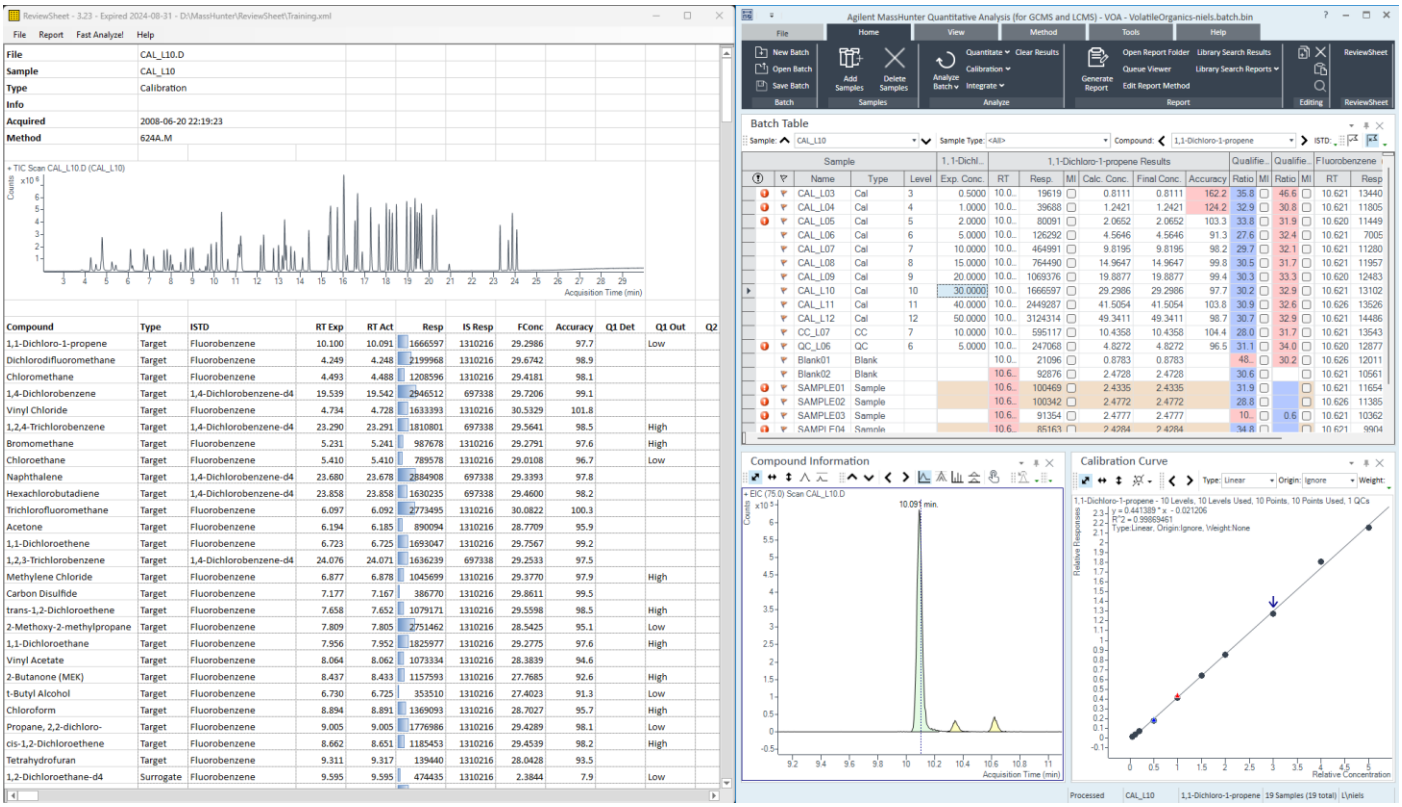
ReviewSheet for MassHunter Quant

User Manual

Developer niels@waleson.eu
Web-page https://waleson.eu/reviewsheet

Purpose

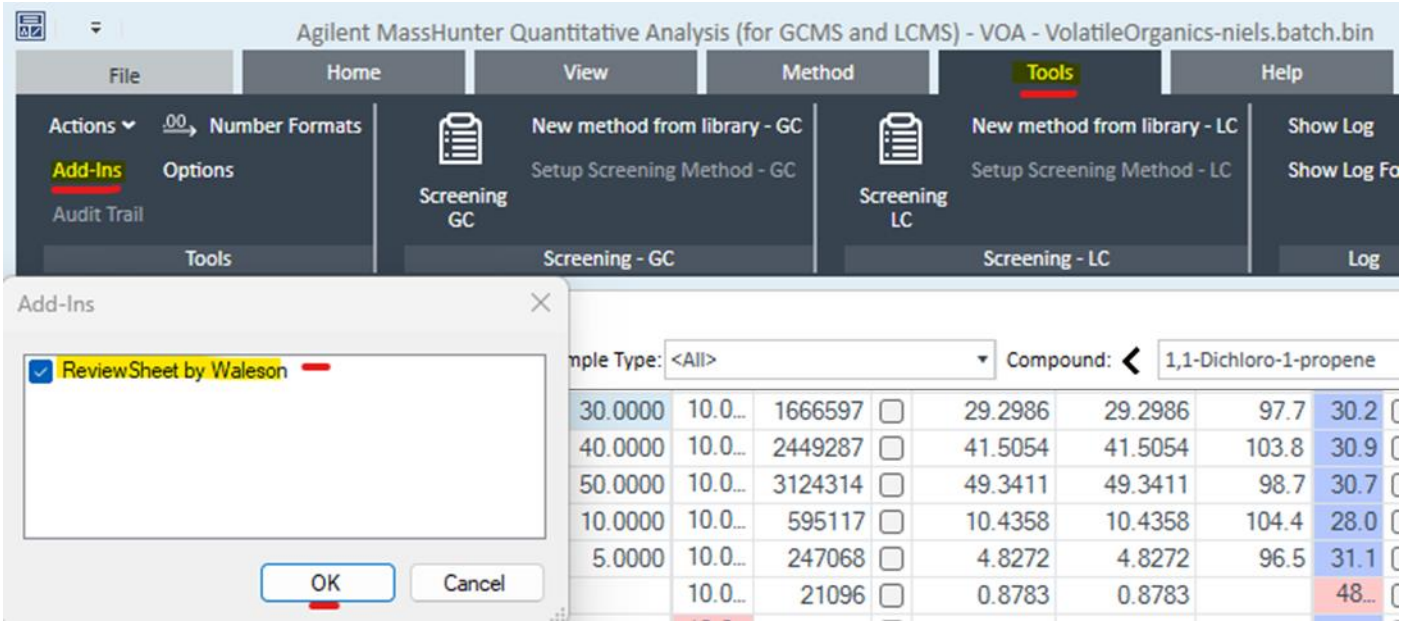
High-throughput reviewing and reporting
Highly customizable Excel like sheets (Excel is not required)



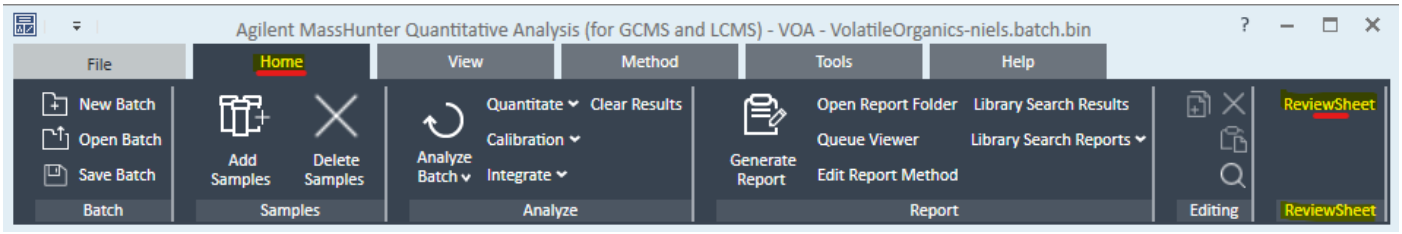
Installation

Download the latest version from https://waleson.eu/reviewsheet
Execute the setup program
Open MassHunter Quant

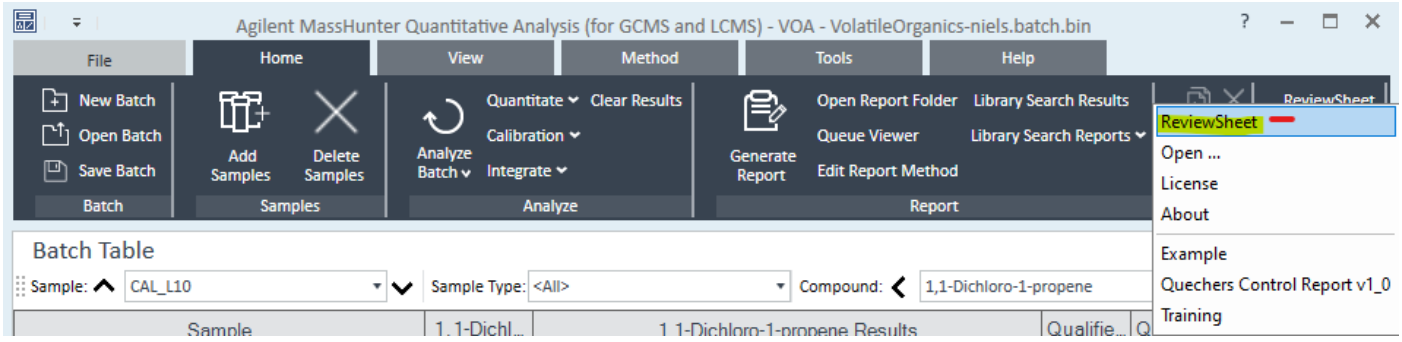
Enable the Add-In



Find the ReviewSheet menu



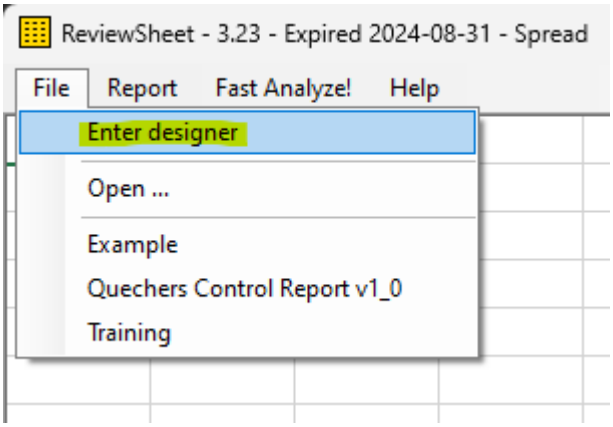
Click ReviewSheet



User mode and designer mode

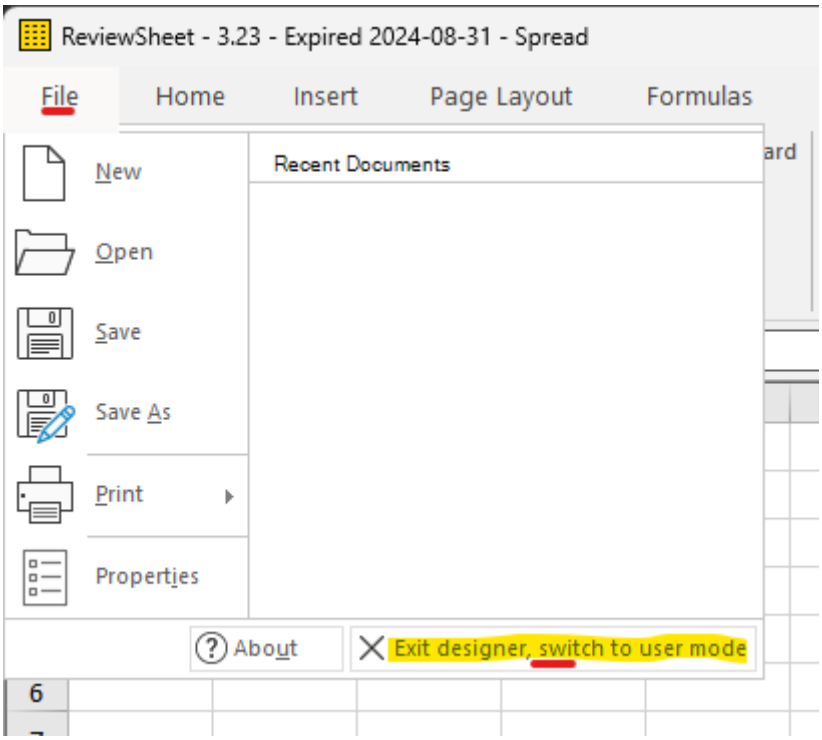
Enter designer

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

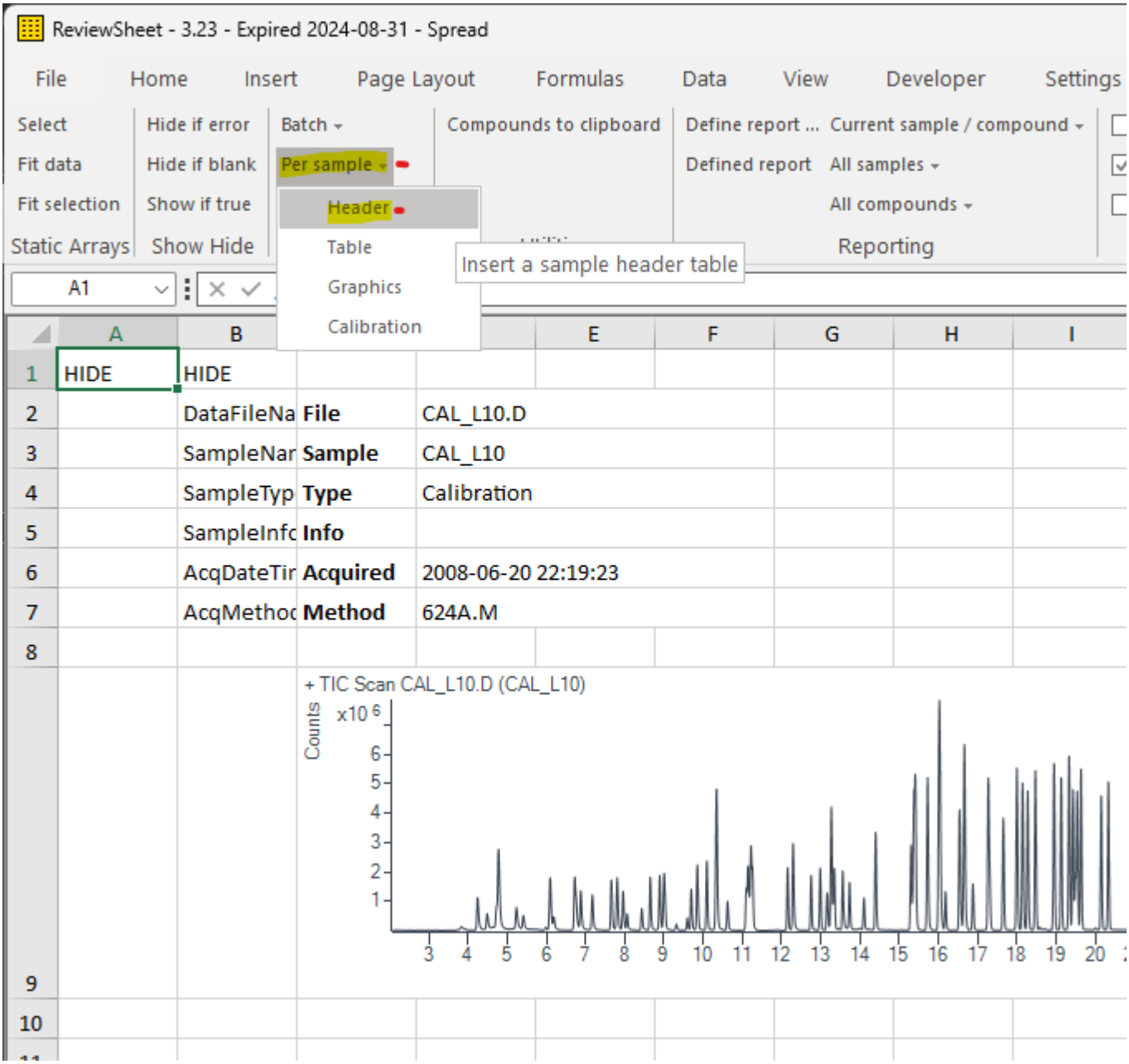
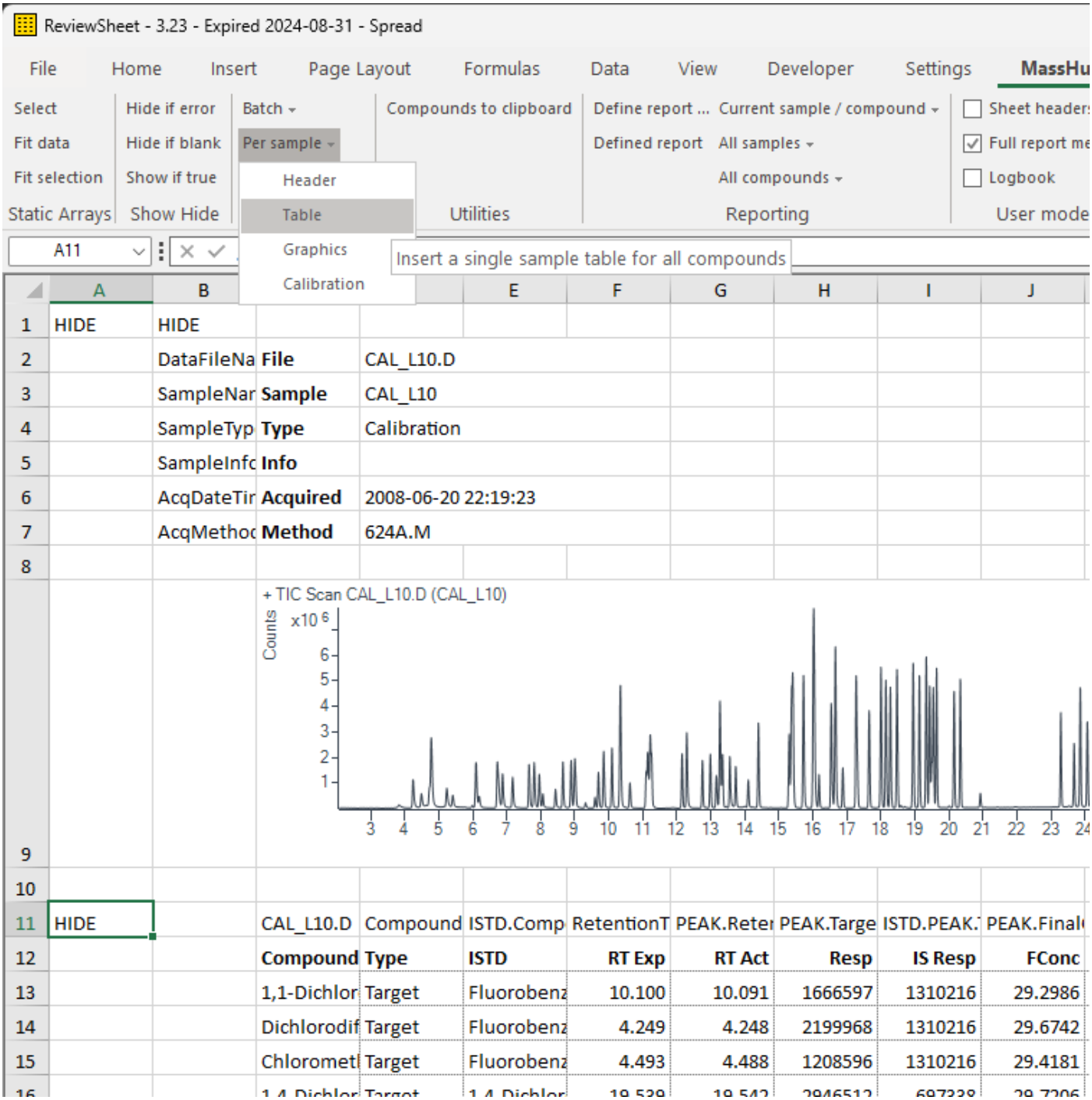


Table of compounds

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



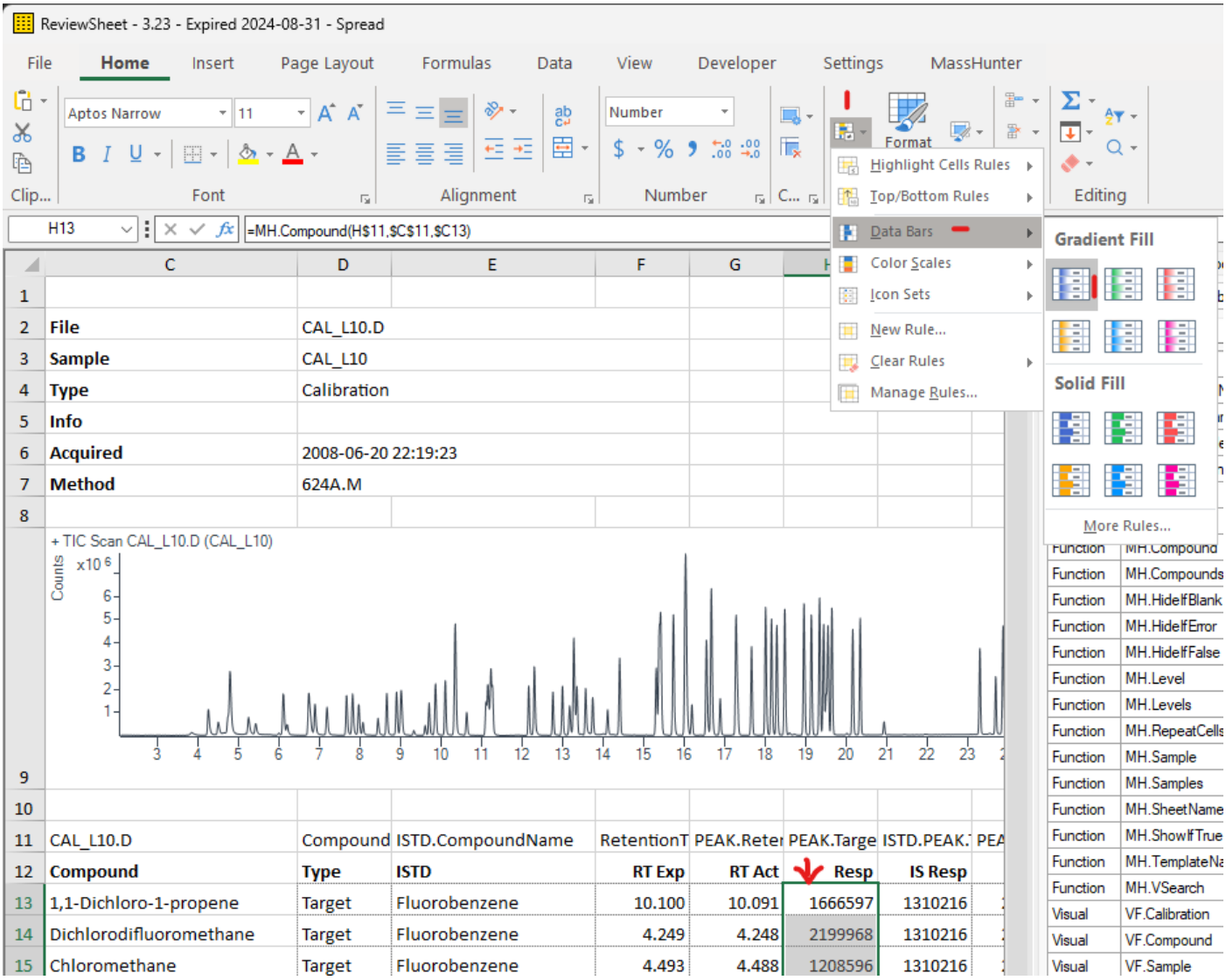
	A	B	C	D	E	F	G	H	I	J
1	HIDE	HIDE								
2		DataFileNa	**File**	CAL_L10.D						
3		SampleNar	**Sample**	CAL_L10						
4		SampleTyp	**Type**	Calibration						
5		SampleInfc	**Info**							
6		AcqDateTir	**Acquired**	2008-06-20 22:19:23						
7		AcqMethoc	**Method**	624A.M						
8										
9										
10										
11	HIDE		CAL_L10.D	Compound	ISTD.Comp	RetentionT	PEAK.Reter	PEAK.Targe	ISTD.PEAK.	PEAK.Final
12			**Compound**	**Type**	**ISTD**	**RT Exp**	**RT Act**	**Resp**	**IS Resp**	**FConc**
13			1,1-Dichlor	Target	Fluorobenz	10.100	10.091	1666597	1310216	29.2986
14			Dichlorodif	Target	Fluorobenz	4.249	4.248	2199968	1310216	29.6742
15			Chloromet	Target	Fluorobenz	4.493	4.488	1208596	1310216	29.4181
16			1,4-Dichlor	Target	1,4-Dichlor	19.539	19.542	2946512	697338	29.7206

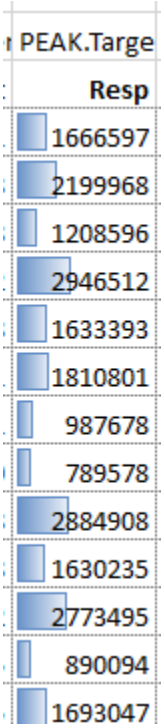
Adjust the width of columns C and E

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



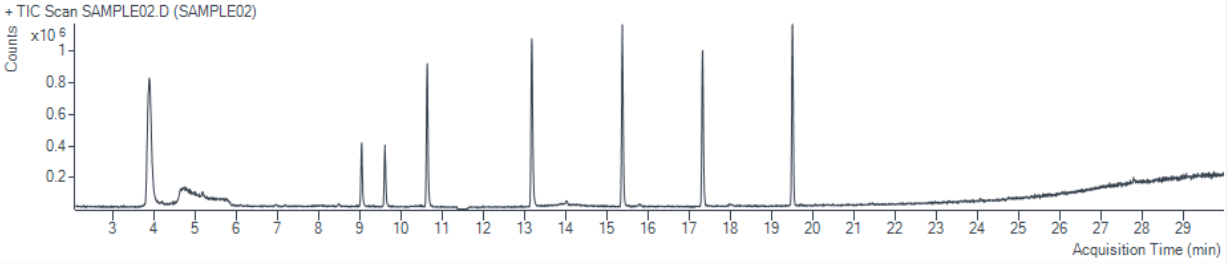


Save and use template

ReviewSheet - 3.23 - Expired 2024-08-31 - D:\MassHunter\ReviewSheet\Training.xml

File Report Fast Analyze! Help

File	SAMPLE02.D
Sample	SAMPLE02
Type	Sample
Info	
Acquired	2008-06-21 03:22:32
Method	624A.M



Compound	Type	ISTD	RT Exp	RT Act	Resp	IS Resp	FConc	Accuracy	Q1 Det	Q1 Out	Q2
1,1-Dichloro-1-propene	Target	Fluorobenzene	10.100	10.626	100342	1138523	2.4772			Low	Low
Dichlorodifluoromethane	Target	Fluorobenzene	4.249	3.418	519	1138523	0.0000			High	
Chloromethane	Target	Fluorobenzene	4.493	5.175	1709	1138523	0.0000		Low		
1,4-Dichlorobenzene	Target	1,4-Dichlorobenzene-d4	19.539	20.153	1165	474424	0.1130			High	
Vinyl Chloride	Target	Fluorobenzene	4.734	4.646	1199	1138523	0.0000			High	
1,2,4-Trichlorobenzene	Target	1,4-Dichlorobenzene-d4	23.290	23.280	2272	474424	0.6580			High	
Bromomethane	Target	Fluorobenzene	5.231	5.328	1306	1138523	0.4746			High	
Chloroethane	Target	Fluorobenzene	5.410	4.711	1441327	1138523	60.8596			Low	
Naphthalene	Target	1,4-Dichlorobenzene-d4	23.680	23.689	7668	474424	0.6620			Low	
Hexachlorobutadiene	Target	1,4-Dichlorobenzene-d4	23.858	23.209	389	474424	0.2592			High	

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

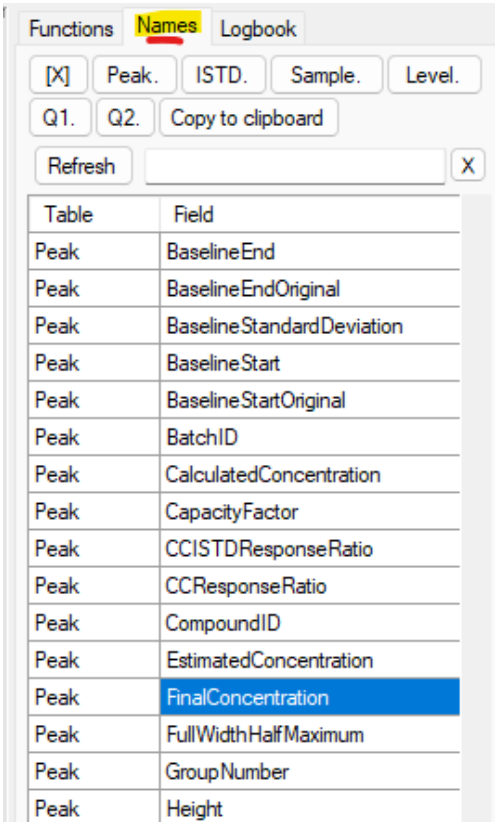
There are 3 **values** set by MassHunter
MH.FirstDataFileName The first data filename in the batch
MH.DataFileName The data filename of the currently selected sample
MH.CompoundName The compound name of the currently selected compound

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

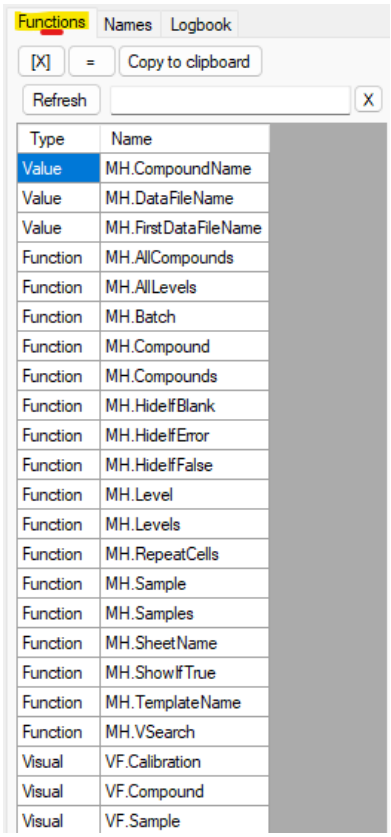
Examples
=MH.Batch("BatchName")
=MH.Sample("SampleName", MH.DataFileName)
=MH.Compound("Peak.FinalConcentration", MH.DataFileName, MH.CompoundName)

	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



More functions



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

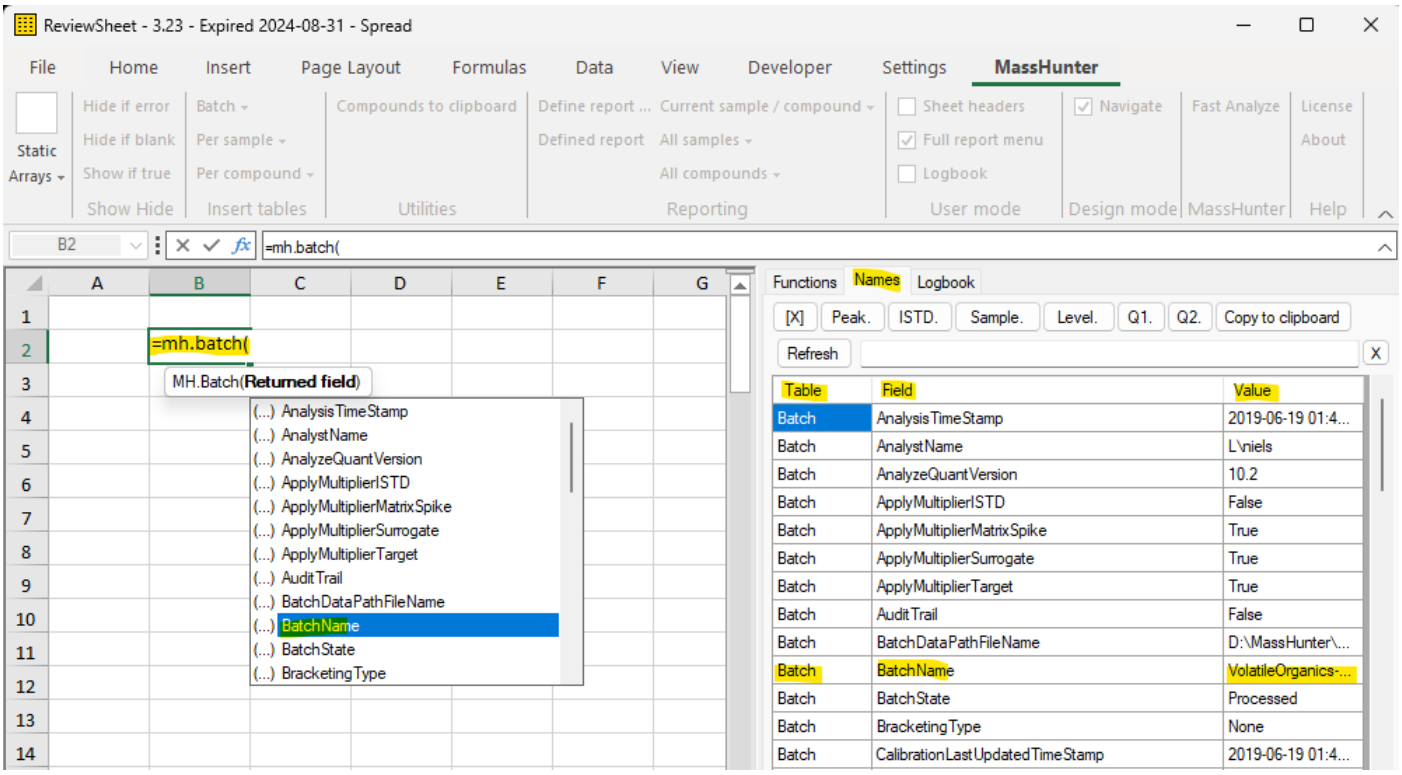
Special functions

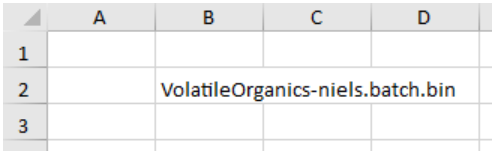
MH.VSearch

Basic functions

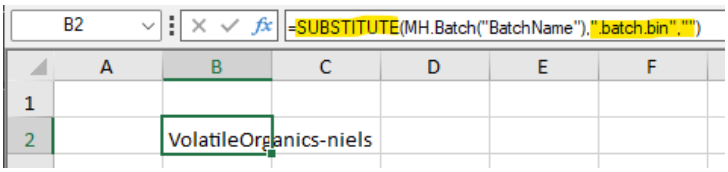
MH.Batch

=MH.Batch(<Returned field>)

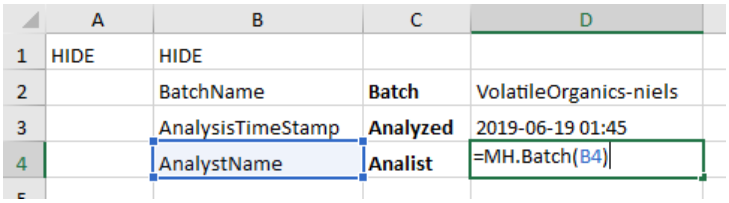




Use the Substitute() function to remove '.batch.bin'
Just like in Excel



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

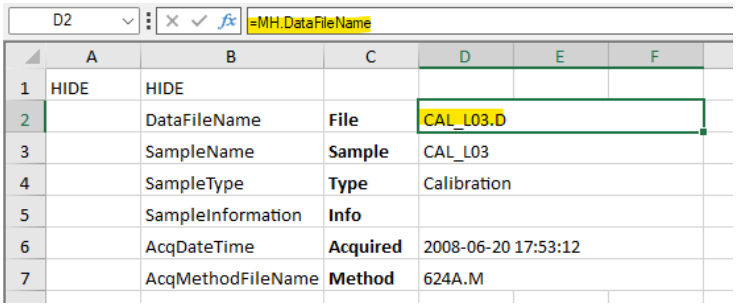


The field names are in the B column (Try double click on the field name in the Names tab)
The C column contains the user friendly name.
The HIDE keyword will hide the columns and rows in User Mode.

MH.Sample

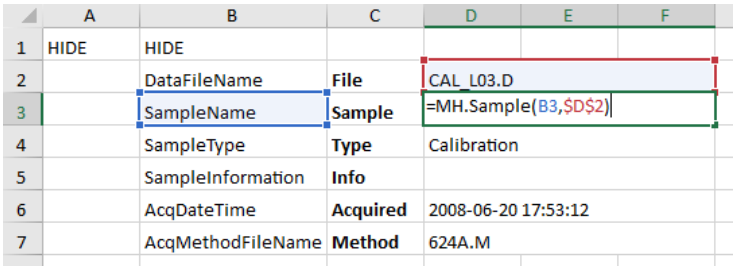
=MH.Sample(<Returned field>, <data filename>)

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,D2)		
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

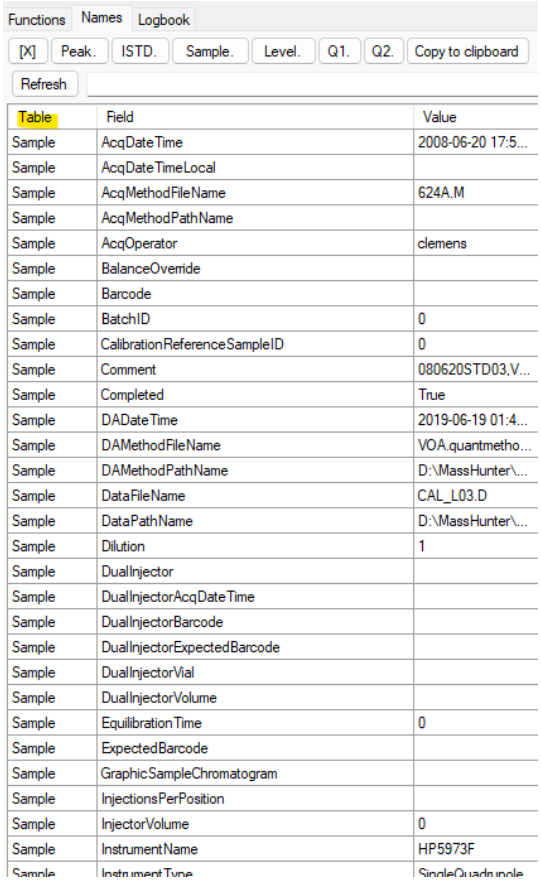
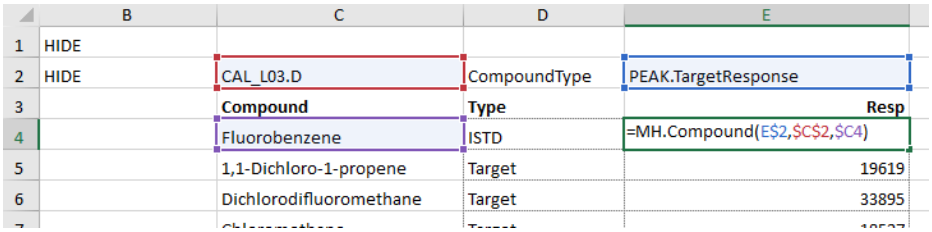


Table	Field	Value
Sample	AcqDateTime	2008-06-20 17:5...
Sample	AcqDateTimeLocal	
Sample	AcqMethodFileName	624A.M
Sample	AcqMethodPathName	
Sample	AcqOperator	clemens
Sample	BalanceOverride	
Sample	Barcode	
Sample	BatchID	0
Sample	CalibrationReferenceSampleID	0
Sample	Comment	080620STD03,V...
Sample	Completed	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	EquilibrationTime	0
Sample	ExpectedBarcode	
Sample	GraphicSampleChromatogram	
Sample	InjectionsPerPosition	
Sample	InjectorVolume	0
Sample	InstrumentName	HP5973F
Sample	InstrumentType	SingleQuadrupole

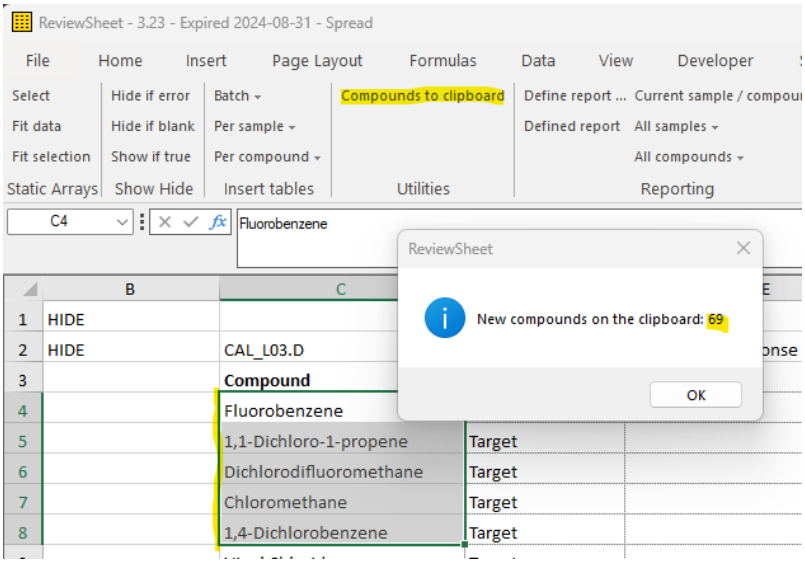
MH.Compound

=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

De formula is E4 use 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.

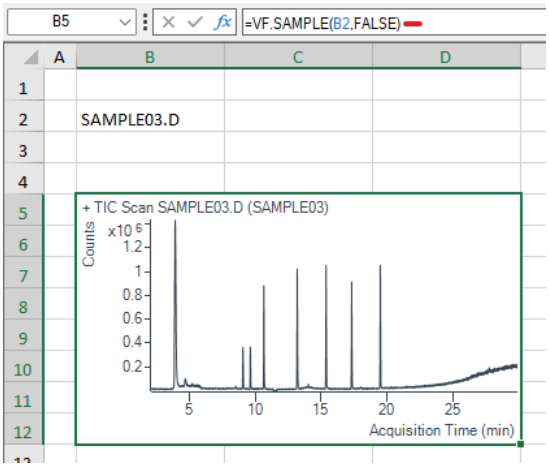


To get peak values for the compound, use the PEAK. Prefix like in cell E2 (see the first image on this page)
There are more prefixes, and they can be chained for example like this:
ISTD.PEAK.TargetResponse
QC.ISTD.PEAK.TargetResponse
Q1.PEAK.OutlierQualifierOutOfLimits

Visual functions

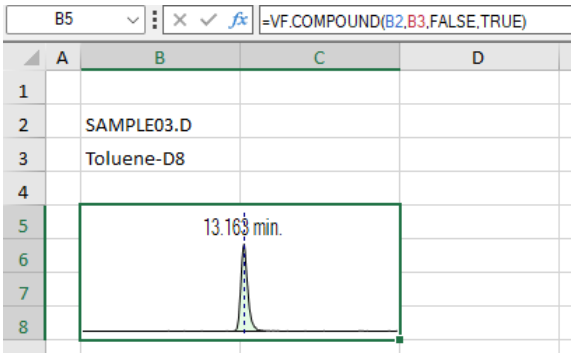
VF.Sample

=VF.SAMPLE(B2,FALSE)



VF.Compound

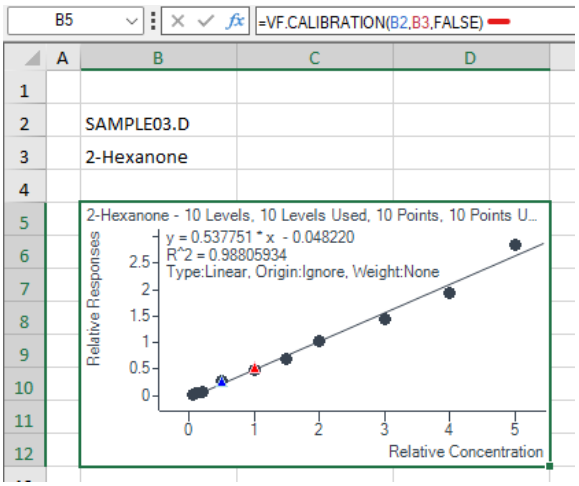
=VF.Compound(<data filename>, <compound name>, <overlay>, <hide axis>)



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

VF.Calibration

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

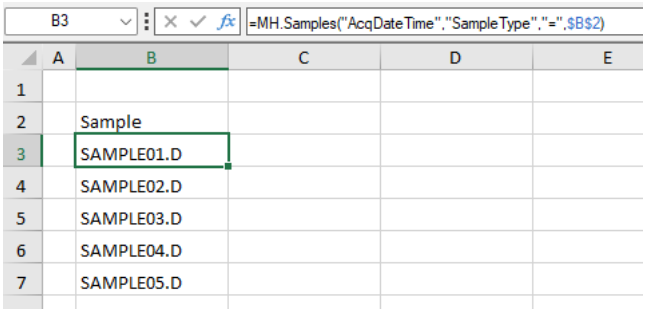


Array functions

MH.Samples

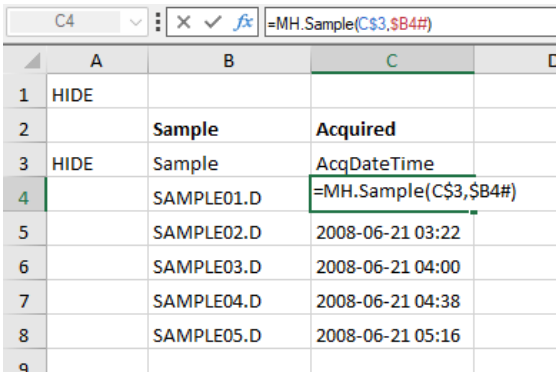
=MH.Samples(<Sort Fields>, <Criteria 1 field>,<Criteria 1 comparator>,<Criteria 1 value>, …)

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



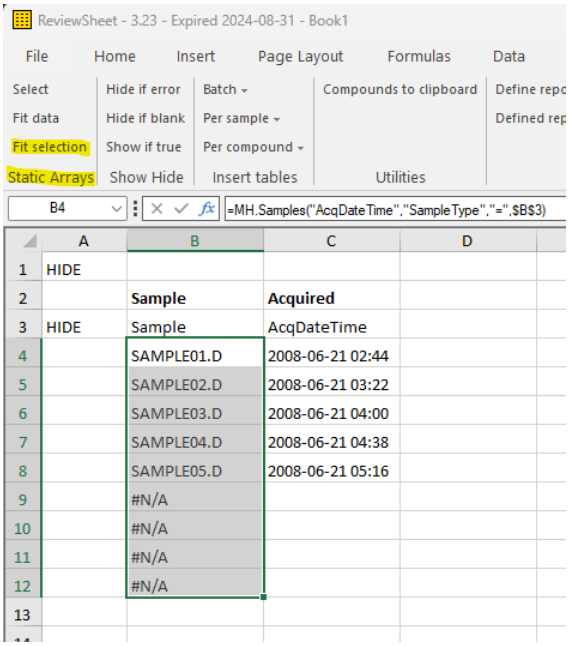
The list is ordered by AcqDateTime
The list is limited to SampleType=Sample (B7)

Because B4 is spilled down, de 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



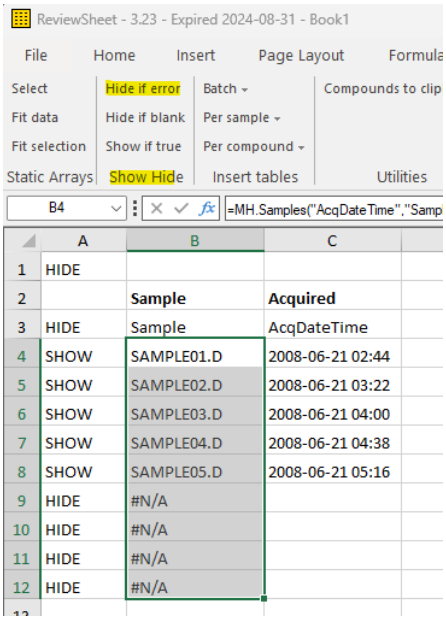
Static array

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



	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



	A	B	C
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	

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.Compounds(<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",">",B3)

	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))
```