

Agilent MassHunter Quantitative Data Analysis Presenters: Howard Sanford

Stephen Harnos

MassHunter Quantitation: Batch Table, Compound Information Setup, Calibration Curve and Globals Settings

> MassHunter Webinar Series 1/17/2018

MassHunter Quantitative Software Review and Quant Method Optimization

Topics

- Brief Review
- Batch Table Navigation
- Compound Information
 - Data review and manual integration
- Calibration Curve
- Working in Compounds At a Glance
- Method Editor Globals Setting
- Tip: Tips are labeled throughout the presentation



Review

Three major views in MassHunter Quantitative Analysis.

- Batch At a Glance
- Method Editor
- Compounds At a Glance

Handling MS/MS data QQQ and QTOF.

Handling accurate mass data TOF and QTOF.



MassHunter Quantitative Software Batch-at-a-Glance View





MassHunter Quantitative Software Method Editor View

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	Open	🐺 Agilent MassHunter Quantitat	Initative Analysis - Method - [C:\MassHuntenData[QuantExample:\MS\VOAI\VOA]	
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612	Validate	Compound Setup	Name Data File Type Level Acq. Method File Acq. Date-Time	â
副	Save	Retention Time Setup	CALLO4 CALLO4 D Cal 4 624A.M 6202008 9.30.	
	Save Ar	Concentration Setup	utomine Name TS Scan Type	
	Save As	X Qualifier Setup		
×	Exit	🛠 Calibration Curve Setup		
	M. H. 101 T. I.	Globals Setup		
	Method Setup Tasks	Save / Exit		
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			+ ED (560) Sean (2015) 1746 min, 35 seare) CALLOAD	
				5 90
	l		Programmer international inter) 3 ISTD (3 total)



MassHunter Quantitative Software Compounds at a Glance View

View > Compounds-at-a-Glance





Editing a Quantitation Method for TOF Mass Extraction Setup



Method > Edit > Advanced Tasks > Mass Extraction Setup

Allows for a mass range for the extraction of the accurate mass (MZ).

C	Juantifier							
	Name	TS	Scan	Туре	Extract Left m/z	MZ	Extract Right m/z	MZ Extraction Window Units
	 Sulfadimethoxine 	1	Scan	ISTD	20.0000	311.0808	20.0000	PPM 🗸
	Caffeine-DAD	1	Scan	Target	20.0000	195.0876	20.0000	PPM
	Sulfadimethoxin	1	Scan	ISTD	20.0000	311.0808	20.0000	PPM

Available MZ Extraction Window Units

MZ Extraction Window Unit	ts
PPM	\sim
Thomsons	
PPM	
Percent	



Editing a Quantitation Method for QTOF Compound Setup & Mass Extraction Setup



QTOF is a combination of MS/MS and accurate mass data

4	uanunei									
	Name	TS	Transition	Scan 🗠	Туре	Precursor Ion	Product Ion	RT	Ion Polarity	Criteria
	Sulfamethizole	1	271.0318 -> 156.0114	Product Ion	Target	271.0318	156.0114	0.620	Positive	Greatest Response
	Sulfachloropyridazine	1	285.0208 -> 156.0114	Product Ion	Target	285.0208	156.0114	0.890	Positive	Greatest Response
	Sulfamethazine	1	279.0910 -> 186.0332, 156.0114, 124.0869	Product Ion	Target	279.0910	186.0332	2.030	Positive	Greatest Response
	Sulfadimethoxine	3	311.0809 -> 156.0768, 218.0230, 245.1030	Product Ion	Target	311.0809	156.0768	2.950	Positive	Greatest Response
	Sulfamethoxazole	2	254.0594 -> 156.0114	Product Ion	ISTD	254.0594	156.0114	0.940	Positive	Greatest Response

Name – Compound name TS – time segments may be multiple Transition – Precursor ion → Product ion scan Scan – Product Ion Type – Target, ISTD, Surrogate or Matrix Spike Precursor Ion – mass of the ion Product Ion – mass of the ion for the target ion to monitor RT – retention time of compound of interest Ion Polarity – usually positive Criteria – Close RT, Close RT with Qualifiers, Greatest Response or Greatest Q-Value

Tip: Enter the Precursor Ion and the Product Ion—Transition auto populates.



Batch Table

Navigation

Bate	ch Tab	le													
	Samp	le:	CAL_LO8		-	Sar	mple Type: <all></all>			Compound	d:	Trichlorofluoromethane	-		
				Sa	mple			Trichlorof		Trichlor	oflu	Trichlorofluoromethane	*	lifie	٢
()	8	Name	Data File	Туре	Level	Acq. Date-Time	Exp. Conc.	RT	Resp. MI	Ca	Acetone	=	0 1	MI
	0	٣	CAL_L03	CAL_L03.D	Cal	3	6/20/2008 5:53 PM	0.5000	6.108	58365 📃		1,1-Dichloroethene		7	
	0	٣	CAL_L04	CAL_L04.D	Cal	4	6/20/2008 6:30 PM	1.0000	6.092	90617 📃		t-Butyl Alcohol		1	
	Θ	٣	CAL_L05	CAL_L05.D	Cal	5	6/20/2008 7:06 PM	2.0000	6.097	173426 📃		t-butyl Alcohol		3	
		٣	CAL_L06	CAL_L06.D	Cal	6	6/20/2008 7:44 PM	5.0000	6.097	248633 📃		Methylene Chloride		0	
		٣	CAL_L07	CAL_L07.D	Cal	7	6/20/2008 8:21 PM	10.0000	6.097	830216 📃		Carbon Disulfide		9	
►		٣	CAL_L08	CAL_L08.D	Cal	8	6/20/2008 9:04 PM	15.0000	6.097	1347631 📃		1.2.0.1		1	
		٣	CAL_L09	CAL_L09.D	Cal	9	6/20/2008 9:41 PM	20.0000	6.092	1781882 📃		trans-1,2-Dicnioroethene		0	
		٣	CAL_L10	CAL_L10.D	Cal	10	6/20/2008 10:19 PM	30.0000	6.092	2773495 📃		2-Methoxy-2-methylpropane	-	7 [
		10	CAL 111	CAL L11 D	C-L	44	C/20/2000 10-57 DM	40,0000	0.007	2020220		AUX A (1911) AUX A (1911) TUT 111	1.4	01	

Click in a sample row to display data on that sample

Click on **Next** and **Previous** icons to move through a batch or use Hotkeys:

Next Sample= Alt + DownNext Compound= Alt + RightPrevious Sample= Alt + UpPrevious Compound= Alt + LeftCompound list are frequently long, try the **Compound** drop down list to godirectly to the desired compound.



Batch Table Alphabetizing the Compound List

		Batcl	h Table									
		Sa	ample: 👔	CAL_L03		-	Sam	ple Type: <all> 👻</all>	Compound: [Acetone	-	-
	Add/Remove Columns				S	ample			Acetone	Acetone	^	
						Туре	Level	Acq. Date-Time	Exp. Conc.	Benzene		Conc
	Restore Default Columns					Cal	3	6/20/2008 11:53 AM	0.5000	Benzene, bromo-		0.208
						Cal	4	6/20/2008 12:30 PM	1.0000	Bromotorm		0.632
	Reset Sort				_		5	6/20/2008 1:06 PM	2.0000	Bromomethane		1.64/
	511.0					Cal	7	6/20/2008 2:21 PM	10,0000	Carbon Disulfide		9 799
4	Fill Down					Cal	8	6/20/2008 3:04 PM	15.0000	Carbon Tetrachloride		4.628
						Cal	9	6/20/2008 3:41 PM	20.0000	Chlorobenzene		9.969
~	Lock Sample/Compound Columns					Cal	10	6/20/2008 4:19 PM	30.0000	Chloroethane		8.454
						Cal	11	6/20/2008 4:57 PM	40.0000	Chloroform		0.289
	Flat Table					Cal	12	6/20/2008 5:35 PM	50.0000	Chloromethane		0.663
	Nanta d Tabla (Ula Garata)						6	6/20/2008 6:13 PM	5 0000	cis-1.2-Dichloroethene		5 269
	Nested Table (Horizontal)					Blank	0	6/20/2008 7:28 PM	5.0000	cis-1,3-Dichloropropene		0.416
	Nected Table (Vertical)					Blank		6/20/2008 8:07 PM		Dibromochloromethane		0.000
	Nesteu Table (Vertical)				D	Sample		6/20/2008 8:44 PM		Dibromomethane		0.000
	Compound Table				D	Sample		6/20/2008 9:22 PM		Dichlorodifluoromethane		0.000
+ ===					D	Sample		6/20/2008 10:00 PM		Dioxane		0.000
	Single Compound/Sample View				D	Sample		6/20/2008 10:38 PM	_	Ethane, 1,1,1,2-tetrachloro-		0.000
	single compound, cample them				U	Sample	I	16/20/2008 T1:16 PM				0.722
	Multiple Compounds/Samples View							From v	vithin	the Batch	18	ab
	Arrange Compounds By		Name					right cl	ick s	alact Arra	nc	
								nyn u	10n, 3		ΠĈ	JE
	Disable Calibration Points		Retent	ion Time				Comp		Du No	100	
								Comp	ouna	IS Dy > INa		e
3	Print Ctrl+P		Mass									
			ISTD									
4	Print Preview		1310									
	Properties		Compo	ound Group				Tip: Alr	ohabe	etize the		
	ropercesii		10									
			ID					Compo	NING	l iet for foe	10	r
			User D	ofined				Compo		LISLIVI 103		
			USELD	enneu				-				



compound access.

Batch Table Messages and Outliers

Sample: 1 CAL_L10	▼	Sa															
			All>		▼ Cor	mpound	d: 🔙 Dich	lorodifluorome	thane	▼ 📄 IS	STD: Fluoro	benzene			📑 🖬 🛛	🛛 🖓 🌱 🌱 🧐 🗱 🚺	
	Sample				Dichlorod		Dichlor	odifluorometha	ne Results		Qualifier	Fluorobe	nzene (L.	Qualifie	Qualifie		
🕐 🌾 Name Data	File Type	Level	Acq. Date-Time	Sample Group	Exp. Conc.	RT	Resp. 1	Il Calc. Conc.	Final Conc.	Accuracy	Ratio MI	RT	Resp.	Ratio MI	Ratio M		
CAL_L03 CAL_L03	03.D Cal	3	6/20/2008 11:53 AM		0.5000	4.237	29715	0.4278	0.4278	85.6	33.6 📃	10.621	1344418	1.9 🔳	9.5 🔳		
0 CAL_L04 CAL_L0	04.D Cal	4	6/20/2008 12:30 PM		1.0000	4.242	66597	1.0238	1.0238	102.4	30.2	10.621	1183924	1.8 🔳	10.1 🔳		
CAL_L05 CAL_L0	05.D Cal	5	6/20/2008 1:06 PM		2.0000	4.247	127904	1.9920	1.9920	99.6	31.6 📃	10.620	1144890	2.0	10.5 🔳		
CAL_L06 CAL_L0	06.D Cal	6	6/20/2008 1:44 PM		5.0000	4.258	203734	5.1178	5.1178	102.4	31.1 🔳	10.621	700587	1.6 📃	9.8 🔳		
CAL_L07 CAL_L0	07.D Cal	7	6/20/2008 2:21 PM		10.0000	4.248	671861	10.4356	10.4356	104.4	32.4 📃	10.621	1128268	2.0 📃	11.0 📃	Soloct	
CAL_L08 CAL_L0	08.D Cal	8	6/20/2008 3:04 PM		15.0000	4.242	1105069	16.1636	16.1636	107.8	31.4 📃	10.621	1196415	2.0 📃	10.9 📃	Select	
CAL_L09 CAL_L0	09.D Cal	9	6/20/2008 3:41 PM		20.0000	4.242	1474827	20.6623	20.6623	103.3	32.0 📃	10.620	1248377	2.0 📃	10.4 📃	_	
CAL_L10 CAL_L	10.D Cal	10	6/20/2008 4:19 PM		30.0000	4.248	2199968	29.3491	29.3491	97.8	33.0	10.621	1310216	1.7	10.3	Outliore	
CAL_L11 CAL_L	11.D Cal	11	6/20/2008 4:57 PM		40.0000	4.247	3126148	40.3840	40.3840	101.0	33.0 📃	10.626	1352547	1.9 📃	10.6 📃	Oullei S	
CAL_L12 CAL_L	12.D Cal	12	6/20/2008 5:35 PM		50.0000	4.247	3975819	47.9439	47.9439	95.9	32.8 📃	10.621	1448684	2.1	10.3 📃		
CC_L07 CC_L0	7.D CC	7	6/20/2008 6:13 PM		10.0000	4.247	802673	10.3859	10.3859	103.9	33.8 📃	10.621	1354419	1.6 📃	10.7 📃	for Dicploy	
🛛 🛛 🖗 QC_L06 QC_L0	6.D QC	6	6/20/2008 6:50 PM		5.0000	4.247	211200	2.9037	2.9037	58.1	32.1 📃	10.620	1288192	1.7 🔳	10.5 📃	IUI DISplay	
🛛 🤻 Blank01 BLANK	01.D Blank		6/20/2008 7:28 PM			4.258	20853	0.3450	0.3450		37.2 📃	10.626	1201381	2.1	10.9 📃		
Plank02 BLANK	02.D Blank		6/20/2008 8:07 PM			4.630	266	0.0464	0.0464		163.6	10.621	1059821	1.9 🔳	10.3 🔳		

Red Outlier – High (above upper limit)

Outlier(s)

Blue Outlier – Low (below lower limit)



\rm Quantitation Message(s)

Dibromomethane: Qualifier M/Z = 93.0: Qualifier peak not found or does not match quantitation criteria Hexachlorobutadiene: Qualifier M/Z = 223.0: Qualifier peak not found or does not match quantitation criteria Hexachlorobutadiene: Qualifier M/Z = 227.0: Qualifier peak not found or does not match quantitation criteria Tetrahydrofuran: Qualifier M/Z = 72.0: Qualifier peak not found or does not match quantitation criteria Vinyl Acetate: Qualifier M/Z = 86.1: Qualifier peak not found or does not match quantitation criteria



Outliers

Messages

Dichlorodifluoromethane: Retention time = 4.630 is outside the allowed range [4.037, 4.462]

Hover cursor over the outlier or message to display details



Batch Table Layout Modification Add/Remove/Move Columns

Bat	ch Tal	ole																						
1	Samp	le: [CAL_LO)3		- T	Sa	mple T _j	/pe: <all></all>		Ŧ	Comp	oun	d: 🔙 Chlor	oform		-	ISTO	: Flu	orobenze	ene			
					Sar	mple				Chlorofor			С	hloroform Res	sults		Qualifie	r Qua	lifier	Fluorob	enzene (L.	Qualifier	Quali	ifier
)	7	Name		Data File	Туре	Level	A	cq. Date-Time	Exp. Conc.	RT	Resp.	MI	Calc. Conc.	Final Conc.	Accuracy	Ratio	MI Rati	o MI	RT	Resp.	Ratio N	1I Ratio	MI
►	0	٣	CAL LOO		CALLAND	C-1	1	1 croop	008 5:53 PM	0.5000	8.891	32587		0.6516	0.6516	130.3	165	9.	4 🗖	10.621	1344418	1.9	9.5	
	Θ	٣	CAL	A	.dd/Remove Co	olumns			008 6:30 PM	1.0000	8.891	49632		1.1376	1.1376	113.8	164	16.	8	10.621	1183924	1.8	10.1	
	Θ	٣	CAL_	R	estore Default	Columns			008 7:06 PM	2.0000	8.885	91234		2.1757	2.1757	108.8	156	17.	7 🔳	10.620	1144890	2.0	10.5	
		٣	CAL_	-					008 7:44 PM	5.0000	8.891	130047		5.0875	5.0875	101.7	170_	14.	7 🔳	10.621	700587	1.6	9.8	
_		٣	CAL_	R	eset Sort				008 8:21 PM	10.0000	8.891	419785		Colum	ns							-		
_		٣	CAL_	Fi	ill Down				008 9:04 PM	15.0000	8.891	649647												
		٣	CAL_	-					008 9:41 PM	20.0000	8.891	893838		Select	Columns From:									
		٣	CAL_	Lo	ock Sample/Co	mpound Col	lumns		008 10:19 PM	30.0000	8.891	1369093		Sample	e		•							
		-	7											Availat	ole Columns:					Show th	nese columns	in the orde	r:	

Use the Add/Remove Columns function to customize the Batch table.

Note that the columns of data in the Batch Table are organized into sections.

Columns can be moved only within a section.

Tip: Select the correct table





Batch Table Layout Modification Single and Multiple Compound Modes

Single Compound Mode

-																						
÷	Samp	le:	CAL_L10		- F	Sa	mple Type: <all></all>		▼ Co	mpoun	i: 🔙 Dici	hloi	rodifluorom	ethane	- 🗭 I	STD: Flu	Joro	benzene				1
					Sample				Dichlorod		Dichlo	proc	difluorometha	ne Results		Qualifi	er	Fluorobe	enzene (L	Qualifi	e	Qualif
	1	7	Name	Data File	Туре	Level	Acq. Date-Time	Sample Group	Exp. Conc.	RT	Resp.	MI	Calc. Conc.	Final Conc.	Accuracy	Ratio	MI	RT	Resp.	Ratio	MI	Ratio
	0		CAL_L03	CAL_L03.D	Cal	3	6/20/2008 11:53 AM		0.5000	4.237	29715		0.4278	0.4278	85.6	33.6		10.621	1344418	1.9		9.5
	0		CAL_L04	CAL_L04.D	Cal	4	6/20/2008 12:30 PM		1.0000	4.242	66597		1.0238	1.0238	102.4	30.2		10.621	1183924	1.8		10.1
	0		CAL_L05	CAL_L05.D	Cal	5	6/20/2008 1:06 PM		2.0000	4.247	127904		1.9920	1.9920	99.6	31.6		10.620	1144890	2.0		10.5
			CAL_L06	CAL_L06.D	Cal	6	6/20/2008 1:44 PM		5.0000	4.258	203734		5.1178	5.1178	102.4	31.1		10.621	700587	1.6		9.8
			CAL_L07	CAL_L07.D	Cal	7	6/20/2008 2:21 PM		10.0000	4.248	671861		10.4356	10.4356	104.4	32.4		10.621	1128268	2.0		11.0
			CAL_L08	CAL_L08.D	Cal	8	6/20/2008 3:04 PM		15.0000	4.242	1105069		16.1636	16.1636	107.8	31.4		10.621	1196415	2.0		10.9
			CAL_L09	CAL_L09.D	Cal	9	6/20/2008 3:41 PM		20.0000	4.242	1474827		20.6623	20.6623	103.3	32.0		10.620	1248377	2.0		10.4
►			CAL_L10	CAL_L10.D	Cal	10	6/20/2008 4:19 PM		30.0000	4.248	2199968		29.3491	29.3491	97.8	33.0		10.621	1310216	1.7		10.3
			CAL_L11	CAL_L11.D	Cal	11	6/20/2008 4:57 PM		40.0000	4.247	3126148		40.3840	40.3840	101.0	33.0		10.626	1352547	1.9		10.6
		٣	CAL_L12	CAL_L12.D	Cal	12	6/20/2008 5:35 PM		50.0000	4.247	3975819		47.9439	47.9439	95.9	32.8		10.621	1448684	2.1		10.3
			CC_L07	CC_L07.D	CC	7	6/20/2008 6:13 PM		10.0000	4.247	802673		10.3859	10.3859	103.9	33.8		10.621	1354419	1.6		10.7
		٣	QC_L06	QC_L06.D	QC	6	6/20/2008 6:50 PM		5.0000	4.247	211200		2.9037	2.9037	58.1	32.1		10.620	1288192	1.7		10.5
		٣	Blank01	BLANK01.D	Blank		6/20/2008 7:28 PM			4.258	20853		0.3450	0.3450		37.2		10.626	1201381	2.1		10.9
		٣	Blank02	BLANK02.D	Blank		6/20/2008 8:07 PM			4.630	266		0.0464	0.0464		163.6		10.621	1059821	1.9		10.3
		٣	SAMPLE01	SAMPLE01.D	Sample		6/20/2008 8:44 PM			4.139	287		0.0463	0.0463		152.6		10.621	1165447	2.0		10.3
		٣	SAMPLE02	SAMPLE02.D	Sample		6/20/2008 9:22 PM			3.418	519		0.0500	0.0500		125.4		10.626	1138631	2.2		10.8
		٣	SAMPLE03	SAMPLE03.D	Sample		6/20/2008 10:00 PM			3.882	662		0.0532	0.0532		160.8		10.621	1036288	2.2		11.1
		٣	SAMPLE04	SAMPLE04.D	Sample		6/20/2008 10:38 PM			4.035	353		0.0482	0.0482		55.8		10.621	990498	2.5		11.8
		٣	SAMPLE05	SAMPLE05.D	Sample		6/20/2008 11:16 PM			4.842	286		0.0462	0.0462		182.8		10.621	1205617	2.1		11.3

Flat Table compounds across the top.

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Multiple Compound Mode

Batch Table																																		-	×
	Sample	: 1	CAL_L10		- I] Sa	mple Type: <all></all>			Compo	und: 🔙	Dichlorodi	fluoromet	hane	👻 📫 - IS	TD: Fluo	robenzer	ne		1		P	• 🕈	777											
				S	ample			1,1,1-T	richloroethar	e Results	1,1,2,2-1	etrachloroeth	ane Re	1,1,2-Tr	ichloroethane	Results	1,1-Dich	loro-1-propen	e Resul	1,1-Di	ichloroethane	Results	1,1-Di	hloroethene	Results	1,2,3-Tricl	hlorobenzen	e Resul	1,2,3-Trie	chloropropan	e Resul	1,2,4-Tric	hlorobenzene	e Resul 1	1,2,4
C	D	7	Name	Data File	Туре	Level	Acq. Date-Time	RT	Final Conc.	Accuracy	RT	Final Conc.	Accuracy	RT	Final Conc. A	Accuracy	RT	Final Conc.	Accuracy	RT	Final Conc.	Accuracy	RT	Final Conc.	Accuracy	RT F	inal Conc.	Accuracy	RT	Final Conc.	Accuracy	RT I	Final Conc. A	Accuracy	R1
	0	۳ (CAL_LO3	CAL_L03.D	Cal	3	6/20/2008 11:53 AM	9.846	0.6074	121.5	16.661	0.4496	89.9	12.989	0.5297	105.9	10.097	0.8125	162.5	7.958	0.8214	164.3	6.730	0.6400	128.0	24.076	0.8497	169.9	17.310	8.2431	1648.6	23.296	1.0907	218.1	19.3
	0	۳ (CAL_L04	CAL_L04.D	Cal	4	6/20/2008 12:30 PM	9.846	1.0299	103.0	16.650	0.9010	90.1	12.983	1.0112	101.1	10.091	1.2425	124.2	7.952	1.3034	130.3	6.714	1.1898	119.0	24.065	1.3603	136.0	16.879	0.0000	0.0	23.290	1.4642	146.4	19.0
	0	۳ (CAL_L05	CAL_L05.D	Cal	5	6/20/2008 1:06 PM	9.857	2.0102	100.5	16.655	1.9043	95.2	12.994	2.1236	106.2	10.091	2.0667	103.3	7.952	2.2506	112.5	6.719	2.0537	102.7	24.071	2.2501	112.5	16.885	0.0000	0.0	23.290	2.3133	115.7	19.3
		۳ (CAL_LOG	CAL_L06.D	Cal	6	6/20/2008 1:44 PM	9.857	4.7230	94.5	16.650	6.2325	124.7	12.978	5.5467	110.9	10.091	4.5658	91.3	7.958	4.9158	98.3	6.725	4.6847	93.7	24.065	5.0702	101.4	16.885	4.8956	97.9	23.296	4.7206	94.4	19.3
		۳ (CAL_L07	CAL_L07.D	Cal	7	6/20/2008 2:21 PM	9.851	9.9647	99.6	16.656	10.0043	100.0	12.983	10.0977	101.0	10.091	9.8186	98.2	7.958	9.9753	99.8	6.725	10.0559	100.6	24.065	9.6899	96.9	16.879	8.5782	85.8	23.290	9.2812	92.8	19.3
		Y (CAL_LO8	CAL_L08.D	Cal	8	6/20/2008 3:04 PM	9.857	15.1405	100.9	16.656	15.2043	101.4	12.983	14.9484	99.7	10.091	14.9581	99.7	7.958	14.6205	97.5	6.725	14.8672	99.1	24.065	14.6137	97.4	16.885	14.2062	94.7	23.291	14.5152	96.8	19.3
		Y (CAL_L09	CAL_L09.D	Cal	9	6/20/2008 3:41 PM	9.851	19.6216	98.1	16.655	20.0773	100.4	12.983	20.6586	103.3	10.091	19.8885	99.4	7.958	19.8200	99.1	6.725	20.0570	100.3	24.071	19.7139	98.6	16.885	19.1484	95.7	23.290	20.0493	100.2	19.3
•		Y (AL_LIO	CAL_LIO.D	Cal	10	6/20/2008 4:19 PM	9.85/	29.6345	98.8	16.656	28.9150	96.4	12.983	28.8907	96.3	10.091	29.2991	97.7	7.952	29.2766	97.6	6.725	29./5/2	99.2	24.071	29.1939	97.3	16.879	29.0618	96.9	23.291	29.4688	98.2	19.
	_	Y (AL_LII	CAL_LIT.D	Cal	10	6/20/2008 4:57 PM	9.85/	42.0349	105.1	16.655	36.8531	92.1	12.983	36.7778	91.9	10.091	41.5072	103.8	7.958	39.5124	98.8	6.725	40.0941	100.2	24.071	40.0495	100.1	16.879	37.2742	93.2	23.290	40.0411	100.1	19.
		۲ (AL_LIZ	CAL_LIZ.D	Cal	12	6/20/2008 5:35 PM	9.851	48.7333	97.5	10.000	52.9585	105.9	12.989	52.9157	105.8	10.091	49.3410	98.7	7.958	51.0040	102.0	6.725	50.1004	100.2	24.071	50.7087	101.4	16.8/9	53.6///	107.4	23.290	50.5555	100.0	19.
	-	Y (00	6	0/20/2000 0:13 FM	0.051	3.0303	07.0	10.000	10.2431	00.0	12.303	E 0550	101.7	10.091	10.4362	05.2	7.552	5.0410	100.0	0.713	4 7070	0.00	24.071	E 5000	110.4	10.000	0.0207	00.3 50.5	23.230	E 2025	106.3	10.1
		v (lank01	RI ANKO1 D	Riank	•	6/20/2008 6.30 FM	5.001	4.0001	37.0	10.000	4.5025	50.0	12.303	0.6991	101.1	10.000	4.7376	50.2	7.932	0.9021	100.2	6.713	4./3/3	30.0	24.000	1.2614	110.4	17 210	2.0207	00.0	23.250	1 2161	105.5	19.0
	-	v -	Blank02	BLANK02 D	Blank	-	6/20/2008 8:07 PM	10.370	0.1851		16.050	0.0000		13 180	1 3919		10.621	2 4606		8 667	0.3021		6.267	0.2944		24.002	0.5752		17.305	8 5789		23.230	0.7753		19.
	-	· ·	SAMPLE01	SAMPLE01 D	Sample		6/20/2008 8:44 PM	10.173	0.1842		15.854	0.0978		13 180	1 3256	_	10.626	2,4000		8.089	0.4310		7.560	0.2900		24.071	0.5083		17.300	8.0261		24.060	0.6785		191
	-	· ·	SAMPLE02	SAMPLE02 D	Sample	-	6/20/2008 9:22 PM	9 344	0 1862		17 294	0.1018		13 185	1 4552	_	10.626	2 4784		8 640	0 4449		6 703	0 2945		24.065	0.4845		17 310	8 4554		24.065	0.6569		19
		· ·	SAMPLE03	SAMPLE03.D	Sample	-	6/20/2008 10:00 PM	9,949	0.1897		16.055	0.0931		13,180	1.4057	_	10.626	2.4790		8.356	0.4503		6.736	0.2944		23.280	0.4325		17.310	8.3269		23.280	0.6246		19.1
		Y 5	SAMPLE04	SAMPLE04.D	Sample	-	6/20/2008 10:38 PM	10.768	0.1869					13.174	1.4943		10.615	2.4298		8.258	0.4437		7.554	0.2937		24.071	0.4794		17.316	8.3527					19.1
		Y 9	SAMPLE05	SAMPLE05.D	Sample		6/20/2008 11:16 PM	9.857	0.2115		17.316	0.1092		13.185	1.5543		10.348	3.9750		7.958	13.2340		7.652	0.4832		24.065	0.5247		16.672	24.4296		22.898	0.6084		19.1
															· · · · · ·																			-	



Batch Table Layout Modification Compound Table Modes

📅 Agilent MassHunter Quantitat	tive Ana	lysis (for C	SCN	1S) - VOA - v	oa_example	.batch.bin										
File Edit View Analyze Me	thod U	pdate R	еро	rt Tools H	elp											
: 🛅 🗁 🛃 🗈 💭 🖓 Analyz	ze Batch	• 🕜	L	ayout: 🔜		_ ∞	Restore	Defa	ault Lay	out						
Batch Table																
Sample: 👔 QC_L06		-	ł	Sample T	ype: <all></all>				-	Compound: Dichlor	odifluoro	methane	-	IST): Flu	orobenzene
Compound Method				QC_L06			Qualifie.	Qı	ualifie	ISTD Method	ISTD	Results	ISTD Q	ISTD (a [−]	Add/Pemous Columns
Name	RT	Resp.	MI	Calc. Conc.	Final Conc.	Accuracy	Ratio M	1I Ra	atio MI	Name	RT	Resp.	Ratio MI	Ratio	N	Add/ Nellove Coldmins
1,1-Dichloro-1-propene	10.0	243136		4.7578	4.7578	95.2	31.6	3	4.5	Fluorobenzene	10.620	1288192	1.7	10.5	Ē.	Add Column
Dichlorodifluoromethane	4.247	211200		2.9037	2.9037	58.1	32.1			Fluorobenzene	10.620	1288192	1.7	10.5		Restore Default Columns
Chloromethane	4.498	194192		4.7682	4.7682	95.4	31.8			Fluorobenzene	10.620	1288192	1.7 🔳	10.5	Ĩ	Auto Fit Columns Ctrl+U
1,4-Dichlorobenzene	19.5	458056		5.2756	5.2756	105.5	64.6	4	3.9 📃	1,4-Dichlorobenzene-d4	19.504	619825	57.6	41.8		
Vinyl Chloride	4.739	232215		4.1548	4.1548	83.1	32.8			Fluorobenzene	10.620	1288192	1.7 🔳	10.5	[Reset Sort
1,2,4-Trichlorobenzene	23.2	259025		5.2625	5.2625	105.3	98.9	2	9.6 🔳	1,4-Dichlorobenzene-d4	19.504	619825	57.6	41.8		Lock Sample/Compound Columns
Bromomethane	5.251	116516		3.9551	3.9551	79.1	98.4 📃			Fluorobenzene	10.620	1288192	1.7 🔳	10.5		cock sample, compound columns
Chloroethane	5.421	135709		5.1361	5.1361	102.7	37.1 🔳			Fluorobenzene	10.620	1288192	1.7 🔳	10.5		Flat Table
Naphthalene	23.6	519274		6.3779	6.3779	127.6	12.0 📃	10	0.9 📃	1,4-Dichlorobenzene-d4	19.504	619825	57.6 📃	41.8		Nested Table (Horizontal)
Hexachlorobutadiene	23.8	227798		5.1452	5.1452	102.9	60.0	5	7.9 🔳	1,4-Dichlorobenzene-d4	19.504	619825	57.6	41.8	L	
Trichlorofluoromethane	6.097	377098		3.8308	3.8308	76.6	65.4	1	0.6 🔳	Fluorobenzene	10.620	1288192	1.7 🔳	10.5		Nested Table (Vertical)
Acetone	6.190	170682		5.2692	5.2692	105.4	27.5			Fluorobenzene	10.620	1288192	1.7 🔳	10.5	↓⊞	Compound Table
1,1-Dichloroethene	6.719	254894		4.7979	4.7979	96.0	61.3	3	8.5 🔳	Fluorobenzene	10.620	1288192	1.7 🔳	10.5		Single Company d/Semale View
1,2,3-Trichlorobenzene	24.0	257316		5.5208	5.5208	110.4	10 🔳	2	9.7 🔳	1,4-Dichlorobenzene-d4	19.504	619825	57.6	41.8	۳	single compound/sample view
Methylene Chloride	6.877	182447		5.1839	5.1839	103.7	64.0			Fluorobenzene	10.620	1288192	1.7 🔳	10.5		Multiple Compounds/Samples View
Carbon Disulfide	7.178	69556		5.8374	5.8374	116.7	69.6			Fluorobenzene	10.620	1288192	1.7 🔳	10.5		Armana Compounds Pu
trans-1,2-Dichloroethene	7.663	165832		5.0298	5.0298	100.6	14 🔳	6	3.8 📃	Fluorobenzene	10.620	1288192	1.7 🔳	10.5		Arrange Compounds By
2-Methoxy-2-methylpropane	7.810	439953		5.1203	5.1203	102.4	15.9			Fluorobenzene	10.620	1288192	1.7 🔳	10.5		Print Ctrl+P
1,1-Dichloroethane	7.952	303201		5.3097	5.3097	106.2	35.0		6.3 🔳	Fluorobenzene	10.620	1288192	1.7 🔳	10.5		Drint Draview
Vinyl Acetate	8.056	130420		4.5381	4.5381	90.8	8.9			Fluorobenzene	10.620	1288192	1.7 🔳	10.5		FILL FIEVIEW
2-Butanone (MEK)	8.438	229534		5.7318	5.7318	114.6	26.2	1	6.5	Fluorobenzene	10.620	1288192	1.7 🔳	10.5		

Compound Table lists by compound rather than sample.

Select **Flat Table** to see list by sample.



Batch Table Compounds Groups

Bato	:h Tal	ole														
	Samp	le:	CAL_L08		-	Sar	mple Type: <all></all>		Ŧ	Compo	ound	1:	Trichlorofluoromethane	-	E	Þ
				Sa	mple			Trichlorof		Tric	hloro	oflu	Trichlorofluoromethane	٠	lifie	er
(D	8	Name	Data File	Туре	Level	Acq. Date-Time	Exp. Conc.	RT	Resp.	MI	Ca	Acetone	=	0	MI
	0	*	CAL_L03	CAL_L03.D	Cal	3	6/20/2008 5:53 PM	0.5000	6.108	58365			1,1-Dichloroethene		7	
	0	٣	CAL_L04	CAL_L04.D	Cal	4	6/20/2008 6:30 PM	1.0000	6.092	90617			t-Butyl Alcohol		1	
	0	٣	CAL_L05	CAL_L05.D	Cal	5	6/20/2008 7:06 PM	2.0000	6.097	173426			Course Alconor		3 [
		٣	CAL_L06	CAL_L06.D	Cal	6	6/20/2008 7:44 PM	5.0000	6.097	248633			Methylene Chloride		0	
		٣	CAL_L07	CAL_L07.D	Cal	7	6/20/2008 8:21 PM	10.0000	6.097	830216			Carbon Disulfide		9	
►		٣	CAL_L08	CAL_L08.D	Cal	8	6/20/2008 9:04 PM	15.0000	6.097	1347631			terre 1.2 Disklass there		1	
		٣	CAL_L09	CAL_L09.D	Cal	9	6/20/2008 9:41 PM	20.0000	6.092	1781882			trans-1,2-Dichloroethene		0	
		٣	CAL_L10	CAL_L10.D	Cal	10	6/20/2008 10:19 PM	30.0000	6.092	2773495			2-Methoxy-2-methylpropane	-	7	
		10	CAL 111	CALLETED.	0-1	44	C/20/2000 10.57 DM	40,0000	C 007	2020220		_	ATT # 211 ATT # 211 111 111 111	1.4	61	

It may be useful to group compounds to organize Batch Table.

Look at parent compound and metabolites.

Group hydrocarbons to Group 1, aromatics to Group 2 and so forth.

Compound groups are generated in the Method Editor.



Batch Table Compounds Groups



Activated with a right click to the right of the 'flags' or **View > Toolbars > Filtering**.





Batch Table Samples Groups

Sample Groups are specified in the Batch Table through **Add/Remove Columns.**

Each Sample is assigned to a group, then only samples specific to a group are displayed and evaluated.



Samples groups are distinctively different from compound groups.



Batch Table Layout Modification

How to change the number of decimal places.

Alter number formats

- 1) Exponential (scientific notation)
- 2) Fixed point
- 3) General
- 4) Significant Figures

Alter Date formats

🙀 Ag	gilent MassHun	ter Quantitative Ar	nalysis (for GC	MS) - VOA	- Vola	atileOr	ganics.ł	oatch.bi	n		
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Formats	s					^	.5000	4.237	29715		0.0019
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10	Calc. Conc.		Exponential	~ 4			[4.237	29715		1.8800E-003
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	Custom Calc. 1		Significant Figu	res <mark>4</mark>				4.258	198094		4.6697E+000
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Batch Table Layout Modification Context Menu Properties

Change the Font size

Properties	×
General:	
Font size:	100 ~ %
Color scheme:	Standard ~
Default OK	Cancel Apply

NEW FEATURE!

Change the Color scheme

Properties			×
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Export Batch Table

ssHunter Quantitative Analysis (for QQQ) - VOA - VolatileOr	ganics.batch.bin
w Analyze Method Update Library Report Tools H	lelp
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ata\Quant Examples\MS\VQA\VolatileQrganics batch.bin	40.0000 4.247 31261
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uant Examples\MS\RI-PEST-MATRIX\TargetDEMO.batch.bir	5.0000 4.247 2112
amples QOQ New\BenzosInUrine\BenzosInUrine.batch.bin	4.630 2
ples OOO New\DrugsOfAbuse\DrugsOfAbuseDemo.batch.	bin 3.418 5
QQ New\DrugsOfAbuse\DrugsOfAbuseDemo-small.batch.h	a.882 6
ssHunter\Data\evaldemo2a.batch.bin	4.035 3
April 2017 test\11_April 2017 Calibration.batch.bin	
amples QQQ New\PEST\Blankoffsetcalculated.batch.bin	

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2	Name	Data File	Туре	Level	Acq. Date-T	ìme	Exp. Conc.	RT	Resp.	MI	Calc. Conc.	Final Conc.	Accuracy	Ratio	MI	RT	Resp.	Ratio	MI	Ratio	MI
з	CAL_L03	CAL_L03.D	Cal	3	6/20/2008 11:53	1	0.5	4.237	29714.96	##	0.00187998	0.00188	0.375995	33.6	#	10.621	1344418	3 1.86	##	9.55	##
4	QC_L06	QC_L06.D	QC	6	6/20/2008 18:50)	5	4.247	211200.4	##	2.54215754	2.5421575	50.84315	32.1	#	10.62	1288192	2 1.69	##	10.5	##
5	CAL_L04	CAL_L04.D	Cal	4	6/20/2008 12:30)	1	4.242	66596.94	##	0.61342523	0.6134252	61.34252	30.2	#	10.621	1183924	1.81	##	10.1	##
6	SAMPLE02	SAMPLE02.D	Sample		6/20/2008 21:22			3.418	518.7985	##	0	0		125	#	10.626	1138631	2.22	##	10.8	##
7	SAMPLE03	SAMPLE03.D	Sample		6/20/2008 22:00)		3.882	662.477	##	0	0		161	#	10.621	1036288	3 2.17	##	11.1	##
8	SAMPLE04	SAMPLE04.D	Sample		6/20/2008 22:38			4.035	353.4815	##	0	0		55.8	#	10.621	990498.4	2.45	##	11.8	##
9	SAMPLE01	SAMPLE01.D	Sample		6/20/2008 20:44			4.139	286.89	##	0	0			#	10.621	1165447	7 1.96	##	10.3	##
10	SAMPLE05	SAMPLE05.D	Sample		6/20/2008 23:16			4.842	286.347	##	0	0		183	#	10.621	1205617	2.09	##	11.3	##
11	Blank02	BLANK02.D	Blank		6/20/2008 20:07	'		4.63	266.178	##	0	0			#	10.621	1059821	1.93	##	10.3	##
12	CAL_L06	CAL_LO6.D	Cal	6	6/20/2008 13:44		5	4.258	198094.3	##	4.66973662	4.6697366	93.39473	31	#	10.621	700587.4	1.59	##	9.82	##
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NEW FEATURE!

CSV Files (*.csv)
CSV Files (*.csv)
Excel Files (*.xlsx)
Tab Delimited Files (*.txt)
Xml Files (*.xml)

Tip: Popular option to Excel based reports. Easy to layout columns and format data, then export into Excel.



Let's take a moment for questions on Batch Table Navigation.



MassHunter Webinar Series 1/17/2018



Time for a demo on Batch Table Navigation

Next up: Compound Information

> MassHunter Webinar Series 1/17/2018

Compound Information

Display and access one compound in one sample at a time.





Compound Information - Toolbar





Manual Integrations and MI Toolbar



Click on the Manual Integration icon to place Compound Information in Manual Integration mode.

Each signal is placed in its own window (no overlay of qualifiers).



Manual Integration Toolbar





Enable Manual Integration – this tool activates the manual integration toolbar.



Clear Manual Integration – this tool becomes active once a manual integration is present.



Zero Peak – this tool sets start and stop to the same value.



Merge Right/Left Peak – this tool merges the peak to the right/left of the selected peak.

🔺 📩

Split Peak and Pick Right/Left – this tool splits the peak and then selects the right or left peak.



Snap Baseline – this tool places start/stop integration points on the baseline.

4

Drop Baseline – this tool finds the lowest end of the peak, then drops the baseline on the other side of the peak from it, thereby creating a flat baseline that avoids negative area.



Compound Information Peak Annotation

Activated from **Tools > Add-Ins...**



NI – The peak was not integrated at all by the computer software.

LT – The peak in question was inappropriately integrated to an area less than what it should be (e.g., Peak area was cut).

GT - The peak in question was inappropriately integrated to an area greater than what it should be (e.g., Peak Tailing).

BA – The baseline had to be adjusted correctly by the analyst.

CO –The analyst had to split to co-eluting peaks apart that were not (or could not be) separated by the computer system.

RT – The retention time for the peak in question has shifted from the expected retention time.

INT – There was electronic interference (e.g., Noise).



Compound Information Peak Annotation

The editable file is located in C:\Program Files\Agilent\MassHunter\Workstation\Quant\bin\AddIns\PeakAnnotations.xml.

Tip: Always create a back-up file before editing a configuration file.



Compound Information Peak Annotation

The Peak Annotation can also be displayed in the Batch Table.

When the batch is saved, the values are retained.

Columns				?	>	<								
Select Columns From:														
Compound Method	~						Dichloro	difluoron	nethane Method		Dichlorodi	fluor	romethane Re	sults
Available Columns:	•	. LLA	Show these columns	in the ord	ier:		Exp. Conc.	RT	User Annotation	RT	Resp.	MI	Calc. Conc.	Final Conc.
Agilent ID Alternative Peak Criteria		Add ->	Liser Apportation				0.5000	4,249	NI	4.237	22897		0.0000	0.0000
Alternative Peak ID		<- Remove	User Armotation				1.0000	4.249	LT	4.242	51949	\leq	0.3941	0.3941
Amt. Limit High Amt. Limit Low		Add All ->>					2.0000	4.249	GT	4.247	98928	\sim	1.1534	1.1534
Area CF Area Cor. m/z		< Remove All					5.0000	4.249	BA	4.307	-3978	\checkmark	0.0000	0.0000
Area Correction Selected MZ							10.0000	4.249	CO	4.248	495112	\leq	7.4664	7.4664
Avg. RF RSD							15.0000	4.249	RT	4.406	-90142	\leq	0.0000	0.0000
Blank Resp. Offset							20.0000	4.249	INT	4.242	1149283	\checkmark	16.0929	16.0929
Calibration Range Filter Capacity Factor Limit							30.0000	4.249		4.248	2199968		29.6758	29.6758
CAS# CAV <	>									-				
			Move Up	Move		T	he MI f	lag	is checl	ked	in the	е	Comp	ound
		OK Res	Default	Са	ncel	F	Results.							



Compound Information Context Menu Integration Parameters



Right click to expose the context menu.

Most of the features are toolbar icons.

Integration Parameters can be used to change the integration parameters.

Applies ONLY to this compound in this sample.

Restore Integration Parameters reverts to the method integration values.



Compound Information Context Menu Properties

Properties allows for customization of the display.

Can change Fill colors.

Can change Peak labels.

Can change Titles.

RT Name Calc. Conc. Final Conc. Height Area Delta RT S/N Cmpd. Group Q. Computed	Ę	 Ion polarity Scan type Collision energy Transition File name Compound name Sample name Instrument Name Acq. Date-Time

	pound Information (2)				
General:			Retention time:		
Background color:	Automatic	\sim	Reference RT:	No display	
Foreground color:	Automatic	\sim	Recognition window:	No display	
Gridlines color:	No display	\sim	Peak purity:		
Time segment boundary:	No display	\sim	Show peak purity		
Chromatogram:			Purity colors		
✓ Baselines					
Baseline calculation p	pints				
Normalize quantifier					
Original baselines after	r manual integration				
Noise regions:	No display	~			
Peak fill:	75% Transparent	~			
r curchit.					
Fill colors					
Fill colors]				



Compound Information Context Menu Properties

Properties (h)	×	
Compound Information Compound Information (2) Qualifiers: Normalize qualifiers Annotations Qualifier colors Uncertainty band: No display Fill peaks: Fill out-of-limits qualifier peaks Fill all qualifier peaks Fill all qualifier peaks Fill target peaks Fill target peaks Fill target peaks Y Response ratio label: Patio and percent of expected ratio Y	Spectrum: MS/MS precursor ion Reference spectrum Reference library source Reference pattern spectrum Override spectrum Show match scores Show mass indicators Manual integration: Show baseline start/end boxes Max. # of panes per row: 3	
[Default OK Cancel Apply	

Qualifier Properties can be changed.

Spectrum Properties can be altered.

Manual integration parameters can be varied.

Tip: Uncheck Normalize qualifiers and display the Uncertainty band for more information about the qualifiers.



Signal to Noise Five algorithms are available

Consult online help for more information on the algorithms. Noise regions can be automatically determined or individually specified.

The Noise regions can be displayed in the Compound Information window under **Properties > Compound** Information (1) > Baseline Calculation Points.

In this example, 2 noise regions were determined—one before the peak and the other after.







Let's take a moment for questions on Compound Information



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Let's take a moment for a demo on the features of Compound Information

Next up:

Calibration Curve and Curve Fit Assistant

> MassHunter Webinar Series 1/17/2018

Calibration Curve



Concentration can be set as relative (to ISTD) or actual.


Calibration Curve Disable calibration points



Click on calibration point once to disable and remove from curve.

Tip: After changing the curve always reanalyze the batch.



Curve Fit Assistant





Curve Fit Assistant Sorting Columns

Best curve fit may be ranked using by R², Standard Error, or Max % Residual.



Curve Fit Assistant calculates the mathematical curves.



Curve Fit Assistant Disabled Points

Calibration Cu	ve											\mathbf{X}
₽ ↔ \$	× - 🛛		Type: Linear		- Origin: I	gnore 👻	Weigh	nt: None 🔻	ISTD QC	CC		
diazepam - 5 Le	evels, 5 Leve 770949 * x = 0.9988658 : Linear, Orig 771976 * x = 1.0000000 Linear, Orig 0 0.5	els Used, 5 - 0.037379 2 gin:Ignore, ' - 0.112636 0 gin:Ignore, ' 1 1.5	Points, 5 Points Used Weight:None Weight:None	5	ICs	5 5.5 6	6.5	7 7.5 8	8.5 9	9.5 10 Relative Co	0 10.5 ncentra	1
Curve Fit												
	Origin V	Weight S	# of Disabled Points	$\overline{\nabla}$	R2 ⊽ 🏹	Standard Erro	r 🏹 Ma	ax % Residual 🏹	Fo	uation	7	
► Linear	lanore	None	(AII)		1.00000000		0.0	0.0	v = 0.77197	76*x - 0.1	12636	
Linear	Ignore	1/x	(Custom)	- 1	1.00000000		0.0	0.0	y = 0.76186	63 * x - 0.01	11506	1
Linear	Ignore	1/x^2	(Blanks)		1.00000000		0.0	0.0	y = 0.5798	29 * x + 0.0	0795	1
Linear	Ignore	1/y	(NonBlanks)		1.00000000		0.0	0.0	y = 0.76186	63*x -0.0	1506	
Linear	Ignore	1/y^2	1		1.00000000		0.0	0.0	y = 0.5798	29 * x + 0.0	0795	
Linear	Ignore	Log	2		1.00000000		0.0	0.0	y = 0.76889	97*x - 0.08	31844	
Linear	Include	1/x	3		1.00000000		0.0	0.0	y = 0.76186	63*x -0.0	11506	
Linear	Include	1/x^2		3	1.00000000		0.0	0.0	y = 0.5798	29 * x + 0.0	0795	
Linear	Include	1/y		3	1.00000000		0.0	0.0	y = 0.76186	53*x - 0.0	1506	
Linear	Include	1/y~2		3	1.00000000		0.0	0.0	y = 0.5/982	29 x + 0.0	J/95	~

of Disabled Points defaults to 3 but column can be filtered.



Curve Fit Assistant Confidence Band





Calibration Curve



NEW FEATURE!



Curve Fit Assistant Accept Assistant Curve

Calibration Curve									\mathbf{X}
🛃 ↔ ‡ 👯 • 💽	Type: Linear	▼ Or	rigin: Ignore 🛛 🔻	Weight:	None 🔻	ISTD QC	CC		
diazepam - 5 Levels, 5 Levels Used, y = 0.770949*x + 0.0373 R^2 = 0.99886582 Type:Linear, Origin:Ignore 6 y = -0.006755*x ^2 + 0.8 F R^2 = 0.99937228 Type:Quadratic, Origin:Ig	5 Points, 5 Points Used, 0 Q 79 9, Weight:None 342446 * x - 0.130065 nore, Weight:None	Cs	Copy Curve Fit Assistant Confidence Band	Ctrl+C					
	2 2.5 3 3.5		Accept Assistant C Relative Concentra Standard Deviation Auto Scale	Curve ation n Bars	7.5 8	8.5 9	9,5 10	10.5	
		+	X - Auto Scale			1	neialive Con	centrati	
Curve Fit		+	Y - Auto Scale						^
Iype Y Origin Y Weight Quadratic Ignore None			X - Log Scale		Residual ¥ 5.1	y = -0.006	quation 755 * x ^ 2 +	¥ 0.8	
Quadratic Include None Linear Include None	0		Y - Log Scale		5.3	y = -0.0044 y = 0.7693	411 * x ^ 2 + 12 * x - 0.025	0.8	
Quadratic Force Log	0		Print	Ctrl+P	19.9	y = -0.003	180*x^2 +	0.7	
Quadratic Blank off Log	0	0	Print Preview		19.9	y = -0.003	180 * x ^ 2 +	0.7	
Linear Ignore None	0	-	Duenenting		4.2	y = 0.7709	49 ° X - 0.03/ 242 * v ^ 2 +	/3/9	
Quadratic Blank off., None	0	1.770	Properties	0.01	31	v = -0.0018	342 * x ^ 2 +	0.7	
Power Ignore None	0	0.998	377784	0.1	3.9	y = 0.7675	19 * x ^ 0.998	791	
Power Force None	0	0.998	377784	0.1	3.9	y = 0.7675	19 * x ^ 0.998	791	~



Calibration Curve Properties

Calibration Curve					
🛃 🕂 🕈 🔅	🔹 💽 📝 Type: Quadratic	▼ Origin: Ignore ▼ V	Veight: None 🔻 ISTD Q	с сс	
diazepan 5 Levels y = -0.000 R^2 = 0.9 7.5 Type:Qua	, 5 Levels Used, 5 Points, 5 Points Used, 0 Q 6755 * x ^ 2 + 0.842446 * x - 0.130065 9937228 adratic, Origin:Ignore, Weight:None	Cs			
80 92 12 15 15 15 15 15 15 15 15 15 15 15 15 15	Copy Ctrl+C	Properties			×
6- 55-	Curve Fit Assistant Confidence Band	Calibration Curve General:		Standard deviation bars: —	
5	Accept Assistant Curve	Background color: Foreground color:	Automatic ~	Show standard deviation Color:	bars
4.5	Standard Deviation Bars	Gridlines color:	Light Gray ~	ISTD responses:	
3.5-	Auto Scale X - Auto Scale	Point size: Calibration curve:	Small ~	ISTD response color:	Green ~
2.5	Y - Auto Scale	Curve color:	Automatic ~	QC: Show QC points	
1.5	X - Log Scale	Auto scale to enabled p	points	Line color: Fill color:	Light Blue ~
0.5-	Print Ctrl+P	Current sample indicator: — Show indicator		CC:	
	Print Preview Properties	Calibration sample:	Dark Blue ~	Line color:	Pink ~
		Sample.		Fill color:	Red ~
				Default OK	Cancel Apply



Let's take a moment for questions on Calibration Curve and Curve Fit Assistant





Time for a demo on Calibration Curve and Curve Fit Assistant

Next up: Compounds at a Glance

> MassHunter Webinar Series 1/17/2018 46

Compounds-at-a-Glance

High throughput data review environment. View compounds across multiple samples. View all compounds within a sample.





MassHunter Webinar Series 1/17/2018

Compounds-at-a-Glance

To start, select View > Compounds-at-a-Glance...

Choose Layout > Predefined Layout



Styples/Targets/Auto Scale
Samples/Targets/Link X Axes + Fit to low CAL
Samples/Targets/Overlay Qualifiers + Link X Axes
Samples/Targets/Overlay ISTDs + Link X, Y Axes
Samples/ISTDs/Overlay Qualifiers + Link X Axes
Samples/Targets/By Compound Wrapped + Fit to low CAL
Samples/Targets/By Sample Wrapped + Fit to Iow CAL
Calibration/Targets/ByCompound Overlapped + Fit to peak
Calibration/ISTDs/ByCompound Overlapped + Fit to peak





Compounds-at-a-Glance Setup Graphics Wizard

To customize select Layout > Setup...

Setup Graphics							
Samples Compounds	Organize	Outlier					

Specify **Samples** to view in Compounds-at-a-Glance then **Compounds**. By default, all samples and all compounds are selected.

Specific samples and order can be modified.

up Graphics				
Samples Cor Samples:	mpounds Organize	Outlier		
Name	Data File	Туре	Level	Sample Group
4				
			(Demous	All
Samples show	n in this order:	nda Mil >>	< nemove	< Nemove All
Name	Data File	Туре	Level	Sample Group
Name Blank-1	Data File CMAMBlk_01.d	Type Blank	Level	Sample Group
Name Blank-1 Calib-L1	Data File CMAMBlk_01.d CMAMCal_L1.d	Type Blank Cal	Level L1	Sample Group
Name Blank-1 Calib-L1 Calib-L2	Data File CMAMBIk_01.d CMAMCal_L1.d CMAMCal_L2.d	Type Blank Cal Cal	Level L1 L2	Sample Group
Name Blank-1 Calib-L1 Calib-L2 Calib-L3	Data File CMAMBIk_01.d CMAMCal_L1.d CMAMCal_L2.d CMAMCal_L3.d	Type Blank Cal Cal Cal	Level L1 L2 L3	Sample Group
Name Blank-1 Calib-L1 Calib-L2 Calib-L3 Calib-L4	Data File CMAMBIk_01.d CMAMCal_L1.d CMAMCal_L2.d CMAMCal_L3.d CMAMCal_L3.d	Type Blank Cal Cal Cal Cal Cal	Level L1 L2 L3 L4	Sample Group
Name Blank-1 Calib-L1 Calib-L2 Calib-L3 Calib-L4 <	Data File CMAMBIk_01.d CMAMCal_L1.d CMAMCal_L2.d CMAMCal_L3.d CMAMCal_L3.d	Type Blank Cal Cal Cal Cal Cal Cal	Level L1 L2 L3 L4	Sample Group
Name Blank-1 Calib-L1 Calib-L2 Calib-L3 Calib-L4 <	Data File CMAMBIk_01.d CMAMCal_L1.d CMAMCal_L2.d CMAMCal_L3.d CMAMCal_L4.d	Type Blank Cal Cal Cal Cal Cal	Level L1 L2 L3 L4 Move Down	Sample Group



Compounds-at-a-Glance Setup Graphics Wizard

amples Compounds Organize Ou	tlier					
rganize Rows by:	Review Mode					
Samples	None None					
y Samples	Sample by Sample					
)verlay:	Compound by Compound					
) None - target only	Compound Group by Compound Group					
) None -target and qualifiers	Pane Dimension					
Qualifiers	5 x 4 🗸 🗸					
) ISTD	Display Options					
) Matrix Spike	Wrap Rows					
) Compound Groups	Baselines					
) Sample Groups	Fill Peaks					
Compounds	Normalize					
) Samples	Uncertainty Band					
	Peak annotations					

Define how to Organize the selected compounds and samples.

Define the Overlay mode.

Review Mode Sample by Sample Compound by Compound Compound Group by Compound Group

Display Options

Dis	play Options
	Wrap Rows
	Baselines
	Fill Peaks
	Normalize
	Uncertainty Band



Compounds-at-a-Glance Setup Graphics Wizard



Finally, define which **Outliers** should be highlighted...

Outliers can also be filtered by Panes without outliers Panes with outliers





Compounds-at-a-Glance Outliers



Outliers are highlighted in red.



Compounds-at-a-Glance Manual Integration Pop Up

Double click for single pane access.

Can be accessed without manual integration being activated.





Compounds-at-a-Glance Print Preview

Select File > Print Preview to create a chromatogram report.



Export Graphics give a graphic image in various formats.

Enhanced Metafiles (*.EMF) Enhanced Metafiles (*.EMF) Bitmap Files (*.BMP;*.DIB;*.RLE) JPEG (*.JPG;*.JPEG;*.JPE;*.JFIF) GIF (*.GIF) TIFF (*.TIF;*.TIFF) PNG (*.PNG)





Compounds-at-a-Glance Properties Properties

From the context menu select **Properties**

Properties				×
Compounds-at-a-Glance				
General:			Peaks:	
Background color:	Automatic	~	Baselines	Area Move Up
Foreground color: Gridlines color:	No display	~	Uncertainty band	Final Conc. RT Height Device
Outlier color:		~	Peak annotations Peak fill:	Delta RT S/N Q. Computed
Pane border: Selected pane border:	Light Gray	~	Fill alternate peaks whe	
Font size:		8 🚔	Retention Time:	 Display annotation names (ex. RT=2.452) Display units for Conc., RT and Delta RT
Chromatogram colors Chromatogram Colors	×		Reference RT:	Response ratio label: Ratio ~
Colors:	Maure Lin		Recognition window:	OK Cancel
	Move Down		Manual integration:	
	Remove		Show baseline start	/end boxes
			Manual integration:	~
	Change		Max. # of panes:	3 📫
	Insert		Navigation:	
Default OK	Cancel		Synchronize Naviga	ation
			Default O	K Cancel Apply



Compounds-at-a-Glance Save Layout



Some settings in the Layout screens are not saved such as compounds, samples, etc.





Time for questions on Compounds at a Glance



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Let's watch a demo on Compounds at a Glance

Next up: Global Settings

> MassHunter Webinar Series 1/17/2018 58

Globals Settings

Component of Method Editor.

Global parameters are critical to proper quantitation.

Globals are method parameters.

Globals apply to the whole batch – all samples and all compounds.



Globals Settings

Globals]	
Apply Multiplier to ISTD				
Apply Multiplier to Matrix Spike 74	\checkmark			
Apply Multiplier to Surrogate	\checkmark			Apply Multiplier's
Apply Multiplier to Target	\checkmark			
Bracketing Type	None		\rightarrow	None or Overlapped or Sample Group
Correlation Window		2.000	\longrightarrow	Associates target and qualifiers in min
Dynamic Background Subtraction			\longrightarrow	Dynamic Background Subtraction
Ignore Peaks Not Found				To evoid flooring torget compounds that about
Library Method				To avoid hagging target compounds that absent
Non Reference Window		200.000		Part of Unified method
Non Reference Window Type	Percent			Peak identification within the extraction window
Reference Library				Spectral Reference Library (reflibrary xml)
Reference Pattern Library		=	$ \longrightarrow $	Spectral Pattern Reference Library (.reflibrary.xml)
Reference Window		80.000		Peak identification within the extraction window
Reference Window Type	Percent			(ISTD with Time Reference Flag checked)
Relative ISTD			\longrightarrow	Semi quant relative to ISTD
Standard Addition			\longrightarrow	Quantitate with Standard Addition



Globals Settings Calculated and Final Concentration

	Sample			1,2,4-Trichl	orobe	1,2,4-Trichlorobenzene Results				ults
Туре		Level	Dil.	Exp. Conc.	Units	RT	Resp.	MI	Calc. Conc.	Final Conc.
	Sample		1.0		ng/ml	23.280	1138		0.6341	0.6341
	Sample		1.0		ng/ml	24.071	പ്പപ്പു074		0.6581	0.6581
	Sample		1.0		ng/ml	23.280	2272		0.6580	0.6580
	Sample		1.0		ng/ml	23.280	5189		0.6964	0.6964

Calculated Concentration (Calc. Conc.)—is the concentration of the compound as calculated from the calibration curve.

Final Concentration (Final Conc.)—is the concentration after the Multiplier has been applied to the Calculated Concentration.

The equations are:

Final Concentration = Calculated Concentration x Multiplier



Globals Settings Multiplier

Multiplier = Dilution x Sample Amount Multiplier where

Sample Amount Multiplier = TotalAmt/Amt

All three of the factors are columns in the Sample section of the Batch Table. By default, they are set to 1, either

explicitly (Dil.) or implicitly (Amt. and Tot. Amt.)

Sample				1,2,4-Trichl	orobe	1,2,4-Trichlorobenzene Results						
	Туре	Level	Dil.	Amt.	Tot. Amt.	Exp. Conc.	Units	RT	Resp.	MI	Calc. Conc.	Final Conc.
	Sample		1.0				ng/ml	23.280	1138		0.6341	0.6341
	Sample		1.0				ng/ml	24.071	2074		0.6581	0.6581
	Sample		1.0				ng/ml	23.280	2272		0.6580	0.6580
	Sample		1.0				ng/ml	23.280	5189		0.6964	0.6964



Globals Settings Multiplier





Globals Settings Bracketing type = None

No (None) Bracketing allows the user to have sample(s) quantitated using the average of **all** the calibration standards in the batch without regard to order.





Globals Settings Bracketing type = Overlapped

Overlapped Bracketing allows the user to have sample(s) quantitated using the average of the calibration standards injected both before and after the samples injection.

Average Calibration (A+B)

Average Calibration (B+C)



Globals Settings Bracketing Type = Sample Group

Used with Stream Select (LC)

When the Bracketing Type Sample Group is implemented, only samples from a specific Sample Group (specified in the Batch Table) are considered in the formation of the calibration curve and quantitation of the samples. This feature would accommodate slight shifts in retention time and/or variations in instrument responses.

Comment	Sample Group	Info.		
	Column 1			
	Column 2			
	Column 1			
	Column 2			

Added from Worklist or Batch Table.



Globals Settings Correlation Window

Indicates the retention time relationship of target and ions to one or more qualifiers.



Tolerance of extracted ions to be considered a single peak.

Default time of 0.5 min is rather wide.

Typically 0.01 to 0.05 min (0.6 sec to 3 sec)



Globals Settings Dynamic Background Subtraction

Removes noise or background ions in TIC, not generally recommended.





Globals Settings Non Reference & Reference Window

Globals			
Apply Multiplier to ISTD			
Apply Multiplier to Matrix Spike		1	
Apply Multiplier to Surrogate		1	
Apply Multiplier to Target		1	
Bracketing Type	None		
CC Maximum Elapsed Time In Hours			0.000
Correlation Window			2.000
Dynamic Background Subtraction			
Ignore Peaks Not Found			
Library Method			
Non Reference Window			0.250
Non Reference Window Type	Minutes		
Reference Library			
Reference Pattern Library			
Reference Window			0.750
Reference Window Type	Minutes		
Relative ISTD			
Standard Addition			

Extract full signal for baseline and noise. Restrict peak selection to smaller RT window.



Quantifier

	Name	TS	Scan	Type 🗠	ISTD Compound Name	ISTD Flag	ISTD Conc.	Time Reference Flag		
•	Fluorobenzene	1	Scan	ISTD	<none></none>	V	10.0000	V		Reference = ISTD + Time Reference
	Chlorobenzene-d5	1	Scan	ISTD	<none></none>	V	10.0000			
	1,4-Dichlorobenzene-d4	1	Scan	ISTD	<none></none>	V	10.0000			
	1,2-Dichloroethane-d4	1	Scan	Surrogate	Fluorobenzene		10.0000			
	Toluene-D8	1	Scan	Surrogate	Chlorobenzene-d5		10.0000			Non Reference = Everything else
	1,1-Dichloro-1-propene	1	Scan	Target	Fluorobenzene		10.0000			
	Dichlorodifluoromethane	1	Scan	Target	Fluorobenzene		10.0000			
	Chloromethane	1	Scan	Target	Fluorobenzene		10.0000			



Option to Display Reference RT and Window Compound Information > Properties > Retention time

Chose which reference points to show and in what color and style.





Globals Settings Reference Library



High level calibrator should be selected before entering Method Editor to obtain better quality spectra for the reference library from the sample.

The Reference Library is activated from Library > Setup Reference Library...

A reference library can be created from a calibrator or existing library and added to the quant method to aid in the identification of compounds.

Setup Reference Library	\times
O Obtain reference spectra from sample	
Obtain reference spectra from lookup library	
Lookup library:	
D:\MassHunter\Library\demo.l Browse.	
Create reference library at:	
D:\MassHunter\Data\QuantExamples\MS\VOA\VolatileOrganics.reflibrary Browse.	
OK Cancel	I



Globals Settings Reference Library




Globals Settings Relative ISTD

A method of semi quantitation.

It is a global parameter and is applied to every sample in the batch.

 $[Phe] = \frac{Intensity of Phe}{Intensity of D_5 Phe} x [D_5 Phe]$

Relative ISTD is a concept where the response factor of the ISTD is used for quantitation.

 $\frac{\textit{Response}}{\textit{ISTDResponse}}*\textit{ISTDConcentration}*\textit{ISTDRelativeMultipler} = Calculate@oncentration$



Globals Settings Standard Addition

Standard Addition is activated in Globals Setup in the Method Editor. The calibration curve is Linear, Ignore Origin and No Weighting. The non-spiked sample MUST precede the calibrators in the Batch Table. Quant assumes that the order samples are acquired are the order in which they are analyzed.

Globals					
Apply Multiplier to ISTD					
Apply Multiplier to Matrix Spike	\checkmark				
Apply Multiplier to Surrogate					
Apply Multiplier to Target					
Bracketing Type	None				
Correlation Window	2.000				
Dynamic Background Subtraction					
Ignore Peaks Not Found					
Library Method					
Non Reference Window	200.000				
Non Reference Window Type	Percent				
Reference Library	D:\MassHunter\Data\QuantE\VolatileOrganics.reflibrary.xml				
Reference Pattern Library					
Reference Window	80.000				
Reference Window Type	Percent				
Relative ISTD					
Standard Addition					

1	Ÿ	Name	Туре	Level
0	٣	Sample 1	Sample	
0	٣	Sample 1 Spike 1	Cal	L1
0	٣	Sample 1 Spike 2	Cal	L2
0	٣	Sample 2	Sample	
0	٣	Sample 2 Spike 1	Cal	L1
0	٣	Sample 2 Spike 2	Cal	L2

Order in Batch Table is imperative. Sample, Cal1, Cal 2....



Training Resources

Training resources that are available.

Convenient Training ⊾

Our team of industry experts delivers a quality learning experience with a high degree of flexibility to fit the needs of your lab – in our classrooms, at your site or online:

- Classroom Training Introductory level to in-depth, hands-on training for lab hardware or software.
- Customized On-Site Training Effective learning environment designed to achieve operational excellence and employee development without the need to travel.
- Online From foundation to expert offerings when and where you need it at your own pace



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Upgraded customer experience:

 Search and find courses that meet your interests and needs in the format they require

Introduce new eLearning capabilities:

- Recorded and video-based learning
- Virtual online classes

Expanded portfolio:

- Foundational subjects
- Intermediate subjects
- Advanced subjects
- Workflow and applications

Helping customers:

- Educate your employees on Agilent instruments and software
- From new hires to the most seasoned scientists







Questions on today's material... Thank you for your attention.



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