

ReviewSheet for MassHunter Quant

User Manual

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Web-page <https://waleson.eu/reviewsheet>

Purpose

High-throughput reviewing and reporting
Highly customizable Excel like sheets (Excel is not required)

The screenshot displays the ReviewSheet software interface, which is designed for high-throughput reviewing and reporting of mass spectrometry data. The interface is divided into several main sections:

- Top Panel:** Contains file information (Sample: CAL_L10.D, Type: Calibration, Acquired: 2008-06-20 22:19:23, Method: 624A.M) and a menu bar with options like File, Report, Fast Analyze, and Help.
- Chromatogram:** A Total Ion Chromatogram (TIC) plot showing detector response versus acquisition time (min). The x-axis ranges from 3 to 25 minutes, and the y-axis is labeled 'Counts x10⁴'. A prominent peak is visible at approximately 10.091 minutes.
- Data Table:** A comprehensive table listing various compounds and their analysis results. The table includes columns for Compound, Type, ISTD, RT Exp, RT Act, Resp, IS Resp, FConc, Accuracy, Q1 Det, and Q1 Out. The table lists numerous compounds such as 1,1-Dichloro-1-propene, Dichlorodifluoromethane, Chloromethane, 1,4-Dichlorobenzene, Vinyl Chloride, 1,2,4-Trichlorobenzene, Bromomethane, Chloroethane, Naphthalene, Hexachlorobutadiene, Trichlorofluoromethane, Acetone, 1,1-Dichloroethene, 1,2,3-Trichlorobenzene, Methylene Chloride, Carbon Disulfide, trans-1,2-Dichloroethane, 2-Methoxy-2-methylpropane, 1,1-Dichloroethane, Vinyl Acetate, 2-Butanone (MEK), t-Butyl Alcohol, Chloroform, Propane, 2,2-dichloro-1,2-Dichloroethene, Tetrahydrofuran, and 1,2-Dichloroethane-d4.
- Batch Table:** A detailed table showing the results for a specific sample (CAL_L10). It includes columns for Sample Name, Type, Level, Exp. Conc., RT, Resp, MI, Calc. Conc., Final Conc., Accuracy, Ratio, and RT. The table lists 19 samples, including various concentrations of 1,1-Dichloro-1-propene and other compounds like Blank01, Blank02, SAMPLE01, SAMPLE02, SAMPLE03, and SAMPL F04.
- Compound Information:** A panel showing the chromatogram for a specific compound (1,1-Dichloro-1-propene) with a peak at 10.091 min. The x-axis is 'Acquisition Time (min)' and the y-axis is 'Counts x10⁴'.
- Calibration Curve:** A plot showing the relationship between Relative Response (y-axis) and Relative Concentration (x-axis) for 1,1-Dichloro-1-propene. The curve is linear, with the equation $y = 0.441389 * x - 0.021206$ and $R^2 = 0.9989461$. The plot includes 10 data points and a linear fit line.

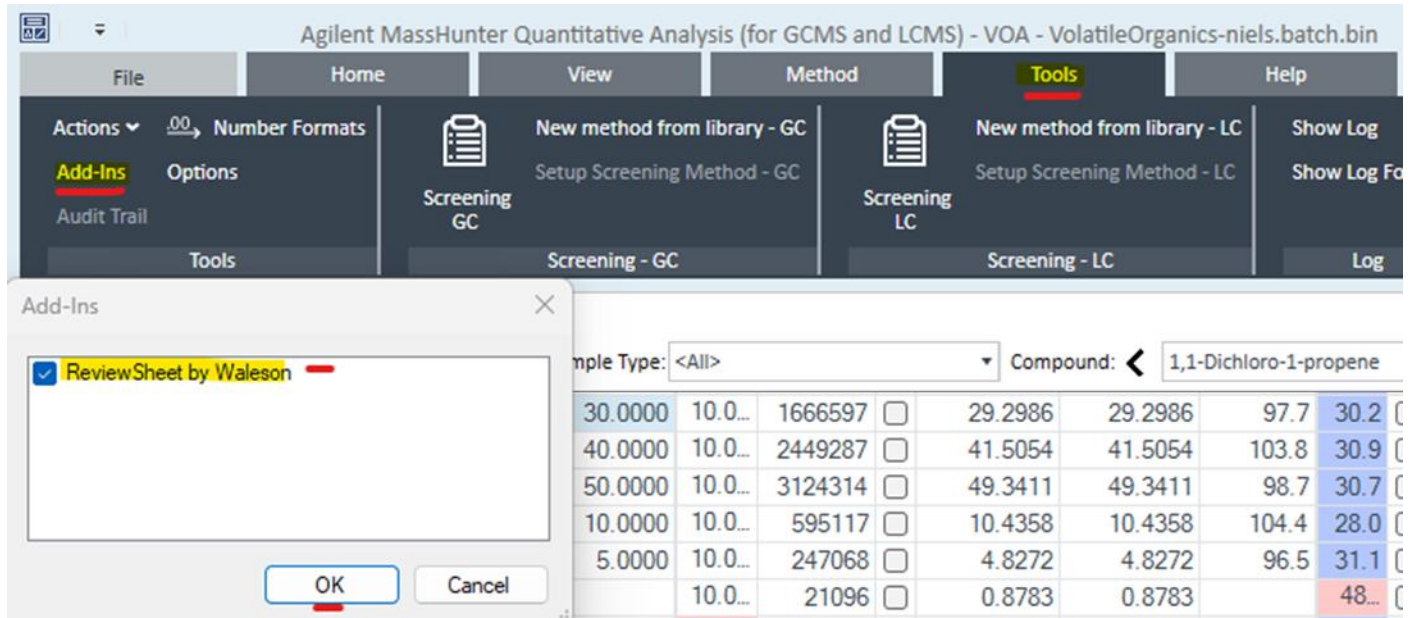
Installation

Download the latest version from <https://waleson.eu/reviewsheet>

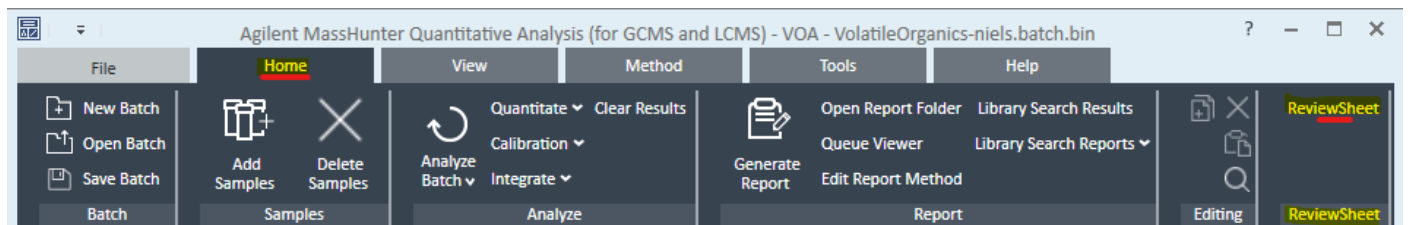
Execute the setup program

Open MassHunter Quant

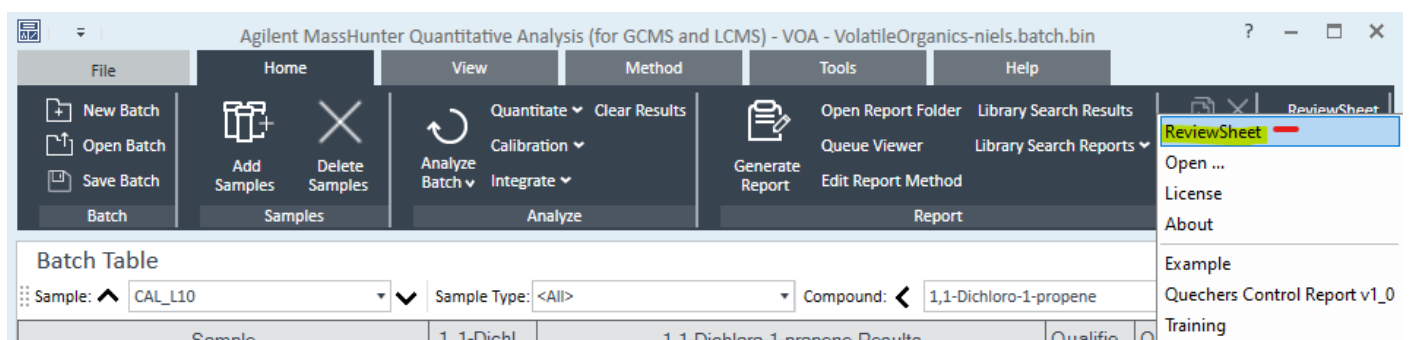
Enable the Add-In



Find the ReviewSheet menu



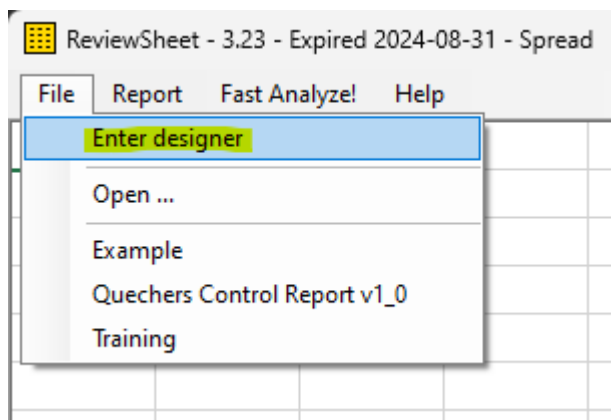
Click ReviewSheet



User mode and designer mode

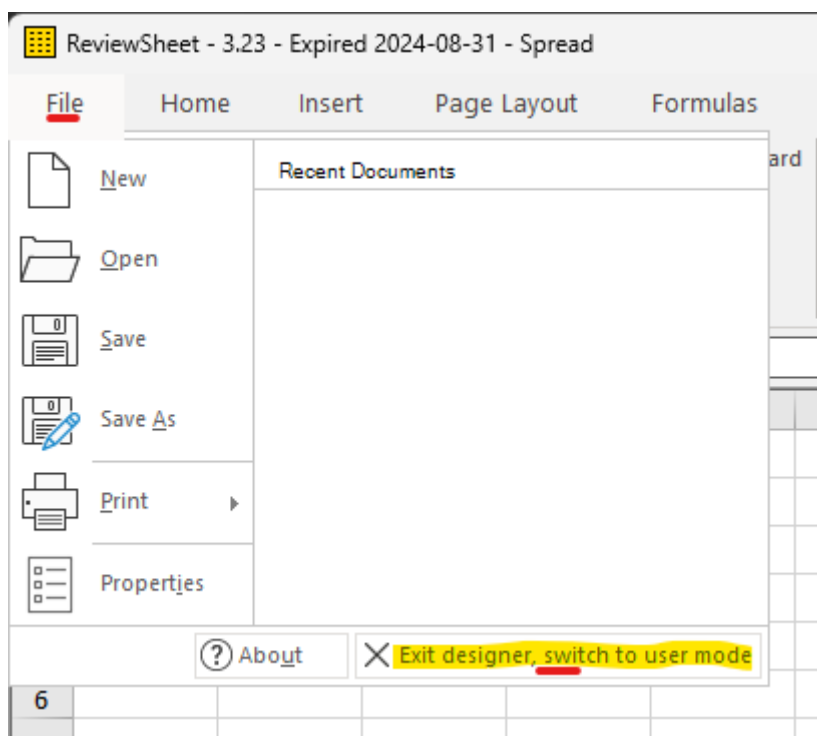
Enter designer

Design and save templates



Switch to user mode

Use templates to review quantitation results



Predefined tables

Create a single sample sheet

Sample header

Select A1 and click: Insert tables - Per sample - Header

The screenshot displays a software interface with a spreadsheet and a chromatogram. The spreadsheet has columns A through I and rows 1 through 11. The 'Insert' menu is open, showing options like 'Table', 'Graphics', and 'Calibration'. A tooltip 'Insert a sample header table' is visible. The sample header table is as follows:

	A	B		E	F	G	H	I
1	HIDE	HIDE						
2		DataFileName	File	CAL_L10.D				
3		SampleName	Sample	CAL_L10				
4		SampleType	Type	Calibration				
5		SampleInfo	Info					
6		AcqDateTime	Acquired	2008-06-20 22:19:23				
7		AcqMethod	Method	624A.M				
8								
9								
10								
11								

The chromatogram, titled '+ TIC Scan CAL_L10.D (CAL_L10)', shows 'Counts x10⁶' on the y-axis (ranging from 0 to 6) and time on the x-axis (ranging from 3 to 20 minutes). The plot displays a complex pattern of peaks, with a significant cluster of peaks between 15 and 20 minutes.

Table of compounds

Select A11 and click: Insert tables - Per sample - Table

The screenshot shows a software interface with a spreadsheet. The 'Insert' menu is open, showing options like 'Header', 'Table', 'Graphics', and 'Calibration'. The 'Table' option is selected, and a tooltip says 'Insert a single sample table for all compounds'. The spreadsheet has columns A through J and rows 1 through 16. Row 11 is highlighted with a green border. A chromatogram plot is visible in the background, showing 'Counts x10⁶' vs. 'Retention Time'.

Retention Time	Peak Name	ISD	RT Exp	RT Act	Resp	IS Resp	FConc
10.100	1,1-Dichloro	Fluorobenz	10.100	10.091	1666597	1310216	29.2986
4.249	Dichlorodif	Fluorobenz	4.249	4.248	2199968	1310216	29.6742
4.493	Chloromet	Fluorobenz	4.493	4.488	1208596	1310216	29.4181
10.520	1,4-Dichlor	1,4-Dichlor	10.520	10.512	2046512	607220	20.7206

Adjust the width of columns C and E

Double click between the header cell C and D, and between E and F

Columns and rows, that start with HIDE, will be hidden in User mode.

Conditional format

ReviewSheet - 3.23 - Expired 2024-08-31 - Spread

File Home Insert Page Layout Formulas Data View Developer Settings MassHunter

Clipboard Font Alignment Number

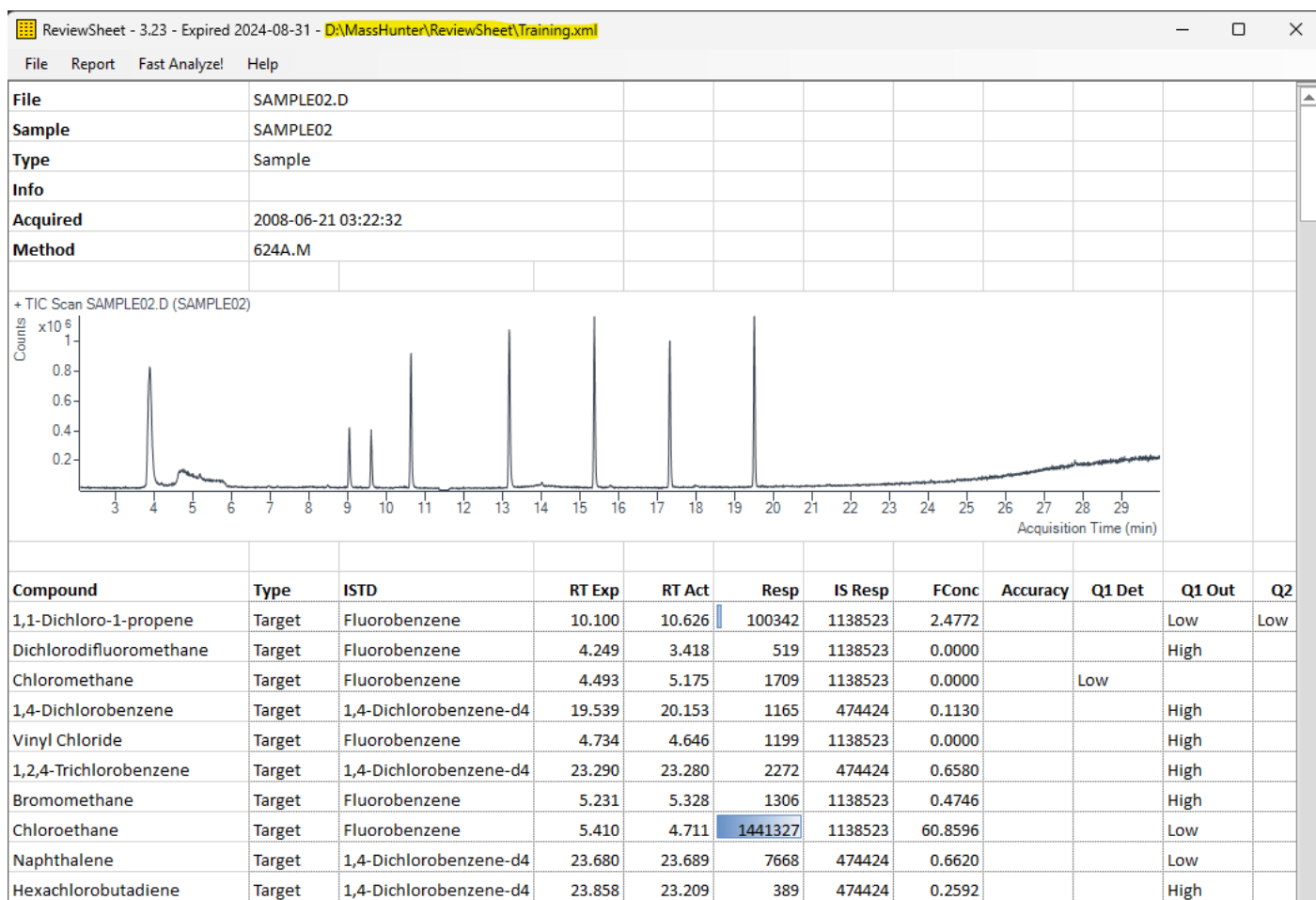
H13 =MH.Compound(H\$11,\$C\$11,\$C13)

1							
2	File	CAL_L10.D					
3	Sample	CAL_L10					
4	Type	Calibration					
5	Info						
6	Acquired	2008-06-20 22:19:23					
7	Method	624A.M					
8							
9							
10							
11	CAL_L10.D	Compound	ISTD.CompoundName	RetentionT	PEAK.Reter	PEAK.Targe	ISTD.PEAK. PEA
12	Compound	Type	ISTD	RT Exp	RT Act	Resp	IS Resp
13	1,1-Dichloro-1-propene	Target	Fluorobenzene	10.100	10.091	1666597	1310216
14	Dichlorodifluoromethane	Target	Fluorobenzene	4.249	4.248	2199968	1310216
15	Chloromethane	Target	Fluorobenzene	4.493	4.488	1208596	1310216

Format: Gradient Fill, Solid Fill, More Rules...

PEAK.Targe
Resp
1666597
2199968
1208596
2946512
1633393
1810801
987678
789578
2884908
1630235
2773495
890094
1693047

Save and use template



The rows and columns started with HIDE, are hidden

Select another sample in MassHunter, the values are updated on the sheet

Select an cell related to a different compound on the sheet, MassHunter navigates to that compound

Perform a manual integration in MassHunter, the sheets shows the new response

Functions

There are 400+ functions equivalent to Excel (without requiring Excel)
ReviewSheet adds about 20 functions

There are 3 **values** set by MassHunter

MH.FirstDataFileName The first data filename in the batch
MH.DataFileName The data filename of the currently selected sample
MH.CompoundName The compound name of the currently selected compound

The 3 **basic functions** to retrieve values from MassHunter are

MH.Batch Get values from the batch, like BatchName
MH.Sample Get values from a sample, like SampleName
MH.Compound Get values from a compound, like FinalConcentration

Examples

=MH.Batch("BatchName")

=MH.Sample("SampleName", MH.DataFileName)

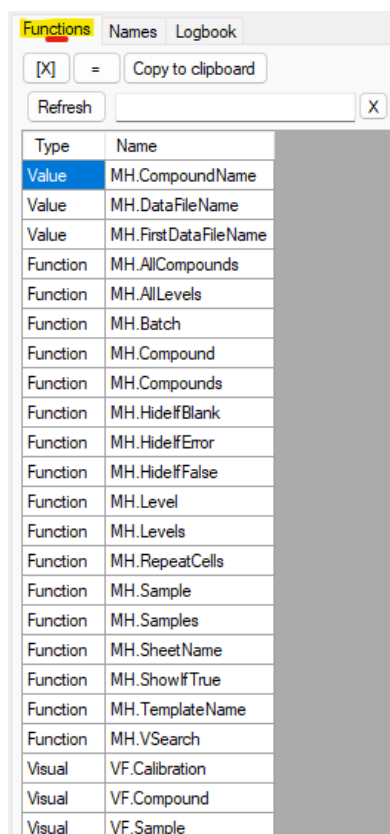
=MH.Compound("Peak.FinalConcentration", MH.DataFileName, MH.CompoundName)

	A	B
1	Formula	Value
2	=MH.FirstDataFileName	CAL_L03.D
3	=MH.DataFileName	SAMPLE05.D
4	=MH.CompoundName	Carbon Disulfide
5	=MH.Batch("BatchName")	VolatileOrganics-niels.batch.bin
6	=MH.Sample("SampleName",MH.DataFileName)	SAMPLE05
7	=MH.Compound("Peak.FinalConcentration",MH.DataFileName,MH.CompoundName)	18.57

Field names

Table	Field
Peak	BaselineEnd
Peak	BaselineEndOriginal
Peak	BaselineStandardDeviation
Peak	BaselineStart
Peak	BaselineStartOriginal
Peak	BatchID
Peak	CalculatedConcentration
Peak	CapacityFactor
Peak	CCISTDResponseRatio
Peak	CCResponseRatio
Peak	CompoundID
Peak	EstimatedConcentration
Peak	FinalConcentration
Peak	FullWidthHalfMaximum
Peak	GroupNumber
Peak	Height

More functions



Type	Name
Value	MH.CompoundName
Value	MH.DataFileName
Value	MH.FirstDataFileName
Function	MH.AllCompounds
Function	MH.AllLevels
Function	MH.Batch
Function	MH.Compound
Function	MH.Compounds
Function	MH.HideIfBlank
Function	MH.HideIfError
Function	MH.HideIfFalse
Function	MH.Level
Function	MH.Levels
Function	MH.RepeatCells
Function	MH.Sample
Function	MH.Samples
Function	MH.SheetName
Function	MH.ShowIfTrue
Function	MH.TemplateName
Function	MH.VSearch
Visual	VF.Calibration
Visual	VF.Compound
Visual	VF.Sample

Visual functions

VF.Sample

VF.Compound

VF.Calibration

Array functions

MH.Samples

MH.Compounds

MH.Levels

MH.AllCompounds

MH.AllLevels

Hide functions

MH.ShowIfTrue

MH.HideIfFalse

MH.HideIfBlank

MH.HideIfError

Information functions

MH.SheetName

MH.TemplateName

Formatting functions

MH.RepeatCells

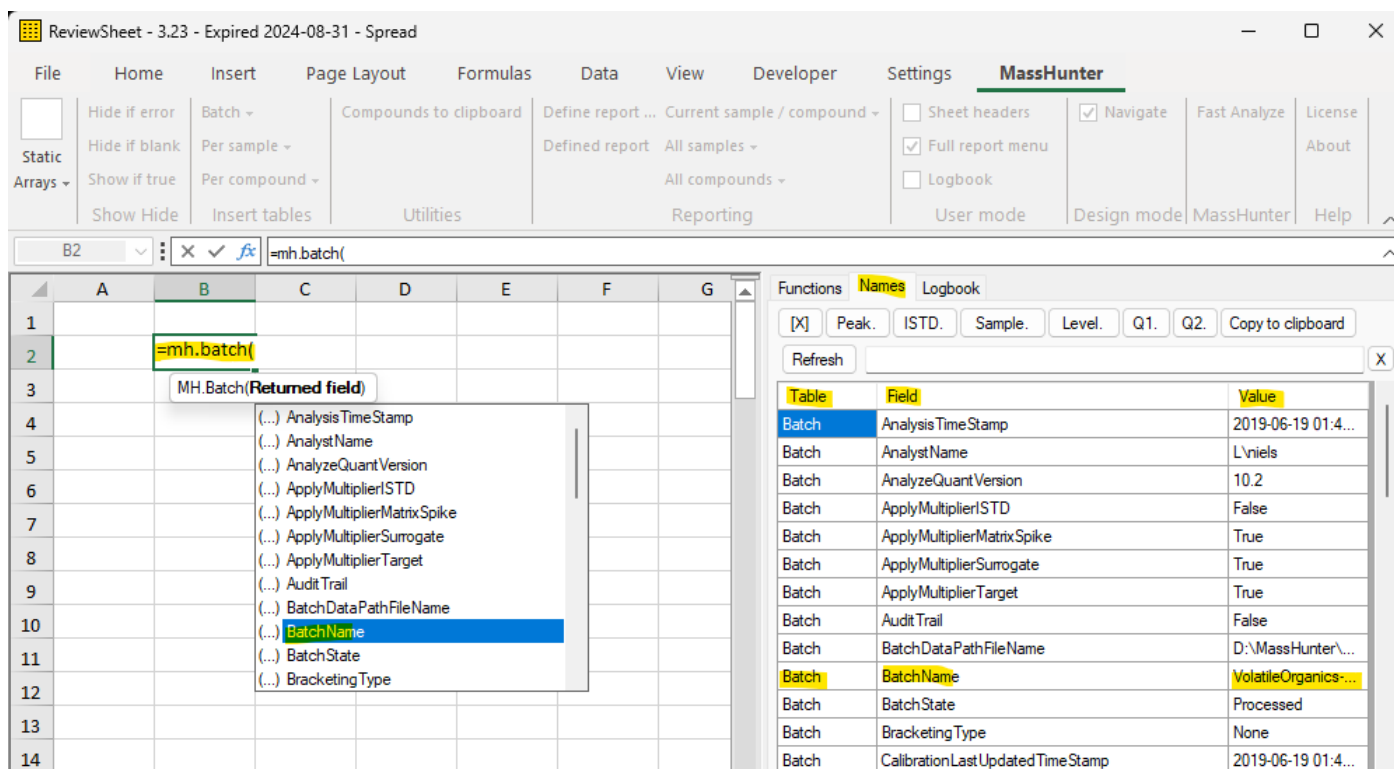
Special functions

MH.VSearch

Basic functions

MH.Batch

=MH.Batch(<Returned field>)

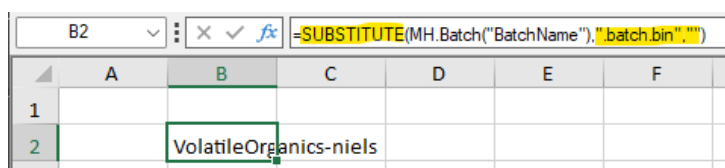


The screenshot shows the MassHunter software interface with a spreadsheet. The formula bar shows the function `=mh.batch()`. A dropdown menu is open, listing various fields such as `AnalysisTimeStamp`, `AnalystName`, `BatchName`, and `BatchState`. The `BatchName` field is highlighted. The Names tab is open, showing a table of fields and their values.

Table	Field	Value
Batch	Analysis Time Stamp	2019-06-19 01:4...
Batch	Analyst Name	L'niels
Batch	Analyze Quant Version	10.2
Batch	Apply Multiplier STD	False
Batch	Apply Multiplier Matrix Spike	True
Batch	Apply Multiplier Surrogate	True
Batch	Apply Multiplier Target	True
Batch	Audit Trail	False
Batch	Batch Data Path File Name	D:\MassHunter\...
Batch	Batch Name	VolatileOrganics-...
Batch	Batch State	Processed
Batch	Bracketing Type	None
Batch	Calibration Last Updated Time Stamp	2019-06-19 01:4...

A	B	C	D
1			
2		VolatileOrganics-niels.batch.bin	
3			

Use the Substitute() function to remove '.batch.bin'
Just like in Excel



The screenshot shows the spreadsheet with the formula `=SUBSTITUTE(MH.Batch("BatchName"), ".batch.bin", "")` in cell B2. The result in cell B2 is `VolatileOrganics-niels`.

In this manual, the field names will be separated like this:

A	B	C	D
HIDE	HIDE		
	BatchName	Batch	VolatileOrganics-niels
	AnalysisTimeStamp	Analyzed	2019-06-19 01:45
	AnalystName	Analist	=MH.Batch(B4)

The field names are in the B column (Try double click on the field name in the Names tab)

The C column contains the user friendly name.

The HIDE keyword will hide the columns and rows in User Mode.

MH.Sample

=MH.Sample(<Returned field>, <data filename>)

Cell D2 contains =MH.DataFileName

This variable contains the data filename of the currently selected sample in MassHunter

	A	B	C	D	E	F
1	HIDE	HIDE				
2		DataFileName	File	CAL_L03.D		
3		SampleName	Sample	CAL_L03		
4		SampleType	Type	Calibration		
5		SampleInformation	Info			
6		AcqDateTime	Acquired	2008-06-20 17:53:12		
7		AcqMethodFileName	Method	624A.M		

The formula in D3 uses the data filename in D2 to retrieve the sample name as specified in cell B3

The \$ prefix works as in Excel, see

<https://www.microsoft.com/en-us/microsoft-365/blog/2011/08/17/making-sense-of-dollar-signs-in-excel>

	A	B	C	D	E	F
1	HIDE	HIDE				
2		DataFileName	File	CAL_L03.D		
3		SampleName	Sample	=MH.Sample(B3,\$D\$2)		
4		SampleType	Type	Calibration		
5		SampleInformation	Info			
6		AcqDateTime	Acquired	2008-06-20 17:53:12		
7		AcqMethodFileName	Method	624A.M		

Available field names are listed in the Names tab

Table	Field	Value
Sample	AcqDateTime	2008-06-20 17:5...
Sample	AcqDate TimeLocal	
Sample	AcqMethodFileName	624A.M
Sample	AcqMethodPathName	
Sample	AcqOperator	ciemens
Sample	BalanceOverride	
Sample	Barcode	
Sample	BatchID	0
Sample	CalibrationReferenceSampleID	0
Sample	Comment	080620STD03,V...
Sample	Completed	True
Sample	DADateTime	2019-06-19 01:4...
Sample	DAMethodFileName	VOA.quantmetho...
Sample	DAMethodPathName	D:\MassHunter\...
Sample	DataFileName	CAL_L03.D
Sample	DataPathName	D:\MassHunter\...
Sample	Dilution	1
Sample	DualInjector	
Sample	DualInjectorAcqDateTime	
Sample	DualInjectorBarcode	
Sample	DualInjectorExpectedBarcode	
Sample	DualInjectorVial	
Sample	DualInjectorVolume	
Sample	Equilibration Time	0
Sample	ExpectedBarcode	
Sample	GraphicSampleChromatogram	
Sample	InjectionsPerPosition	
Sample	InjectorVolume	0
Sample	InstrumentName	HP5973F
Sample	InstrumentType	SingleQuadrupole

MH.Compound

=MH.Compound(<Returned field>, <data filename>)

	B	C	D	E
1	HIDE			
2	HIDE	CAL_L03.D	CompoundType	PEAK.TargetResponse
3		Compound	Type	Resp
4		Fluorobenzene	ISTD	=MH.Compound(E\$2,\$C\$2,\$C4)
5		1,1-Dichloro-1-propene	Target	19619
6		Dichlorodifluoromethane	Target	33895
7				

The formula in E4 uses the data filename in C2 (it is the data file of the currently selected sample in MassHunter). And it uses the compound name in C4 and the field name in E2.

The \$ prefix allows the formula to be copied down or right while maintaining the desired cell references.

The name in C4 could be the currently selected compound in MassHunter: =MH.CompoundName, but here we use a fixed list of compound names. It is probably the easiest way to develop a sample report.

If new compounds are added to the MassHunter method, select the currently compound list on the template, and click 'Compounds to clipboard' to get a list of the missing compounds.

The screenshot shows a spreadsheet application window titled 'ReviewSheet - 3.23 - Expired 2024-08-31 - Spread'. The 'Formulas' menu is open, and the 'Compounds to clipboard' option is highlighted. Below the menu, the spreadsheet content is visible, showing a table with columns B, C, D, and E. The table contains data for various compounds, including Fluorobenzene, 1,1-Dichloro-1-propene, Dichlorodifluoromethane, Chloromethane, and 1,4-Dichlorobenzene. A dialog box titled 'ReviewSheet' is overlaid on the spreadsheet, displaying an information icon and the text 'New compounds on the clipboard: 69' with an 'OK' button.

To get peak values for the compound, use the PEAK. Prefix like in cell E2 (see the first image on this page)

There are more prefixes, and they can be chained for example like this:

ISTD.PEAK.TargetResponse

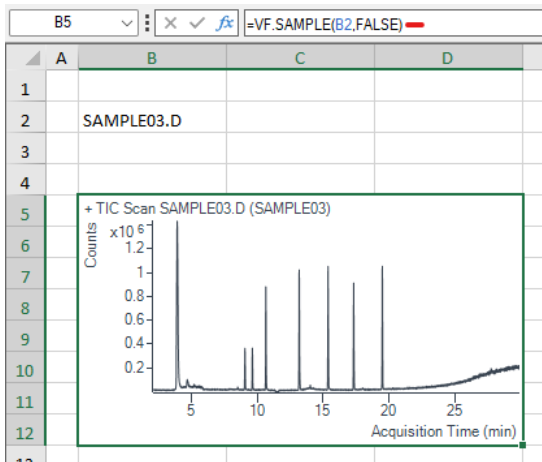
QC.ISTD.PEAK.TargetResponse

Q1.PEAK.OutlierQualifierOutOfLimits

Visual functions

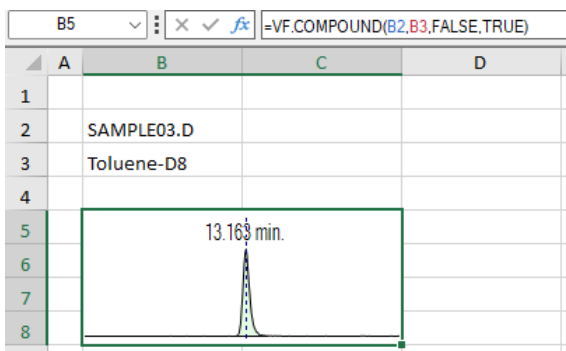
VF.Sample

=VF.SAMPLE(B2,FALSE)



VF.Compound

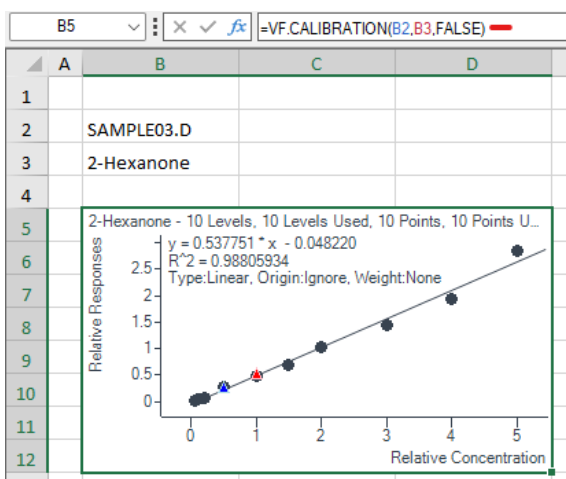
=VF.Compound(<data filename>, <compound name>, <overlay>, <hide axis>)



Cells B5:C8 are merged and contain formula =VF.Compound(B2,B3,False,True)

VF.Calibration

=VF.CALIBRATION(<data filename>, <compound name>, <hide axis>)



Array functions

MH.Samples

=MH.Samples(<Sort Fields>, <Criteria 1 field>, <Criteria 1 comparator>, <Criteria 1 value>, ...)

Cell B3 contains a formula that spills multiple values down to B7

The screenshot shows an Excel spreadsheet with the following data:

	A	B	C	D	E
1					
2		Sample			
3		SAMPLE01.D			
4		SAMPLE02.D			
5		SAMPLE03.D			
6		SAMPLE04.D			
7		SAMPLE05.D			

The list is ordered by AcqDateTime

The list is limited to SampleType=Sample (B7)

Because B4 is spilled down, the function in C4 can also spill down by the # appendix.

The # suffix works as in Excel, see

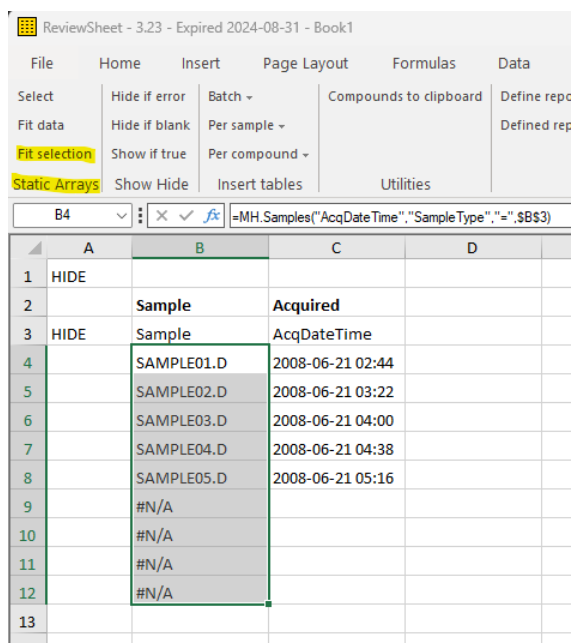
<https://support.microsoft.com/en-us/office/dynamic-array-formulas-and-spilled-array-behavior-205c6b06-03ba-4151-89a1-87a7eb36e531>

The screenshot shows an Excel spreadsheet with the following data:

	A	B	C	D
1	HIDE			
2		Sample	Acquired	
3	HIDE	Sample	AcqDateTime	
4		SAMPLE01.D	=MH.Sample(C\$3,\$B4#)	
5		SAMPLE02.D	2008-06-21 03:22	
6		SAMPLE03.D	2008-06-21 04:00	
7		SAMPLE04.D	2008-06-21 04:38	
8		SAMPLE05.D	2008-06-21 05:16	

Static array

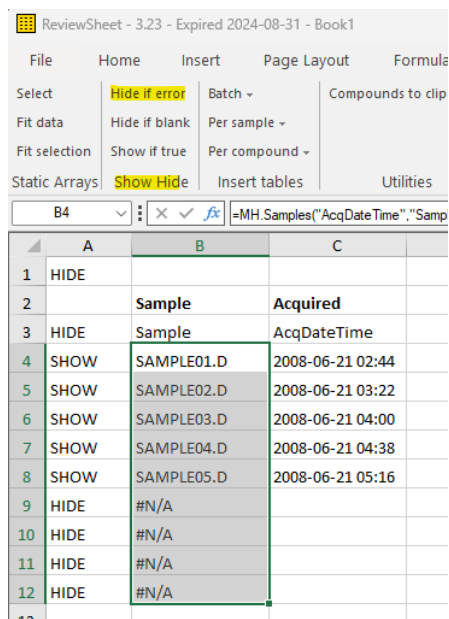
Or reserve a large enough range of cells for the array in B4 to accommodate all the samples in future larger batches. Then click Stat Arrays - Fit selection



The screenshot shows the Excel ribbon with the 'Static Arrays' menu open. The 'Fit selection' option is highlighted in yellow. The formula bar shows the formula: `=MH.Samples("AcqDateTime","SampleType", "=", B3)`. The spreadsheet data is as follows:

	A	B	C	D
1	HIDE			
2		Sample	Acquired	
3	HIDE	Sample	AcqDateTime	
4		SAMPLE01.D	2008-06-21 02:44	
5		SAMPLE02.D	2008-06-21 03:22	
6		SAMPLE03.D	2008-06-21 04:00	
7		SAMPLE04.D	2008-06-21 04:38	
8		SAMPLE05.D	2008-06-21 05:16	
9		#N/A		
10		#N/A		
11		#N/A		
12		#N/A		
13				

And click Show Hide – Hide if error



The screenshot shows the Excel ribbon with the 'Show Hide' option highlighted in yellow in the 'Static Arrays' menu. The formula bar shows the formula: `=MH.Samples("AcqDateTime","Samp`. The spreadsheet data is as follows:

	A	B	C	D
1	HIDE			
2		Sample	Acquired	
3	HIDE	Sample	AcqDateTime	
4	SHOW	SAMPLE01.D	2008-06-21 02:44	
5	SHOW	SAMPLE02.D	2008-06-21 03:22	
6	SHOW	SAMPLE03.D	2008-06-21 04:00	
7	SHOW	SAMPLE04.D	2008-06-21 04:38	
8	SHOW	SAMPLE05.D	2008-06-21 05:16	
9	HIDE	#N/A		
10	HIDE	#N/A		
11	HIDE	#N/A		
12	HIDE	#N/A		
13				

Column A cells contain a formula that return HIDE if a B column cell contains an error. In User mode, the rows with the HIDE will be hidden. The sheet is now independent of the number of samples in the batch.

MH.Compounds

=MH.Compounds(<Sort Fields>, <DataFileName>, <Criteria 1 field>,<Criteria 1 comparator>,<Criteria 1 value>, ...)

This function returns a list of compound names for the sample with the specified data filename.

MH.AllCompounds

=MH.AllCompounds(<Sort Fields>, <DataFileName>, <Criteria 1 field>,<Criteria 1 comparator>,<Criteria 1 value>, ...)

Returns an array of data filename and compound names that fulfill the criteria

In the example below, all compounds in just the samples that have a final concentration of more than 50 are shown.

B4		=MH.AllCompounds(,"SAMPLE.SampleType","=","Sample","Peak.FinalConcentration",">",\$B\$3)			
	A	B	C	D	E
1	HIDE				
2		Data file	Compound	Conc	
3	HIDE	50		PEAK.FinalConcentration	
4		SAMPLE02.D	Chloroethane	60.86	
5		SAMPLE05.D	1,2,4-Trimethylbenzene	146.24	
6		SAMPLE05.D	1,3,5-Trimethylbenzene	65.09	
7		SAMPLE05.D	2-Butanone (MEK)	137.62	
8		SAMPLE05.D	Benzene	69.20	
9		SAMPLE05.D	Ethylbenzene	225.78	
10		SAMPLE05.D	M&P-Xylenes	343.13	
11		SAMPLE05.D	Naphthalene	160.34	
12		SAMPLE05.D	O-Xylene	224.10	
13		SAMPLE05.D	Tetrahydrofuran	937.35	
14		SAMPLE05.D	Toluene	713.83	
15		SAMPLE05.D	trans-1,3-Dichloropropene	82.09	
16		SAMPLE05.D	Vinyl Acetate	111.40	

The formula in B4

=MH.AllCompounds(,"SAMPLE.SampleType","=","Sample","Peak.FinalConcentration",">",\$B\$3)

The formula in D4

=MH.Compound(D\$3,CHOOSECOLS(\$B4#,1),CHOOSECOLS(\$B4#,2))