



Moving From MSD ChemStation to MassHunter EnviroQuant

Workflow Guide



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Notices

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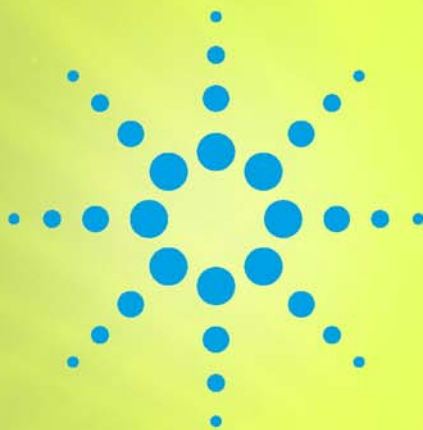
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1 Introduction

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This book contains a brief description of some of MassHunter EnviroQuant features as they relate to Environmental Data Analysis.

For those individuals moving from MSD ChemStation to MassHunter EnviroQuant, we identify some features that are improvements over MSD ChemStation workflows.



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MassHunter EnviroQuant

MassHunter Quantitative Analysis, running in Environmental Quant Mode (hereafter called EnviroQuant), is designed to facilitate the implementation of EPA methods in an environmental laboratory.

Reviewing the typically large amount of information generated by target analysis is easily done in EnviroQuant. Here you can choose to view your batch results on a sample-by-sample basis or on a compound-by-compound basis. In both views, quality test outliers are flagged, using a color code, to improve efficiency when reviewing results.

Additionally, there are templates included that are specific to EPA reporting requirements and they are customizable for individual laboratory needs.

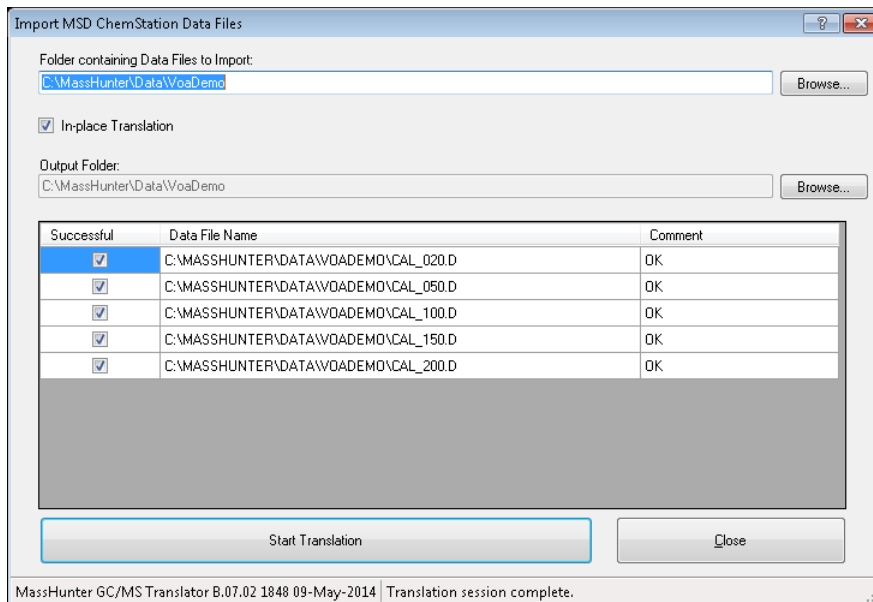
Translator



Import ChemStation Data Files

For those individuals moving from MSD ChemStation Data Analysis to EnviroQuant, the GC MSD Translator easily converts your ChemStation methods and sample data for use with EnviroQuant.

Here is an example of the screen you will see when importing MSD ChemStation data files.



Export MSD ChemStation Quant Database

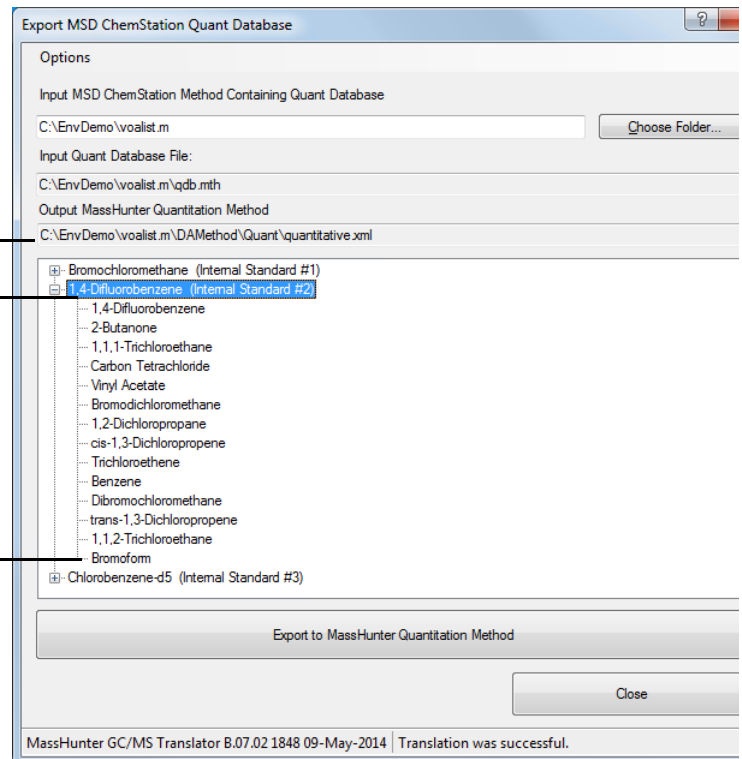
This is what you will see when exporting an MSD ChemStation Quant Database to the MassHunter format.

MassHunter EnviroQuant, like MSD ChemStation, uses a Unified Method that contains the Data Acquisition, Quantitative Analysis, Unknowns Analysis, and Qualitative Analysis parts of the method. (The .m method file.)

When the MSD ChemStation method is converted, MassHunter creates a new path in which the quant part of the Data Analysis method is saved, as shown in the example below.

Quantitative Part of the method

Compounds using ISTD #2



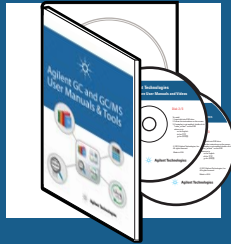
Notice of successful translation

Centralized Documentation

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

- MassHunter software installation disks
- GC/MS Software Information USB (G1701-60172)

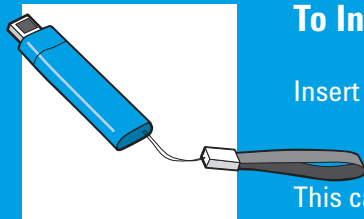
Take a look at what is included in these libraries. They contain a vast amount of valuable information.



To Install Your Hardware Library

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

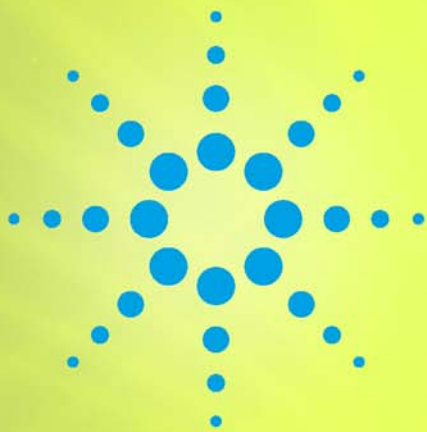
This can be installed by anyone who has authority to copy information onto the receiving computer.



To Install Your Software Library

Insert the memory stick into a USB port and follow the prompts.

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



2 Batch View

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Overview

Batch Table - Viewed by Sample

You may view your results in the Batch Table by sample or by compound.

In MassHunter EnviroQuant, when you view the Batch Table by sample, each row represents the analysis of a single sample. Here you may select any sample and scroll through the results by targeted compounds in that sample. Also, you can easily spot quality outliers, identified by blue and red colored cells.

The layout shown in this example is for illustration purposes only. You may easily customize your view by adding or removing columns or rearranging how the sections are displayed.

- 1 Selected sample
- 2 Next and Previous compound arrows
- 3 Selected compound
- 4 Displays the Table in Sample view
- 5 Quantitation results (shaded area)
- 6 TIC of selected sample
- 7 Target peak
- 8 Compound qualifier peaks
- 9 Library Match Score
- 10 Compound spectrum
- 11 Calibration curve



Batch Table - Viewed by Compound

When you view the Batch Table by compound, each row represents the analysis of a target compound. Here you may select any target compound and scroll through the results by sample. Also, you can easily spot quality outliers, identified by blue and red colored cells.

Displays the Table in Compound view

The screenshot displays the Agilent MassHunter software interface. The main window shows a 'Batch Table' for 'Sample 02' with 'Compound: Chlorobenzene' and 'ISTD: Chlorobenzene-d5'. The table lists various compounds and their analysis results across multiple samples. The table is organized into columns for 'Compound Method', 'Sample 02', 'Sample 02', 'Sample 02', 'Qualifier 1 Results', 'Qualifier 2 Results', and 'ISTD Method'. The table is viewed in 'Compound view', showing results for Chlorobenzene-d5. The table is organized into columns for 'Compound Method', 'Sample 02', 'Sample 02', 'Sample 02', 'Qualifier 1 Results', 'Qualifier 2 Results', and 'ISTD Method'. The table is viewed in 'Compound view', showing results for Chlorobenzene-d5. The table is organized into columns for 'Compound Method', 'Sample 02', 'Sample 02', 'Sample 02', 'Qualifier 1 Results', 'Qualifier 2 Results', and 'ISTD Method'. The table is viewed in 'Compound view', showing results for Chlorobenzene-d5.





Compound Method	Sample 02	Sample 02	Sample 02	Qualifier 1 Results	Qualifier 2 Results	ISTD Method															
Name	Acq. Date-Time	RT	Resp.	MI	Calc. Conc.	Final Conc.	Accuracy	Int. Metric	ISTD Resp. % Dev.	Ratio	MI	Int. Metric	Ratio	MI	Int. Metric	Name	Avg. RF	Avg. RF RSD	CF R2	RT	Resp.
Chloromethane	7/1/2014 12:45 PM															Bromochloromethane	0.0000	NaN		7.921	12605
Bromomethane	7/1/2014 12:45 PM															Bromochloromethane	0.0000	NaN		7.921	12605
Vinyl Chloride	7/1/2014 12:45 PM															Bromochloromethane	0.0000	NaN		7.921	12605
Chloroethane	7/1/2014 12:45 PM															Bromochloromethane	0.0000	NaN		7.921	12605
Methylene Chloride	7/1/2014 12:45 PM	4.587	1656		3.1567	3.1567		Accepted		183.3		Accepted	58.6		Accepted	Bromochloromethane	0.0000	NaN		7.921	12605
Acetone	7/1/2014 12:45 PM	5.324	563		5.0625	5.0625		Accepted								Bromochloromethane	0.0000	NaN		7.921	12605
Carbon Disulfide	7/1/2014 12:45 PM															Bromochloromethane	0.0000	NaN		7.921	12605
1,1-Dichloroethene	7/1/2014 12:45 PM	7.378	28470		61.2760	61.2760		Accepted		209.9		Accepted	63.3		Accepted	Bromochloromethane	0.0000	NaN		7.921	12605
1,1-Dichloroethane	7/1/2014 12:45 PM															Bromochloromethane	0.0000	NaN		7.921	12605
1,2-Dichloroethene (total)	7/1/2014 12:45 PM															Bromochloromethane	0.0000	NaN		7.921	12605
Chloroform	7/1/2014 12:45 PM															Bromochloromethane	0.0000	NaN		7.921	12605
1,2-Dichloroethane-d4	7/1/2014 12:45 PM	10.751	32687		53.6483	53.6483		Accepted		19.6		Accepted				Bromochloromethane	0.0000	NaN		7.921	12605
1,2-Dichloroethane	7/1/2014 12:45 PM															Bromochloromethane	0.0000	NaN		7.921	12605
2-Butanone	7/1/2014 12:45 PM	10.790	2048		8.4995	8.4995		Accepted								1,4-Difluorobenzene	0.0000	NaN		18.157	73033
1,1,1-Trichloroethane	7/1/2014 12:45 PM															1,4-Difluorobenzene	0.0000	NaN		18.157	73033
Carbon Tetrachloride	7/1/2014 12:45 PM															1,4-Difluorobenzene	0.0000	NaN		18.157	73033
Vinyl Acetate	7/1/2014 12:45 PM															1,4-Difluorobenzene	0.0000	NaN		18.157	73033
Bromodichloromethane	7/1/2014 12:45 PM															1,4-Difluorobenzene	0.0000	NaN		18.157	73033
1,2-Dichloropropane	7/1/2014 12:45 PM															1,4-Difluorobenzene	0.0000	NaN		18.157	73033
cis-1,3-Dichloropropene	7/1/2014 12:45 PM															1,4-Difluorobenzene	0.0000	NaN		18.157	73033
Trichloroethene	7/1/2014 12:45 PM	15.171	33939		55.1714	55.1714		Accepted		97.6		Accepted	115.0		Accepted	1,4-Difluorobenzene	0.0000	NaN		18.157	73033
Benzene	7/1/2014 12:45 PM	15.598	90501		51.5585	51.5585		Accepted								1,4-Difluorobenzene	0.0000	NaN		18.157	73033
Dibromochloromethane	7/1/2014 12:45 PM															1,4-Difluorobenzene	0.0000	NaN		18.157	73033
trans-1,3-Dichloropropene	7/1/2014 12:45 PM	15.598	1718		3.1733	3.1733		Accepted		1238.4		Accepted				1,4-Difluorobenzene	0.0000	NaN		18.157	73033
1,1,2-Trichloroethane	7/1/2014 12:45 PM															1,4-Difluorobenzene	0.0000	NaN		18.157	73033
Bromoform	7/1/2014 12:45 PM															1,4-Difluorobenzene	0.0000	NaN		18.157	73033
4-Methyl-2-Pentanone	7/1/2014 12:45 PM															Chlorobenzene-d5	0.0000	NaN		22.926	64338
2-Hexanone	7/1/2014 12:45 PM	20.367	98		0.2244	0.2244		Accepted								Chlorobenzene-d5	0.0000	NaN		22.926	64338
Tetrachloroethene	7/1/2014 12:45 PM	20.716	2262		4.3440	4.3440		Accepted		144.2		Accepted				Chlorobenzene-d5	0.0000	NaN		22.926	64338

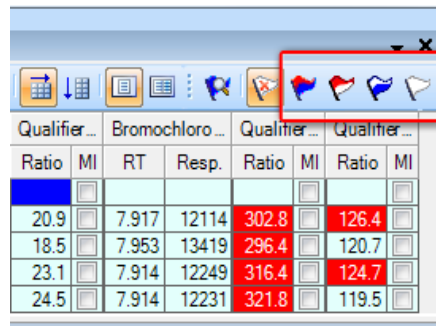
The screenshot also shows 'Compound Information' with chromatograms and a 'Calibration Curve' for Chlorobenzene-d5. The calibration curve shows a linear relationship between Relative Response and Relative Concentration, with the equation $y = 1.055631 \cdot x$ and $R^2 = 0.9995887$. The table at the bottom indicates 'Processed Sample 02 Chlorobenzene 37 Compounds (40 total including ISTDs) TW/ijt'.

Outliers Icons

Outlier icons act as filters that control which rows display in your batch table.

Outliers values are indicated by red cells for a high values and blue cells for low values. These Outlier icons are toggles. When selected, they will:



-  Display rows with **both** high and low outliers
-  Display rows with **high** outliers only
-  Display rows with **low** outliers only
-  Display rows containing **no** outliers

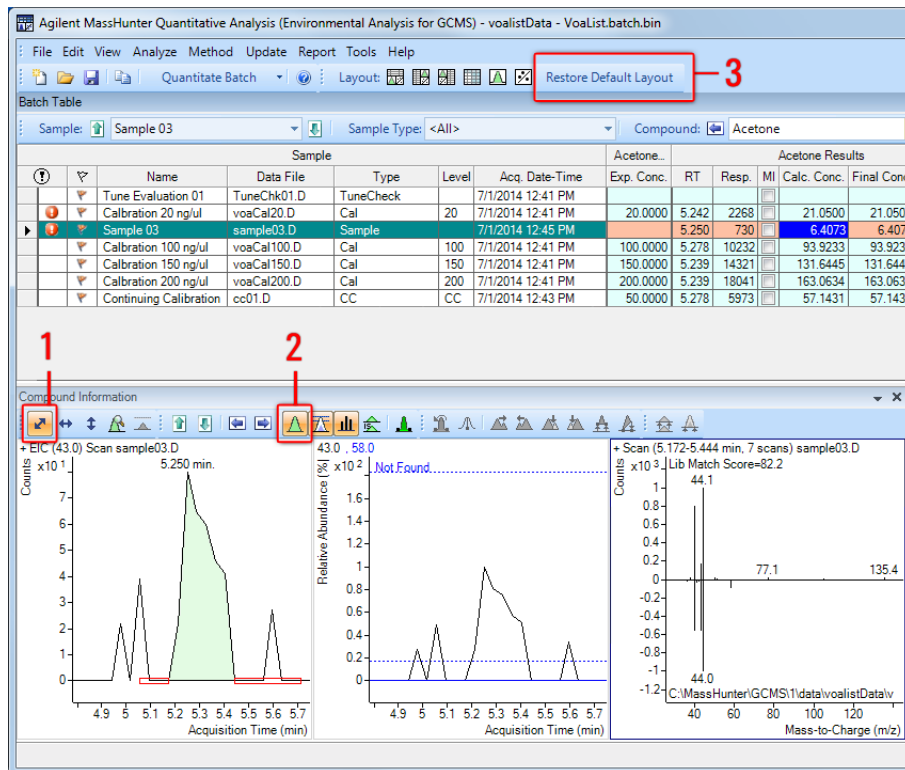


Qualifier...	Bromochloro...	Qualifier...	Qualifier...
Ratio	MI	RT	Resp.
20.9	7.917	12114	302.8
18.5	7.953	13419	296.4
23.1	7.914	12249	316.4
24.5	7.914	12231	321.8

Chromatograms, Autoscale, and Default Icons

Other commonly used icons are those shown in this example. You can use the icons highlighted in this example to:

1.  Turn on/off Autoscale
2.  Show/Hide Chromatogram
3. **Restore Default Layout** Restores Default Layout





Manual Integration

In MassHunter EnviroQuant, unlike ChemStation, if you delete or manually integrate a peak, then re-quantitate the batch, your edits remain, unless you clear the edit, no matter how often you re-quantitate the batch.

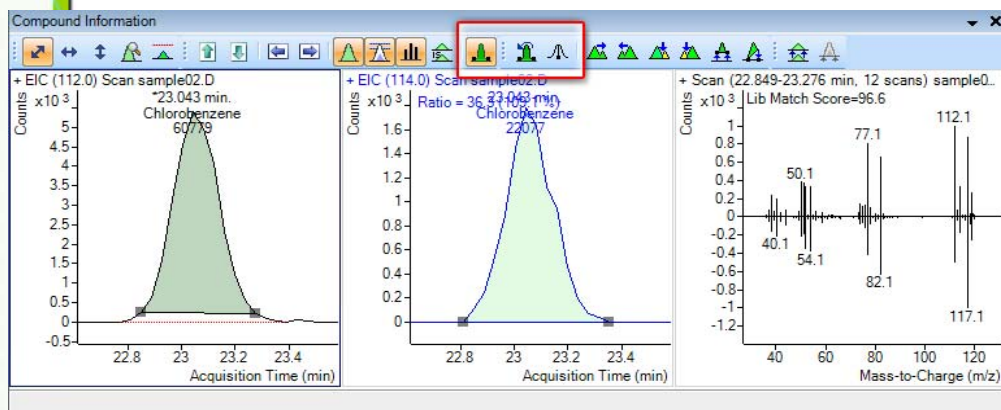
Highlighted below are some of the icons used for manual integration:

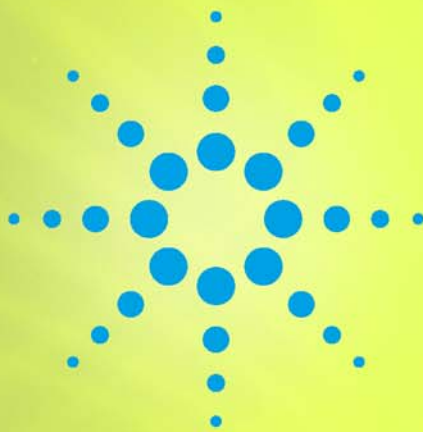
 Manual Integration icon

 Clear Manual Integration icon

 Zero Peak icon (Delete Peak)

Cursor over any other icon to see its function displayed in a tool tip.





3 Method Editor View

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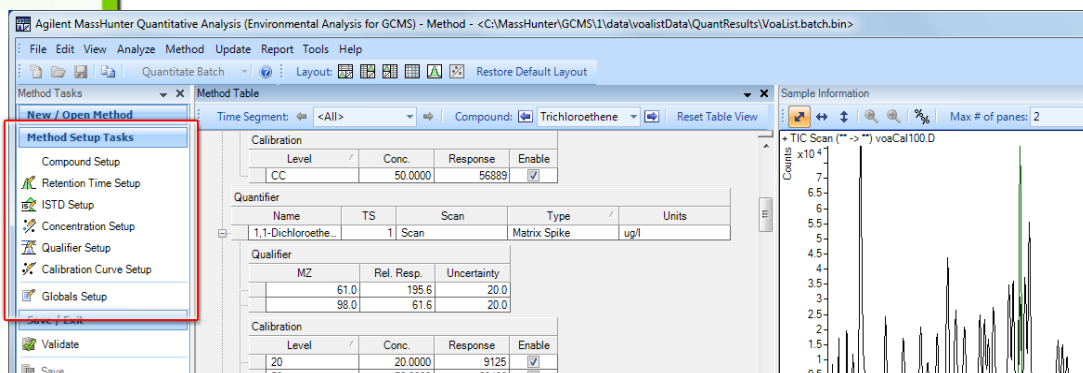


Overview

In the Method Editor view you create a database of target compounds and their qualifiers. Here you can also specify quality control parameters to comply with EPA regulations for example, or for your own internal quality control.

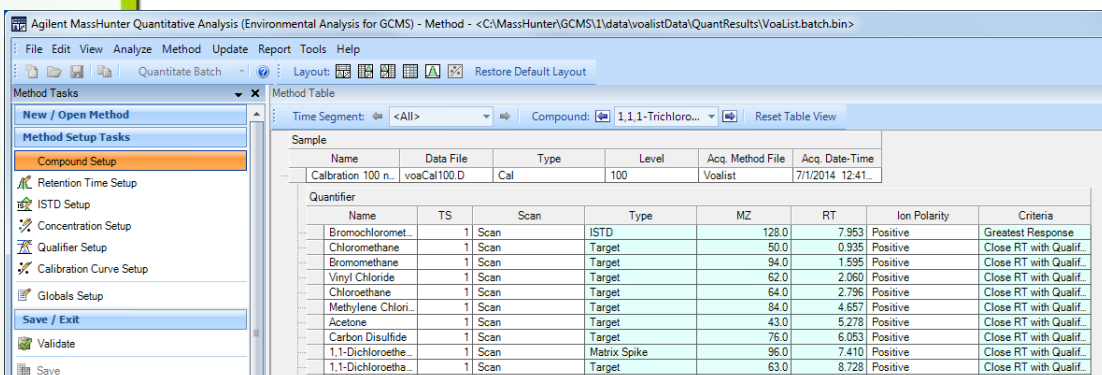
Quantitation Database

Under the Method Setup Tasks area you will set up the quantitation database. Here you specify parameters ranging from the compound name to its calibration curve.

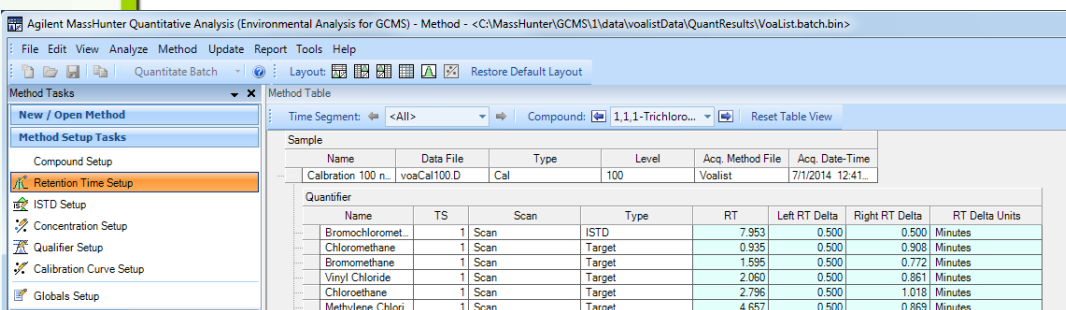


Below are a few sample screens from the Method Setup Tasks area.

Compound Setup



Retention Time Setup



ISTD Setup

Name	Data File	Type	Level	Acq. Method File	Acq. Date-Time
Calibration 100 n...	voaCal100.D	Cal	100	Voalist	7/1/2014 12:41...

Name	TS	Scan	Type	ISTD Compound Name	ISTD Flag	ISTD Conc.	Time Reference Flag
Bromochloromet...	1	Scan	ISTD	<None>	<input checked="" type="checkbox"/>	50.0000	<input checked="" type="checkbox"/>
Chloromethane	1	Scan	Target	Bromochloromethane	<input type="checkbox"/>	50.0000	<input type="checkbox"/>
Bromomethane	1	Scan	Target	Bromochloromethane	<input type="checkbox"/>	50.0000	<input type="checkbox"/>
Vinyl Chloride	1	Scan	Target	Bromochloromethane	<input type="checkbox"/>	50.0000	<input type="checkbox"/>
Chloroethane	1	Scan	Target	Bromochloromethane	<input type="checkbox"/>	50.0000	<input type="checkbox"/>
Methylene Chlori...	1	Scan	Target	Bromochloromethane	<input type="checkbox"/>	50.0000	<input type="checkbox"/>
Acetone	1	Scan	Target	Bromochloromethane	<input type="checkbox"/>	50.0000	<input type="checkbox"/>
Carbon Disulfide	1	Scan	Target	Bromochloromethane	<input type="checkbox"/>	50.0000	<input type="checkbox"/>

Concentration Setup

Name	Data File	Type	Level	Acq. Method File	Acq. Date-Time
Calibration 100 n...	voaCal100.D	Cal	100	Voalist	7/1/2014 12:41...

Name	TS	Scan	Type	Units
Chloromethane	1	Scan	Target	ug/l

Level	Conc.	Response	Enable
20	20.0000	8376	<input checked="" type="checkbox"/>
50	50.0000	22832	<input checked="" type="checkbox"/>
100	100.0000	42588	<input checked="" type="checkbox"/>
150	150.0000	62878	<input checked="" type="checkbox"/>
200	200.0000	83223	<input checked="" type="checkbox"/>
CC	50.0000	22897	<input checked="" type="checkbox"/>

Qualifier Setup

Name	Data File	Type	Level	Acq. Method File	Acq. Date-Time
Calibration 100 n...	voaCal100.D	Cal	100	Voalist	7/1/2014 12:41...

Name	TS	Scan	Type	MZ	Uncertainty
Chloromethane	1	Scan	Target	50.0	Absolute

MZ	Rel. Resp.	Uncertainty	Area Sum
52.0	32.3	20.0	<input type="checkbox"/>

Name	TS	Scan	Type	MZ	Uncertainty
Bromomethane	1	Scan	Target	94.0	Absolute

EPA Method Requirements

List of Outliers

Unique to MassHunter EnviroQuant

Applied on a Compound-by- Compound Basis

MassHunter EnviroQuant running in environmental mode, provides specialized method parameters to track EPA regulated criteria. These method parameters are known as outliers.

In the Outliers section of the Method Editor view, you can setup ranges of parameters that represent acceptable results. Results outside these acceptable limits are considered outliers. MassHunter EnviroQuant monitors the outliers found in compounds present in every sample, and then presents these as color-coded results graphically in tables.

Shown below is a list of outliers available in MassHunter EnviroQuant.

Outlier Setup Tasks	
Retention Time	
Relative Retention Time	
Peak Resolution	
Peak Symmetry	
Peak Full Width Half Maximum	
Peak Purity	
Signal-to-Noise Ratio	
Limit Of Detection	
Limit Of Quantitation	
Method Detection Limit	
Qualifier Ratio	
ISTD Response	
ISTD Response Percent Deviation	
Sample Amount	
Sample RSD	
Blank Concentration	
Blank Response	
Accuracy	
Average Response Factor	
Average Response Factor RSD	
Curve Fit R ²	
Relative Response Factor	
Response Factor	
QC	
QC Relative Standard Deviation	
CC Average Response Factor	
CC ISTD Response Ratio	
CC Relative Response Factor	
CC Response Ratio	
CC Retention Time	
Matrix Spike	
Matrix Spike Percent Difference	
Matrix Spike Percent Recovery	
Matrix Spike Group Recovery	
Surrogate	
Surrogate Percent Recovery	
Response Check	
Mass Accuracy	
Custom Calculation	

Some of these parameters are monitored in both the MSD ChemStation and MassHunter EnviroQuant. Others, such as the *Average Response Factor*, and *Curve Fit R²* are available in MassHunter only.

Unlike the process used in the MSD ChemStation, in MassHunter EnviroQuant these parameters can be applied on a compound-by-compound-basis. For example, you can set the Method Detection Limit, Average Response Factor RSD, and Curve Fit R² for each compound individually.

Commonly Used Outliers

The following are just a few examples of the Method Editor data entry screens for commonly used outliers, included here for illustration purposes only. For EPA compliance, your methods will include many more.

Method Detection Limit

Name	TS	Scan	Type	MDL
Bromochloromet...	1	Scan	ISTD	
Chloromethane	1	Scan	Target	0.5000
Bromomethane	1	Scan	Target	0.5000
Vinyl Chloride	1	Scan	Target	0.5000
Chloroethane	1	Scan	Target	0.5000
Methylene Chlori...	1	Scan	Target	0.5000
Acetone	1	Scan	Target	0.5000
Carbon Disulfide	1	Scan	Target	0.5000
1,1-Dichloroethe...	1	Scan	Matrix Spike	0.5000
1,1-Dichloroetha...	1	Scan	Target	0.5000
1,2-Dichloroethe...	1	Scan	Target	0.5000
Chloroform	1	Scan	Target	0.5000
1,2-Dichloroetha...	1	Scan	Surrogate	0.5000
1,2-Dichloroetha...	1	Scan	Target	0.5000

Average Response Factor RSD

In MSD ChemStation this was only available if you had a compound type C. In MassHunter EnviroQuant this is compound type independent.

Name	TS	Scan	Type	Max. Avg. RF RSD
Chloromethane	1	Scan	Target	20.000000
Bromomethane	1	Scan	Target	20.000000
Vinyl Chloride	1	Scan	Target	20.000000
Chloroethane	1	Scan	Target	20.000000
Methylene Chlori...	1	Scan	Target	20.000000
Acetone	1	Scan	Target	20.000000
Carbon Disulfide	1	Scan	Target	20.000000
1,1-Dichloroethe...	1	Scan	Matrix Spike	20.000000
Bromochloromet...	1	Scan	ISTD	
Dichloroetha...	1	Scan	Target	20.000000
1,2-Dichloroethe...	1	Scan	Target	20.000000
Chloroform	1	Scan	Target	20.000000
1,2-Dichloroetha...	1	Scan	Surrogate	20.000000
2-Butanone	1	Scan	Target	20.000000

Curve Fit R^2

The Curve Fit R^2 was not available in MSD ChemStation. So if your curve fit was outside your laboratory's acceptable limits, there was no way to indicate this. In MassHunter EnviroQuant you can use the Curve Fit R^2 Outlier for this.

Agilent MassHunter Quantitative Analysis (Environmental Analysis for GCMS) - Method - <C:\MassHunter\GCMS\1\data\voalistData\QuantResults\VoalList.batch.bin>

File Edit View Analyze Method Update Report Tools Help

Quantitate Batch Layout: Restore Default Layout

Method Tasks

- Qualifier Ratio
- ISTD Response
- ISTD Response Percent Deviation
- Sample Amount
- Sample RSD
- Blank Concentration
- Blank Response
- Accuracy
- Average Response Factor
- Average Response Factor RSD
- Curve Fit R2**
- Relative Response Factor
- Response Factor
- QC

Method Table

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

Sample						
Name	Data File	Type	Level	Acq. Method File	Acq. Date-Time	
Calibration 100 n...	voaCal100.D	Cal	100	Voalist	7/1/2014 12:41...	
Quantifier						
Name	TS	Scan	Type	CF Min. R2		
Chloromethane	1	Scan	Target	0.97000000		
Bromomethane	1	Scan	Target	0.97000000		
Vinyl Chloride	1	Scan	Target	0.97000000		
Chloroethane	1	Scan	Target	0.97000000		
Methylene Chlori...	1	Scan	Target	0.97000000		
Acetone	1	Scan	Target	0.97000000		
Carbon Disulfide	1	Scan	Target	0.97000000		
1,1-Dichloroeth...	1	Scan	Matrix Spike	0.97000000		
Bromochloromet...	1	Scan	ISTD	0.97000000		
1,1-Dichloroetha...	1	Scan	Target	0.97000000		
1,2-Dichloroeth...	1	Scan	Target	0.97000000		
Chloroform	1	Scan	Target	0.97000000		
1,2-Dichloroetha...	1	Scan	Surrogate	0.97000000		
2-Butanone	1	Scan	Target	0.97000000		

Outlier - Curve Fit R2

Relative Response Factor

Agilent MassHunter Quantitative Analysis (Environmental Analysis for GCMS) - Method - <C:\MassHunter\GCMS\1\data\voalistData\QuantResults\VoalList.batch.bin>

File Edit View Analyze Method Update Report Tools Help

Quantitate Batch Layout: Restore Default Layout

Method Tasks

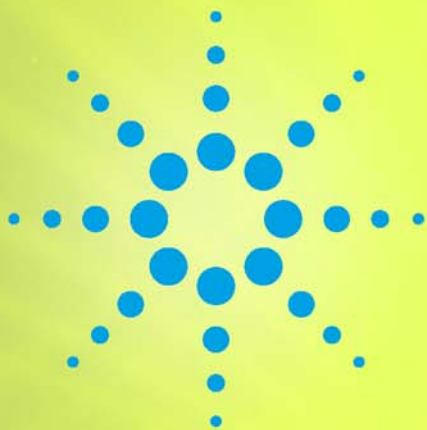
- Qualifier Ratio
- ISTD Response
- ISTD Response Percent Deviation
- Sample Amount
- Sample RSD
- Blank Concentration
- Blank Response
- Accuracy
- Average Response Factor
- Average Response Factor RSD
- Curve Fit R2
- Relative Response Factor**
- Response Factor
- QC

Method Table

Time Segment: <All> Compound: Chlorobenzen... Reset Table View

Sample						
Name	Data File	Type	Level	Acq. Method File	Acq. Date-Time	
Calibration 100 n...	voaCal100.D	Cal	100	Voalist	7/1/2014 12:41...	
Quantifier						
Name	TS	Scan	Type	RRF Max. % Dev.		
Chloromethane	1	Scan	Target	20.0		
Bromomethane	1	Scan	Target	20.0		
Vinyl Chloride	1	Scan	Target	20.0		
Chloroethane	1	Scan	Target	20.0		
Methylene Chlori...	1	Scan	Target	20.0		
Acetone	1	Scan	Target	20.0		
Carbon Disulfide	1	Scan	Target	20.0		
1,1-Dichloroeth...	1	Scan	Matrix Spike	20.0		
Bromochloromet...	1	Scan	ISTD			
1,1-Dichloroetha...	1	Scan	Target	20.0		
1,2-Dichloroeth...	1	Scan	Target	20.0		
Chloroform	1	Scan	Target	20.0		
1,2-Dichloroetha...	1	Scan	Surrogate	20.0		
2-Butanone	1	Scan	Target	20.0		

Outlier - Relative Response Factor



4 Compounds at a Glance

View up to 100 Compounds at a Glance 22

Read Outlier Messages 22

Manually Integrate Compounds 23

Display Qualifiers and Ion Ratios 23

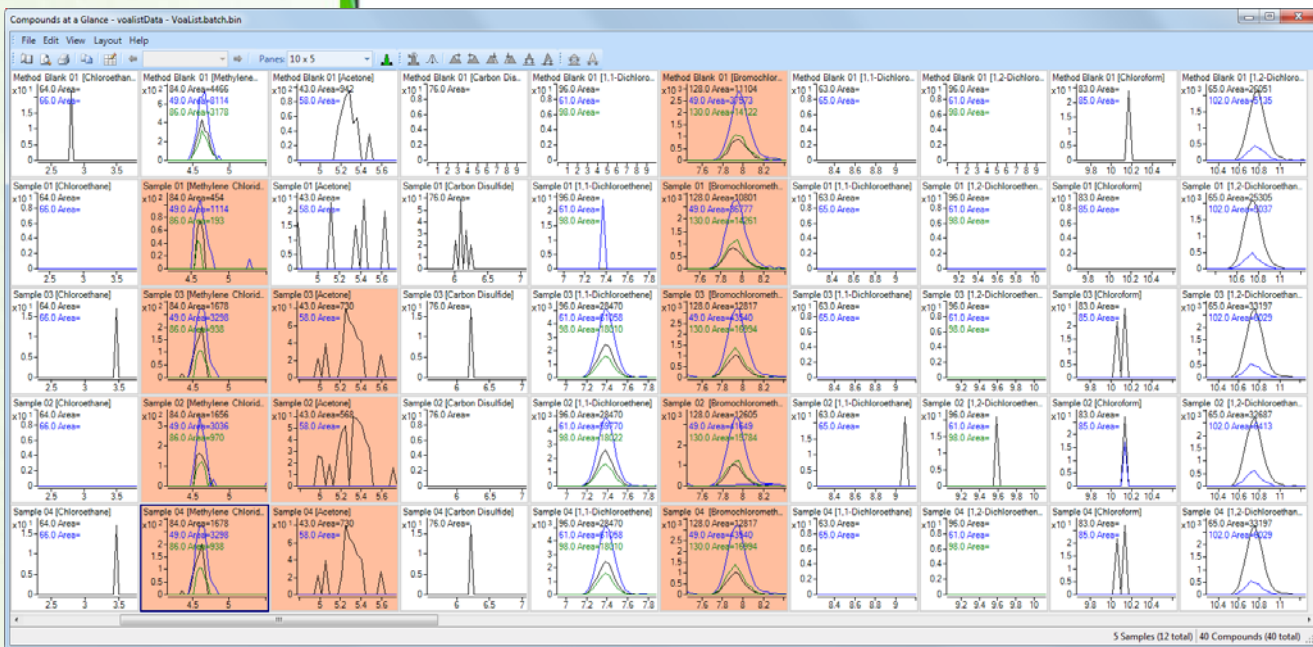


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View up to 100 Compounds at a Glance

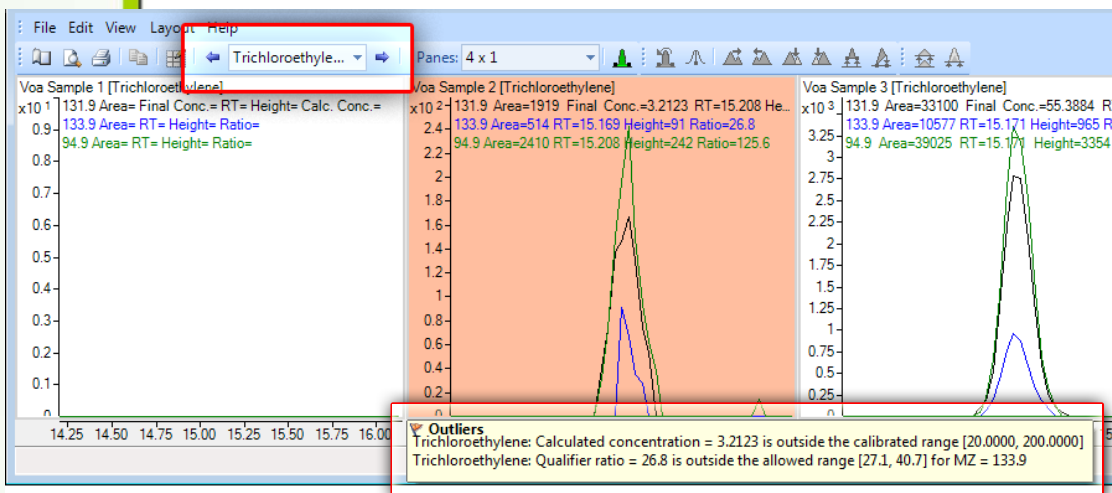
In the Compounds at a Glance view (**View > Compounds-at-a-Glance**) you can view up to 100 compound chromatograms at a time, by compound name, or by sample.

The compound peak may show overlaid qualifiers, ISTDs, a matrix spike, and more. In this example, compounds with outliers are highlighted in orange for easy identification.



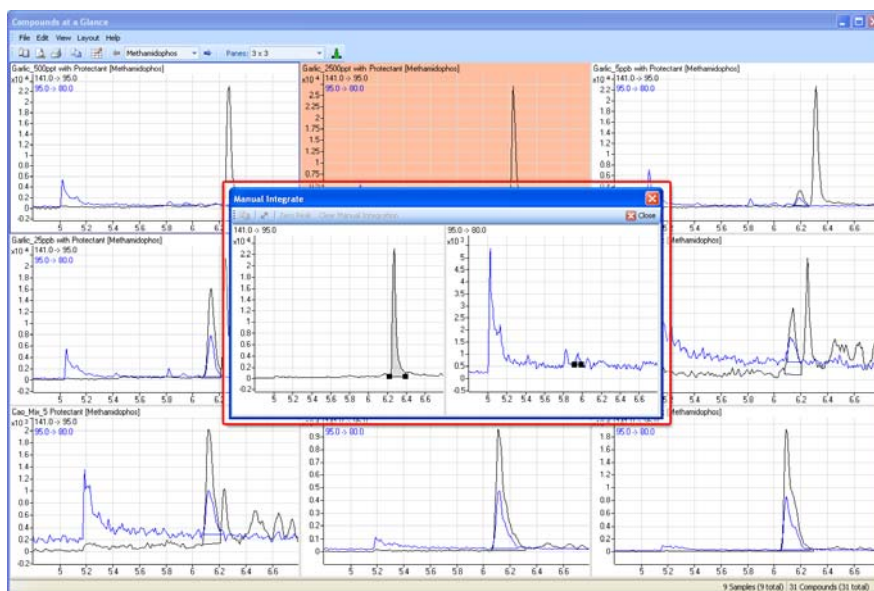
Read Outlier Messages

When you mouse over the highlighted pane you will see Outlier messages for the analyzed results. In this example you can see that the calculated concentration is outside the calibration range and the qualifier ratio is also outside its allowable range.



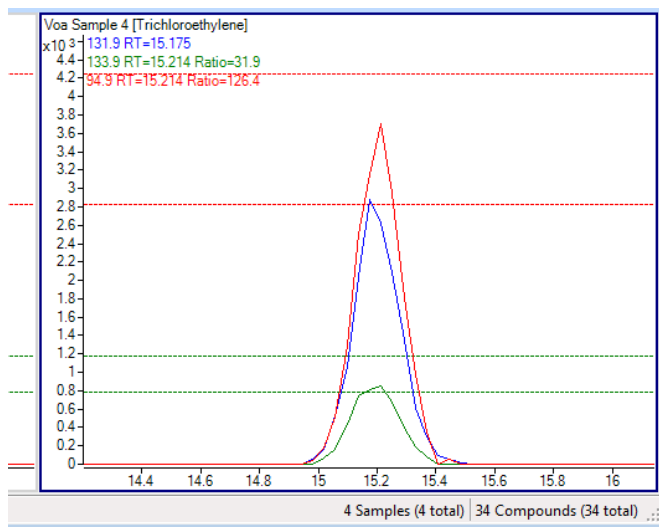
Manually Integrate Compounds

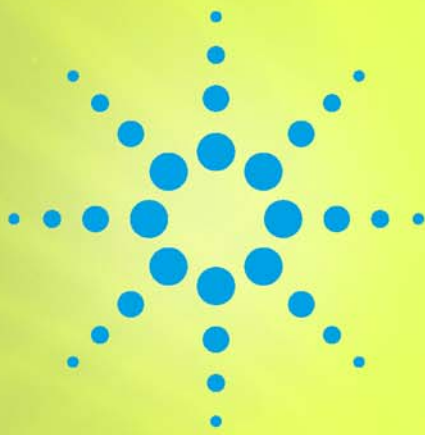
In the Compounds at a Glance view, if you double-click on a compound, you can manually integrate it in this window.



Display Qualifiers and Ion Ratios

In this example, the target compound, its qualifiers, and lines representing their allowable ion ratios are color coded for easy identification.





5 Tune Evaluation

Tune Evaluation Tool 26

Tune Evaluation Results 27



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Tune Evaluation Tool

The Tune Evaluation Tool in MassHunter EnviroQuant makes it easy to enter EPA required analyzer tune and GC performance criteria. Once the criteria are entered and saved, this becomes part of the run method.

When the tune evaluation sample is the first sample in the batch, a failed evaluation will cause the sequence to stop automatically and prevent the remaining samples from running on an out-of-spec instrument.

Below are the Tune Evaluation Method screens provided in MassHunter EnviroQuant to enter this criteria.

Tune Evaluation Method

Tune Evaluation | GC Performance Evaluation

Tune Evaluation

Method Title: DFTPP

Spectral Evaluation

Manual Auto

Manual Options

Spectrum Extraction: Apex

Background Subtraction: None

Within: 20 Scans + 20 Scans

Criteria

Base MZ: 198 Alternate Base MZ: 0

Mass	Rel. To MZ	% Low	% High	Alt. Base OK
51	198	30	60	<input type="checkbox"/>
68	69	0	2	<input type="checkbox"/>
70	69	0	2	<input type="checkbox"/>
127	198	40	60	<input type="checkbox"/>
197	198	0	1	<input type="checkbox"/>
198	198	100	100	<input type="checkbox"/>
199	198	5	9	<input type="checkbox"/>
275	198	10	30	<input type="checkbox"/>
365	198	1	100	<input type="checkbox"/>
441	443	1E-10	100	<input type="checkbox"/>
442	198	40	100	<input type="checkbox"/>
443	442	17	23	<input type="checkbox"/>

Apply Cancel Help

Tune Evaluation Method

Tune Evaluation | GC Performance Evaluation

Breakdown

Compound Name	Expected RT	Delta RT	Parent Compound	Parent CompoundName	Quant Ion	Qual Ions	Breakdown Limit
4,4'-DDT	7.1	0.2	<input checked="" type="checkbox"/>	4,4'-DDT	235	165,237	15
4,4'-DDD	6	0.2	<input type="checkbox"/>	4,4'-DDT	235	237,165	15
4,4'-DDE	5.6	0.2	<input type="checkbox"/>	4,4'-DDT	246	248,176	15

Tailing Factor

Compound Name	Expected RT	Delta RT	Quant Ion	Qual Ions	Tailing Factor Limit
Pentachlorophenol	4.9	0.5	266	264,268	5
Benzidine	6.3	0.5	184	92,185	3

Apply Cancel Help

Tune Evaluation Results

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

Online Results

The screenshot displays the Tune Evaluation Tool interface with the following components:

- Top Window (DFTPP.D TIC):** Shows a Total Ion Chromatogram (TIC) with peaks at approximately 9.2, 10.5, 13.5, and 15.0 minutes. The y-axis is labeled $\times 10^5$.
- Mass Spectrum (Scan 10.582-10.670 min):** Shows a mass spectrum with a base peak at m/z 197.9 and other significant peaks at 51.0, 77.0, 110.0, 127.0, 254.9, 274.9, and 441.9. The y-axis is labeled $\times 10^3$.
- Table 1 (Tune Eval Results):**

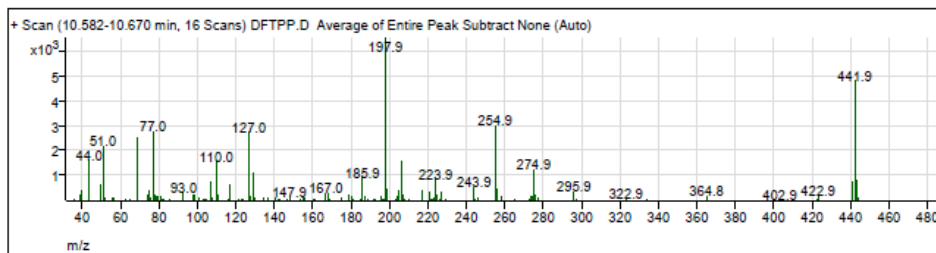
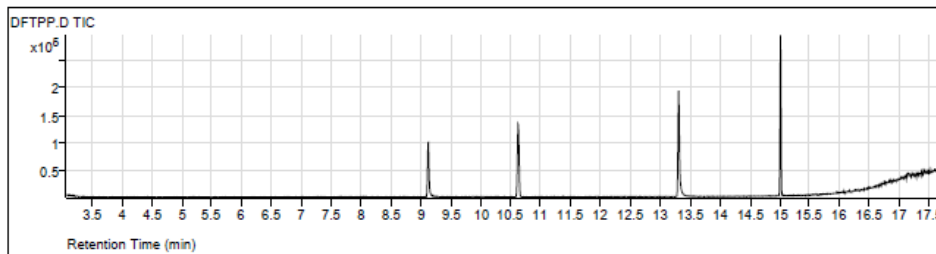
Target Mass	Rel. to Mass	Lower Limit %	Upper
51	198	30	60
68	69	0	2
70	69	0	2
127	198	40	60
197	198	0	1
198	198	100	100
199	198	5	9
275	198	10	30
365	198	1	100
441	443	1E-10	100
442	198	40	100
443	442	17	23
- Bottom Window (DFTPP.D TIC):** Shows a zoomed-in TIC with a peak at 15.012 minutes. The y-axis is labeled $\times 10^5$.
- Mass Spectrum (Scan 15.012 min):** Shows a mass spectrum for the peak at 15.012 min with a base peak at m/z 234.9 and other peaks at 50.0, 63.0, 75.0, 88.0, 135.9, 150.0, 165.0, 176.0, 212.0, 246.0, 261.9, 281.9, 317.9, and 353.8. The y-axis is labeled $\times 10^4$.
- Table 2 (Tune Eval Results):**

Compound Name	Exp. RT	obs. RT	TIC Area	Breakdown %	Tailing Factor	Pass/Fail
4,4'-DDT	15.000	15.012	325703	0.0	N/A	Pass
4,4'-DDD	14.500	0.000	0	N/A	N/A	
4,4'-DDE	14.000	0.000	0	N/A	N/A	
Pentachlorophenol	9.200	9.125	N/A	N/A	1.1	Pass

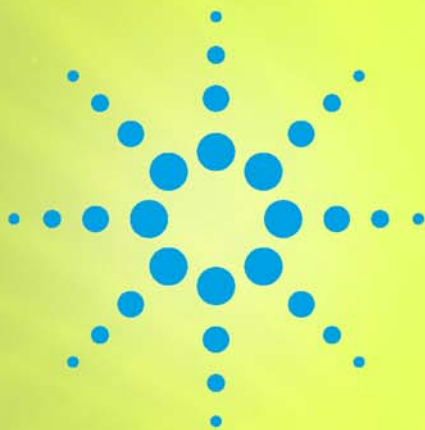
Tune Evaluation Report

Tune Evaluation Report

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



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



6 Reports

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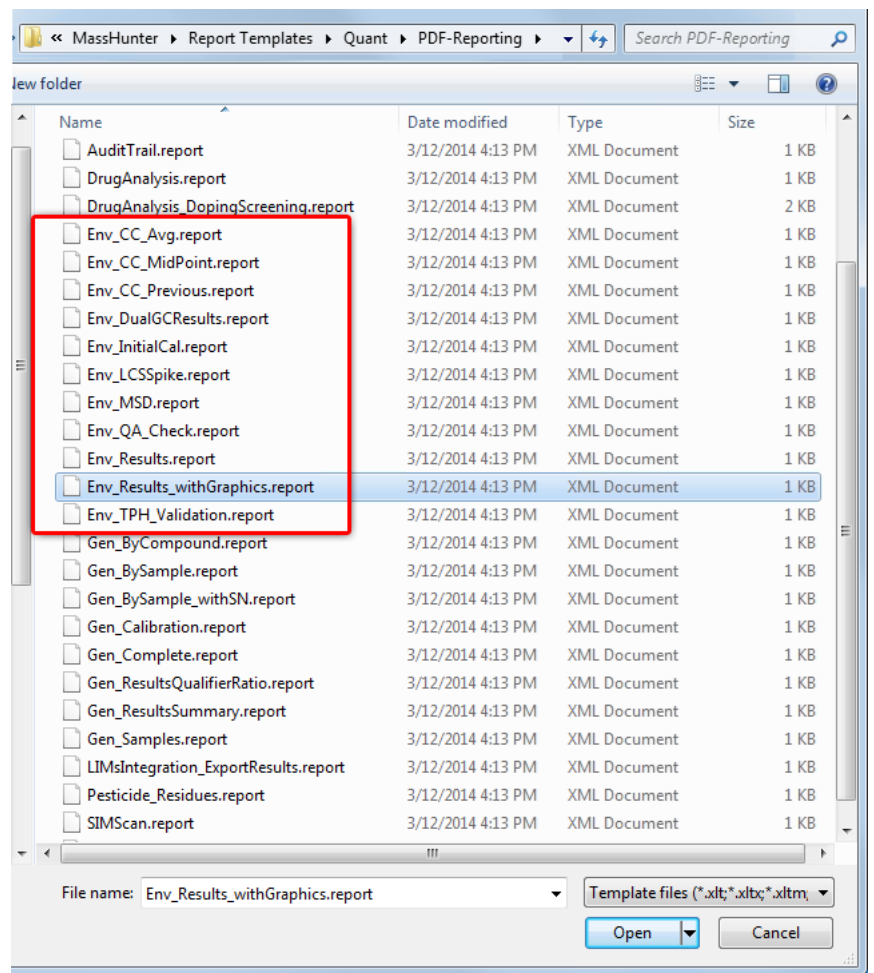
Report Templates

PDF Report Templates

MassHunter uses both Excel-based report templates and fast generating PDF report templates. Both types include many Environmental reports, and several include reporting features not found in MSD ChemStation.

To speed report generation, MassHunter EnviroQuant provides PDF report templates. PDF report templates generate reports 10 times faster than the Excel-based templates, however they are not customizable.

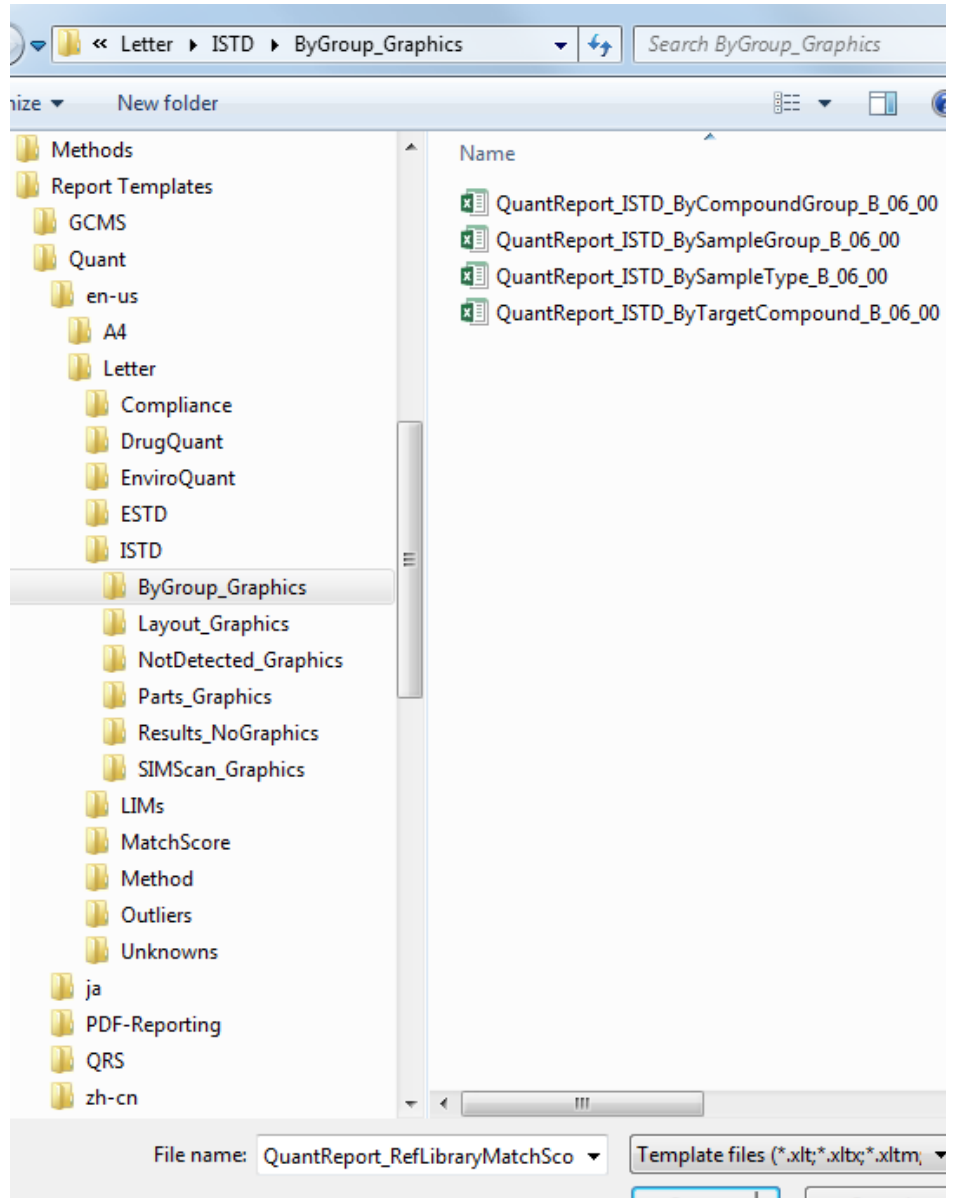
A partial list of MassHunter PDF report templates is shown below. Those designed specifically for Environmental reporting are shown in the red box. These templates are generally saved in: **MassHunter/Report Templates/Quant/PDF Reporting**.



Excel-based Report Templates

MassHunter EnviroQuant reporting is built on Microsoft Excel and is driven by Excel templates. This provides a great deal of flexibility in the reporting options, from layout and formatting to custom calculations and interactions with other software applications like LIMS.

A partial list of MassHunter's Excel Templates is shown here. So they can be easily located, these templates are grouped by report type. These templates are generally saved in: **MassHunter/Report Templates/Quant/....**



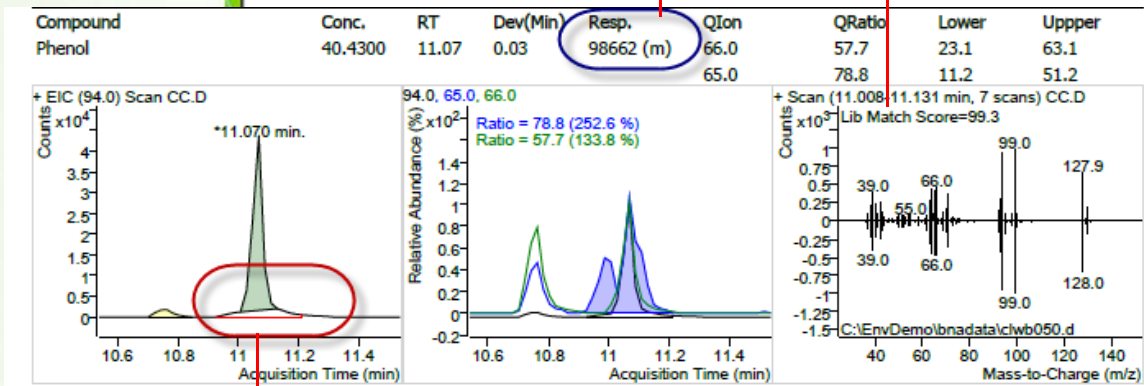
Before and After

To improve your data review process, in MassHunter EnviroQuant, both the before and after manual integration results are shown on the same report.

Manually Integrated Baseline

In this example you can see the red baseline, which is the baseline before manual integration, the manual integration indicator, and the Library Match Score.

(m) = Manual Integration Library Match Score

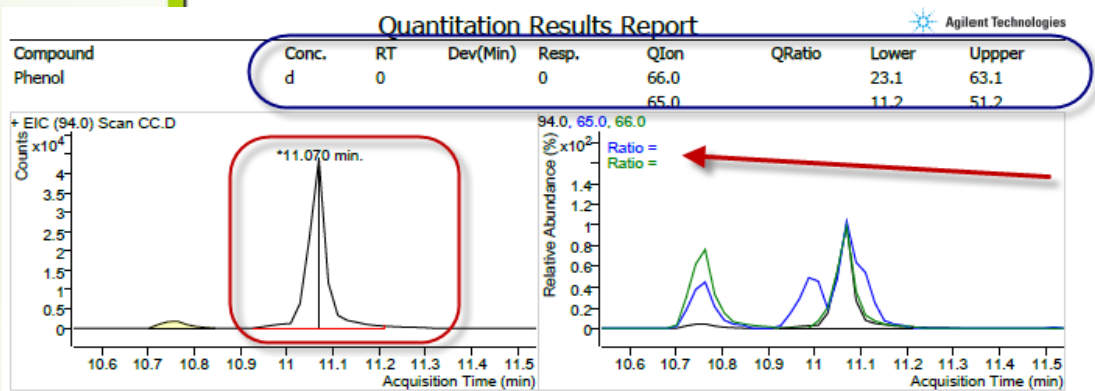


Red line = baseline before manual integration

Peak Removed

Here you can see how a removed peak will be shown in your reports. This is shown as a straight line through the apex of the peak, in the red circled area below.

Also, because the peak was deleted, the qualifier ratios are undefined, pointed to by the red arrow.



Bookmarks

Individual Samples

The bookmarks included with your PDF reports allow you to very quickly move through large reports to exactly the compound of interest. If they are not already displayed, click the bookmark icon to show the bookmarks that are automatically generated with your report.

The opening bookmarks list individual samples.

Bookmark icon

Data File	: methodBlank
Operator	: HP Chemist
Acq. Method	: Voalst
Acq. Date-Time	: 7/1/2014 12:4
Sample Name:	: Method Blank
Vial	: 17
Multiplier	: 1
Sample Info	:
...	...

Compounds Within Samples

When you select one of the samples, the bookmarks for the compounds within that sample are displayed. Click any one to jump directly to that compound.

Compound	Conc.	RT	Dev(Min)	Resp.	QIon	QRatio	Lower	Upper
Toluene-d8	48.9325	21.72	-0.07	67304	100.0	64.1	40.1	80.1

Quantitation Results Report

Compound: Toluene-d8, Conc.: 48.9325, RT: 21.72, Dev(Min): -0.07, Resp.: 67304, QIon: 100.0, QRatio: 64.1, Lower: 40.1, Upper: 80.1

Ratio = 64.1 (106.7%)

Three Continuing Calibration Reports

In MassHunter EnviroQuant there are three PDF versions of Continuing Calibration reports designed to measure the internal standard criteria as required by each method.

- **Env_CC_Avg.report.xml** measures the continuing calibration internal standard responses, against the average of the iCal internal standard responses.
- **Env_CC_MidPoint.report.xml** measures the continuing calibration internal standard responses, against the midpoint of the iCal.
- **Env_CC_Previous.report.xml** measures the continuing calibration internal standard responses to the previous ConCal and to the mid or average of the iCal, as is required for EPA method 525.3, for example.

Env_CC_Average Report

In this sample Continuing Calibration Report, the red entry represents an outlier.

Also, this report includes multiple curve types (e.g., Avg RF and Linear) reported. This type of reporting was not available in MSD ChemStation. In MSD ChemStation, a separate report would have to have been generated for each curve type.

A = measured against the Average

Outlier

Multiple curve fits

Continuing Calibration Report								Agilent Technologies
Batch Name	C:\MassHunter\GCMS\1\data\ConCal8260C\QuantResults\2014 Mar 26 1729 8260C.batch.bin							
Method File	C:\MassHunter\GCMS\1\methods\8260C.m							
Daily CC	C:\MassHunter\GCMS\1\DATA\ConCal8260C\CC.D							
Level name	Injection Time	Calibration Files						
20	3/26/2014 6:09:01 AM	C:\MassHunter\GCMS\1\DATA\ICAL8260C\20PPB.D						
50	3/26/2014 6:09:02 AM	C:\MassHunter\GCMS\1\DATA\ICAL8260C\50PPB.D						
100	3/26/2014 6:09:03 AM	C:\MassHunter\GCMS\1\DATA\ICAL8260C\100PPB.D						
150	3/26/2014 6:10:04 AM	C:\MassHunter\GCMS\1\DATA\ICAL8260C\150PPB.D						
200	3/26/2014 6:10:05 AM	C:\MassHunter\GCMS\1\DATA\ICAL8260C\200PPB.D						
CC	3/26/2014 6:29:08 PM	C:\MassHunter\GCMS\1\data\ConCal8260C\CC.D <=====						
ISTD Compound:	Avg Resp	Mid Resp	CC Resp	Area%			A/M	
Bromochloromethane	12491	13419	11753	94.10			A	
1,4-Difluorobenzene	67469	70129	66432	98.46			A	
Chlorobenzene-d5	57456	59487	56912	99.05			A	
Target Compound	AvgRF/R2	CC RF	Exp. Conc	Calc. Conc	%Dev	Area%	Curve Fit	
Bromochloromethane	-----ISTD-----							
Chloromethane	1.7066	1.9311	50.00	56.58	13.16	48.31	Avg RF	
Bromomethane	1.6991	1.7108	50.00	50.34	0.69	53.72	Avg RF	
Vinyl Chloride	1.9588	2.0730	50.00	52.91	5.83	51.10	Linear	
Chloroethane	1.2063	1.3481	50.00	55.88	11.15	48.18	Avg RF	
Methylene Chloride	2.0650	2.1558	50.00	52.20	4.40	50.86	Avg RF	
Acetone	0.4080	0.5082	50.00	62.20	24.58 #	40.56	Avg RF	
Carbon Disulfide	5.8963	5.7533	50.00	48.79	2.43	56.08	Avg RF	
1,1-Dichloroethene	1.8290	1.9146	50.00	52.34	4.68	52.23	Linear	
1,1-Dichloroethane	4.5032	4.5746	50.00	50.79	1.58	53.10	Avg RF	
1,2-Dichloroethene (total)	4.0099	4.1738	50.00	52.04	4.09	51.66	Avg RF	
Chloroform	4.4776	4.6252	50.00	51.65	3.30	52.38	Avg RF	
1,2-Dichloroethane-d4	2.4261	2.3782	50.00	49.01	1.98	7.57	Avg RF	
1,2-Dichloroethane	2.9877	2.9695	50.00	49.70	0.61	54.68	Avg RF	
1,4-Difluorobenzene	-----ISTD-----							
2-Butanone	0.1654	0.1594	50.00	48.18	3.65	52.63	Avg RF	
1,1,1-Trichloroethane	0.6655	0.6402	50.00	48.10	3.80	53.84	Avg RF	
Carbon Tetrachloride	0.5585	0.5250	50.00	47.00	6.00	55.40	Avg RF	
Vinyl Acetate	1.1716	1.1530	50.00	49.21	1.58	53.07	Avg RF	

Env_CC_MidPoint.Report

M = measured against the Mid

Continuing Calibration Report						Agilent Technologies	
Batch Name	C:\MassHunter\GCMS\1\data\ConCal8260C\QuantResults\2014 Mar 26 1729 8260C.batch.bin						
Method File	C:\MassHunter\GCMS\1\methods\8260C.m						
Daily CC	C:\MassHunter\GCMS\1\DATA\ConCal8260C\CC.D						
Level name	Injection Time	Calibration Files					
20	3/26/2014 6:09:01 AM	C:\MassHunter\GCMS\1\DATA\ICAL8260C\20PPB.D					
50	3/26/2014 6:09:02 AM	C:\MassHunter\GCMS\1\DATA\ICAL8260C\50PPB.D					
100	3/26/2014 6:09:03 AM	C:\MassHunter\GCMS\1\DATA\ICAL8260C\100PPB.D					
150	3/26/2014 6:10:04 AM	C:\MassHunter\GCMS\1\DATA\ICAL8260C\150PPB.D					
200	3/26/2014 6:10:05 AM	C:\MassHunter\GCMS\1\DATA\ICAL8260C\200PPB.D					
CC	3/26/2014 6:29:08 PM	C:\MassHunter\GCMS\1\data\ConCal8260C\CC.D <=====					
ISTD Compound:	Avg Resp	Mid Resp	CC Resp	Area%	A/M		
Bromochloromethane	12491	13419	11753	12.42	M		
1,4-Difluorobenzene	67469	70129	66432	5.27	M		
Chlorobenzene-d5	57456	59487	56912	4.33	M		
Target Compound	AvgRF/R2	CC RF	Exp. Conc	Calc. Conc	%Dev	Area%	Curve Fit
Bromochloromethane	-----ISTD-----						
Chloromethane	1.7066	1.9311	50.00	56.58	13.16	0.59	Avg RF
Bromomethane	1.6991	1.7108	50.00	50.34	0.69	11.61	Avg RF
Vinyl Chloride	1.9588	2.0730	50.00	52.91	5.83	8.30	Avg RF
Chloroethane	1.2063	1.3481	50.00	55.88	11.75	5.38	Avg RF
Methylene Chloride	2.0650	2.1558	50.00	52.20	4.40	8.32	Avg RF
Acetone	0.4080	0.5082	50.00	62.29	24.58 #	-10.93	Avg RF
Carbon Disulfide	5.8963	5.7533	50.00	48.79	2.43	12.39	Avg RF
1,1-Dichloroethene	1.8290	1.9146	50.00	52.34	4.68	4.22	Avg RF
1,1-Dichloroethane	4.5032	4.5746	50.00	50.79	1.58	8.22	Avg RF

Env_CC_Previous.Report

Reports both Average and Linear Curve Fit data in one report

Continuing Calibration Report								Agilent Technologies		
Batch Name	C:\MassHunter\GCMS\1\DATA\ConCal525_3nextday\QuantResults\2014 Mar 25 0546 525_3.batch.bin									
Method File	C:\MassHunter\GCMS\1\methods\525_3.M									
Daily CC	C:\MassHunter\GCMS\1\DATA\ConCal525_3nextday\CC.D									
Level name	Injection Time	Calibration Files								
20	3/24/2014 7:11:01 AM	C:\MassHunter\GCMS\1\DATA\ICAL525_3\20NG.D								
50	3/24/2014 7:11:02 AM	C:\MassHunter\GCMS\1\DATA\ICAL525_3\50NG.D								
80	3/24/2014 7:12:03 AM	C:\MassHunter\GCMS\1\DATA\ICAL525_3\80NG.D								
120	3/24/2014 7:12:04 AM	C:\MassHunter\GCMS\1\DATA\ICAL525_3\120NG.D								
160	3/24/2014 7:12:05 AM	C:\MassHunter\GCMS\1\DATA\ICAL525_3\160NG.D								
CC	3/24/2014 7:48:08 AM	C:\MassHunter\GCMS\1\data\ConCal525_3\CC.D <=====								
ISTD Compound:	Avg Resp	Mid Resp	CC Resp	CC Resp Prev	Area%_A	Area%_P	A/M/P			
1,4-Dichlorobenzene-d4	41409	41425	54869	53162	32.50	-3.22	A, P			
Naphthalene-d8	160277	160933	210899	190927	31.58	-11.66	A, P			
Acenaphthene-d10	100754	95509	132274	121563	31.28	-11.11	A, P			
Phenanthrene-d10	181317	182653	231297	205519	27.56	-11.54	A, P			
Chrysene-d12	138081	130281	152556	143703	10.48	-11.66	A, P			
Perylene-d12	205130	202925	233158	242481	13.66	3.61	A, P			
Target Compound	AvgRF/R2	CC RF	Exp. Conc	Calc. Conc	%Dev	Area%	Curve Fit			
1,4-Dichlorobenzene-d4	-----ISTD-----									
2-Fluorophenol	1.3031	1.3497	50.00	51.79	3.57	16.37	Avg RF			
bis(2-Chloroethyl)ether	1.5759	1.7034	50.00	54.05	8.09	9.52	Avg RF			
Phenol-d5	1.6859	1.8275	50.00	54.20	8.40	7.59	Avg RF			
Phenol	1.6428	1.8796	50.00	57.21	14.41	1.43	Avg RF			
2-Chlorophenol	1.2560	1.3322	50.00	53.03	6.07	9.86	Avg RF			
1,3-Dichlorobenzene	1.3737	1.4731	50.00	53.62	7.23	10.27	Avg RF			
1,4-Dichlorobenzene	1.3360	1.4909	50.00	55.80	11.59	5.87	Avg RF			

Initial Calibration Report

Initial Calibration Report								Agilent Technologies
Method Path								
Method File								
Batch Name C:\EnvDemo\bnadata\QuantResults\bnadata_01.batch.bin								
Last Calib Update 3/11/2014 3:26:09 AM								
Level Name	Calibration Files	Acq. Date-Time			Level Last Update Time			
20	C:\EnvDemo\bnadata\clwb020.d	1/28/1991 2:16:00 PM			3/11/2014 3:26:09 AM			
80	C:\EnvDemo\bnadata\clwb080.d	1/28/1991 3:11:00 PM			3/11/2014 3:26:09 AM			
120	C:\EnvDemo\bnadata\clwb120.d	1/28/1991 4:06:00 PM			3/11/2014 3:26:09 AM			
160	C:\EnvDemo\bnadata\clwb160.d	1/28/1991 5:01:00 PM			3/11/2014 3:26:09 AM			
50	C:\EnvDemo\bnadata\clwb050.d	1/28/1991 5:56:00 PM			3/11/2014 3:26:09 AM			
Compound	20	80	120	160	50	Avg RF	%RSD	
I 1,4-Dichlorobenzene-d4	----- ISTD -----							
S 2-Fluorophenol	1.2826	1.3675	1.3077	1.1766	1.3812	1.3031	6.268	
T bis(2-Chloroethyl)ether	1.8237	1.6684	1.4883	1.3200	1.5792	1.5759	12.002	
S Phenol-d5	1.9668	1.7185	1.5199	1.3675	1.8568	1.6859	14.472	
M Phenol	2.0332	1.6681	1.4639	1.3112	1.7377	1.6428	16.782 #	
M 2-Chlorophenol	1.4549	1.3096	1.1235	1.0279	1.3642	1.2560	14.003	
T 1,3-Dichlorobenzene	1.4976	1.4352	1.2435	1.1775	1.5149	1.3737	11.189	
M 1,4-Dichlorobenzene	1.5014	1.3018	1.2324	1.1325	1.5119	1.3360	12.503	
T 1,2-Dichlorobenzene	1.5499	1.3935	1.2822	1.1473	1.4674	1.3681	11.542	
T Benzyl alcohol	0.9071	0.9841	0.9651	0.8555	0.9008	0.9225	5.633	
T bis(2-chloroisopropyl)ether	2.0542	2.2180	2.1602	1.9017	2.0764	2.0821	5.780	
T 2-Methylphenol	1.4214	1.3229	1.2882	1.1782	1.3464	1.3114	6.792	
T Hexachloroethane	0.5495	0.5455	0.4947	0.4413	0.5620	0.5186	9.695	
M N-Nitroso-di-n-propylamine	1.2713	1.3040	1.5031	1.0896	1.2185	1.2773	11.771	
T 4-Methylphenol	1.4716	1.3545	1.2259	1.1286	1.3737	1.3109	10.245	
I Naphthalene-d8	----- ISTD -----							
S Nitrobenzene-d5	0.4347	0.4441	0.4049	0.3919	0.4400	0.4231	5.502	
T Nitrobenzene	0.4347	0.4001	0.4020	0.3476	0.3975	0.3964	7.880	
T Isophorone	0.9300	0.9138	0.8740	0.7878	0.8533	0.8718	6.430	
T 2-Nitrophenol	0.2213	0.2328	0.2337	0.2028	0.2126	0.2206	6.007	
T 2,4-Dimethylphenol	0.3642	0.3777	0.3496	0.3295	0.3464	0.3535	5.181	
T bis(2-Chloroethoxy)methane	0.4761	0.4918	0.4710	0.4370	0.4864	0.4725	4.539	
T 2,4-Dichlorophenol	0.3068	0.2867	0.2688	0.2368	0.2961	0.2791	9.824	
M 1,2,4-Trichlorobenzene	0.3316	0.3257	0.2944	0.2706	0.3240	0.3093	8.401	
T Naphthalene	1.0936	0.9722	0.8512	0.7610	0.9860	0.9328	13.816	
T 4-Chloroaniline	0.3501	0.3905	0.3818	0.3664	0.3621	0.3701	4.336	
T Hexachlorobutadiene	0.1811	0.1530	0.1499	0.1246	0.1660	0.1549	13.528	
M 4-Chloro-3-methylphenol	0.3723	0.3711	0.3338	0.3049	0.3672	0.3499	8.498	
T 2-Methylnaphthalene	1.0290	0.8461	0.7728	0.7284	0.9669	0.8686	14.647	
I Acenaphthene-d10	----- ISTD -----							
T Hexachlorocyclopentadiene	0.2080	0.2525	0.2191	0.1962	0.2283	0.2208	9.690	
T 2,4,6-Trichlorophenol	0.3876	0.3549	0.3329	0.3031	0.3915	0.3540	10.538	
T 2,4,5-Trichlorophenol	0.4387	0.3592	0.3061	0.2702	0.4282	0.3605	20.490	
S 2-Fluorobiphenyl	1.3735	0.9759	0.9248	0.8498	1.2211	1.0690	20.564	
T 2-Chloronaphthalene	1.2485	0.9535	0.9461	0.8500	1.1571	1.0310	16.025	
T 2-Nitroaniline	0.4642	0.4498	0.4552	0.4138	0.4727	0.4511	5.018	
T Dimethylphthalate	1.5065	1.1533	1.0743	1.0188	1.2722	1.2050	16.061	
M Acenaphthylene	1.9827	1.4204	1.2367	1.1352	1.5884	1.4727	22.669	
T 2,6-Dinitrotoluene	0.3944	0.3503	0.3381	0.2971	0.3602	0.3480	10.156	
T 3-Nitroaniline	0.3205	0.2879	0.2738	0.2583	0.3415	0.2964	11.503	
T Acenaphthene	1.1240	0.8258	0.7584	0.6908	1.0219	0.8842	20.630	
T 2,4-Dinitrophenol	0.1244	0.2305	0.2319	0.2013	0.2065	0.1989	22.057	

Matrix Spike Report

Matrix Spike/Duplicate Recover and RPD Summary Report



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

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

Matrix Spike Group Soil, Type B Results:

Compound	Sample Conc	Spike Amt	Spike Res	Dup Res	Spike Rec	Dup Rec	RPD	QC RPD	Limits %Rec
1,1-Dichloroethene	0.000	50.000	61.743	60.723	123.49	121.45	1.67	5	70 - 130
Trichloroethene	2.985	50.000	52.122	50.707	104.24	101.41	2.60	5	70 - 130
Benzene	0.094	50.000	52.186	53.709	104.37	107.42	2.87	5	70 - 130
Toluene	0.000	0.000	51.161	52.253			2.11 #		0 - 0
Chlorobenzene	0.000	0.000	49.061	51.952			5.72 #		0 - 0

Matrix Spike Group Water, Type A Results:

Compound	Sample Conc	Spike Amt	Spike Res	Dup Res	Spike Rec	Dup Rec	RPD	QC RPD	Limits %Rec
1,1-Dichloroethene	0.000	50.000	61.743	60.723	123.49	121.45	1.67	5	70 - 130
Trichloroethene	0.000	50.000	55.107	53.692	110.21	107.38	2.60	5	70 - 130
Benzene	0.000	50.000	52.281	53.803	104.56	107.61	2.87	5	70 - 130
Toluene	0.000	0.000	51.161	52.253			2.11 #		0 - 0
Chlorobenzene	0.000	0.000	49.061	51.952			5.72 #		0 - 0

(#) = out of Range

Quantitation Results Report

The Quantitation Results Report contains the Library Match Score between the know and the reference spectra as well as before and after manual integration lines.

Quantitation Results Report							Agilent Technologies		
Data File	: CC.D								
Operator	: HP Chemist								
Acq. Method	: 8260C								
Acq. Date-Time	: 3/26/2014 6:29:08 PM								
Sample Name:	: CC								
Vial	: 2								
Multiplier	: 1								
Sample Info	:								
DA Method File	: 8260C.M								
Tune File	:								
Tune Date	:								
Batch Name	: 2014 Mar 26 1741 8260C.batch.bin								
Last Calib Update	: 3/26/2014 5:36:18 PM								
Compound	RT	QIon	Resp.	Conc.	Units		Dev(Min)		
Internal Standards									
Bromochloromethane	7.953	128.0	11753	50.0000	ug/l	#	0.000		
1,4-Difluorobenzene	18.189	114.0	66432	50.0000	ug/l		0.000		
Chlorobenzene-d5	22.959	117.0	56912	50.0000	ug/l		0.000		
System Monitoring Compounds									
1,2-Dichloroethane-d4	10.783	65.0	27951	49.0124	ug/l		0.000		
Spiked Amount: 50.000	Range: 70.0 - 130.0%			Recovery = 98.02%					
Toluene-d8	21.795	98.0	57736	46.9910	ug/l		0.000		
Spiked Amount: 50.000	Range: 70.0 - 130.0%			Recovery = 93.98%					
Bromofluorobenzene	26.720	95.0	60889	47.8139	ug/l		0.000		
Spiked Amount: 50.000	Range: 70.0 - 130.0%			Recovery = 95.63%					
Target Compounds									
Chloromethane	0.935	50.0	22697	56.5783	ug/l		QValue 96		
Bromomethane	1.595	94.0	20107	50.3441	ug/l		94		
Vinyl Chloride	2.060	62.0	24364	52.9130	ug/l		100		
Chloroethane	2.796	64.0	15845	55.8761	ug/l		95		
Methylene Chloride	4.657	84.0	25338	52.1980	ug/l		94		
Acetone	5.278	43.0	5973	62.2877	ug/l		97		
Carbon Disulfide	6.053	76.0	67619	48.7868	ug/l		100		
1,1-Dichloroethene	7.410	96.0	22503	52.3404	ug/l		97		
1,1-Dichloroethane	8.728	63.0	53766	50.7923	ug/l		95		
1,2-Dichloroethene (total)	9.542	96.0	49055	52.0435	ug/l		96		
Chloroform	10.163	83.0	54361	51.6489	ug/l		94		
2-Butanone	10.822	43.0	10586	48.1767	ug/l		94		
1,2-Dichloroethane	10.900	62.0	34902	49.6957	ug/l		96		
1,1,1-Trichloroethane	12.063	97.0	42530	48.1024	ug/l		94		
Carbon Tetrachloride	12.451	117.0	34876	46.9982	ug/l		98		
Vinyl Acetate	12.722	43.0	76597	49.2078	ug/l		100		
Bromodichloromethane	13.148	83.0	50509	48.2418	ug/l		94		
1,2-Dichloropropane	14.350	63.0	38472	48.2057	ug/l		99		
cis-1,3-Dichloropropene	14.661	75.0	55677	49.2258	ug/l		98		
Trichloroethene	15.242	130.0	27706	49.4570	ug/l		98		
Benzene	15.630	78.0	76861	48.8134	ug/l		100		
Dibromochloromethane	15.902	129.0	31823	47.9801	ug/l		98		
trans-1,3-Dichloropropene	15.979	75.0	21542	44.7259	ug/l		74		
1,1,2-Trichloroethane	15.979	97.0	24769	51.5477	ug/l		99		
Bromoform	18.577	173.0	18220	45.8956	ug/l		92		
4-Methyl-2-Pentanone	18.926	43.0	29316	47.7556	ug/l		97		
2-Hexanone	20.438	43.0	18294	48.1704	ug/l		95		
Tetrachloroethene	20.787	164.0	21623	46.3880	ug/l		98		
CC.D			Page 1 of 16		Generated at 5:56 PM on 3/26/2014				



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