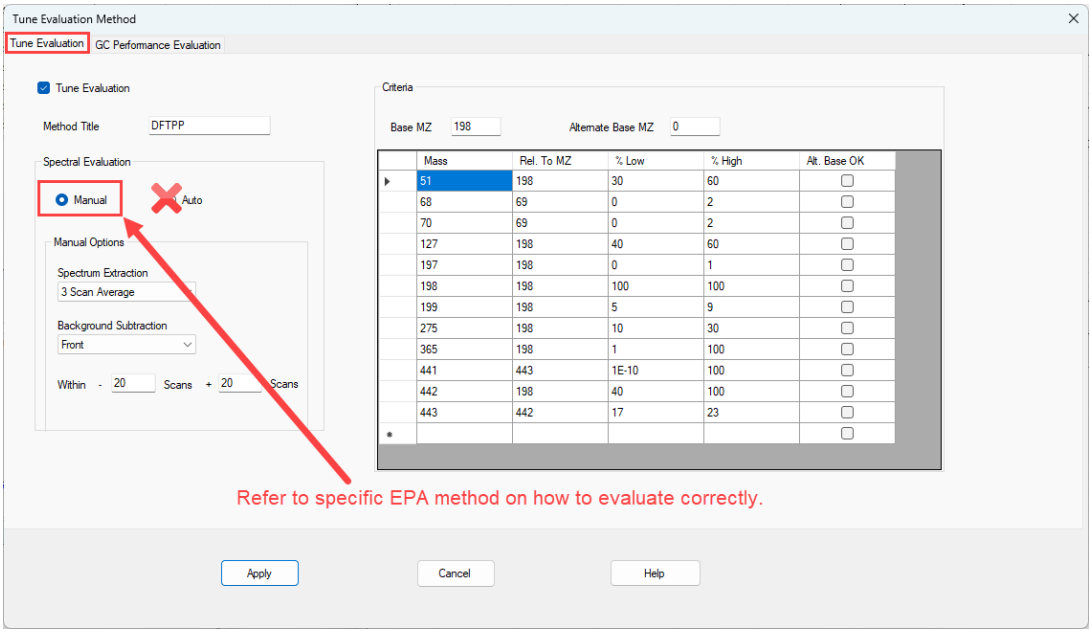
If the **Level** fields have not yet been populated, they can be entered after returning to the batch table. Attempting to proceed directly with **Exit --> Quantify** will result in an error because the calibration has not yet been updated. To proceed, select **Exit --> Integrate**, replace the calibration, and then select **Quantify**. This workflow updates both the calibration and the results fields.

EPA tune checks

For users following EPA guidelines, the Environmental configuration of Quant provides a dedicated tool that simplifies reviewing BFB tune checks for EPA 8260 and DFTPP tune checks for EPA 8270. In Environmental Quant, the **Tools** menu includes a **Tune Evaluation** option in the first panel. Selecting this option opens a set of controls that evaluate BFB, DFTPP, or other customizable method criteria against any injection loaded into the batch, with clear pass/fail results displayed for each check. The tune checks can be exported as a report.

NOTE

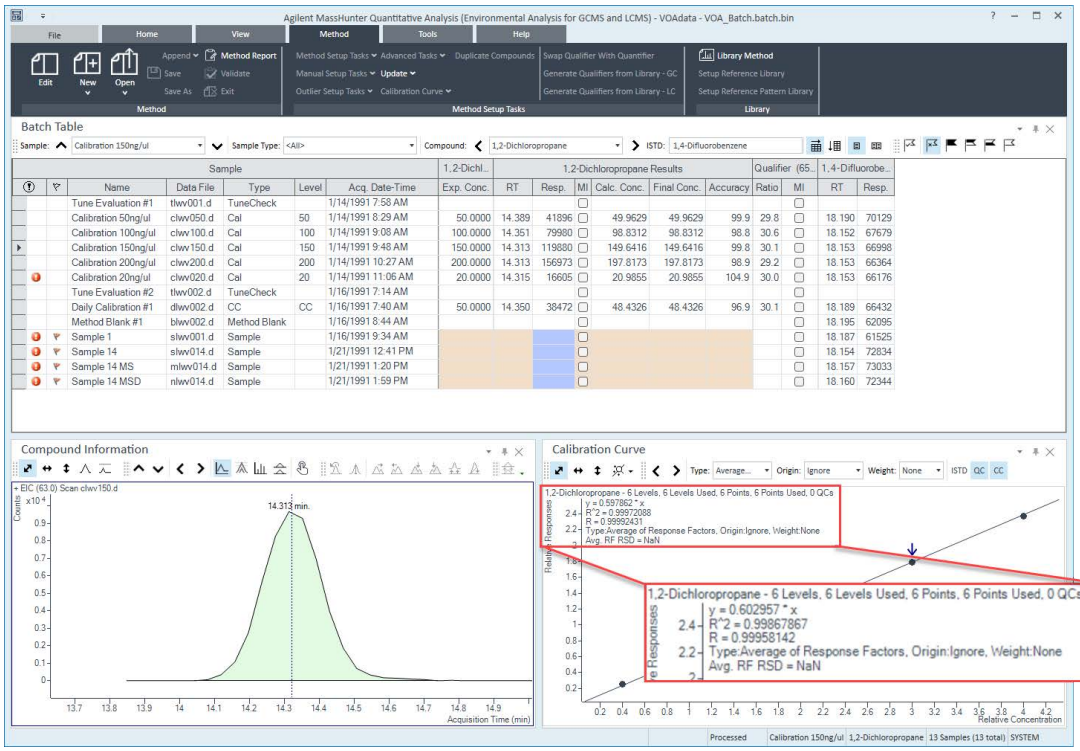
Choosing "Auto" will enable all possible combinations of spectrum extraction and background subtraction to try and pass tune check criteria. If one of them passes, it shows that result. However, this does not comply with EPA regulations for tune checks. It is important you select "Manual" and set it to the method requirements in order to comply with EPA regulations.



Calibration curves

When migrating to a new software platform, generating comparable data is critical to acceptance. Because MSD ChemStation and MassHunter Quantitative Analysis use different integration algorithms, some differences in raw peak areas and resulting calibration curves should be expected. The following steps detail how to review MassHunter generated results from ChemStation translated data.

Open the batch containing the translated data and apply the translated method.



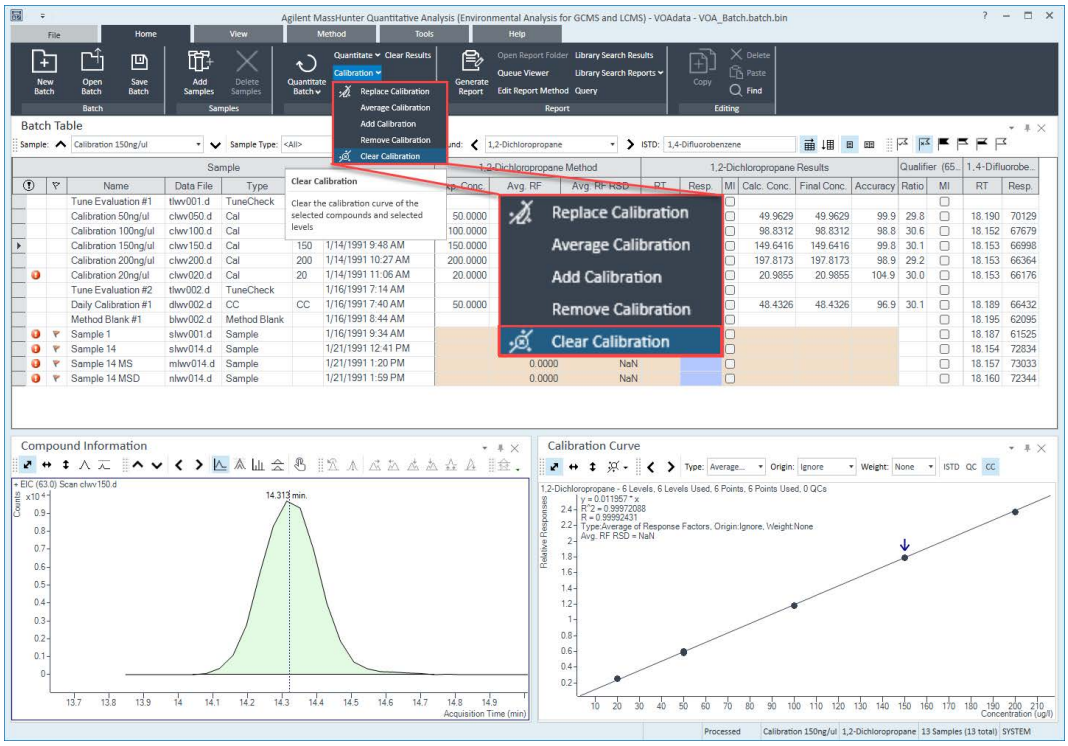
In this example, the MSD ChemStation method was calibrated using the Average of Response Factors (Avg RF) algorithm. Although the MassHunter calibration curve window displays a linear regression, the **Avg RF RSD** field shows **NaN** (not a number) instead of a percent RSD. In addition, calculated concentration and accuracy values are missing, and no error message is provided.

This behavior can occur when migrating calibration data from other software platforms, but the fix is straightforward. The calibration curve must be cleared, and the data reprocessed so MassHunter can rebuild the curve correctly.

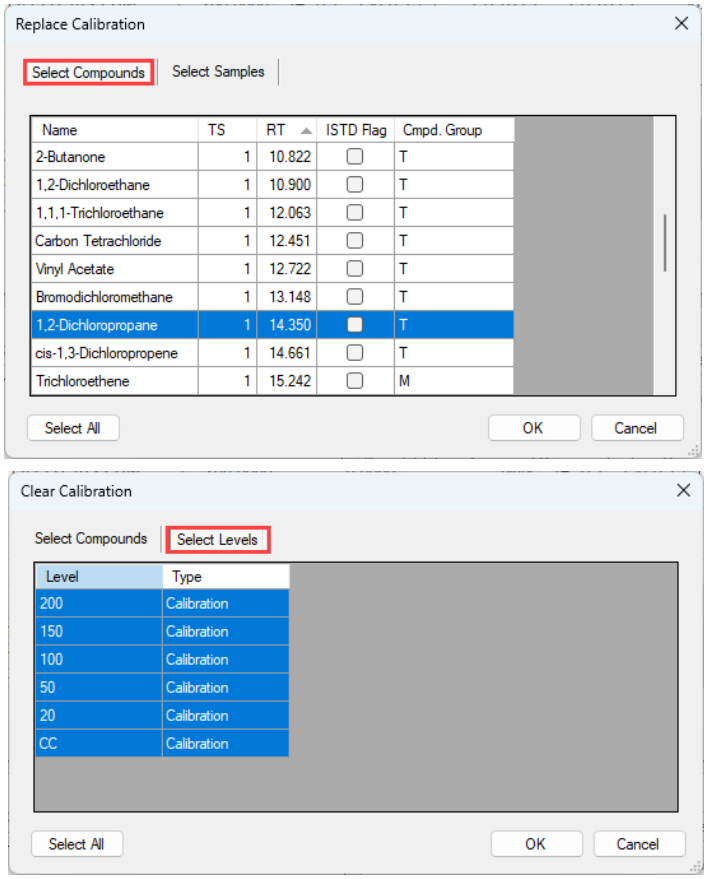
The steps to do this are nearly identical in both the standard Quant-My-Way and Environmental Quant interfaces; however, the screen captures shown are taken from the Environmental configuration.

Clearing and rebuilding the calibration curve

1 Under the **Home** tab, find the **Calibration** drop-down under the **Analyze** section and select **Clear Calibration**.

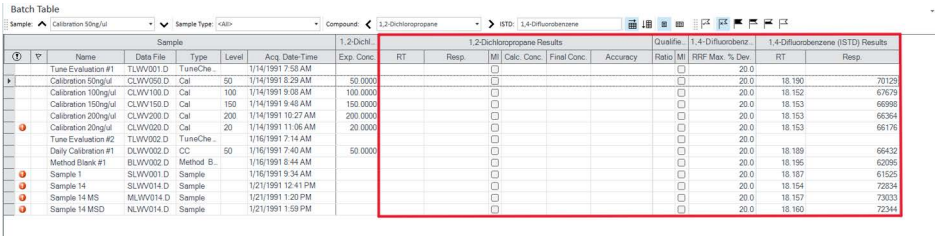


A dialogue box will appear to choose which compounds to clear. In this case, only one compound is selected, 1,2-dichloropropane. The second tab allows the user to choose which levels of the calibration to clear. In this case, all levels are selected.

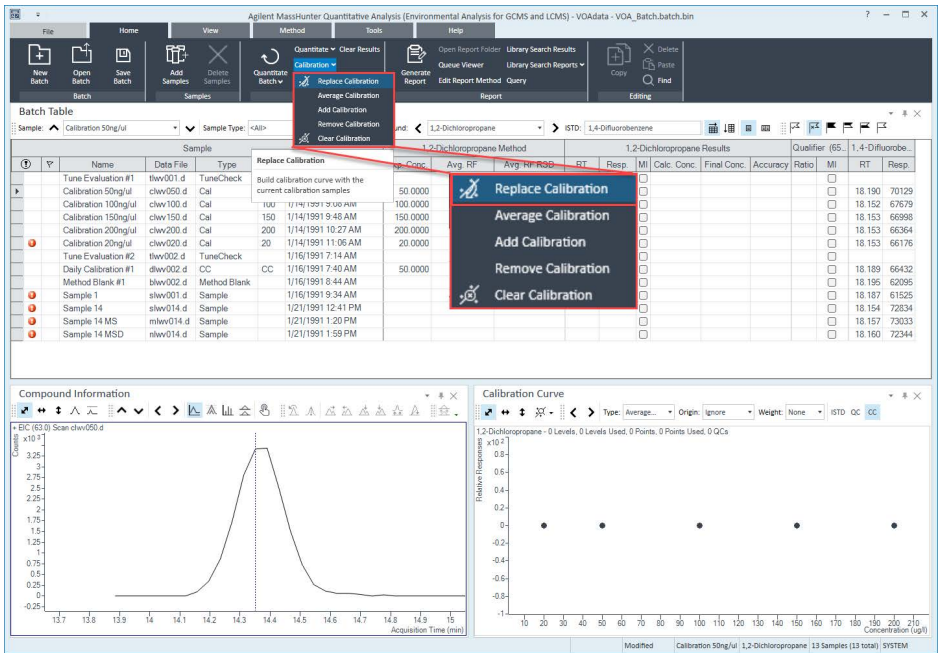


2 Click **OK** to clear the levels.

The table will be cleared of all retention time and integrated results for the compound(s) selected. In this view, the results for 1,2-dichloropropane are cleared, but the internal standard remains unaltered.

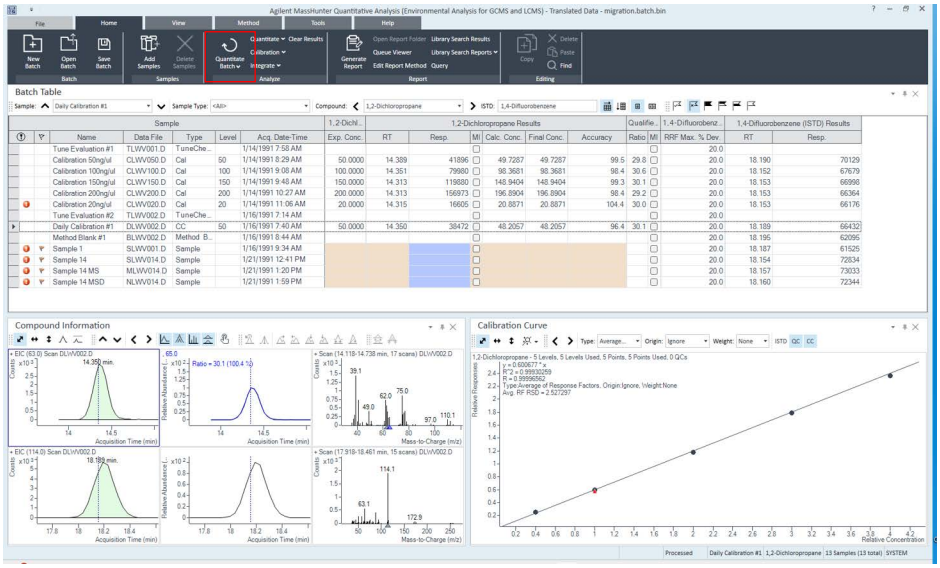


3 To re-establish the calibration curve, select the **Calibration** drop-down from the **Analyze** section of the ribbon and choose **Replace Calibration**. This rebuilds the calibration curve from the current file instead of results from the legacy method.



The same dialogue boxes will appear to select the compounds and levels needed to rebuild the calibration curve. Now, a value exists in the calibration curve for the **Avg RF RSD**, but that calibration curve has not yet been applied to the samples, so no accuracies are observed.

4 Select **Quantitate Batch** to apply the calibration curve to the batch and observe the results.



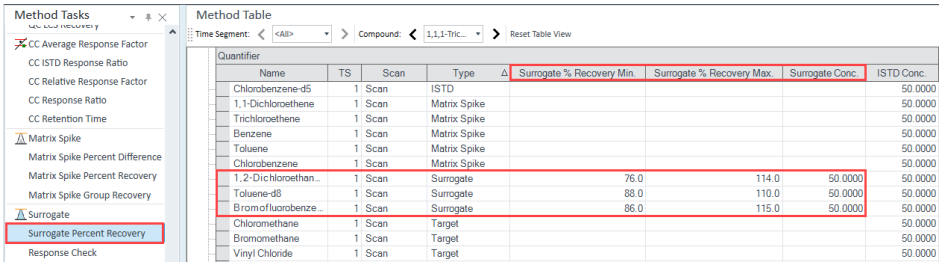
Calibration Parameter	GC/MS ChemStation	Quant-My-Way	Environmental Quant-My-Way
Avg RF RSD	2.677%	2.53%	2.53%
Linear Term	0.5979	0.6007	0.6007

Customizing Quant method with outliers

In many labs, there are different types of QC that have specific pass/fail requirements. These can be added to the Quant method under the **Outlier Setup Tasks**.

1 To access the outliers panel from the batch, select **Method/Edit**, and scroll down until the **Outliers** section is visible.

2 Scroll to the appropriate sample type, in this case, **Surrogates**, enter the limits into the table for the associated compounds.



Building these limits into the Quant method allows for a reviewer to catch nonconformities in the data both in the batch table and the resulting report. The outliers are configured and set in the Quant method, but only the applicable outliers will be pulled into the included reports. In many cases, outlier limits and boundaries may be added to the batch table for easy export into other software not using the Quant reports.

3 In the batch table, right-click and select **Add/Remove Columns** to add the fields.

Table 1 includes commonly applied outliers for environmental workflows, but outliers can be customized for all laboratory operations:

Table 1 Common outliers for environmental workflows.

Report Type	Common Outliers		
Calibrations (iCal, ConCal)	Curve fit type	% RSD	Avg RF
Matrix Spike	% Recovery min	% Recovery max	% Dev
QA Check	Surrogate recovery	Time since tune	ISTD precision

Most result-based outlier settings are configured in the **Outliers Setup** section of the Quant Method Editor. However, some criteria, particularly those based on information outside the data file itself, are found under **Globals Setup**.

For example, a laboratory may require frequent instrument tuning as part of its QA or regulatory procedures. In this case, a time limit (in hours) is specified in the **CC Maximum Elapsed Time in Hours** field to have the QA Check Report flag any samples run outside that window.

In the example shown, the QA report fails because the migrated data is significantly older than the most recent tune, triggering the elapsed-time criterion.

Sample

Name	Data File	Type	Level	Acq. Method File	Acq. Date-Time
Calibration 50ng...	CLWV050.D	Cal	50	DANNY	1/14/1991 8:29 A...

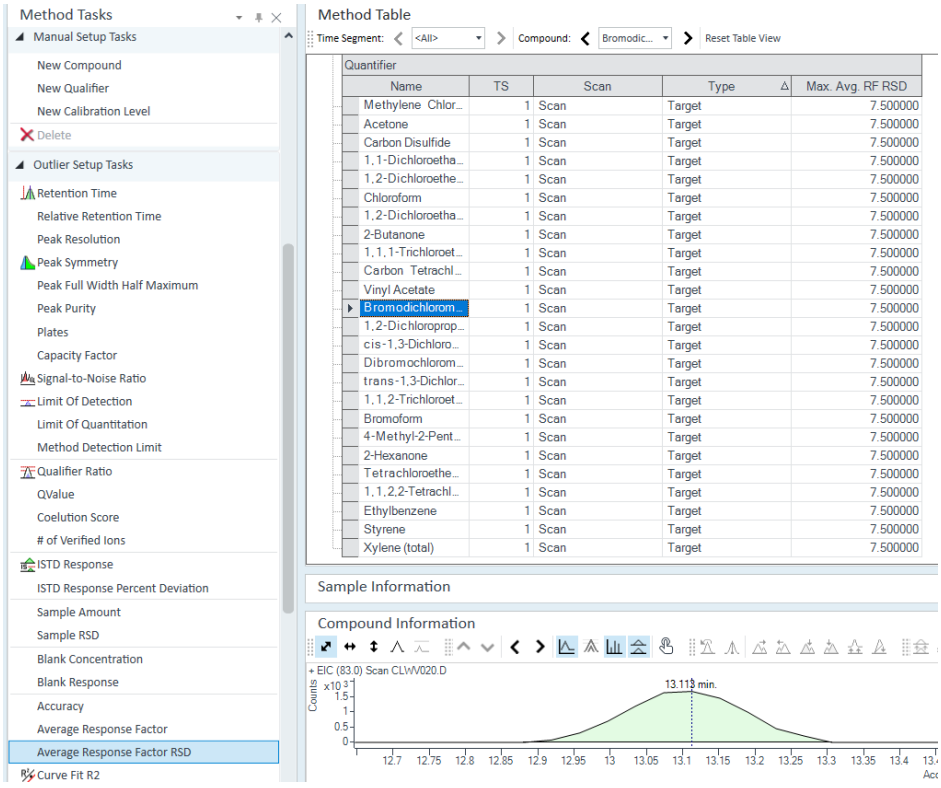
Globals

Apply Multiplier to ISTD	☐
Apply Multiplier to Matrix Spike	☑
Apply Multiplier to Surrogate	☑
Apply Multiplier to Target	☑
Bracketing Type	None
CC Maximum Elapsed Time In Hours	24.000
Correlation Window	0.100
Dynamic Background Subtraction	☐
Ignore Peaks Not Found	☐
Library Method	
Non Reference Window	70.000
Non Reference Window Type	Percent
Reference Library	
Reference Pattern Library	
Reference Window	80.000
Reference Window Type	Percent
Relative ISTD	☐
Standard Addition	☐

Another commonly used report in environmental labs is the **Initial Calibration (iCal)** report. While the report itself will generate calculations based on the data files, applying outliers can improve the review process and provide visual cues that a result needs attention.

To demonstrate how outliers affect the appearance of a report, two iCal reports are generated: one with outliers configured in the Quant method and one without.

The outlier parameter configured is %RSD maximum of 7.5 for curve fits of Avg RF.



While the steps required to generate the iCal report will be demonstrated in the next section, two versions of the iCal report are shown below, the first one without applying the outlier and the second with the outlier boundary applied.

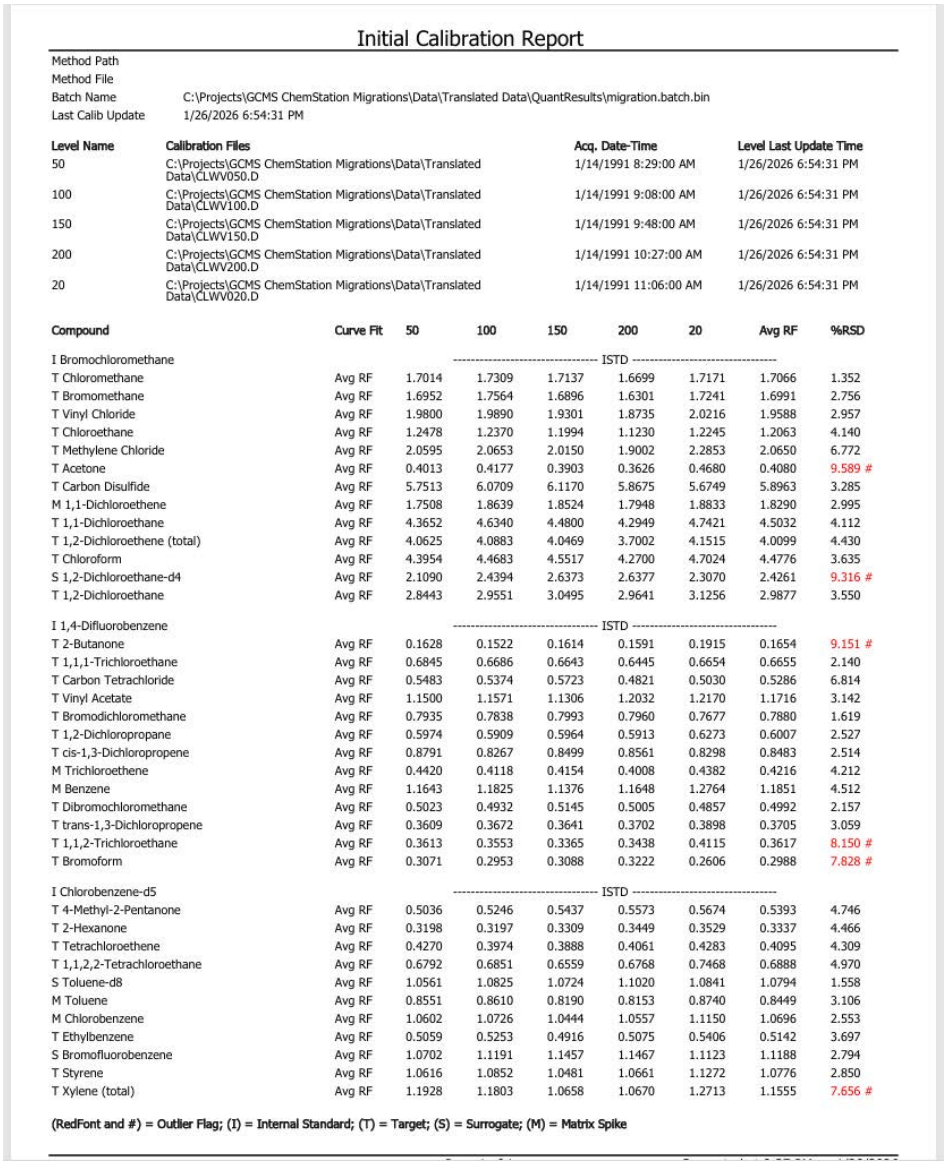
Initial Calibration Report

Method Path
Method File
Batch Name C:\Projects\GCMS ChemStation Migrations\Data\Translated Data\QuantResults\migration.batch.bin
Last Calib Update 1/26/2026 6:54:31 PM

Level Name	Calibration Files	Acq. Date-Time	Level Last Update Time
50	C:\Projects\GCMS ChemStation Migrations\Data\Translated Data\CLWV050.D	1/14/1991 8:29:00 AM	1/26/2026 6:54:31 PM
100	C:\Projects\GCMS ChemStation Migrations\Data\Translated Data\CLWV100.D	1/14/1991 9:08:00 AM	1/26/2026 6:54:31 PM
150	C:\Projects\GCMS ChemStation Migrations\Data\Translated Data\CLWV150.D	1/14/1991 9:48:00 AM	1/26/2026 6:54:31 PM
200	C:\Projects\GCMS ChemStation Migrations\Data\Translated Data\CLWV200.D	1/14/1991 10:27:00 AM	1/26/2026 6:54:31 PM
20	C:\Projects\GCMS ChemStation Migrations\Data\Translated Data\CLWV020.D	1/14/1991 11:06:00 AM	1/26/2026 6:54:31 PM

Compound	Curve Fit	50	100	150	200	20	Avg RF	%RSD
I Bromochloromethane		---------- ISTD ----------						
T Chloromethane	Avg RF	1.7014	1.7309	1.7137	1.6699	1.7171	1.7066	1.352
T Bromomethane	Avg RF	1.6952	1.7564	1.6896	1.6301	1.7241	1.6991	2.756
T Vinyl Chloride	Avg RF	1.9800	1.9890	1.9301	1.8735	2.0216	1.9588	2.957
T Chloroethane	Avg RF	1.2478	1.2370	1.1994	1.1230	1.2245	1.2063	4.140
T Methylene Chloride	Avg RF	2.0595	2.0653	2.0150	1.9002	2.2853	2.0650	6.772
T Acetone	Avg RF	0.4013	0.4177	0.3903	0.3626	0.4680	0.4080	9.589
T Carbon Disulfide	Avg RF	5.7513	6.0709	6.1170	5.8675	5.6749	5.8963	3.285
M 1,1-Dichloroethene	Avg RF	1.7508	1.8639	1.8524	1.7948	1.8833	1.8290	2.995
T 1,1-Dichloroethane	Avg RF	4.3652	4.6340	4.4800	4.2949	4.7421	4.5032	4.112
T 1,2-Dichloroethene (total)	Avg RF	4.0625	4.0883	4.0469	3.7002	4.1515	4.0099	4.430
T Chloroform	Avg RF	4.3954	4.4683	4.5517	4.2700	4.7024	4.4776	3.635
S 1,2-Dichloroethane-d4	Avg RF	2.1090	2.4394	2.6373	2.6377	2.3070	2.4261	9.316
T 1,2-Dichloroethane	Avg RF	2.8443	2.9551	3.0495	2.9641	3.1256	2.9877	3.550
I 1,4-Difluorobenzene		---------- ISTD ----------						
T 2-Butanone	Avg RF	0.1628	0.1522	0.1614	0.1591	0.1915	0.1654	9.151
T 1,1,1-Trichloroethane	Avg RF	0.6845	0.6686	0.6643	0.6445	0.6654	0.6655	2.140
T Carbon Tetrachloride	Avg RF	0.5483	0.5374	0.5723	0.4821	0.5030	0.5286	6.814
T Vinyl Acetate	Avg RF	1.1500	1.1571	1.1306	1.2032	1.2170	1.1716	3.142
T Bromodichloromethane	Avg RF	0.7935	0.7838	0.7993	0.7960	0.7677	0.7880	1.619
T 1,2-Dichloropropane	Avg RF	0.5974	0.5909	0.5964	0.5913	0.6273	0.6007	2.527
T cis-1,3-Dichloropropene	Avg RF	0.8791	0.8267	0.8499	0.8561	0.8298	0.8483	2.514
M Trichloroethene	Avg RF	0.4420	0.4118	0.4154	0.4008	0.4382	0.4216	4.212
M Benzene	Avg RF	1.1643	1.1825	1.1376	1.1648	1.2764	1.1851	4.512
T Dibromochloromethane	Avg RF	0.5023	0.4932	0.5145	0.5005	0.4857	0.4992	2.157
T trans-1,3-Dichloropropene	Avg RF	0.3609	0.3672	0.3641	0.3702	0.3898	0.3705	3.059
T 1,1,2-Trichloroethane	Avg RF	0.3613	0.3553	0.3365	0.3438	0.4115	0.3617	8.150
T Bromoform	Avg RF	0.3071	0.2953	0.3088	0.3222	0.2606	0.2988	7.828
I Chlorobenzene-d5		---------- ISTD ----------						
T 4-Methyl-2-Pentanone	Avg RF	0.5036	0.5246	0.5437	0.5573	0.5674	0.5393	4.746
T 2-Hexanone	Avg RF	0.3198	0.3197	0.3309	0.3449	0.3529	0.3337	4.466
T Tetrachloroethene	Avg RF	0.4270	0.3974	0.3888	0.4061	0.4283	0.4095	4.309
T 1,1,2,2-Tetrachloroethane	Avg RF	0.6792	0.6851	0.6559	0.6768	0.7468	0.6888	4.970
S Toluene-d8	Avg RF	1.0561	1.0825	1.0724	1.1020	1.0841	1.0794	1.558
M Toluene	Avg RF	0.8551	0.8610	0.8190	0.8153	0.8740	0.8449	3.106
M Chlorobenzene	Avg RF	1.0602	1.0726	1.0444	1.0557	1.1150	1.0696	2.553
T Ethylbenzene	Avg RF	0.5059	0.5253	0.4916	0.5075	0.5406	0.5142	3.697
S Bromofluorobenzene	Avg RF	1.0702	1.1191	1.1457	1.1467	1.1123	1.1188	2.794
T Styrene	Avg RF	1.0616	1.0852	1.0481	1.0661	1.1272	1.0776	2.850
T Xylene (total)	Avg RF	1.1928	1.1803	1.0658	1.0670	1.2713	1.1555	7.656

(RedFont and #) = Outlier Flag; (I) = Internal Standard; (T) = Target; (S) = Surrogate; (M) = Matrix Spike



Initial Calibration Report

Method Path
Method File
Batch Name C:\Projects\GCMS ChemStation Migrations\Data\Translated Data\QuantResults\migration.batch.bin
Last Calib Update 1/26/2026 6:54:31 PM

Level Name	Calibration Files	Acq. Date-Time	Level Last Update Time
50	C:\Projects\GCMS ChemStation Migrations\Data\Translated Data\CLWV050.D	1/14/1991 8:29:00 AM	1/26/2026 6:54:31 PM
100	C:\Projects\GCMS ChemStation Migrations\Data\Translated Data\CLWV100.D	1/14/1991 9:08:00 AM	1/26/2026 6:54:31 PM
150	C:\Projects\GCMS ChemStation Migrations\Data\Translated Data\CLWV150.D	1/14/1991 9:48:00 AM	1/26/2026 6:54:31 PM
200	C:\Projects\GCMS ChemStation Migrations\Data\Translated Data\CLWV200.D	1/14/1991 10:27:00 AM	1/26/2026 6:54:31 PM
20	C:\Projects\GCMS ChemStation Migrations\Data\Translated Data\CLWV020.D	1/14/1991 11:06:00 AM	1/26/2026 6:54:31 PM

Compound	Curve Fit	50	100	150	200	20	Avg RF	%RSD
I Bromochloromethane		---------- ISTD ----------						
T Chloromethane	Avg RF	1.7014	1.7309	1.7137	1.6699	1.7171	1.7066	1.352
T Bromomethane	Avg RF	1.6952	1.7564	1.6896	1.6301	1.7241	1.6991	2.756
T Vinyl Chloride	Avg RF	1.9800	1.9890	1.9301	1.8735	2.0216	1.9588	2.957
T Chloroethane	Avg RF	1.2478	1.2370	1.1994	1.1230	1.2245	1.2063	4.140
T Methylene Chloride	Avg RF	2.0595	2.0653	2.0150	1.9002	2.2853	2.0650	6.772
T Acetone	Avg RF	0.4013	0.4177	0.3903	0.3626	0.4680	0.4080	9.589 #
T Carbon Disulfide	Avg RF	5.7513	6.0709	6.1170	5.8675	5.6749	5.8963	3.285
M 1,1-Dichloroethene	Avg RF	1.7508	1.8639	1.8524	1.7948	1.8833	1.8290	2.995
T 1,1-Dichloroethane	Avg RF	4.3652	4.6340	4.4800	4.2949	4.7421	4.5032	4.112
T 1,2-Dichloroethene (total)	Avg RF	4.0625	4.0883	4.0469	3.7002	4.1515	4.0099	4.430
T Chloroform	Avg RF	4.3954	4.4683	4.5517	4.2700	4.7024	4.4776	3.635
S 1,2-Dichloroethane-d4	Avg RF	2.1090	2.4394	2.6373	2.6377	2.3070	2.4261	9.316 #
T 1,2-Dichloroethane	Avg RF	2.8443	2.9551	3.0495	2.9641	3.1256	2.9877	3.550
I 1,4-Difluorobenzene		---------- ISTD ----------						
T 2-Butanone	Avg RF	0.1628	0.1522	0.1614	0.1591	0.1915	0.1654	9.151 #
T 1,1,1-Trichloroethane	Avg RF	0.6845	0.6686	0.6643	0.6445	0.6654	0.6655	2.140
T Carbon Tetrachloride	Avg RF	0.5483	0.5374	0.5723	0.4821	0.5030	0.5286	6.814
T Vinyl Acetate	Avg RF	1.1500	1.1571	1.1306	1.2032	1.2170	1.1716	3.142
T Bromodichloromethane	Avg RF	0.7935	0.7838	0.7993	0.7960	0.7677	0.7880	1.619
T 1,2-Dichloropropane	Avg RF	0.5974	0.5909	0.5964	0.5913	0.6273	0.6007	2.527
T cis-1,3-Dichloropropene	Avg RF	0.8791	0.8267	0.8499	0.8561	0.8298	0.8483	2.514
M Trichloroethene	Avg RF	0.4420	0.4118	0.4154	0.4008	0.4382	0.4216	4.212
M Benzene	Avg RF	1.1643	1.1825	1.1376	1.1648	1.2764	1.1851	4.512
T Dibromochloromethane	Avg RF	0.5023	0.4932	0.5145	0.5005	0.4857	0.4992	2.157
T trans-1,3-Dichloropropene	Avg RF	0.3609	0.3672	0.3641	0.3702	0.3898	0.3705	3.059
T 1,1,2-Trichloroethane	Avg RF	0.3613	0.3553	0.3365	0.3438	0.4115	0.3617	8.150 #
T Bromoform	Avg RF	0.3071	0.2953	0.3088	0.3222	0.2606	0.2988	7.828 #
I Chlorobenzene-d5		---------- ISTD ----------						
T 4-Methyl-2-Pentanone	Avg RF	0.5036	0.5246	0.5437	0.5573	0.5674	0.5393	4.746
T 2-Hexanone	Avg RF	0.3198	0.3197	0.3309	0.3449	0.3529	0.3337	4.466
T Tetrachloroethene	Avg RF	0.4270	0.3974	0.3888	0.4061	0.4283	0.4095	4.309
T 1,1,2,2-Tetrachloroethane	Avg RF	0.6792	0.6851	0.6559	0.6768	0.7468	0.6888	4.970
S Toluene-d8	Avg RF	1.0561	1.0825	1.0724	1.1020	1.0841	1.0794	1.558
M Toluene	Avg RF	0.8551	0.8610	0.8190	0.8153	0.8740	0.8449	3.106
M Chlorobenzene	Avg RF	1.0602	1.0726	1.0444	1.0557	1.1150	1.0696	2.553
T Ethylbenzene	Avg RF	0.5059	0.5253	0.4916	0.5075	0.5406	0.5142	3.697
S Bromofluorobenzene	Avg RF	1.0702	1.1191	1.1457	1.1467	1.1123	1.1188	2.794
T Styrene	Avg RF	1.0616	1.0852	1.0481	1.0661	1.1272	1.0776	2.850
T Xylene (total)	Avg RF	1.1928	1.1803	1.0658	1.0670	1.2713	1.1555	7.656 #

(RedFont and #) = Outlier Flag; (I) = Internal Standard; (T) = Target; (S) = Surrogate; (M) = Matrix Spike

NOTE All compounds with an Avg RF RSD result exceeding 7.5 are shown with red text and also denoted with a hash mark for more attention.

Reporting

Once the calibration curve meets the lab criteria, and the tune check has passed for labs following EPA guidelines, a comparison of sample data is warranted. This batch contains a method blank and four different samples for comparison.

For this example, sample 14 will be used for comparison. In MSD ChemStation, using the EPA template associated with the method, the following results are obtained.

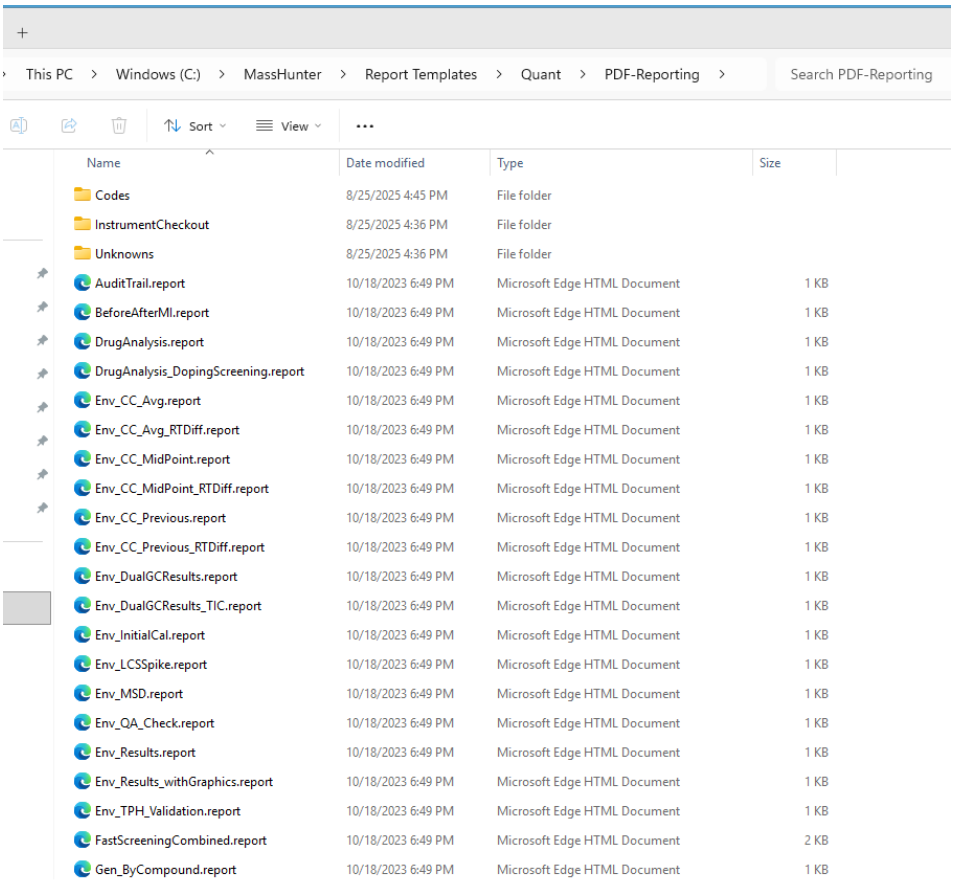
C:\EnvDemo\voadata\mlwv014.d\epatemp.txt

Compound	R.T.	QIon	Response	Conc	Units	Dev(Min)
Internal Standards						
1) Bromochloromethane	7.921	128	12701	50.00	ug/l	#-0.03
15) 1,4-Difluorobenzene	18.157	114	73001	50.00	ug/l	-0.03
29) Chlorobenzene-d5	22.926	117	64313	50.00	ug/l	-0.03
System Monitoring Compounds						
13) 1,2-Dichloroethane-d4	10.751	65	32686	53.07	ug/l	-0.03
Spiked Amount 50.000	Range 76 - 114		Recovery = 106.14%			
34) Toluene-d8	21.724	98	67281	48.44	ug/l	-0.07
Spiked Amount 50.000	Range 88 - 110		Recovery = 96.88%			
38) Bromofluorobenzene	26.649	95	72049	50.07	ug/l	-0.07
Spiked Amount 50.000	Range 86 - 115		Recovery = 100.14%			
Target Compounds						Qvalue
2) Chloromethane	0.942	50	105	0.24	ug/l #	42
3) Bromomethane	0.000		0	N.D.		
4) Vinyl Chloride	2.067	62	47	0.09	ug/l #	22
5) Chloroethane	0.000		0	N.D.		
6) Methylene Chloride	4.587	84	1656	3.16	ug/l #	80
7) Acetone	5.246	43	344	3.14	ug/l #	51
8) Carbon Disulfide	0.000		0	N.D.		
9) 1,1-Dichloroethene	7.378	96	28466	61.28	ug/l	99
10) 1,1-Dichloroethane	0.000		0	N.D.		
11) 1,2-Dichloroethene (to...	9.588	96	49	0.05	ug/l #	1
12) Chloroform	10.131	83	63	0.05	ug/l	92
14) 1,2-Dichloroethane	0.000		0	N.D.		
16) 2-Butanone	10.790	43	2047	8.44	ug/l	59
17) 1,1,1-Trichloroethane	0.000		0	N.D.		
18) Carbon Tetrachloride	0.000		0	N.D.		
19) Vinyl Acetate	12.690	43	47	0.03	ug/l	100
20) Bromodichloromethane	0.000		0	N.D.		
21) 1,2-Dichloropropane	0.000		0	N.D.		
22) cis-1,3-Dichloropropene	0.000		0	N.D.		
23) Trichloroethene	15.171	130	33931	55.08	ug/l	94
24) Benzene	15.598	78	90492	51.43	ug/l	100
25) Dibromochloromethane	0.000		0	N.D.		
26) trans-1,3-Dichloropropene	15.598	75	1438	2.62	ug/l #	1
27) 1,1,2-Trichloroethane	15.637	97	44	0.08	ug/l #	22
28) Bromoform	0.000		0	N.D.		
30) 4-Methyl-2-Pentanone	19.010	43	67	0.10	ug/l #	46
31) 2-Hexanone	20.367	43	98	0.22	ug/l #	45
32) Tetrachloroethene	20.716	164	2331	4.42	ug/l	89
33) 1,1,2,2-Tetrachloroethane	20.871	83	35	0.04	ug/l #	28
35) Toluene	21.918	92	55697	51.25	ug/l	92
36) Chlorobenzene	23.043	112	67848	49.12	ug/l	100
37) Ethylbenzene	0.000		0	N.D.		
39) Styrene	0.000		0	N.D.		
40) Xylene (total)	28.355	106	35	0.02	ug/l #	1

While the core requirements of loading report templates and creating a report method are very similar across all configurations of MassHunter Quant, the **Environmental** option will be used in the screen captures.

Copying report templates to the project folder

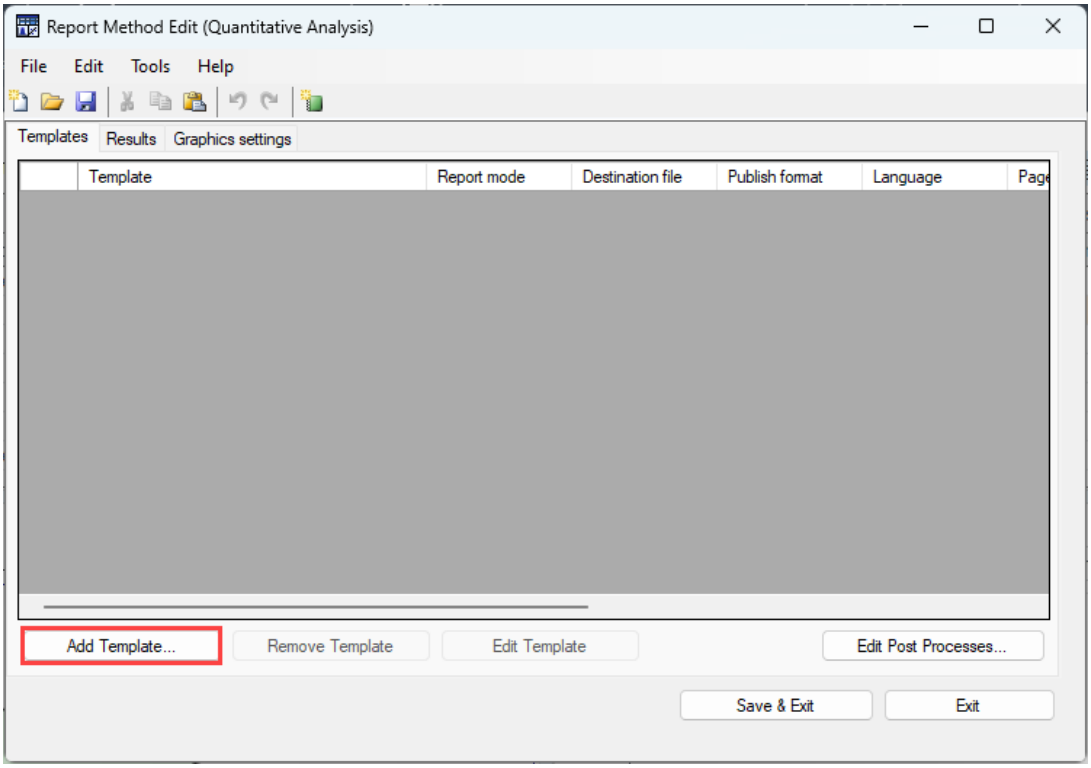
The environmental report templates are in the **MassHunter/Report Templates/Quant/PDF-Reporting** folder. Copy the entire contents of this folder to the **Project/Report Templates** folder. Additional templates are available one level up in the **Quant** folder, such as the **PDF Report Builder Templates**. This folder is shown because the template equivalent to the **MSD ChemStation** report is located here.



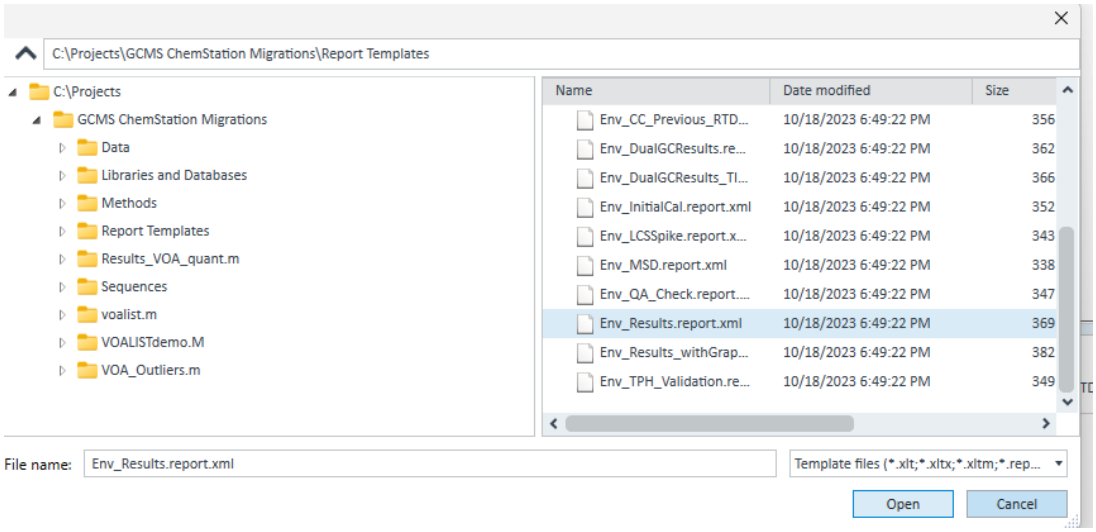
Creating a report method

To select a specific report template, a report method must be created to associate the report with the method.

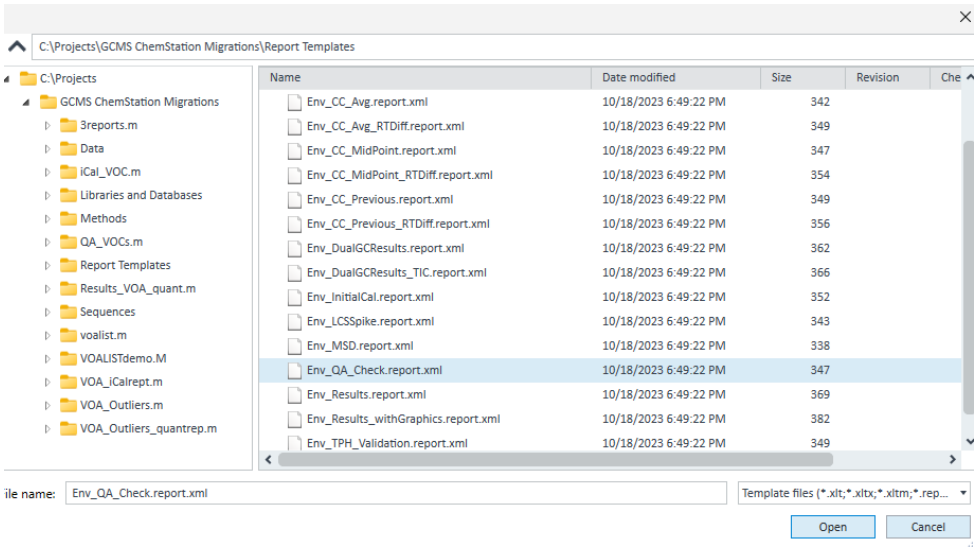
1 In the **Batch Table** view, under the **Home** tab, **Report** segment, select **Edit Report Method**. The following box will appear.



2 Click **Add Template** and browse to the template needed, in this case, the **ENV_Results.report.xml**. Click **Open**.

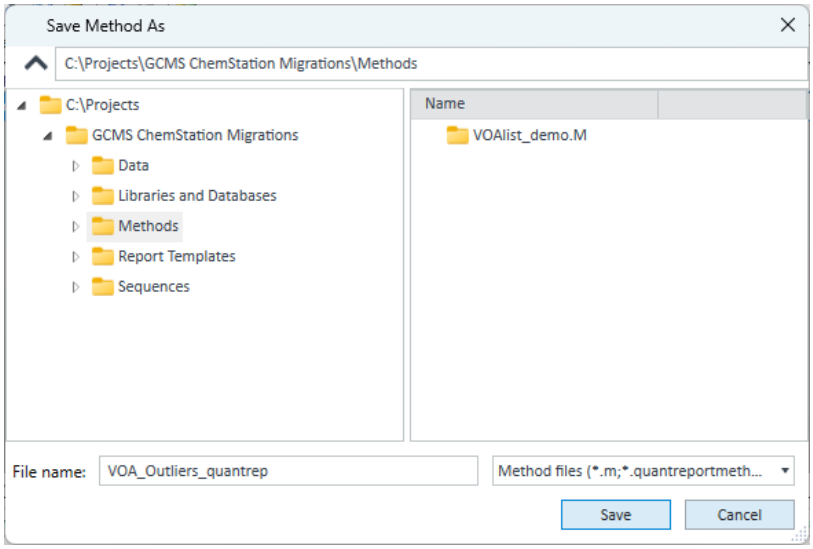


Multiple report templates can be created to process data if the workflow requires more than one type of output. For example, a process may include verifying both an iCal report, a QA report, and a quantitative report. The Quant method must include all outlier set points required for each report type before the reports are generated.



The next window will display a prompt to save the Report Method. This is different than the data analysis method, so the recommendation is to save the method as a similar name with a modifier.

3 Add the modifier to the method name, in this case, the extension **_quantrep** was added at the end to indicate which report is associated with the method.



4 Once the correct template is selected, and the other selections are confirmed, click **Save**.

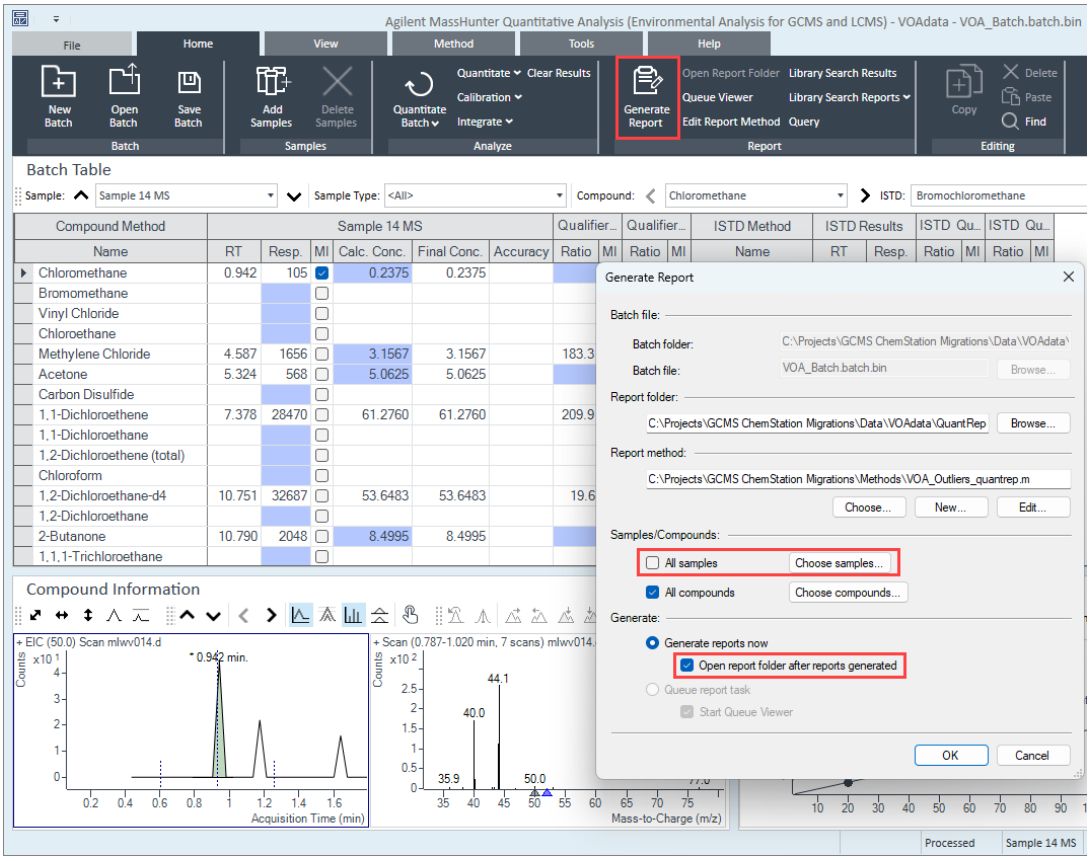
Generating a quantitation report

1 Using the method created in the previous steps, select **Generate Report**.

2 Verify the paths are correct.

In this example, only one sample requires a report to compare against the GC/MS ChemStation report, so the specific sample 14 MS file was chosen. Selecting **All Samples** would create an individual quantitation report for each sample in the batch.

3 Check **Open report folder after reports generated** for quick access to the report file.



Comparison of Results

Two comparable reports have been generated using the same calibration data set and sample files. As noted earlier, the two software platforms apply different integration algorithms. MSD ChemStation uses the RTE integrator, while MassHunter Quant uses the Agile parameterless integrator. The integrators can be changed if wanted. These differences explain the slight variations observed in the quantitative results; however, the discrepancies are minor, typically less than 2% within the calibrated range.

The two reports are shown, followed by a summary comparing the results from both software platforms.

C:\EnvDemo\voadata\mlwv014.d\epatemp.txt

Compound	R.T.	QIon	Response	Conc	Units	Dev(Min)
Internal Standards						
1) Bromochloromethane	7.921	128	12701	50.00	ug/l	#-0.03
15) 1,4-Difluorobenzene	18.157	114	73001	50.00	ug/l	-0.03
29) Chlorobenzene-d5	22.926	117	64313	50.00	ug/l	-0.03
System Monitoring Compounds						
13) 1,2-Dichloroethane-d4	10.751	65	32686	53.07	ug/l	-0.03
Spiked Amount 50.000	Range 76 - 114		Recovery = 106.14%			
34) Toluene-d8	21.724	98	67281	48.44	ug/l	-0.07
Spiked Amount 50.000	Range 88 - 110		Recovery = 96.88%			
38) Bromofluorobenzene	26.649	95	72049	50.07	ug/l	-0.07
Spiked Amount 50.000	Range 86 - 115		Recovery = 100.14%			
Target Compounds						Qvalue
2) Chloromethane	0.942	50	105	0.24	ug/l #	42
3) Bromomethane	0.000		0	N.D.		
4) Vinyl Chloride	2.067	62	47	0.09	ug/l #	22
5) Chloroethane	0.000		0	N.D.		
6) Methylene Chloride	4.587	84	1656	3.16	ug/l #	80
7) Acetone	5.246	43	344	3.14	ug/l #	51
8) Carbon Disulfide	0.000		0	N.D.		
9) 1,1-Dichloroethene	7.378	96	28466	61.28	ug/l	99
10) 1,1-Dichloroethane	0.000		0	N.D.		
11) 1,2-Dichloroethene (to...	9.588	96	49	0.05	ug/l #	1
12) Chloroform	10.131	83	63	0.05	ug/l	92
14) 1,2-Dichloroethane	0.000		0	N.D.		
16) 2-Butanone	10.790	43	2047	8.44	ug/l	59
17) 1,1,1-Trichloroethane	0.000		0	N.D.		
18) Carbon Tetrachloride	0.000		0	N.D.		
19) Vinyl Acetate	12.690	43	47	0.03	ug/l	100
20) Bromodichloromethane	0.000		0	N.D.		
21) 1,2-Dichloropropane	0.000		0	N.D.		
22) cis-1,3-Dichloropropene	0.000		0	N.D.		
23) Trichloroethene	15.171	130	33931	55.08	ug/l	94
24) Benzene	15.598	78	90492	51.43	ug/l	100
25) Dibromochloromethane	0.000		0	N.D.		
26) trans-1,3-Dichloropropene	15.598	75	1438	2.62	ug/l #	1
27) 1,1,2-Trichloroethane	15.637	97	44	0.08	ug/l #	22
28) Bromoform	0.000		0	N.D.		
30) 4-Methyl-2-Pentanone	19.010	43	67	0.10	ug/l #	46
31) 2-Hexanone	20.367	43	98	0.22	ug/l #	45
32) Tetrachloroethene	20.716	164	2331	4.42	ug/l	89
33) 1,1,2,2-Tetrachloroethane	20.871	83	35	0.04	ug/l #	28
35) Toluene	21.918	92	55697	51.25	ug/l	92
36) Chlorobenzene	23.043	112	67848	49.12	ug/l	100
37) Ethylbenzene	0.000		0	N.D.		
39) Styrene	0.000		0	N.D.		
40) Xylene (total)	28.355	106	35	0.02	ug/l #	1

Quantitation Results Report (Not Reviewed)

Data File	MLWV014.D	Operator	HP Chemist
Acq. Method	DANNY	Acq. Date-Time	1/21/1991 1:20:00 PM
Sample Name	Sample 14 MS	Vial	0
Multiplier	1	Sample Info	
DA Method File		Tune File	
Tune Date		Batch Name	migration.batch.bin

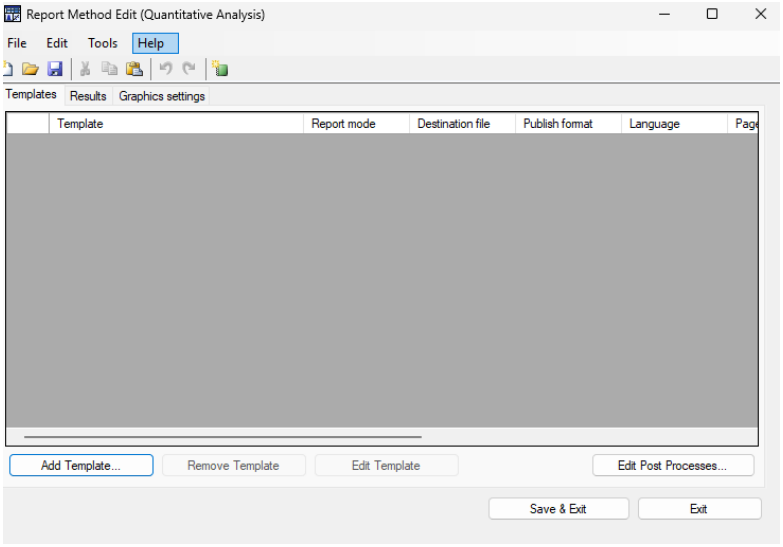
Compound	RT	QIon	Resp.	Conc.	Units		Dev(Min)
Internal Standards							
1) Bromochloromethane	7.921		12605	50.0000	ug/l	#	0.004
15) 1,4-Difluorobenzene	18.157		73033	50.0000	ug/l		0.004
29) Chlorobenzene-d5	22.926		64338	50.0000	ug/l		0.004
System Monitoring Compounds							
13) 1,2-Dichloroethane-d4	10.751		32687	53.4414	ug/l		0.043
Spiked Amount: 50.000	Range: 76.0 - 114.0%			Recovery = 106.88%			
34) Toluene-d8	21.724		67304	48.4555	ug/l		0.004
Spiked Amount: 50.000	Range: 88.0 - 110.0%			Recovery = 96.91%			
38) Bromofluorobenzene	26.649		71997	50.0117	ug/l		-0.035
Spiked Amount: 50.000	Range: 86.0 - 115.0%			Recovery = 100.02%			
Target Compounds							QValue
2) Chloromethane	0.942		105	0.2433	ug/l	m	41
3) Bromomethane	0.000		0	N.D.			
4) Vinyl Chloride	2.067		47	0.0942	ug/l	m	41
5) Chloroethane	0.000		0	N.D.			
6) Methylene Chloride	4.587		1656	3.1815	ug/l		96
7) Acetone	5.246		300	2.9174	ug/l	m	55
8) Carbon Disulfide	0.000		0	N.D.			
9) 1,1-Dichloroethene	7.378		28470	61.7434	ug/l		96
10) 1,1-Dichloroethane	0.000		0	N.D.			
11) 1,2-Dichloroethene (total)	0.000		0	N.D.			
12) Chloroform	10.131		63	0.0557	ug/l	m	19
16) 2-Butanone	10.790		2048	8.4759	ug/l		75
14) 1,2-Dichloroethane	0.000		0	N.D.			
17) 1,1,1-Trichloroethane	0.000		0	N.D.			
18) Carbon Tetrachloride	0.000		0	N.D.			
19) Vinyl Acetate	12.690		47	0.0272	ug/l	m	100
20) Bromodichloromethane	0.000		0	N.D.			
21) 1,2-Dichloropropane	0.000		0	N.D.			
22) cis-1,3-Dichloropropene	0.000		0	N.D.			
23) Trichloroethene	15.171		33939	55.1070	ug/l		96
24) Benzene	15.598		90501	52.2805	ug/l		100
25) Dibromochloromethane	0.000		0	N.D.			
26) trans-1,3-Dichloropropene	15.598		1792	3.3113	ug/l	#	1
27) 1,1,2-Trichloroethane	0.000		0	N.D.			
28) Bromoform	0.000		0	N.D.			
30) 4-Methyl-2-Pentanone	0.000		0	N.D.			
31) 2-Hexanone	20.367		98	0.2275	ug/l		41
32) Tetrachloroethene	20.716		2262	4.2921	ug/l		95
33) 1,1,2,2-Tetrachloroethane	0.000		0	N.D.			
35) Toluene	21.918		55620	51.1608	ug/l		97
36) Chlorobenzene	23.043		66103	48.0304	ug/l		99
37) Ethylbenzene	0.000		0	N.D.			
39) Styrene	0.000		0	N.D.			
40) Xylene (total)	28.432		47	0.0313	ug/l	m	1

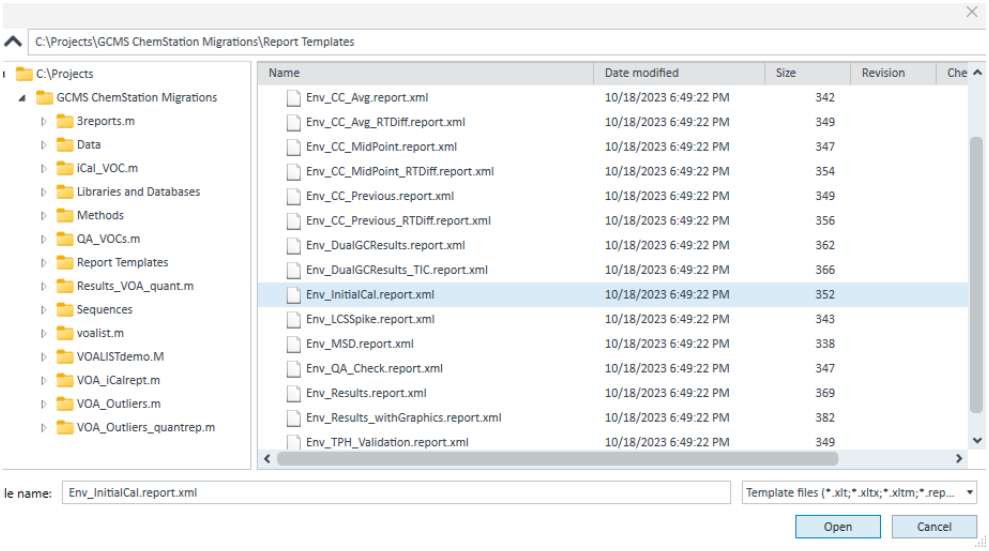
Compound Name	MSD ChemStation Result	GC/MS MassHunter Quant Result	Difference
1,2-Dichlorethane-*d*4	53.07	53.44	0.70%
Toluene-*d*8	48.44	48.46	0.04%
Bromofluorobenzene	50.07	50.01	-0.12%
1,1-Dichloroethene	61.28	61.74	0.75%
Trichloroethene	55.08	55.11	0.05%
Benzene	51.43	52.28	1.65%
Toluene	51.25	51.16	-0.18%
Chlorobenzene	49.12	48.03	-2.22%

Generating an iCal Report

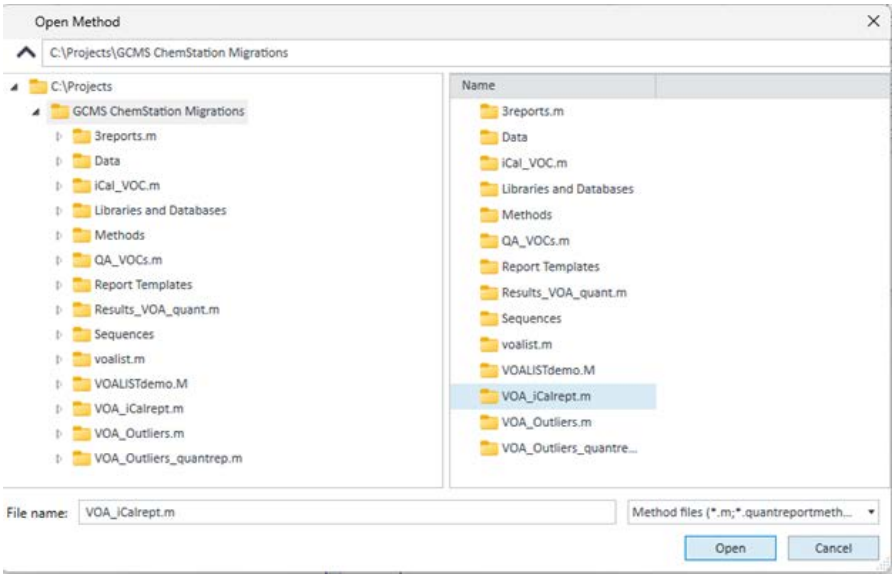
Generating an iCal report follows the same steps already outlined. Verify that the outliers have been entered in the Quant method and save the batch.

1 In the batch view, **Home** tab, select **Create Report Method**, and select the **InitialCal** report template.





2 Save this method with something that ties the Quant method to the report template. In this case, the report method is called **VOA_iCalrept.m**.



3 Click **Generate Report**, and select the method just created to apply to the batch and view the iCal report.

Conclusion

This user guide outlines the steps required to migrate acquisition methods, data files, and data analysis workflows from MSD ChemStation to GC/MS MassHunter, and demonstrates that both platforms can produce highly comparable results. The updated tools built into the MassHunter architecture along with additional utilities located in supporting folders help ensure that migrations are performed correctly and provide users with immediate confirmation when translations are successful.

The guide also highlights useful tips for configuring outlier checks in the various GC/MS MassHunter Quantitative Analysis environments, enabling faster identification of nonconformities and improving overall review efficiency in high throughput laboratory operations.

www.agilent.com

DE-014676

© Agilent Technologies, Inc. 2026

First edition, April 2026

5994-9072EN

Agilent