Moving From MSD ChemStation to MassHunter EnviroQuant

Workflow Guide

Agilent Technologies

Notices

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Contents

1 Introduction

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.

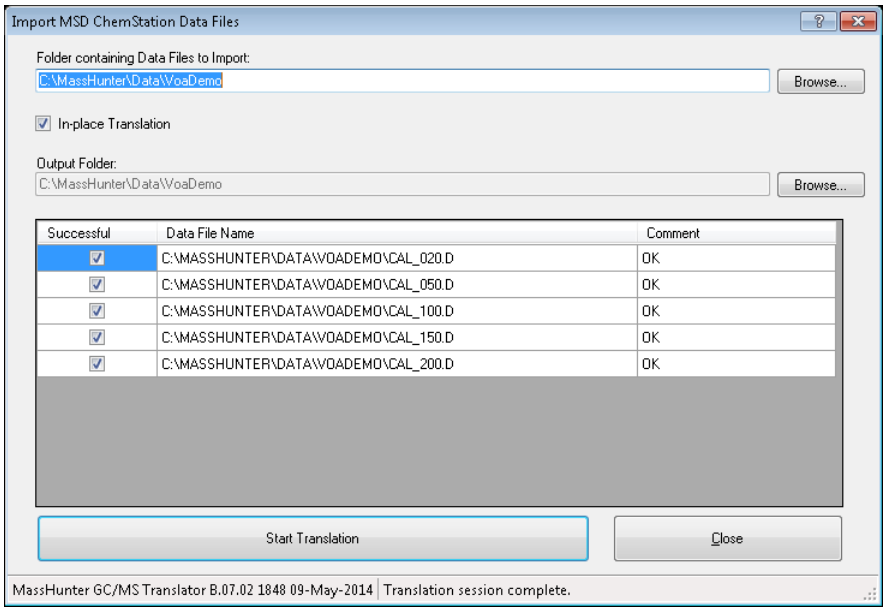
Additionally, there are templates included that are specific to EPA reporting requirements and they are customizable for individual laboratory needs.

Translator

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.

Import ChemStation Data Files

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

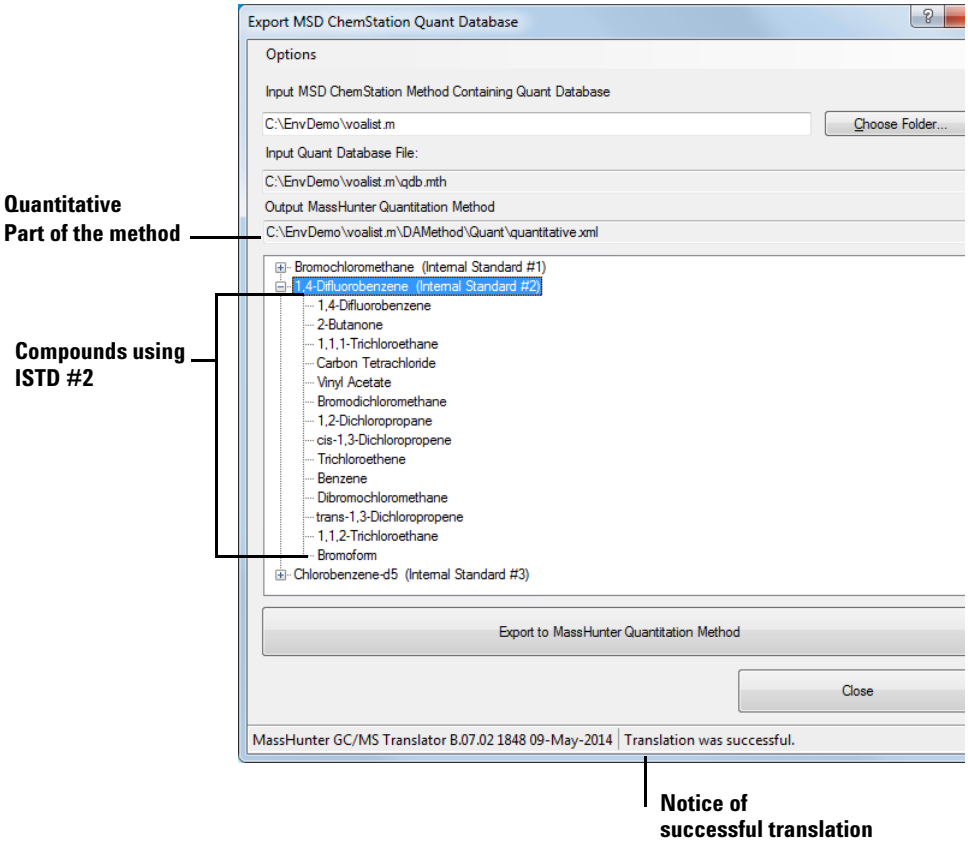


Export MSD ChemStation Quant Database

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.



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:

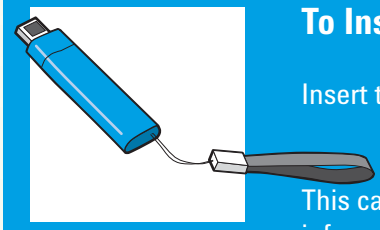
- MassHunter software installation disks
- GC/MS Software Information USB (G1701-60172)

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

Outliers Icons

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

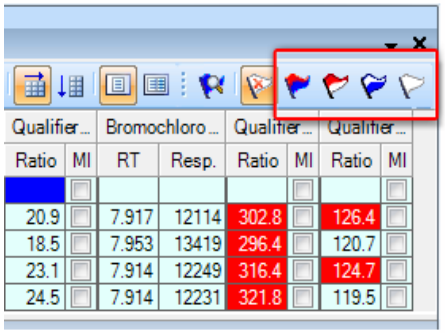
Outliers values are indicated by red cells for a high values and blue cells for low values. These Outlier icons are toggles. When selected, they will:


Display rows with **both** high and low outliers


Display rows with **high** outliers only


Display rows with **low** outliers only

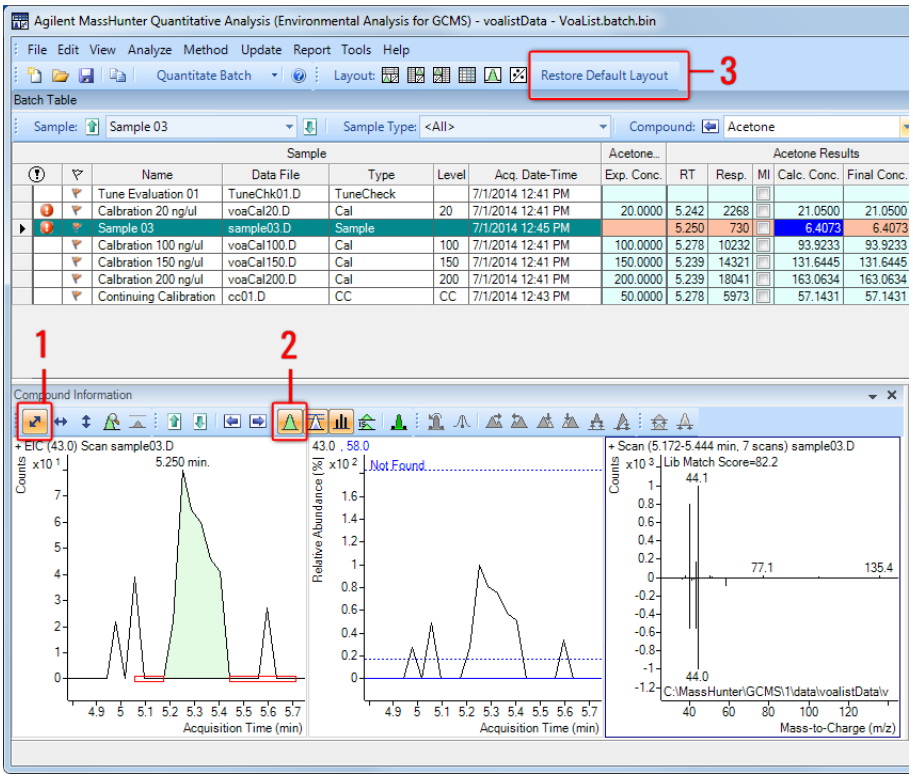

Display rows containing **no** outliers



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.

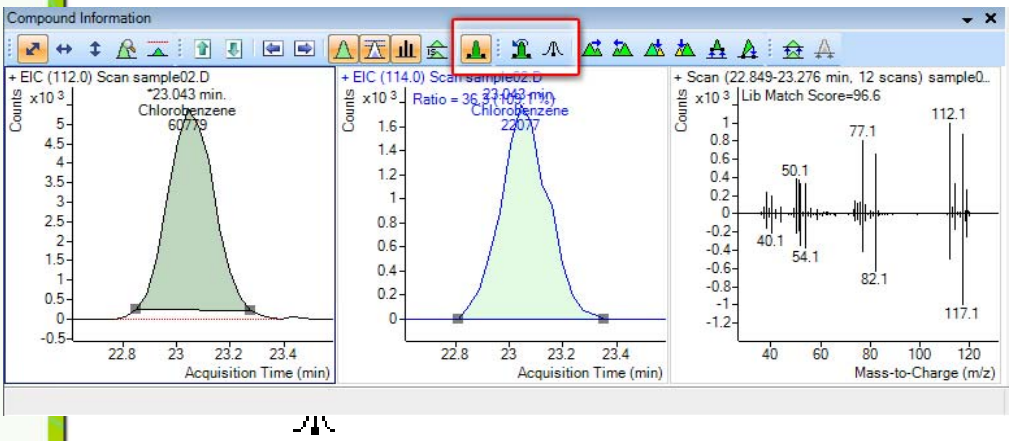
Highlighted below are some of the icons used for manual integration:


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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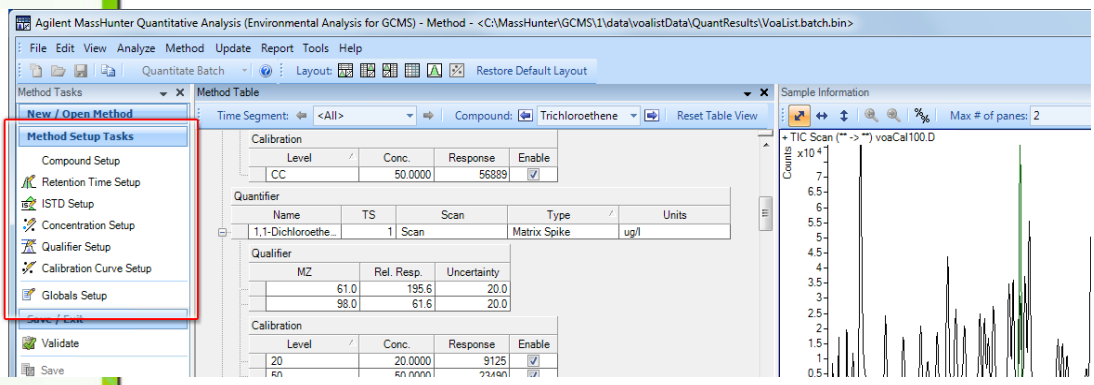
Overview

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.

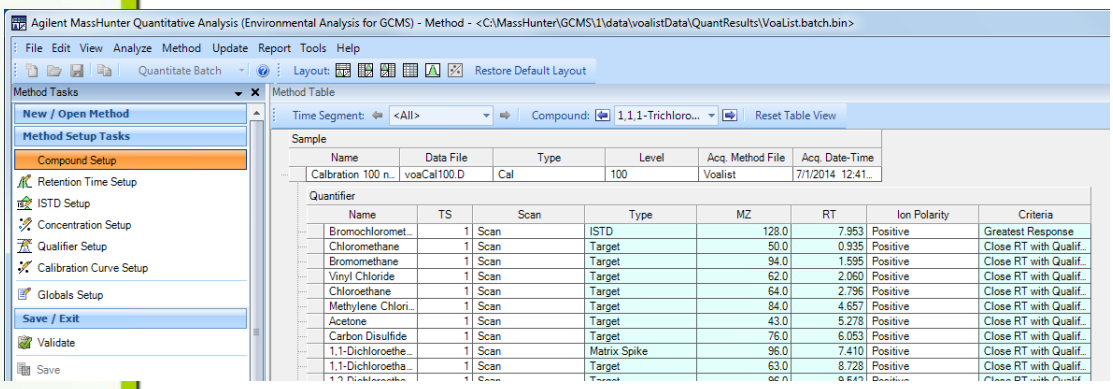
Quantitation Database

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.

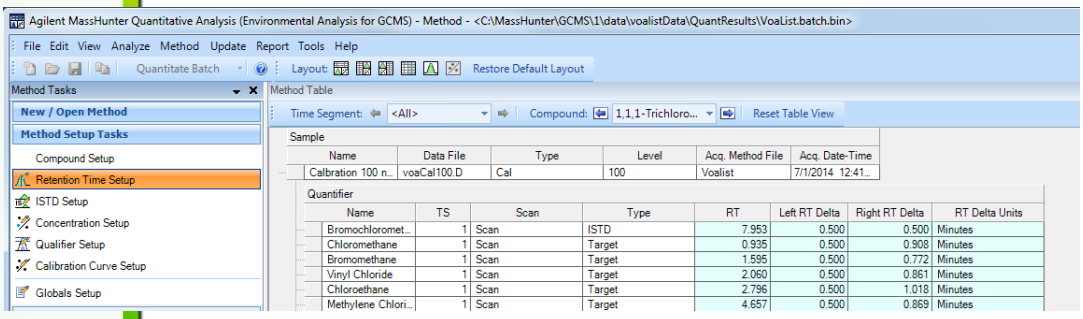


Below are a few sample screens from the Method Setup Tasks area.

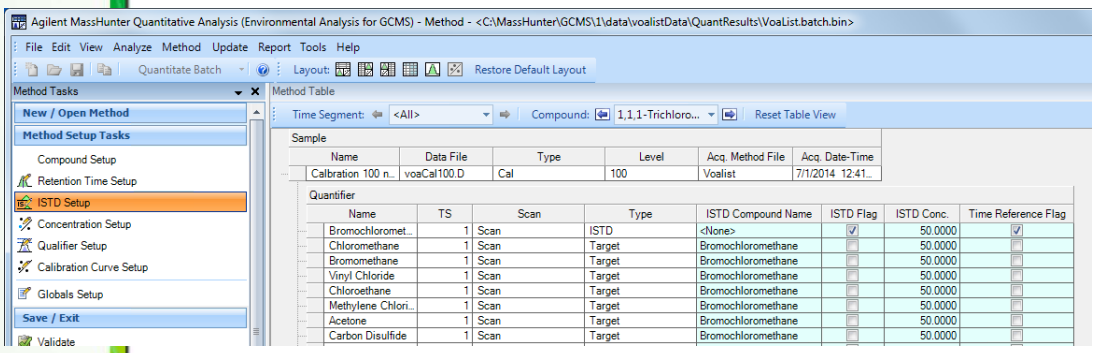
Compound Setup



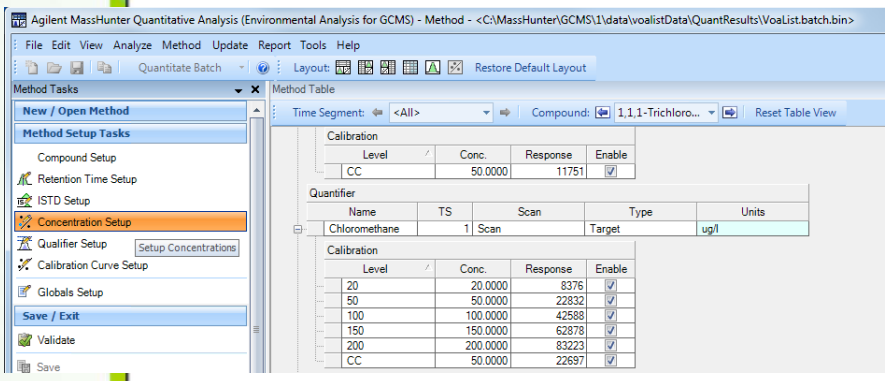
Retention Time Setup



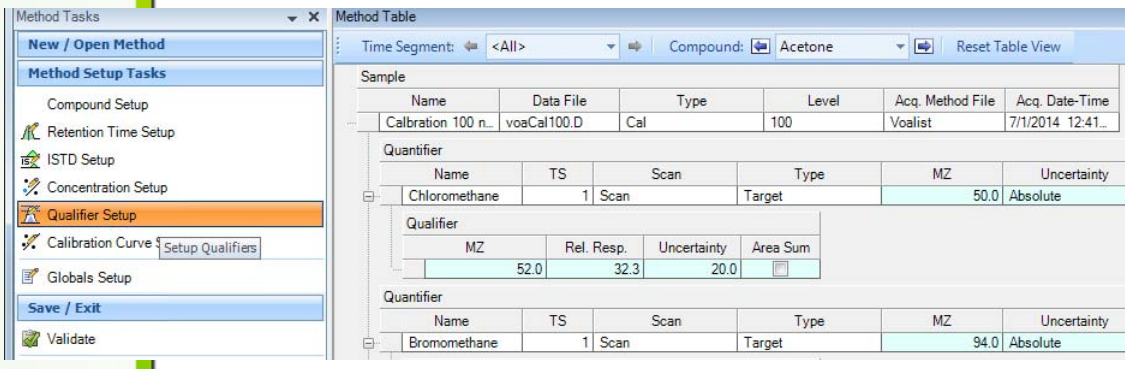
ISTD Setup



Concentration Setup



Qualifier Setup



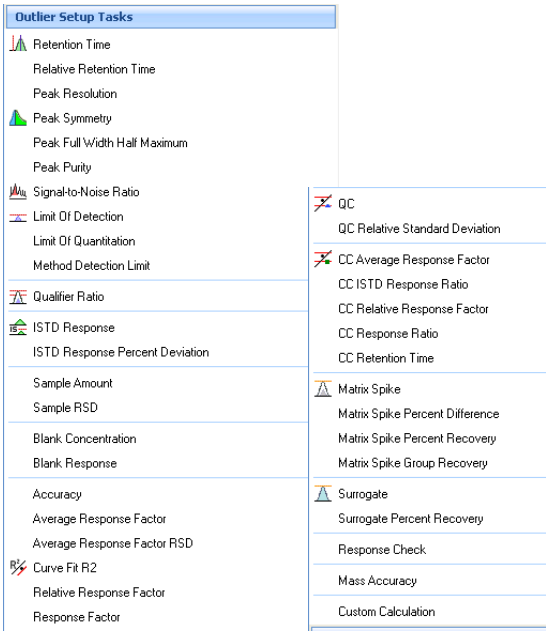
EPA Method Requirements

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.

List of Outliers

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



Unique to MassHunter EnviroQuant

Some of these parameters are monitored in both the MSD ChemStation and MassHunter EnviroQuant. Others, such as the *Average Response Factor*, and *Curve Fit* R^2 are available in MassHunter only.

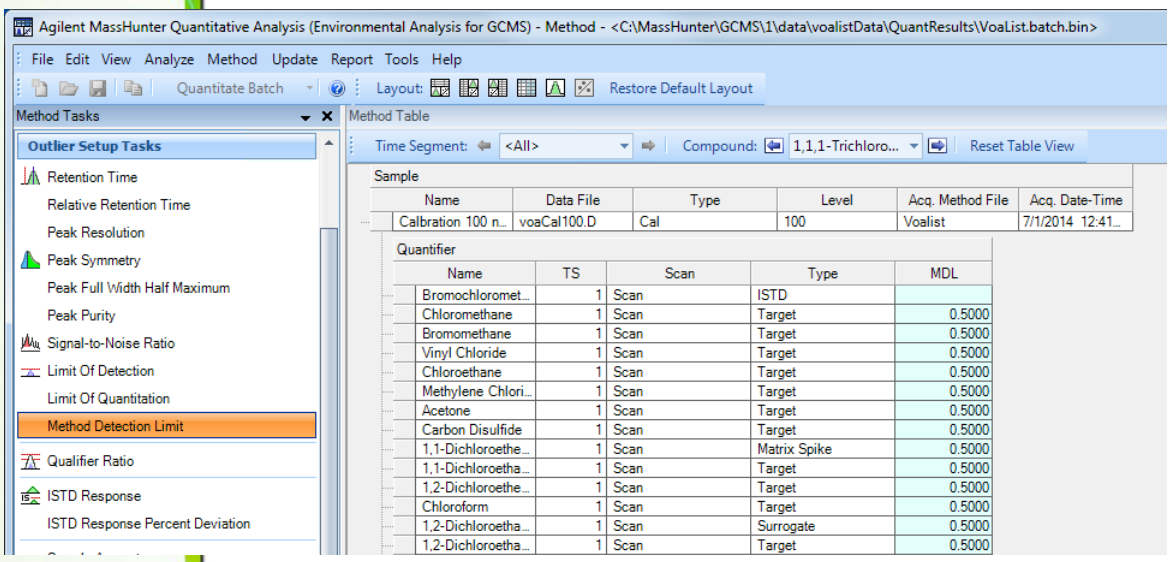
Applied on a Compound-by-Compound Basis

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 R^2 for each compound individually.

Commonly Used Outliers

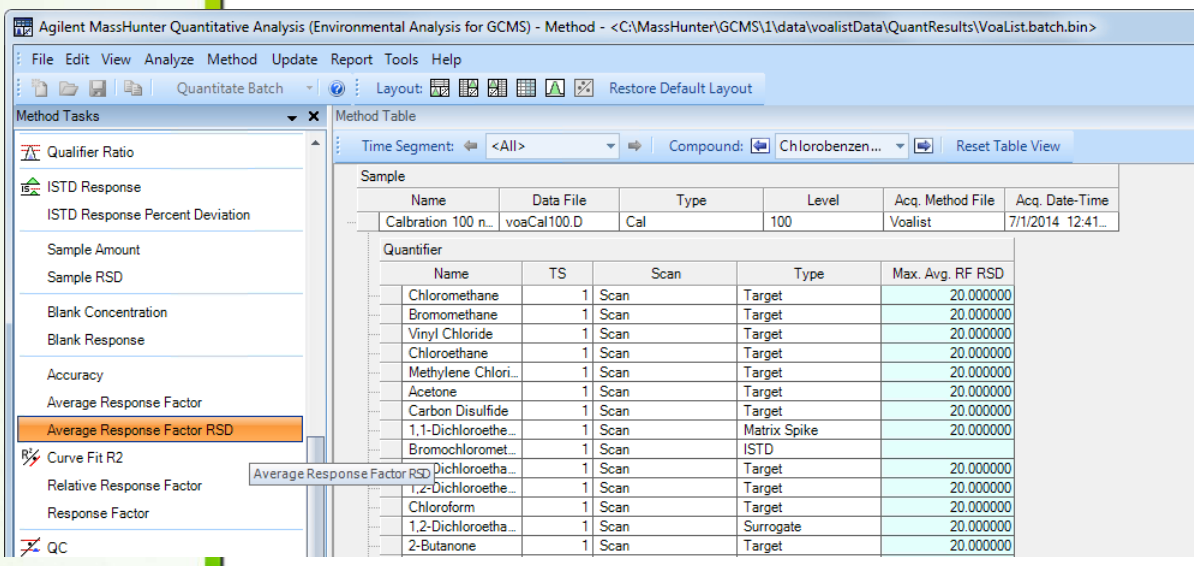
The following are just a few examples of the Method Editor data entry screens for commonly used outliers, included here for illustration purposes only. For EPA compliance, your methods will include many more.

Method Detection Limit



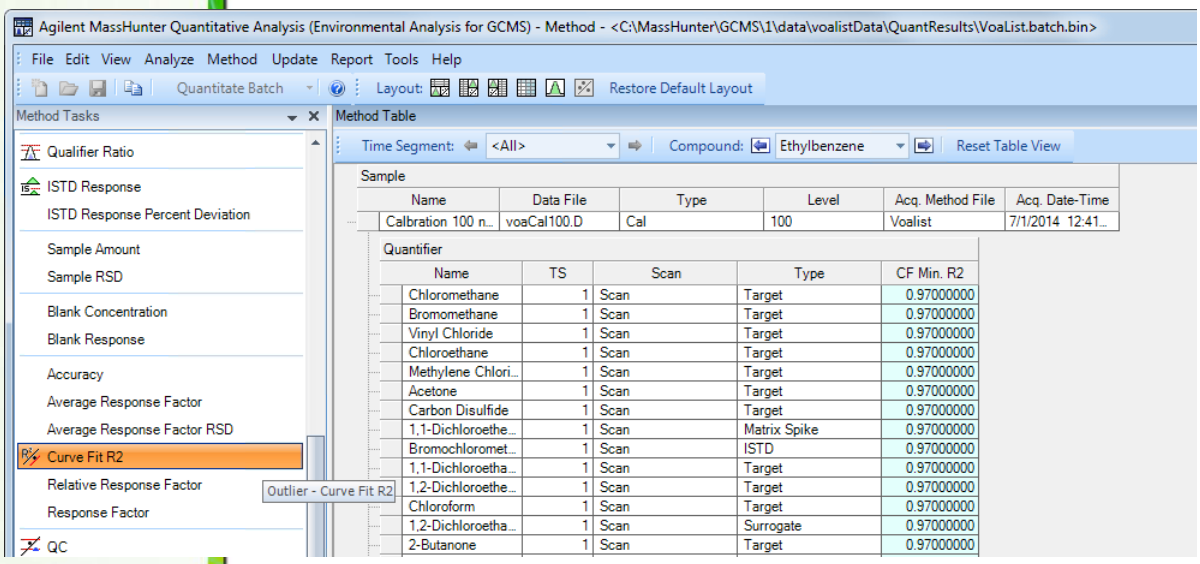
Average Response Factor RSD

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

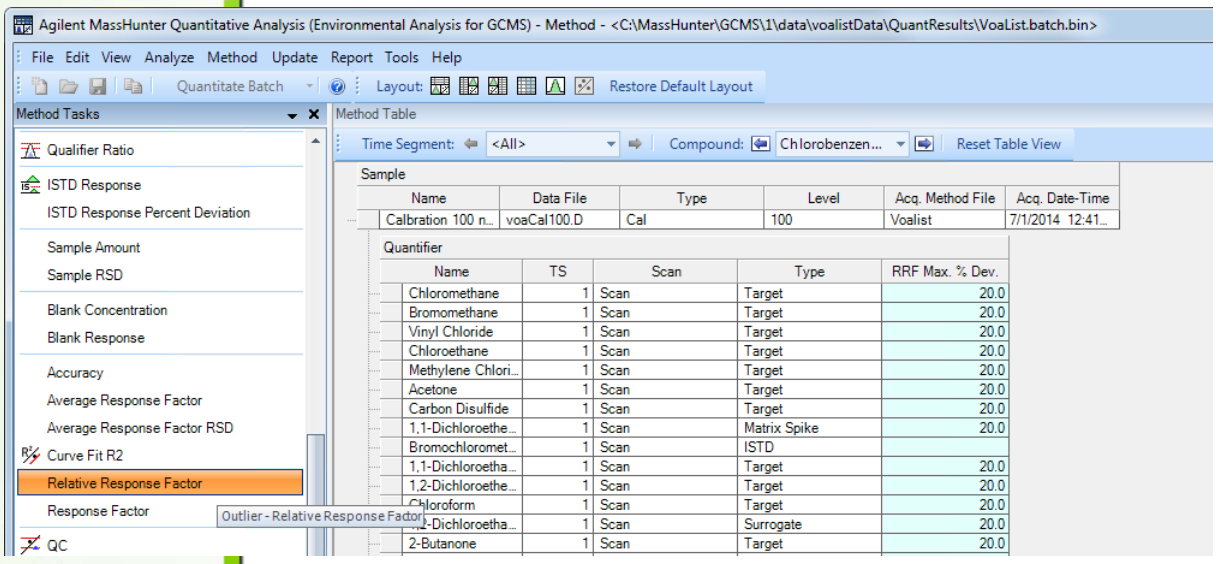


Curve Fit R^2

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.



Relative Response Factor



4
Compounds at a Glance

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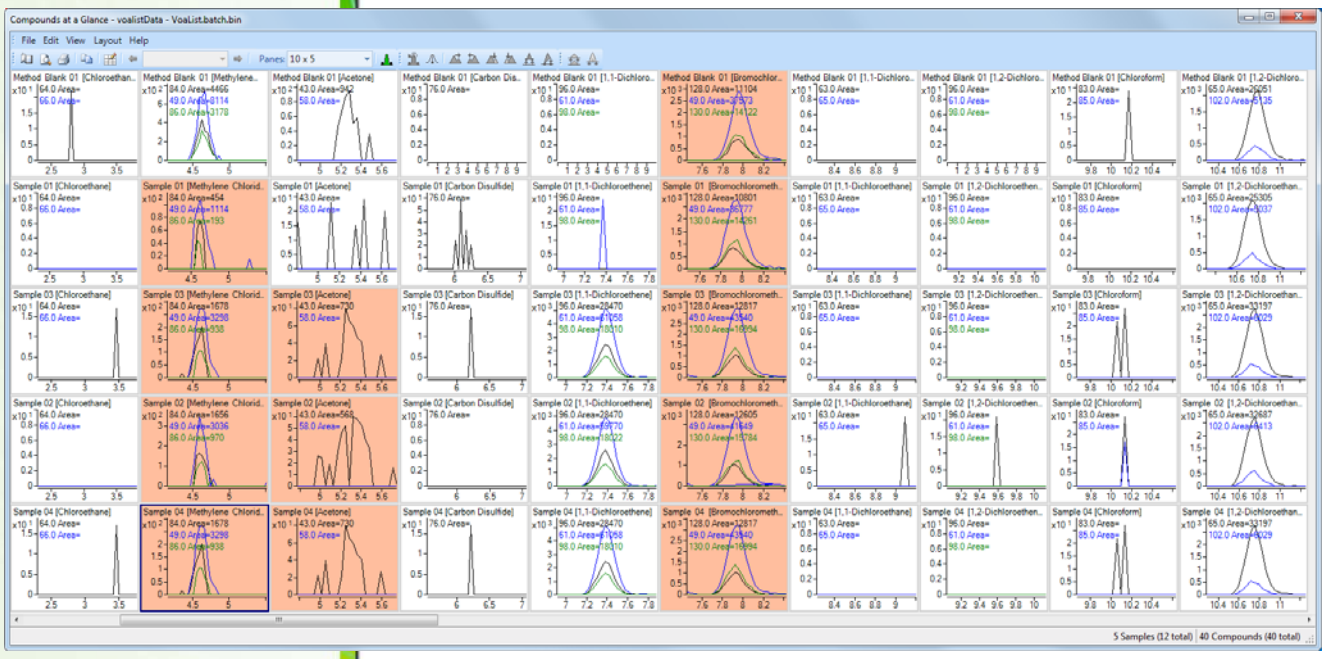
View up to 100 Compounds at a Glance

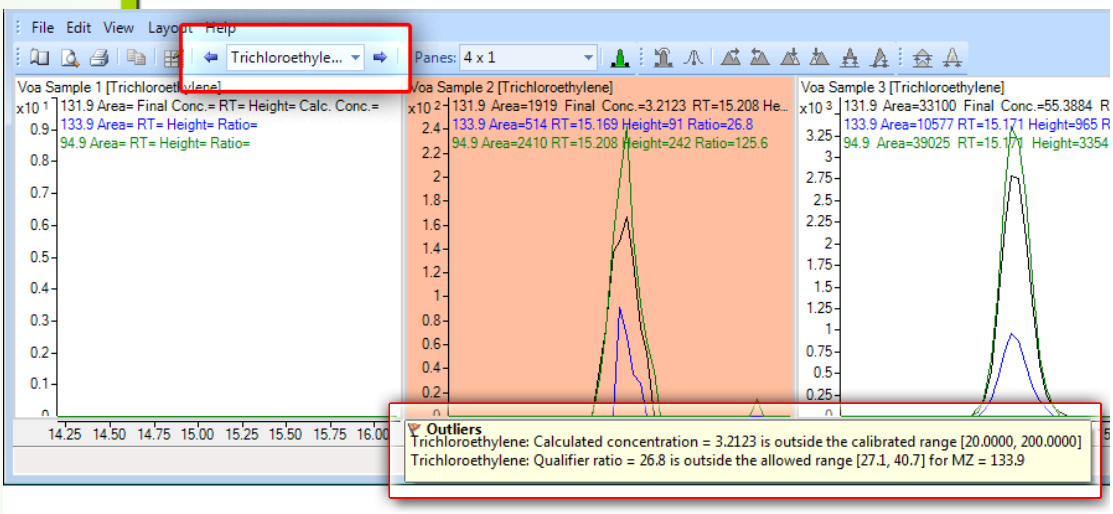
In the Compounds at a Glance view (**View > Compounds-at-a-Glance**) you can view up to 100 compound chromatograms at a time, by compound name, or by sample.

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.



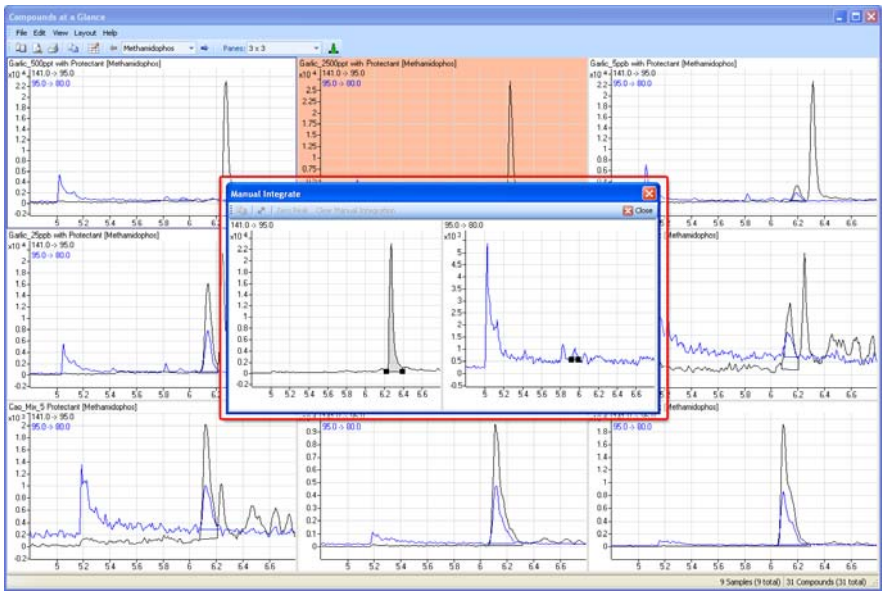
Read Outlier Messages

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.



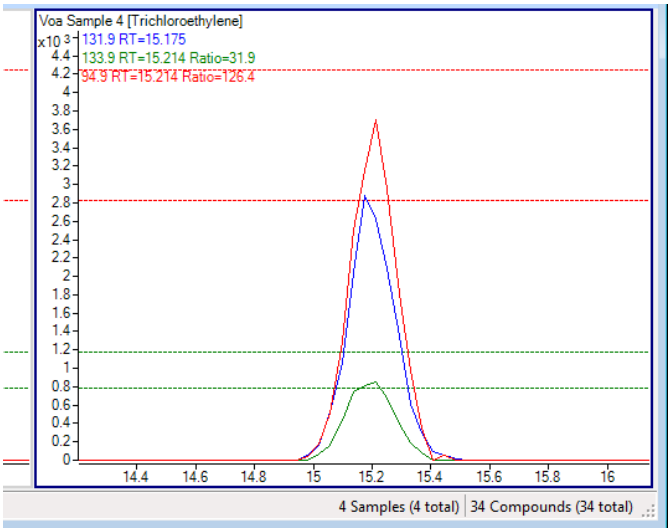
Manually Integrate Compounds

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

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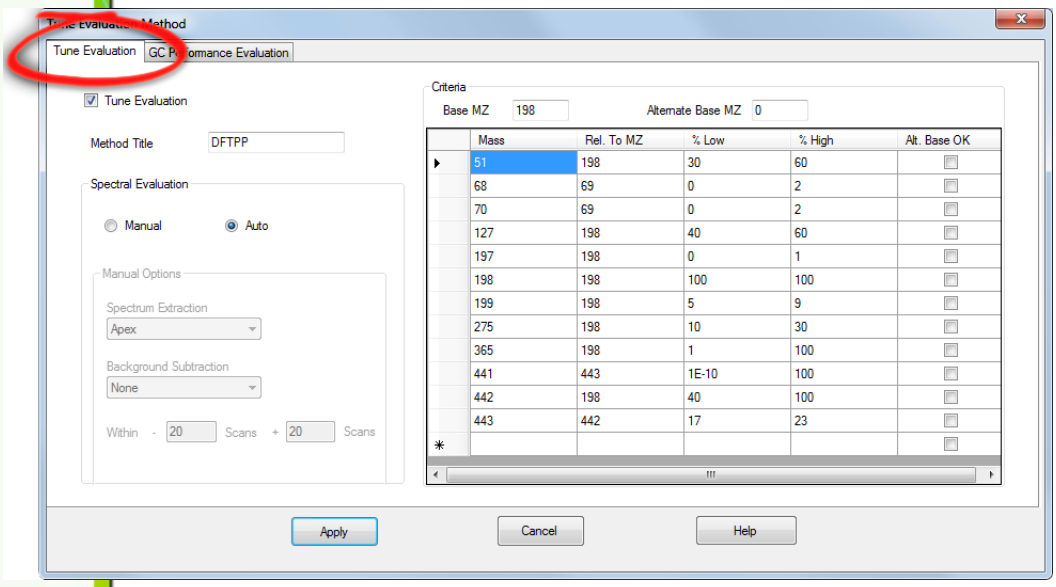
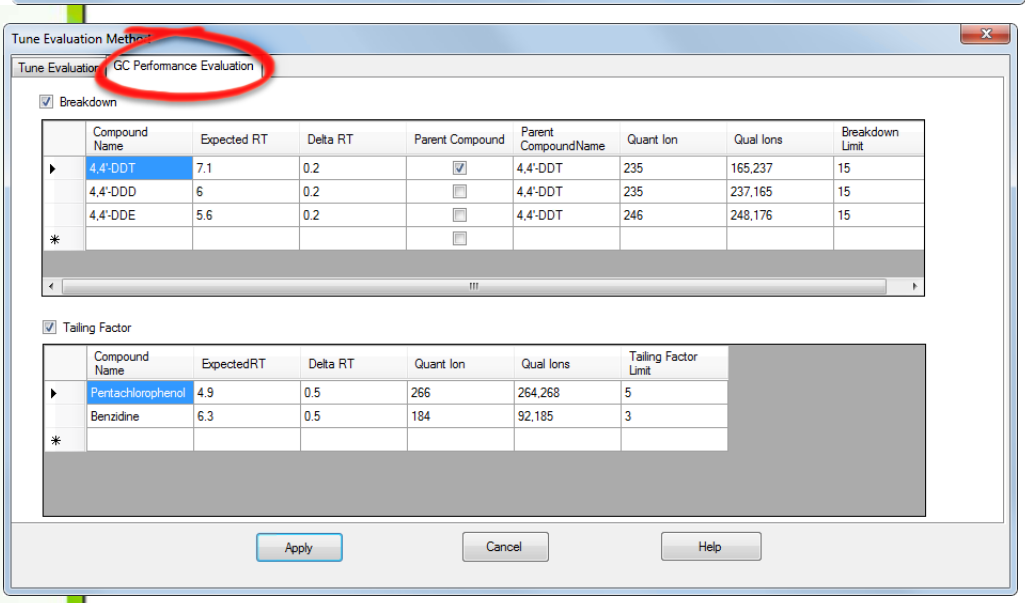
Tune Evaluation Tool

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.

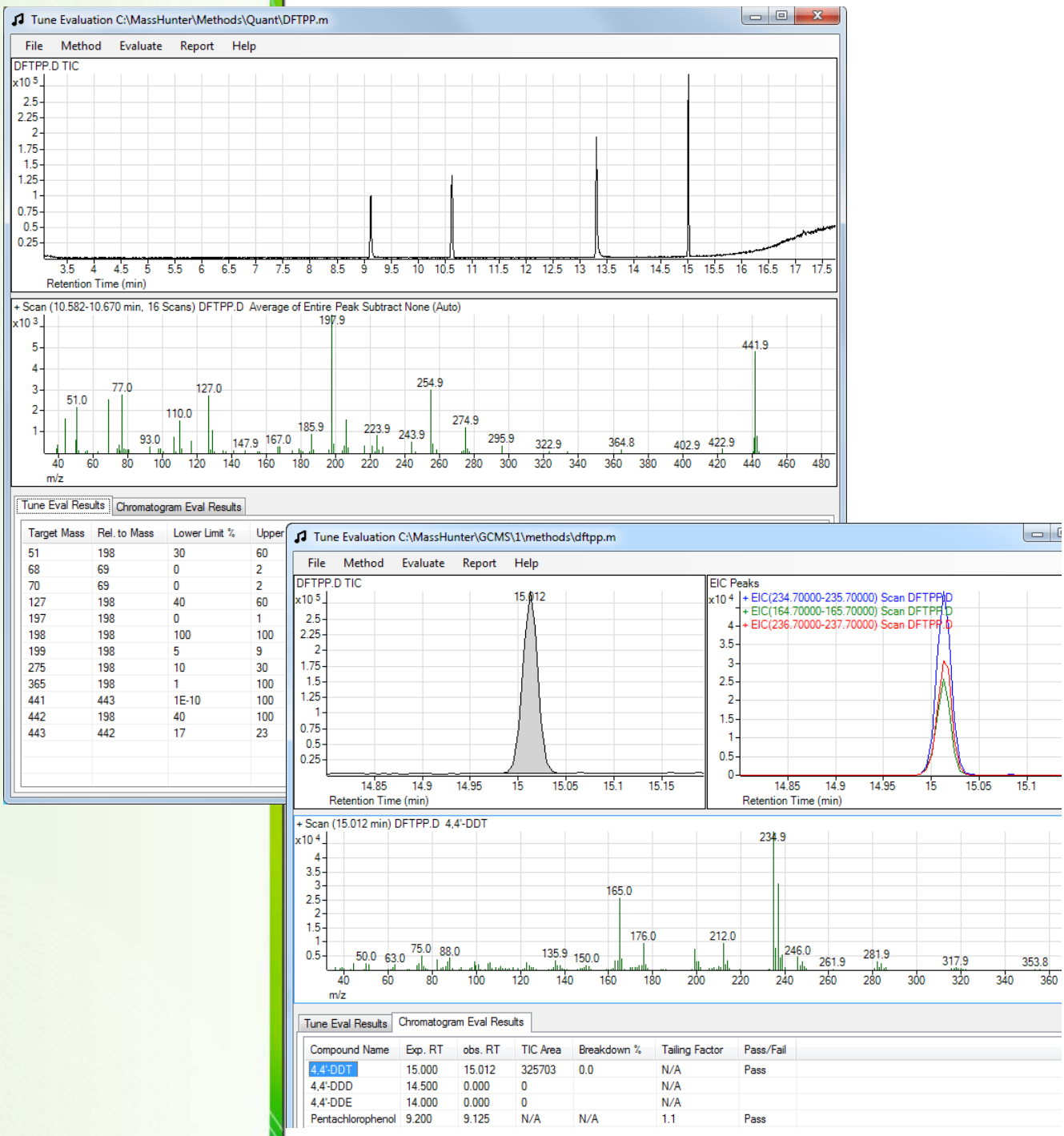




Tune Evaluation Results

Online Results

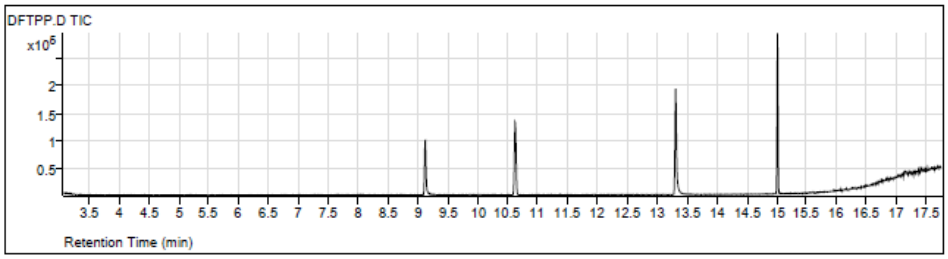
Tune evaluation results can be viewed interactively in the Tune Evaluation Tool, shown below, or can be generated as one of the printed reports for the batch.

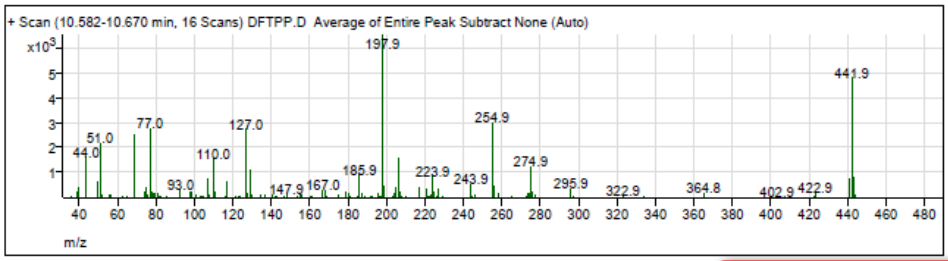


Tune Evaluation Report

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

C:\MassHunter\GCMS\1\DATA\ConCal8270\DFTPP.D 1 Generated

6
Reports

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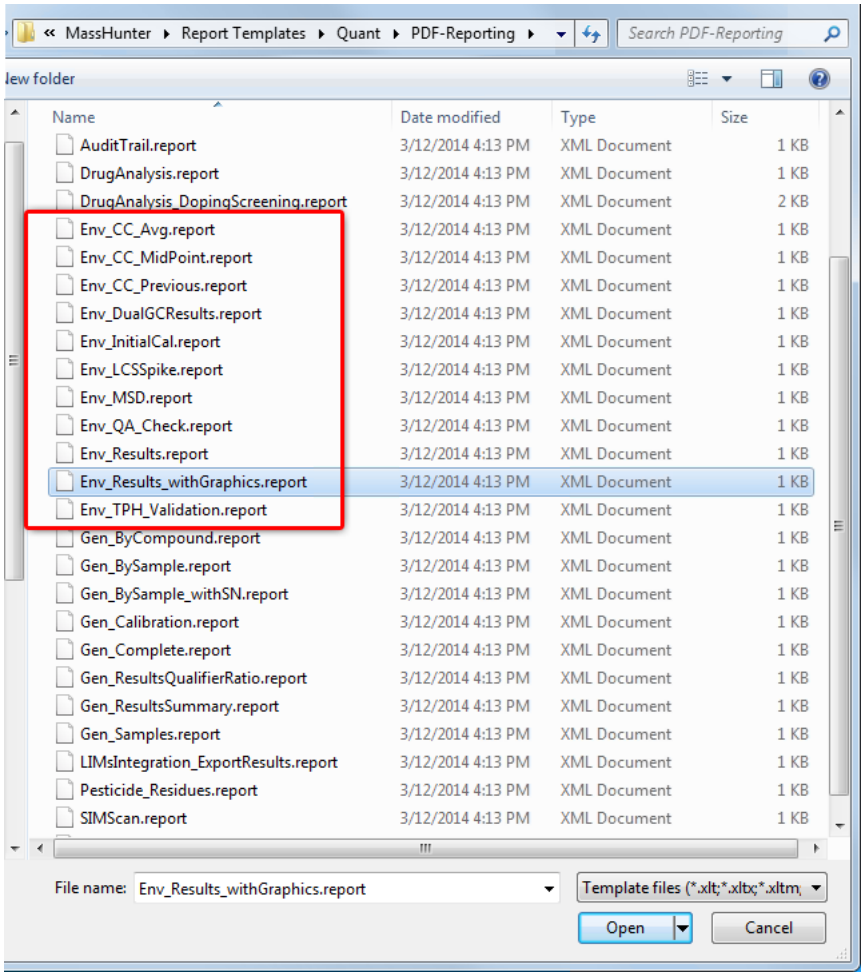
Report Templates

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.

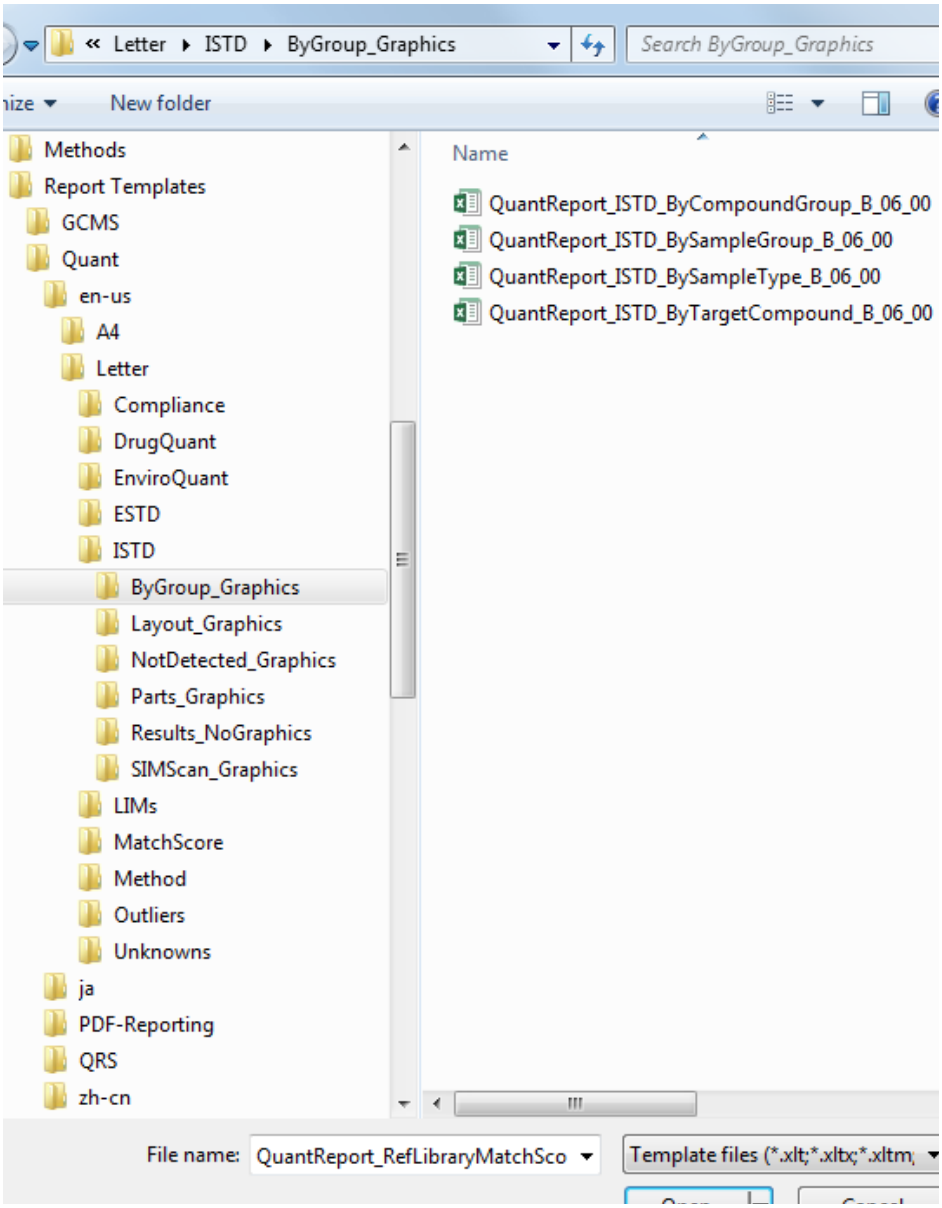
A partial list of MassHunter PDF report templates is shown below. Those designed specifically for Environmental reporting are shown in the red box. These templates are generally saved in: **MassHunter/Report Templates/Quant/PDF Reporting.**



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/....**

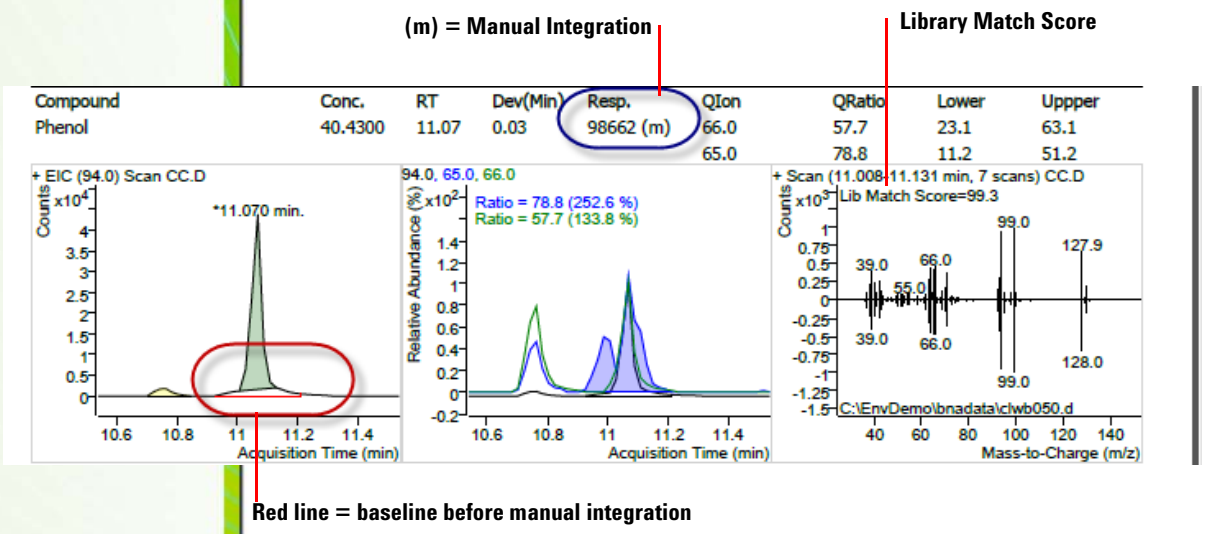


Before and After

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

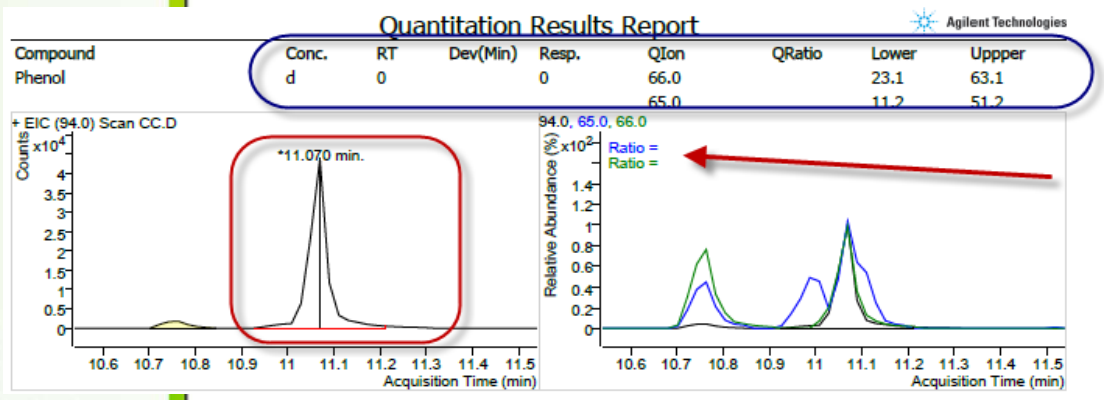
In this example you can see the red baseline, which is the baseline before manual integration, the manual integration indicator, and the Library Match Score.



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.

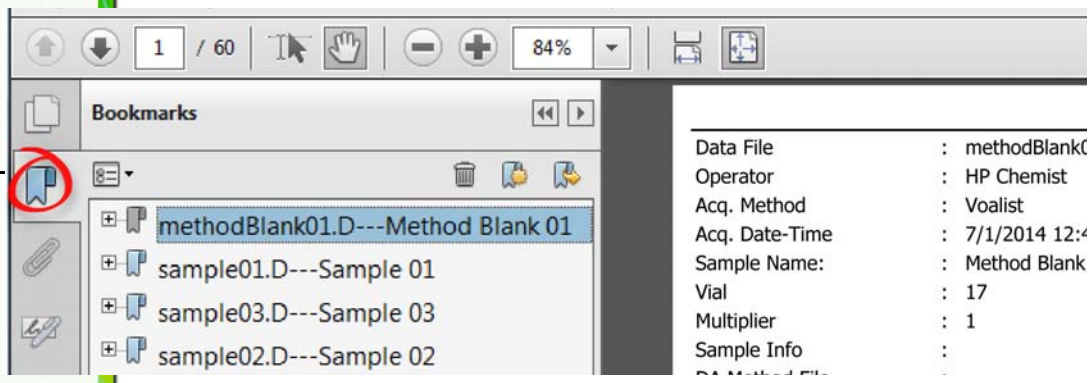


Bookmarks

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.

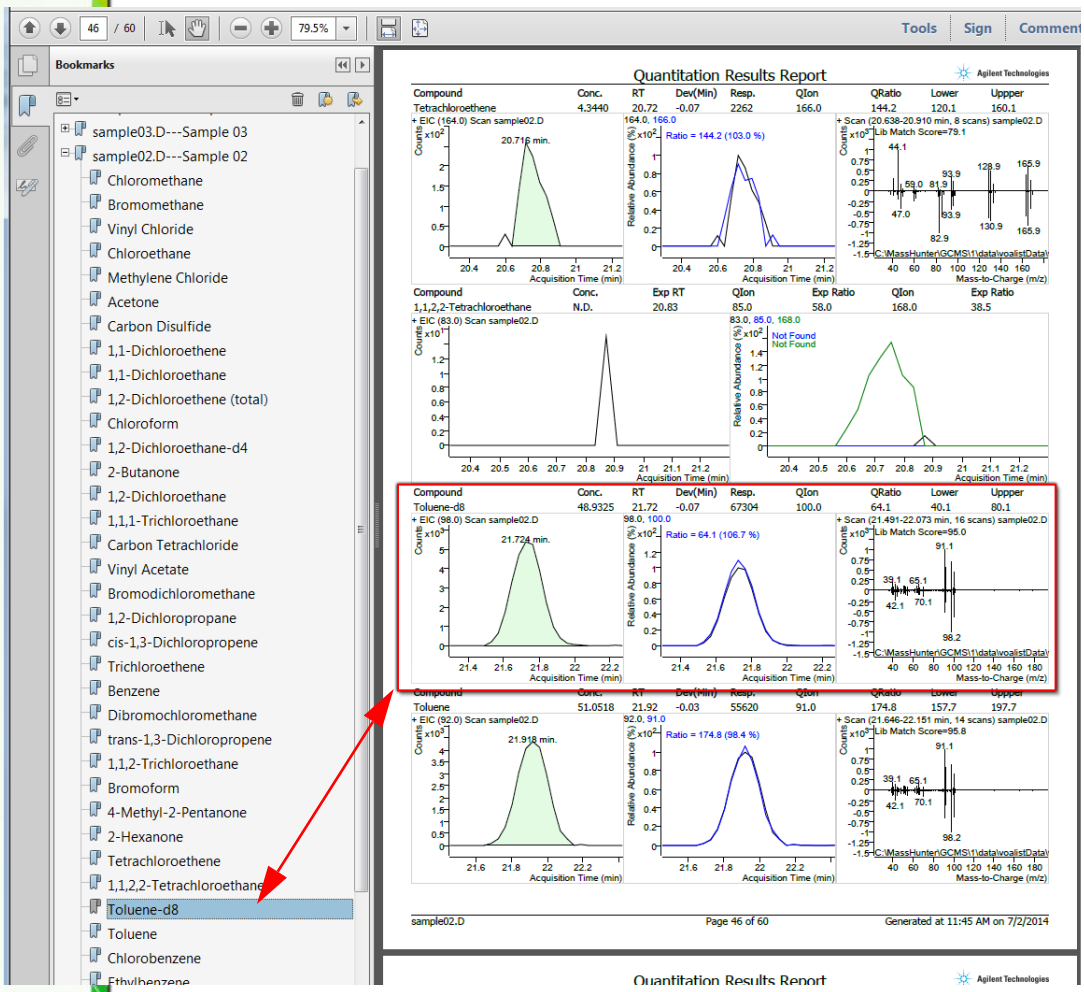
Individual Samples

The opening bookmarks list individual samples.



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.



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.[illegible]	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	62.29	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%	A/M/P
1,4-Dichlorobenzene-d4	41409	41425	54869	53162	32.50	-3.2	A, P
Naphthalene-d8	160277	160933	210899	190927	31.58	-1	A, P
Acenaphthene-d10	100754	95509	132274	121563	31.28		A, P
Phenanthrene-d10	181317	182653	231297	205519	27.56	.54	A, P
Chrysene-d12	138081	130281	152556	143703	10.48		A, P
Perylene-d12	205130	202925	233158	242481	13.66	3.	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

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Matrix Spike Report

Matrix Spike/Duplicate Recover and RPD Summary Report

Agilent Technologies

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							QValue
Chloromethane	0.935	50.0	22697	56.5783	ug/l		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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