



Agilent MassHunter Quantitative Data Analysis

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

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

Review

Three major views in MassHunter Quantitative Analysis.

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

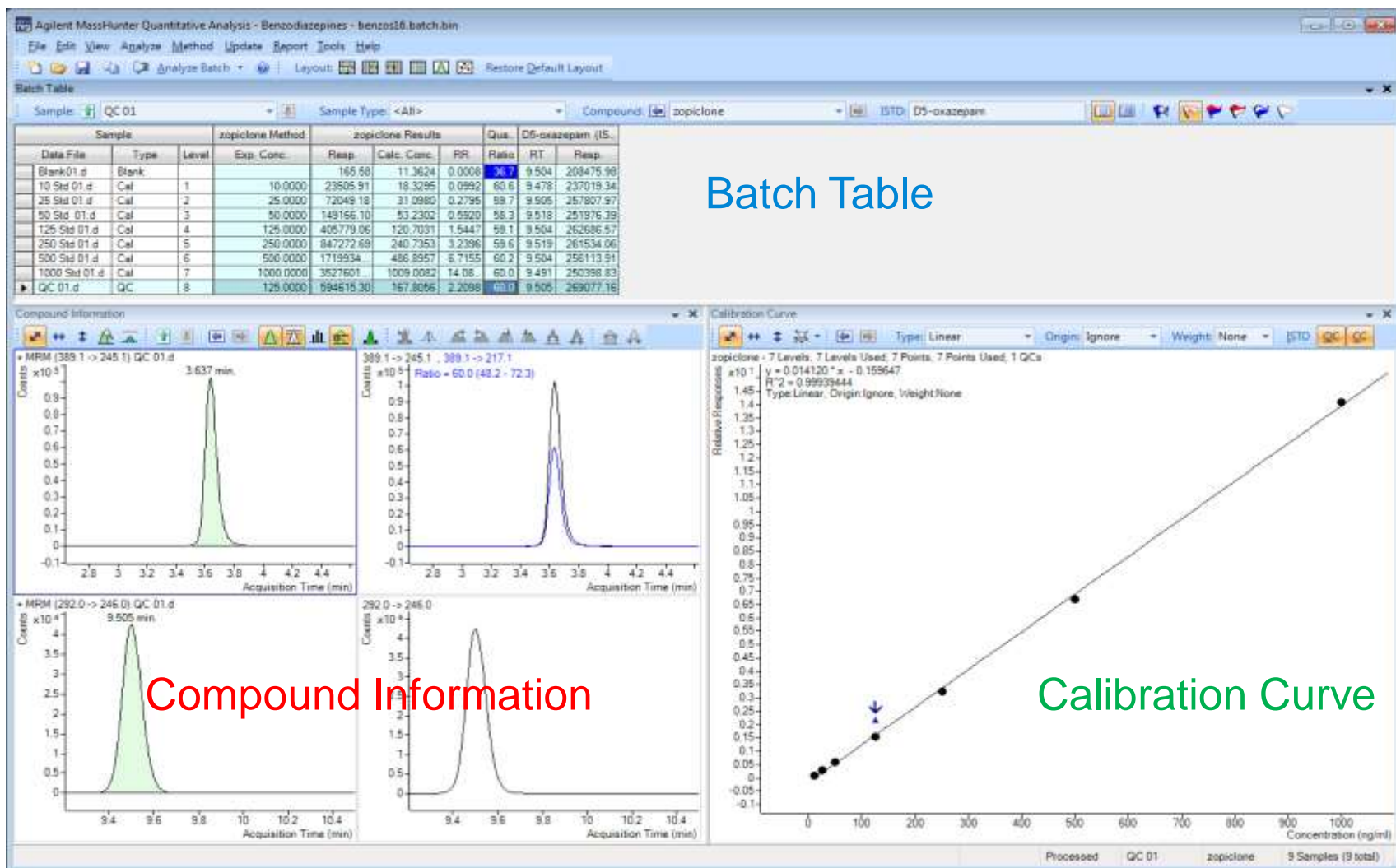
Handling MS/MS data QQQ and QTOF.

Handling accurate mass data.



MassHunter Quantitative Software

Batch-at-a-Glance View



MassHunter Quantitative Software

Method Editor View

Method > Edit menu or F10 key

Method Table

Sample
Information

Compound Information

Method
Tasks

Method Update Report Tools Help

New

Open

Append

Edit

Validate

Save

Save As...

Exit

Method Setup Tasks

Manual Setup Tasks

Outlier Setup Tasks

Advanced Tasks

Copy Calibration Levels To...

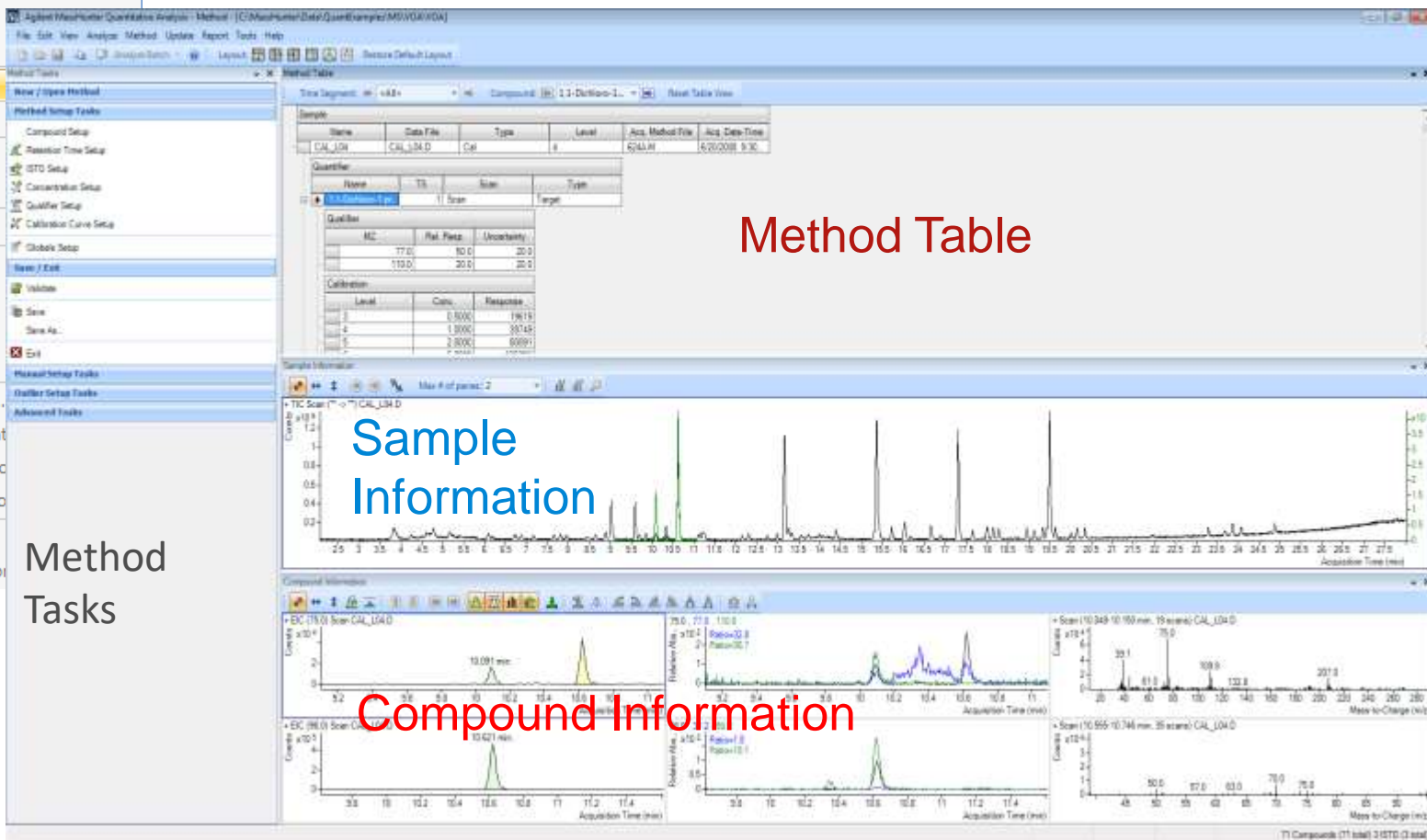
Average Calibration Replicates

Create Levels from Calibration

Import Calibration Levels from

Setup Reference Library...

Setup Reference Pattern Library



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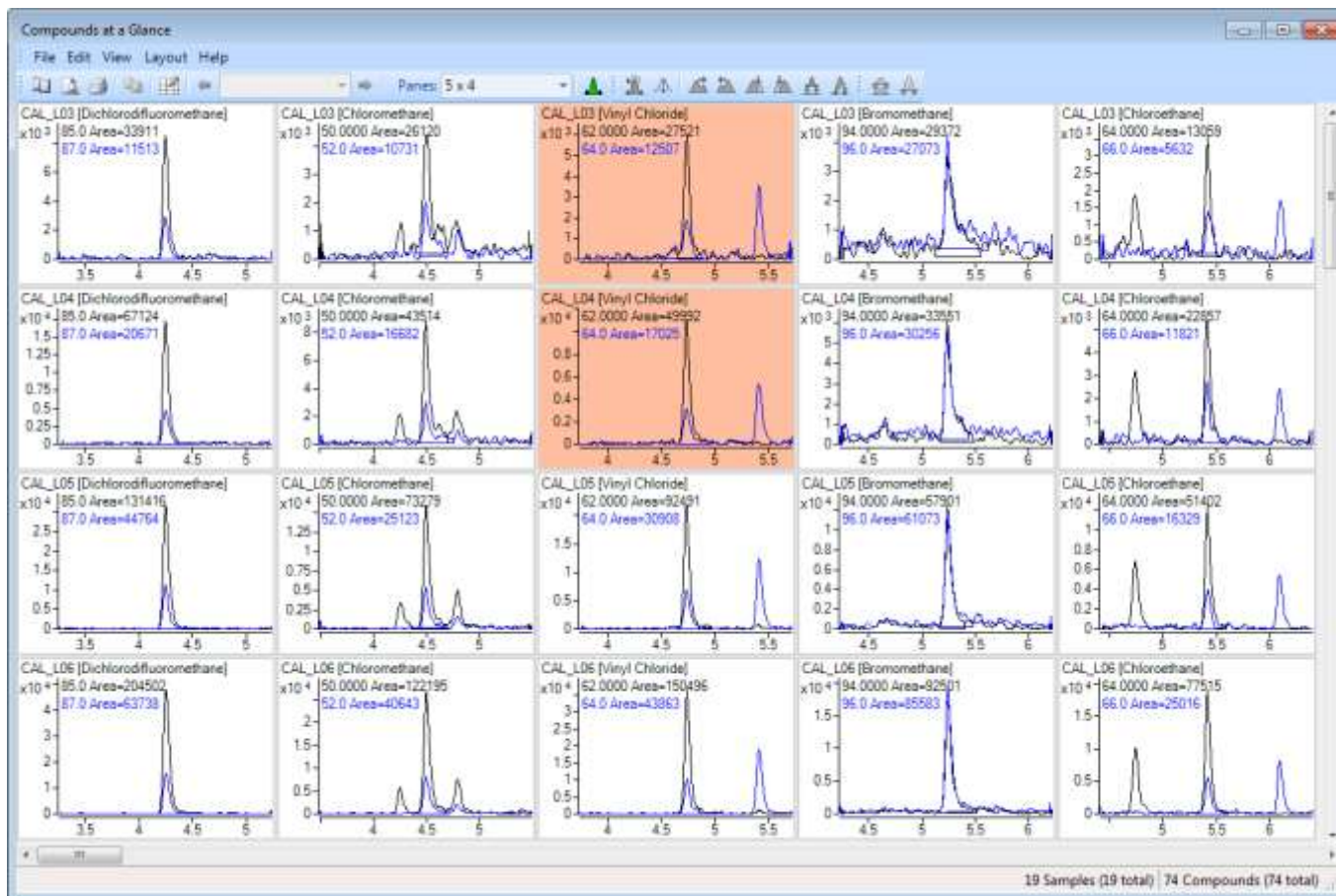
9/13/2017

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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).

Quantifier							
Name	TS	Scan	Type	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 Units
PPM
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

Quantifier									
Name	TS	Transition	Scan	Type	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

Batch Table

Sample:  CAL_L08  Sample Type: <All> Compound:  Trichlorofluoromethane 

Sample							Trichlorofluoromethane	Trichlorofluoromethane				Trichlorofluoromethane	Qualifier...
?	▼	Name	Data File	Type	Level	Acq. Date-Time	Exp. Conc.	RT	Resp.	MI	Ca		
	!	CAL_L03	CAL_L03.D	Cal	3	6/20/2008 5:53 PM	0.5000	6.108	58365			Acetone	7
	!	CAL_L04	CAL_L04.D	Cal	4	6/20/2008 6:30 PM	1.0000	6.092	90617			1,1-Dichloroethene	1
	!	CAL_L05	CAL_L05.D	Cal	5	6/20/2008 7:06 PM	2.0000	6.097	173426			t-Butyl Alcohol	3
	!	CAL_L06	CAL_L06.D	Cal	6	6/20/2008 7:44 PM	5.0000	6.097	248633			Methylene Chloride	0
	!	CAL_L07	CAL_L07.D	Cal	7	6/20/2008 8:21 PM	10.0000	6.097	830216			Carbon Disulfide	9
▶	!	CAL_L08	CAL_L08.D	Cal	8	6/20/2008 9:04 PM	15.0000	6.097	1347631			trans-1,2-Dichloroethene	1
	!	CAL_L09	CAL_L09.D	Cal	9	6/20/2008 9:41 PM	20.0000	6.092	1781882			2-Methoxy-2-methylpropane	0
	!	CAL_L10	CAL_L10.D	Cal	10	6/20/2008 10:19 PM	30.0000	6.092	2773495				7
	!	CAL_L11	CAL_L11.D	Cal	11	6/20/2008 10:57 PM	40.0000	6.097	3830330				0

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 + Down Next Compound = Alt + Right

Previous Sample = Alt + Up Previous Compound = Alt + Left

Compound list are frequently long, try the **Compound** drop down list to go directly to the desired compound.

Batch Table

Alphabetizing the Compound List

The screenshot shows the 'Batch Table' application window. At the top, there are dropdown menus for 'Sample:' (set to 'CAL_L08'), 'Sample Type:' (set to '<All>'), and 'Compound:' (set to 'Trichlorofluoromethane'). Below these is a table with columns 'Sample', 'Trichloroflu...', and 'Trichloroflu...'. The 'Trichloroflu...' column is expanded, showing a list of compounds: Acetone, 1,1-Dichloroethene, t-Butyl Alcohol, Methylene Chloride, Carbon Disulfide, trans-1,2-Dichloroethene, and 2-Methoxy-2-methylpropane. A context menu is open over the table, with 'Arrange Compounds By' selected. This menu has a sub-menu with the following options: Name (checked), Retention Time, Mass, ISTD, Compound Group, ID, and User Defined. Other options in the main menu include 'Add/Remove Columns...', 'Restore Default Columns', 'Reset Sort', 'Fill Down', 'Lock Sample/Compound Columns', 'Flat Table', 'Nested Table (Horizontal)', 'Nested Table (Vertical)', 'Compound Table', 'Single Compound/Sample View', 'Multiple Compounds/Samples View', 'Disable Calibration Points...', 'Print...', 'Print Preview...', and 'Properties...'. The 'Print...' option has a keyboard shortcut 'Ctrl+P'.

From within the Batch Table right click, select **Arrange Compounds By > Name**

Tip: Alphabetize the Compound List for faster compound access.



Batch Table

Messages and Outliers

Batch Table

Sample: CAL_L10 Sample Type: <All> Compound: Dichlorodifluoromethane ISTD: Fluorobenzene

Sample							Dichlorod...	Dichlorodifluoromethane Results						Qualifier...	Fluorobenzene (L		Qualifie...	Qualifie...				
		Name	Data File	Type	Level	Acq. Date-Time	Sample Group	Exp. Conc.	RT	Resp.	MI	Calc. Conc.	Final Conc.	Accuracy	Ratio	MI	RT	Resp.	Ratio	MI	Ratio	MI
		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	
		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	
		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	
		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	
		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	
		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	
		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	

Select Outliers for Display

Select
Outliers
for Display

Red Outlier – High
(above upper limit)

Blue Outlier – Low
(below lower limit)



Messages

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

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

Hover cursor over the outlier or message to display details



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Batch Table Layout Modification

Add/Remove/Move Columns

Batch Table

Sample: CAL_L03 Sample Type: <All> Compound: Chloroform ISTD: Fluorobenzene

Sample							Chloroform Results							Qualifier...		Qualifier...		Fluorobenzene (L...		Qualifier...		Qualifier...	
?		Name	Data File	Type	Level	Acq. Date-Time	Exp. Conc.	RT	Resp.	MI	Calc. Conc.	Final Conc.	Accuracy	Ratio	MI	Ratio	MI	RT	Resp.	Ratio	MI	Ratio	MI
		CAL_L03	CAL_L03.D	Cal	2	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	
		CAL_L03				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	
		CAL_L03				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	
		CAL_L03				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	
		CAL_L03				008 8:21 PM	10.0000	8.891	419785														
		CAL_L03				008 9:04 PM	15.0000	8.891	649647														
		CAL_L03				008 9:41 PM	20.0000	8.891	893838														
		CAL_L03				008 10:19 PM	30.0000	8.891	1369093														

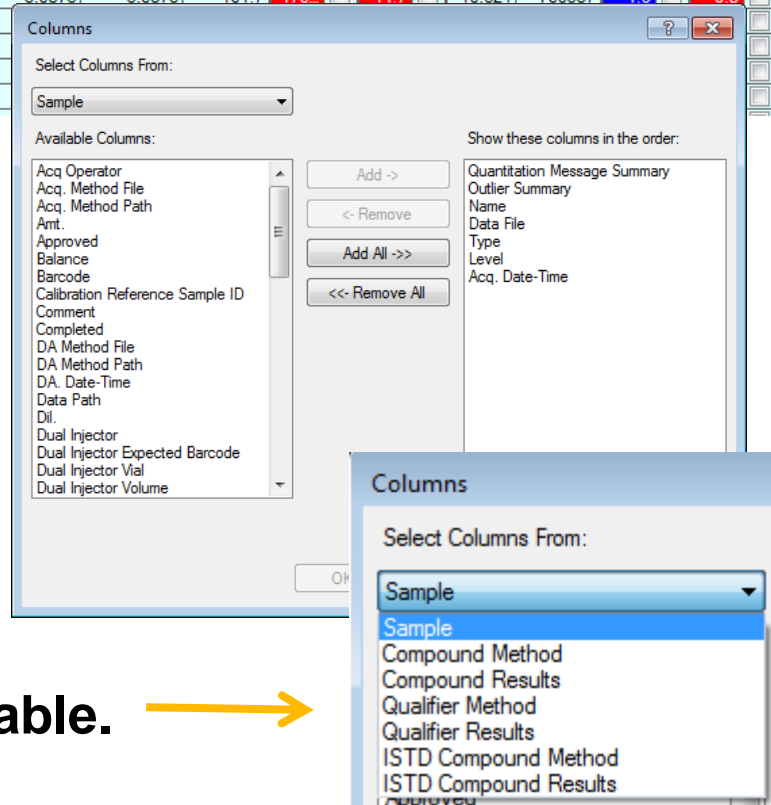
Context menu options:

- Add/Remove Columns...
- Restore Default Columns
- Reset Sort
- Fill Down
- Lock Sample/Compound Columns

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.



Select correct table. →

Batch Table Layout Modification

Single and Multiple Compound Modes

Single Compound Mode

Flat Table compounds across the top.

Flat Table compounds across the top.

Multiple Compound Mode

[illegible]

Batch Table Layout Modification

Compound Table Modes

Agilent MassHunter Quantitative Analysis (for GCMS) - VOA - voa_example.batch.bin

File Edit View Analyze Method Update Report Tools Help

Analyze Batch Layout: Restore Default Layout

Batch Table

Sample: QC_L06 Sample Type: <All> Compound: Dichlorodifluoromethane ISTD: Fluorobenzene

Compound Method		QC_L06						Qualifie...		Qualifie...		ISTD Method		ISTD Results		ISTD Q...		ISTD Q...	
Name	RT	Resp.	MI	Calc. Conc.	Final Conc.	Accuracy	Ratio	MI	Ratio	MI	Name	RT	Resp.	Ratio	MI	Ratio	MI	Ratio	MI
1,1-Dichloro-1-propene	10.0...	243136		4.7578	4.7578	95.2	31.6		34.5		Fluorobenzene	10.620	1288192	1.7		10.5			
Dichlorodifluoromethane	4.247	211200		2.9037	2.9037	58.1	32.1				Fluorobenzene	10.620	1288192	1.7		10.5			
Chloromethane	4.498	194192		4.7682	4.7682	95.4	31.8				Fluorobenzene	10.620	1288192	1.7		10.5			
1,4-Dichlorobenzene	19.5...	458056		5.2756	5.2756	105.5	64.6		43.9		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			
1,2,4-Trichlorobenzene	23.2...	259025		5.2625	5.2625	105.3	98.9		29.6		1,4-Dichlorobenzene-d4	19.504	619825	57.6		41.8			
Bromomethane	5.251	116516		3.9551	3.9551	79.1	98.4				Fluorobenzene	10.620	1288192	1.7		10.5			
Chloroethane	5.421	135709		5.1361	5.1361	102.7	37.1				Fluorobenzene	10.620	1288192	1.7		10.5			
Naphthalene	23.6...	519274		6.3779	6.3779	127.6	12.0		10.9		1,4-Dichlorobenzene-d4	19.504	619825	57.6		41.8			
Hexachlorobutadiene	23.8...	227798		5.1452	5.1452	102.9	60.0		57.9		1,4-Dichlorobenzene-d4	19.504	619825	57.6		41.8			
Trichlorofluoromethane	6.097	377098		3.8308	3.8308	76.6	65.4		10.6		Fluorobenzene	10.620	1288192	1.7		10.5			
Acetone	6.190	170682		5.2692	5.2692	105.4	27.5				Fluorobenzene	10.620	1288192	1.7		10.5			
1,1-Dichloroethene	6.719	254894		4.7979	4.7979	96.0	61.3		38.5		Fluorobenzene	10.620	1288192	1.7		10.5			
1,2,3-Trichlorobenzene	24.0...	257316		5.5208	5.5208	110.4	10...		29.7		1,4-Dichlorobenzene-d4	19.504	619825	57.6		41.8			
Methylene Chloride	6.877	182447		5.1839	5.1839	103.7	64.0				Fluorobenzene	10.620	1288192	1.7		10.5			
Carbon Disulfide	7.178	69556		5.8374	5.8374	116.7	69.6				Fluorobenzene	10.620	1288192	1.7		10.5			
trans-1,2-Dichloroethene	7.663	165832		5.0298	5.0298	100.6	14...		63.8		Fluorobenzene	10.620	1288192	1.7		10.5			
2-Methoxy-2-methylpropane	7.810	439953		5.1203	5.1203	102.4	15.9				Fluorobenzene	10.620	1288192	1.7		10.5			
1,1-Dichloroethane	7.952	303201		5.3097	5.3097	106.2	35.0		6.3		Fluorobenzene	10.620	1288192	1.7		10.5			
Vinyl Acetate	8.056	130420		4.5381	4.5381	90.8	8.9				Fluorobenzene	10.620	1288192	1.7		10.5			
2-Butanone (MEK)	8.438	229534		5.7318	5.7318	114.6	26.2		16.5		Fluorobenzene	10.620	1288192	1.7		10.5			

Add/Remove Columns...
 Add Column
 Restore Default Columns
 Auto Fit Columns Ctrl+U
 Reset Sort
 Lock Sample/Compound Columns
 Flat Table
 Nested Table (Horizontal)
 Nested Table (Vertical)
 Compound Table
 Single Compound/Sample View
 Multiple Compounds/Samples View
 Arrange Compounds By
 Print... Ctrl+P
 Print Preview...

Compound Table lists by compound rather than sample.

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

Batch Table

Compounds Groups

Batch Table

Sample: ↑ CAL_L08 ↓ Sample Type: <All> Compound: ← Trichlorofluoromethane →

Sample							Trichloroflu...	Trichloroflu				Trichlorofluoromethane	lifier...
?	▼	Name	Data File	Type	Level	Acq. Date-Time	Exp. Conc.	RT	Resp.	MI	C	Acetone	MI
?	▼	CAL_L03	CAL_L03.D	Cal	3	6/20/2008 5:53 PM	0.5000	6.108	58365			1,1-Dichloroethene	7
?	▼	CAL_L04	CAL_L04.D	Cal	4	6/20/2008 6:30 PM	1.0000	6.092	90617			t-Butyl Alcohol	1
?	▼	CAL_L05	CAL_L05.D	Cal	5	6/20/2008 7:06 PM	2.0000	6.097	173426			Methylene Chloride	3
	▼	CAL_L06	CAL_L06.D	Cal	6	6/20/2008 7:44 PM	5.0000	6.097	248633			Carbon Disulfide	0
	▼	CAL_L07	CAL_L07.D	Cal	7	6/20/2008 8:21 PM	10.0000	6.097	830216			trans-1,2-Dichloroethene	9
▶	▼	CAL_L08	CAL_L08.D	Cal	8	6/20/2008 9:04 PM	15.0000	6.097	1347631			2-Methoxy-2-methylpropane	1
	▼	CAL_L09	CAL_L09.D	Cal	9	6/20/2008 9:41 PM	20.0000	6.092	1781882				0
	▼	CAL_L10	CAL_L10.D	Cal	10	6/20/2008 10:19 PM	30.0000	6.092	2773495				7
	▼	CAL_L11	CAL_L11.D	Cal	11	6/20/2008 10:57 PM	40.0000	6.097	3838336				

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

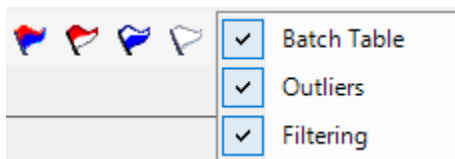
Look at parent compound and metabolites.

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

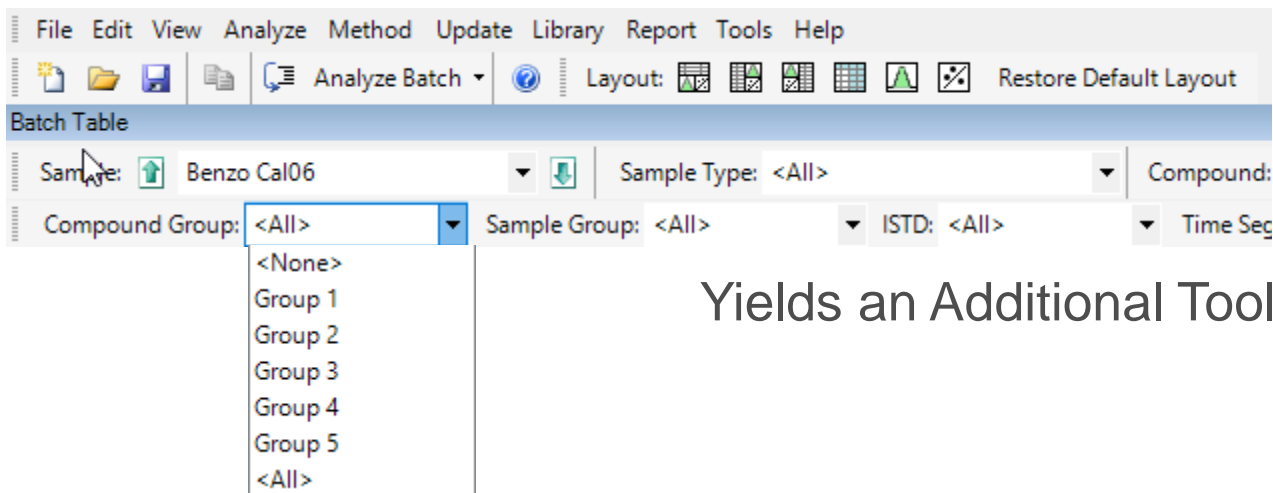
Compound groups are generated in the Method Editor.

Batch Table

Compounds Groups



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



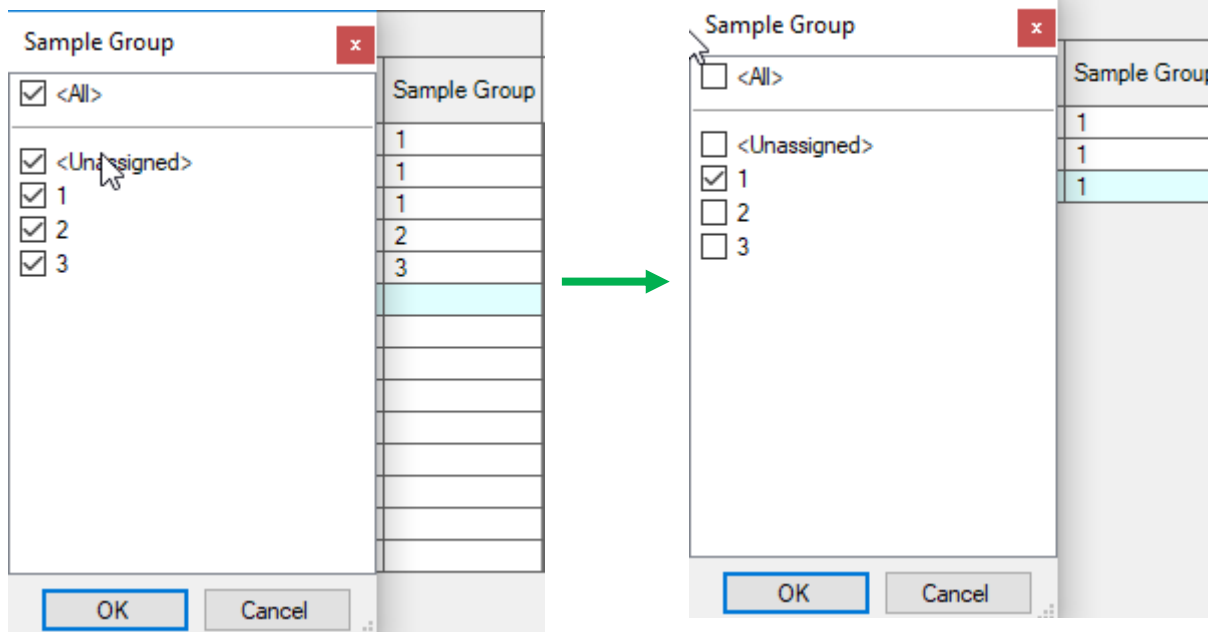
Yields an Additional Toolbar.

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

Format Columns

How to change the number of decimal places.

Alter number formats

- 1) Exponential
- 2) Fixed point
- 3) General

Alter Date formats

Agilent MassHunter Quantitative Analysis - VOA - VolatileOrganics.batch.bin

File Edit View Analyze Method Update Report Tools Help

Analyze Batch Lay

Batch Table

Sample: CC_L07

Compound: 1,2-Dichloroethane

1,2-Dichloroethane Results

RT	Resp.	MI	Calc. Conc.	Final Conc.
9.699	27066		0.3190	0.3190
9.693	53608		0.8626	0.8626
9.693	106105		1.8873	1.8873
9.698	167472		5.0515	5.0515
9.698	547595		10.3761	10.3761
9.693	842997		15.1102	15.1102

Formats

Commonly used

Format pattern Precision

MZ Fixed point 1

RT Fixed point 3

Final Conc. Fixed point 4

All other numbers

Name	Format Pattern	Precision
Category: Concentration		
Calc. Conc.	Fixed point	1
Conc.	Fixed point	4
Custom Calc.	Fixed point	4
Dil. High Conc.	Fixed point	4
Exp. Conc.	Fixed point	4

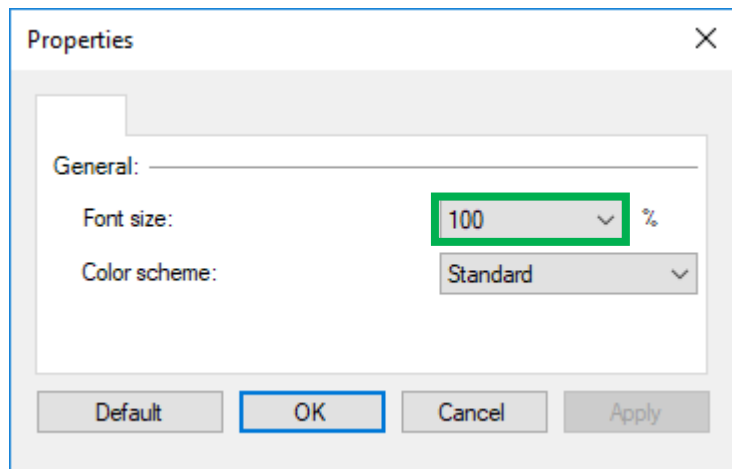
All other date/time

Name	Format
Category: DateTime	
Acq. Date-Time	2/25/2012 5:40 PM
Analysis Time Stamp	2/25/2012 5:40 PM

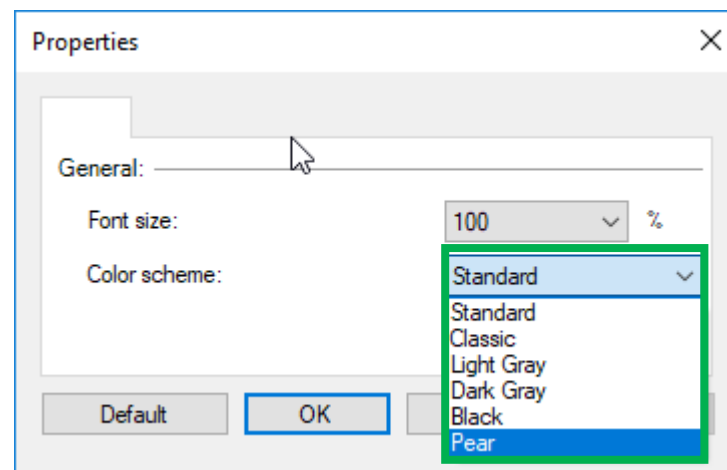
Default OK Cancel Apply

Batch Table Layout Modification Properties

Change the Font size



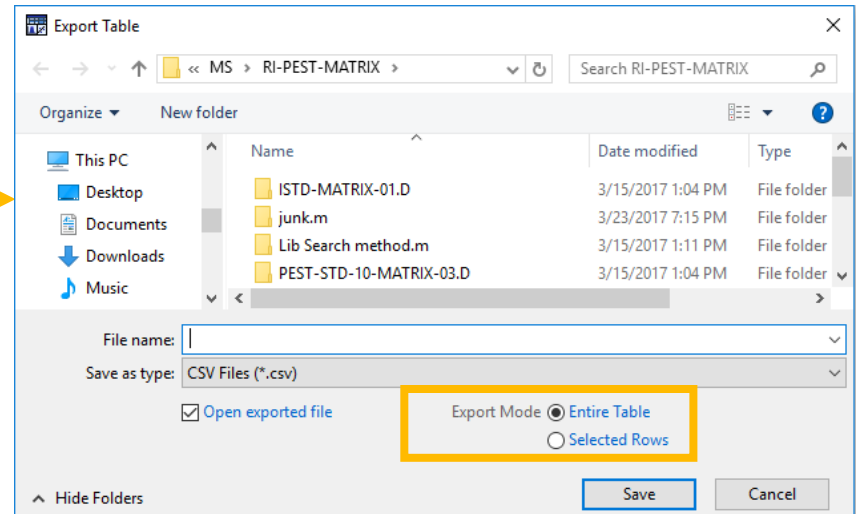
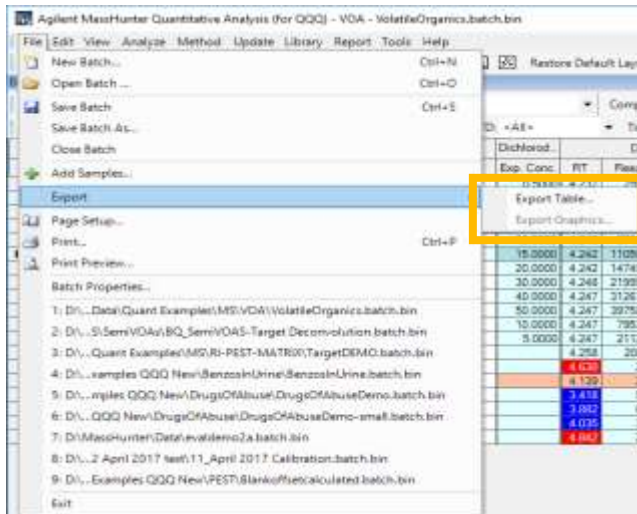
Change the Color scheme



NEW FEATURE!



Export Batch Table



Sample	Data File	Type	Label	Acq. Date/Time	Exp. Conc.	RT	Reten. MI	Calc. Conc.	Final Conc.	Accuracy	Ratio MI	RT	Reten. MI	Ratio MI	Ratio MI
CAL_103	CAL_103.D	Cal	5	6/20/2008 11:53	0.5	4.237	2074.96	0.02187558	0.00160	0.37555	33.6	10.621	1344419	1.96	2.59
QC_104	QC_104.D	QC	6	6/20/2008 18:50	5	4.247	211200.4	2.54215754	2.54215754	90.84315	32.7	10.62	1288192	1.69	10.70
CAL_104	CAL_104.D	Cal	4	6/20/2008 12:30	1	4.242	60996.94	0.01342523	0.01342523	87.34252	30.2	10.621	1183924	1.81	10.71
SAMPLE02	SAMPLE02.D	Sample		6/20/2008 21:22		3.418	518.7885	0	0		125	10.628	1138831	2.22	10.61
SAMPLE03	SAMPLE03.D	Sample		6/20/2008 22:00		3.882	902.477	0	0		161	10.621	1036288	2.17	11.1
SAMPLE04	SAMPLE04.D	Sample		6/20/2008 22:38		4.555	353.4815	0	0		95.8	10.621	990490.4	2.45	11.8
SAMPLE05	SAMPLE05.D	Sample		6/20/2008 22:48		4.139	208.89	0	0		2	10.621	1165443	1.96	10.7
SAMPLE06	SAMPLE06.D	Sample		6/20/2008 23:16		4.842	286.347	0	0		183	10.621	1205617	2.09	11.3
Blank02	BLANK02.D	Blank		6/20/2008 23:07		4.83	266.178	0	0		2	10.621	1058821	1.93	10.7
CAL_106	CAL_106.D	Cal	6	6/20/2008 13:44	5	4.258	198054.3	4.0073302	4.0073302	93.15473	31	10.621	100587.4	1.59	9.62

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.

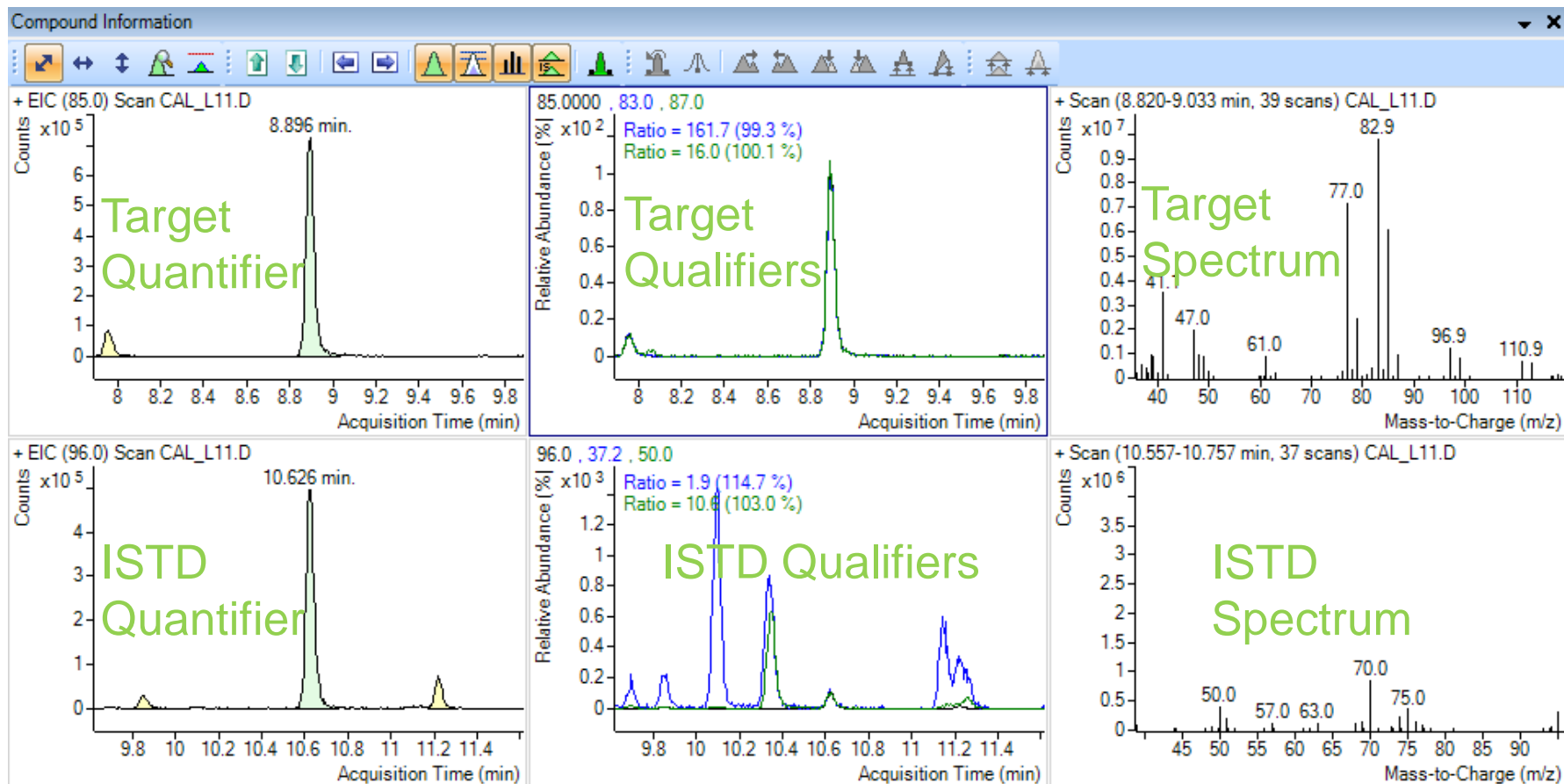


Let's take a moment
for questions on Batch
Table navigation.

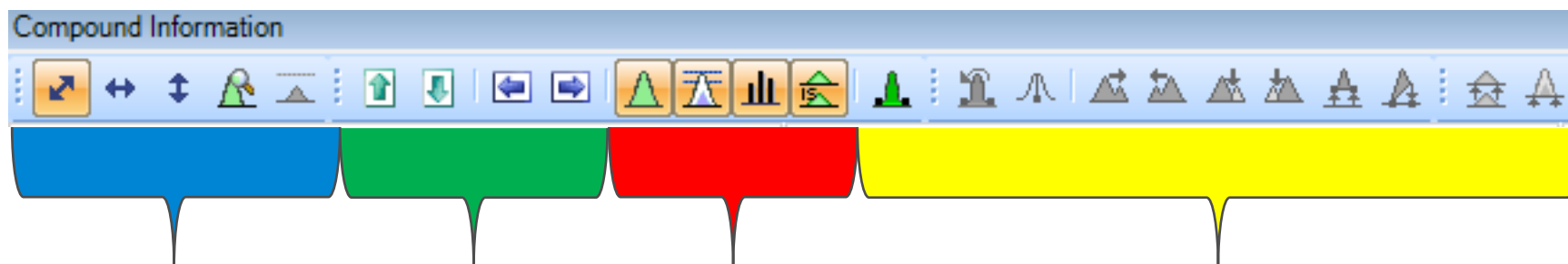
Next up:
Compound Information

Compound Information

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



Compound Information - Toolbar



Un-zooms,
Peak scaling,
Auto Scales x
and y axes

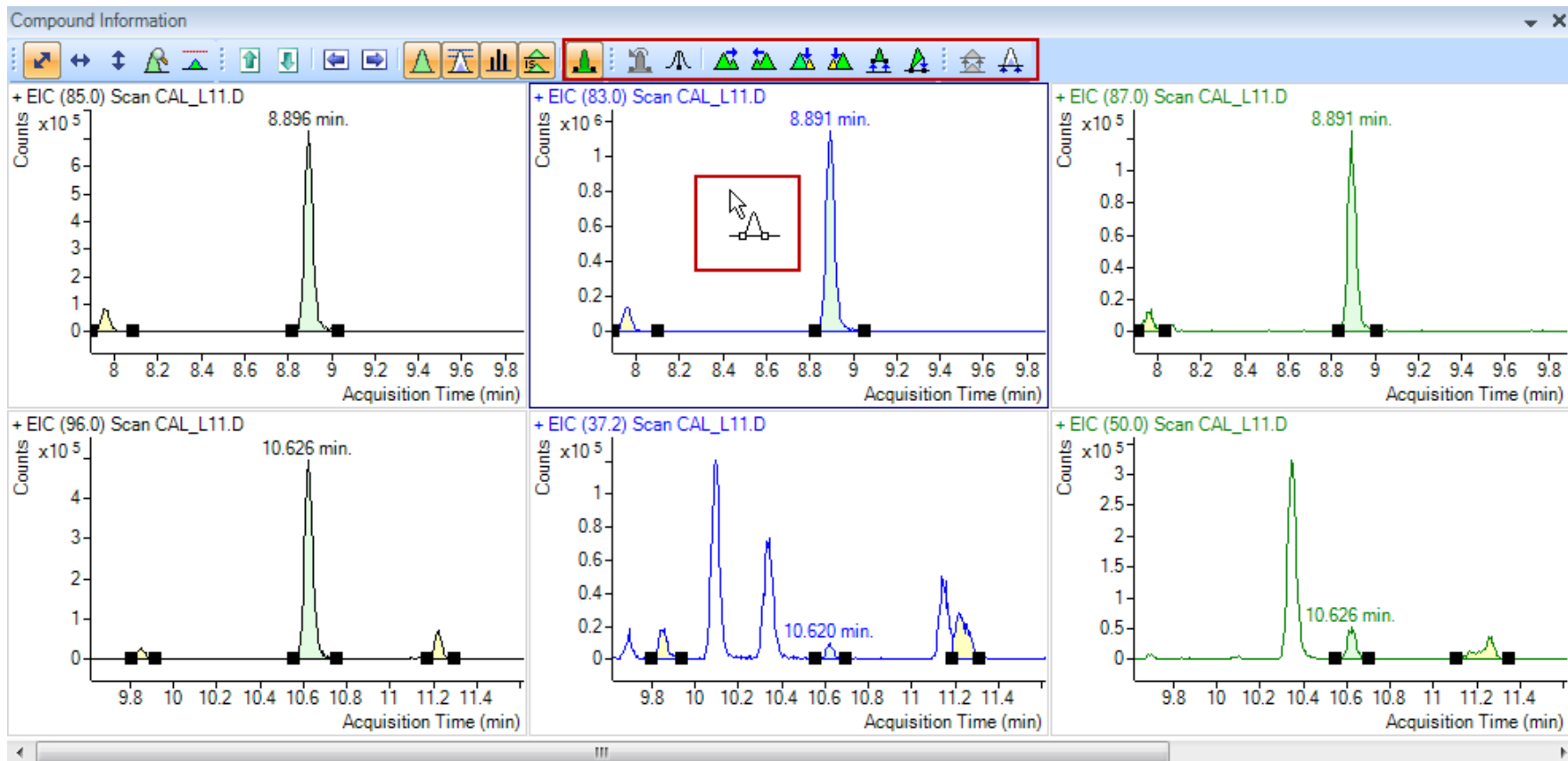
Sample
and
Compound
Navigation
Next /
Previous

Display/Hide
Target,
Qualifiers,
Spectra,
ISTD

Manual Integration
Functions



Manual Integrations and MI Toolbar

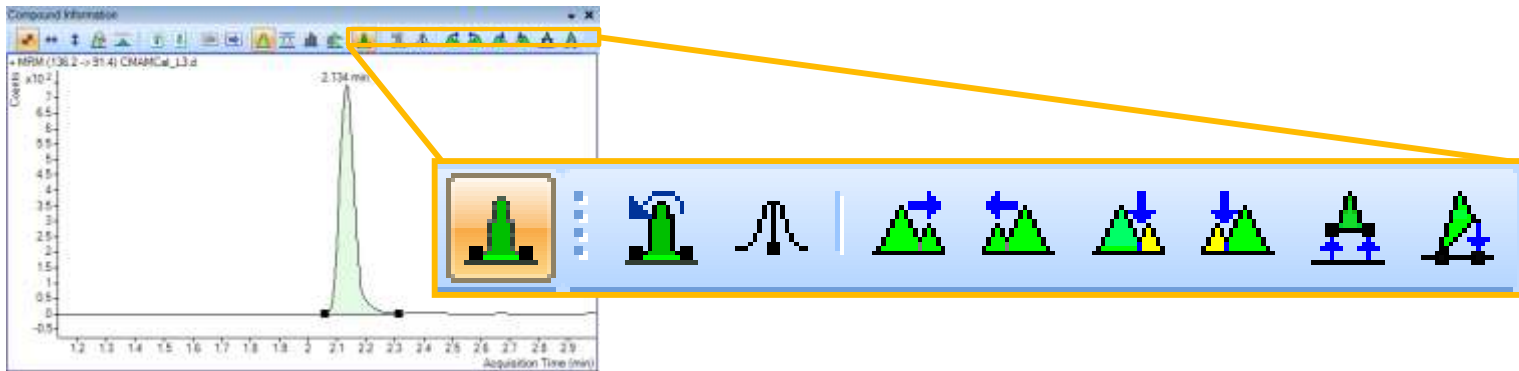


Click on the Manual Integration icon to place Compound Information in Manual Integration mode.

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



Manual Integration Toolbar



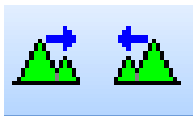
Enable Manual Integration – this tool activates the manual integration toolbar.



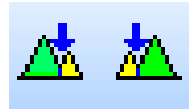
Clear Manual Integration – this tool becomes active once a manual integration is present.



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.



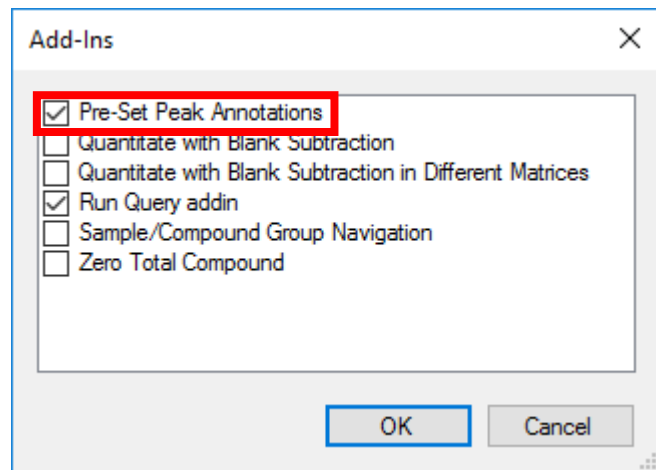
Drop Baseline – this tool finds the lowest end of the peak, then drops the baseline on the other side of the peak from it, thereby creating a flat baseline that avoids negative area.



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.

```
<?xml version="1.0" encoding="utf-8" ?>
<AnnotationButtons>
  <Button ID="NI" DisplayText="NI" Value="NI" Tooltip="The peak was not integrated at all by the computer software."/>
  <Button ID="LT" DisplayText="LT" Value="LT" Tooltip="The peak in question was inappropriately integrated to an area less than what it should be (e.g., Peak area was cut)."/>
  <Button ID="GT" DisplayText="GT" Value="GT" Tooltip="The peak in question was inappropriately integrated to an area greater than what it should be (e.g., Peak tailing)."/>
  <Button ID="BA" DisplayText="BA" Value="BA" Tooltip="The baseline had to be adjusted correctly by the analyst."/>
  <Button ID="CO" DisplayText="CO" Value="CO" Tooltip="The analyst had to split two co-eluting peaks apart that were not (or could not be) separated by the computer system."/>
  <Button ID="RT" DisplayText="RT" Value="RT" Tooltip="The retention time for the peak in question has shifted from the expected retention time."/>
  <Button ID="INT" DisplayText="INT" Value="INT" Tooltip="There was electronic interference (e.g., Noise)."/>
</AnnotationButtons>
```

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

Available Columns:

Accuracy Max. % Dev.
Agilent ID
Alternative Peak Criteria
Alternative Peak ID
Amt. Limit High
Amt. Limit Low
Area CF
Area Cor. m/z
Area Correction Selected MZ
Avg. RF
Avg. RF RSD
Avg. RRT
Blank Resp. Offset
Calibration Range Filter
Capacity Factor Limit
CAS#
CAV

Add ->

<- Remove

Add All ->>

<<- Remove All

Show these columns in the order:

Exp. Conc.
RT
User Annotation

Move Up

Move Down

OK

Reset

Default

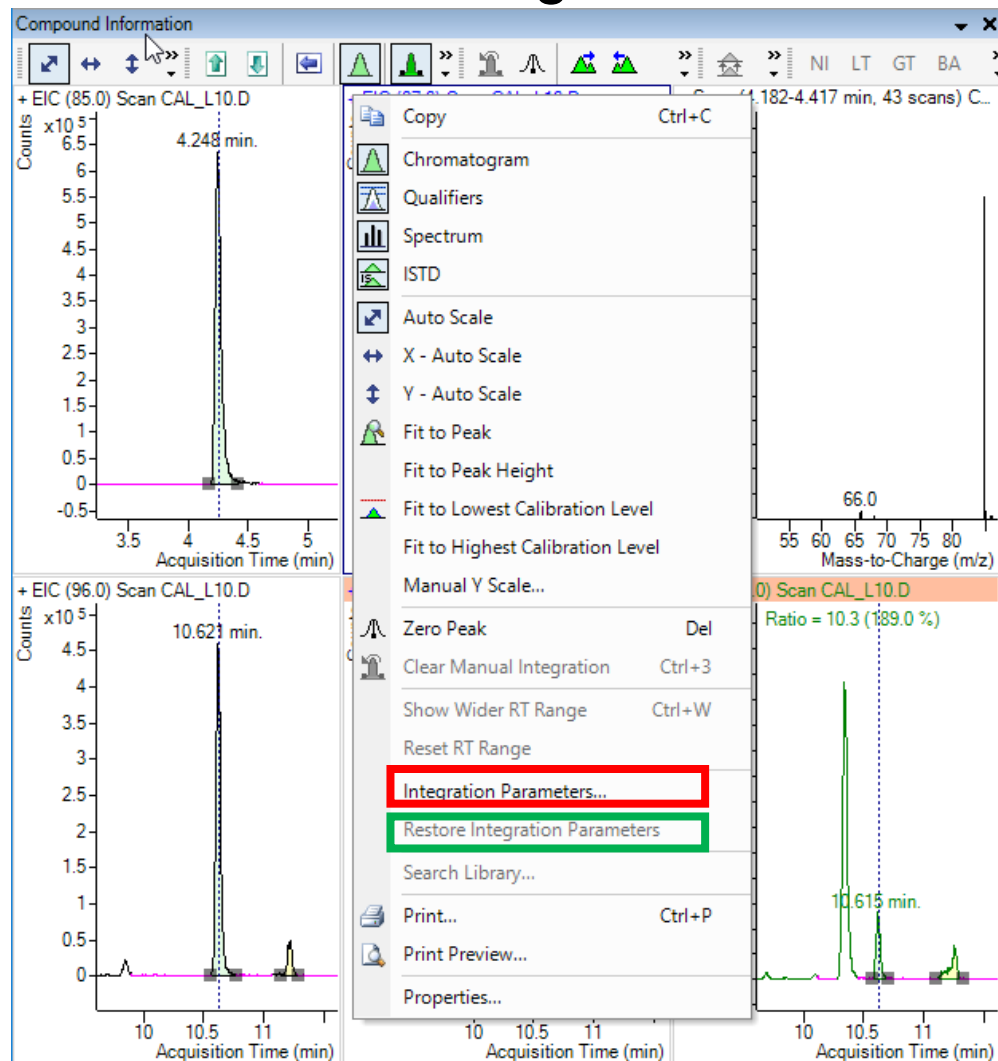
Cancel

Dichlorodifluoromethane Method			Dichlorodifluoromethane Results				
Exp. Conc.	RT	User Annotation	RT	Resp.	MI	Calc. Conc.	Final Conc.
0.5000	4.249	NI	4.237	22897	<input checked="" type="checkbox"/>	0.0000	0.0000
1.0000	4.249	LT	4.242	51949	<input checked="" type="checkbox"/>	0.3941	0.3941
2.0000	4.249	GT	4.247	98928	<input checked="" type="checkbox"/>	1.1534	1.1534
5.0000	4.249	BA	4.307	-3978	<input checked="" type="checkbox"/>	0.0000	0.0000
10.0000	4.249	CO	4.248	495112	<input checked="" type="checkbox"/>	7.4664	7.4664
15.0000	4.249	RT	4.406	-90142	<input checked="" type="checkbox"/>	0.0000	0.0000
20.0000	4.249	INT	4.242	1149283	<input checked="" type="checkbox"/>	16.0929	16.0929
30.0000	4.249		4.248	2199968	<input type="checkbox"/>	29.6758	29.6758

The MI flag is checked in the Compound 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.



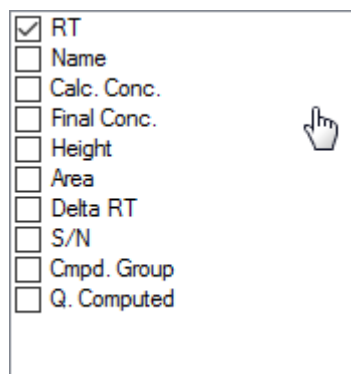
Compound Information Context Menu Properties

Properties allows for customization of the display.

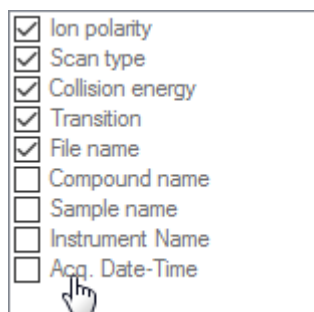
Can change Fill colors.

Can change Peak labels.

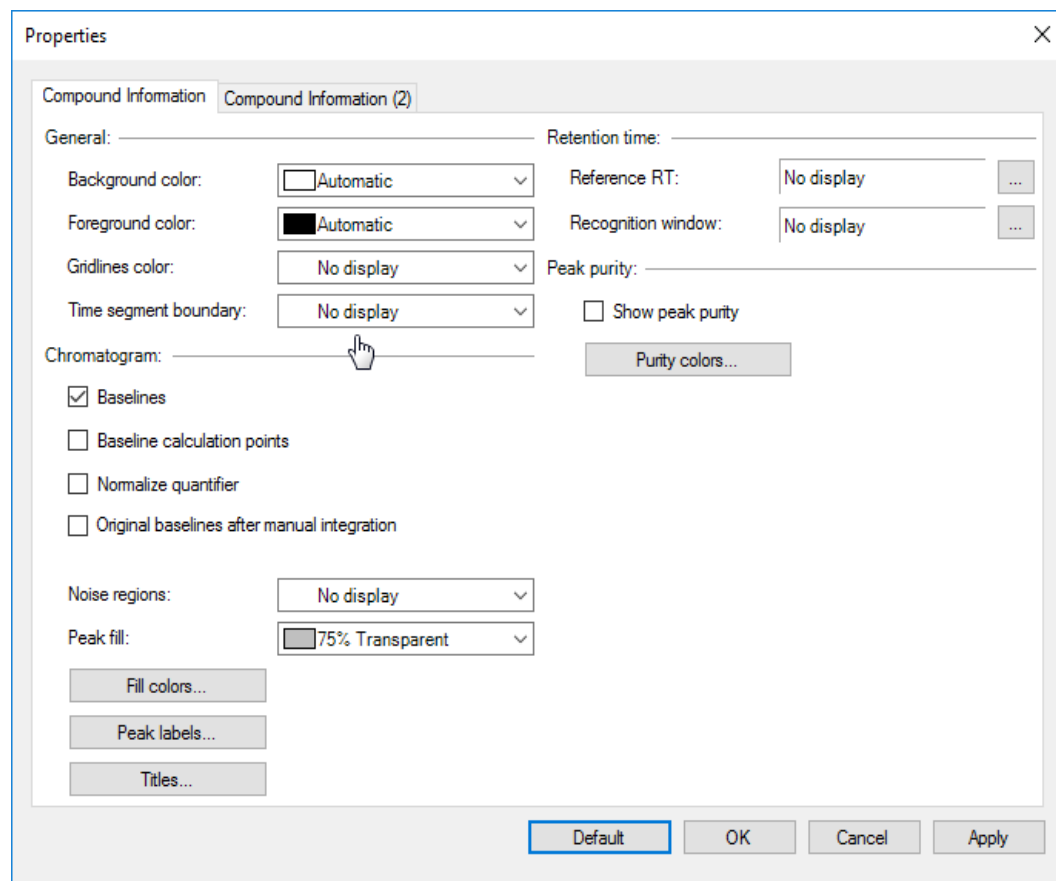
Can change Titles.



- ☒ RT
- ☐ Name
- ☐ Calc. Conc.
- ☐ Final Conc.
- ☐ Height
- ☐ Area
- ☐ Delta RT
- ☐ S/N
- ☐ Cmpd. Group
- ☐ Q. Computed



- ☒ Ion polarity
- ☒ Scan type
- ☒ Collision energy
- ☒ Transition
- ☒ File name
- ☐ Compound name
- ☐ Sample name
- ☐ Instrument Name
- ☐ Acq. Date-Time



Properties

Compound Information Compound Information (2)

General:

Background color: Retention time:

Foreground color: Reference RT:

Gridlines color: Recognition window:

Time segment boundary: Peak purity: ☐ Show peak purity

Chromatogram: Purity colors...

☒ Baselines

☐ Baseline calculation points

☐ Normalize quantifier

☐ Original baselines after manual integration

Noise regions:

Peak fill:

Fill colors...

Peak labels...

Titles...

Default OK Cancel Apply



Compound Information

Context Menu Properties

Properties

Compound Information Compound Information (2)

Qualifiers: Spectrum:

☒ Normalize qualifiers ☒ Reference spectrum

☒ Annotations ☒ Reference library source

Qualifier colors... ☐ Reference pattern spectrum

Uncertainty band: No display ☐ Override spectrum

Fill peaks: ☒ Show match scores

☒ Fill out-of-limits qualifier peaks ☒ Show mass indicators

☐ Fill all qualifier peaks

☐ No qualifier peak fill

☐ Fill target peaks

Manual integration: ☒ Show baseline start/end boxes

Fill transparency: 75% Transparent Max. # of panes per row: 3

Response ratio label: Ratio and percent of expected ratio

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

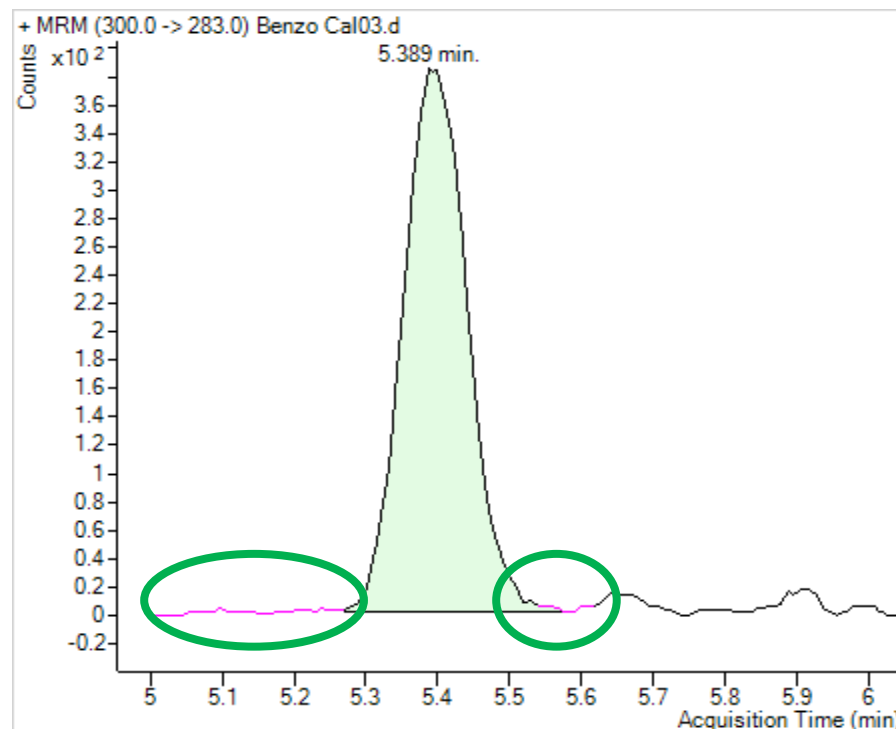
Five algorithms are available

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.

Peak-to-Peak
Peak-to-Peak from Drift
ASTM
RMS
Auto-RMS





Let's take a moment
for questions on
Compound Information

Next up:
Calibration Curve and
Curve Fit Assistant

Calibration Curve

View ISTD Responses ■

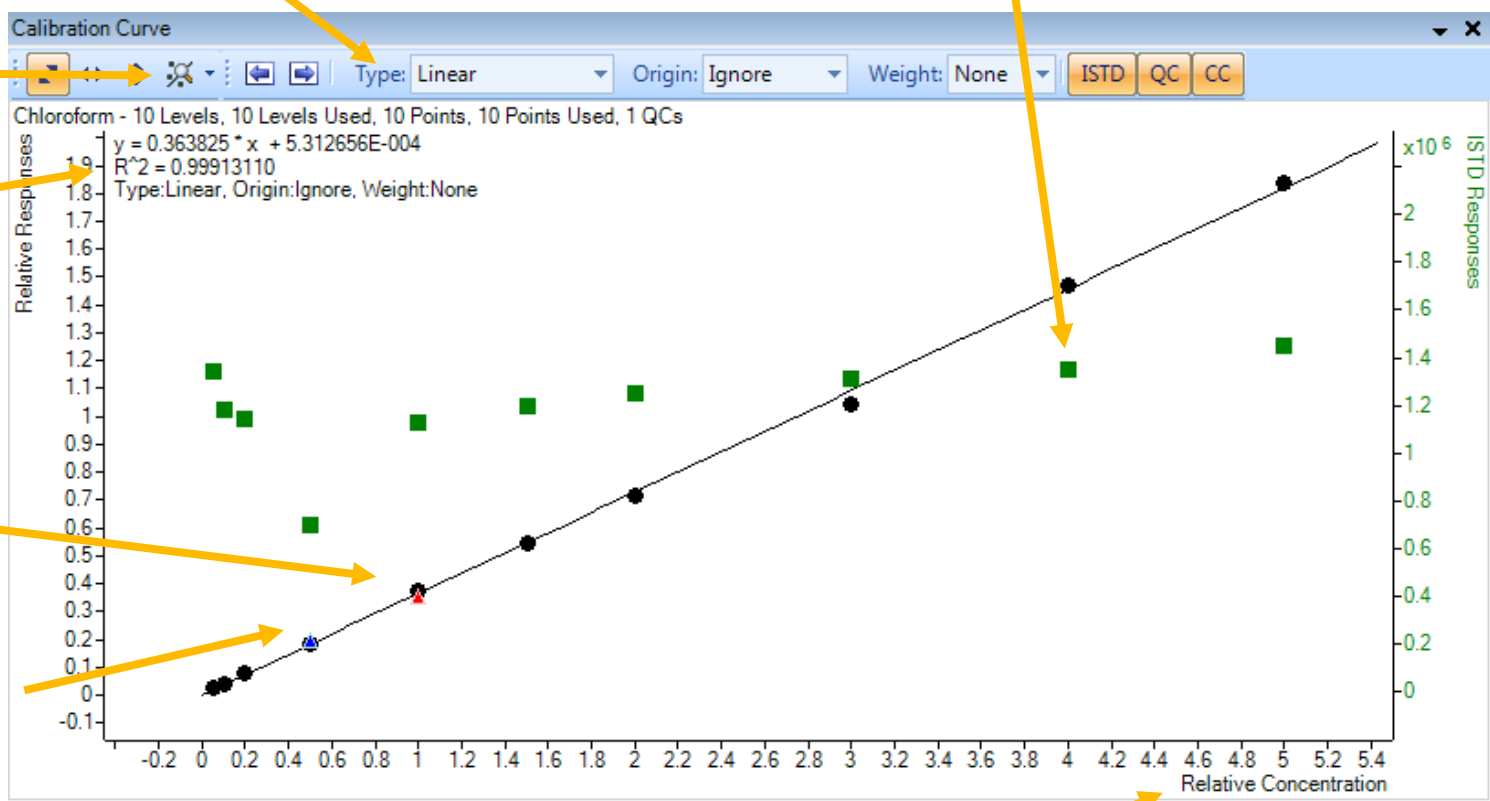
Change Curve Fit.

Fit to Levels (Scaling)

R²

CC Levels ▲

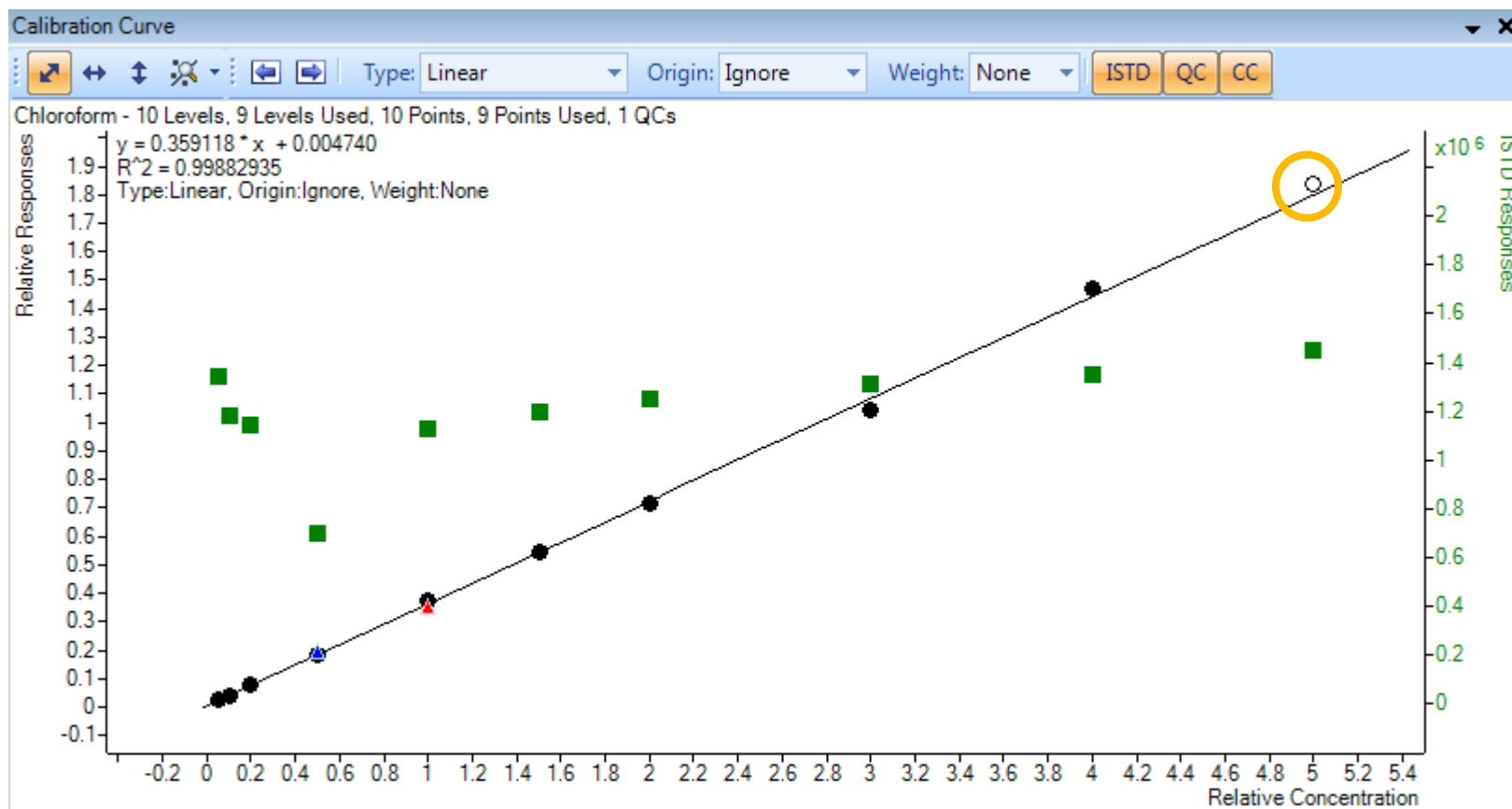
QC Samples ▲



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

Calibration Curve

Disable calibration points

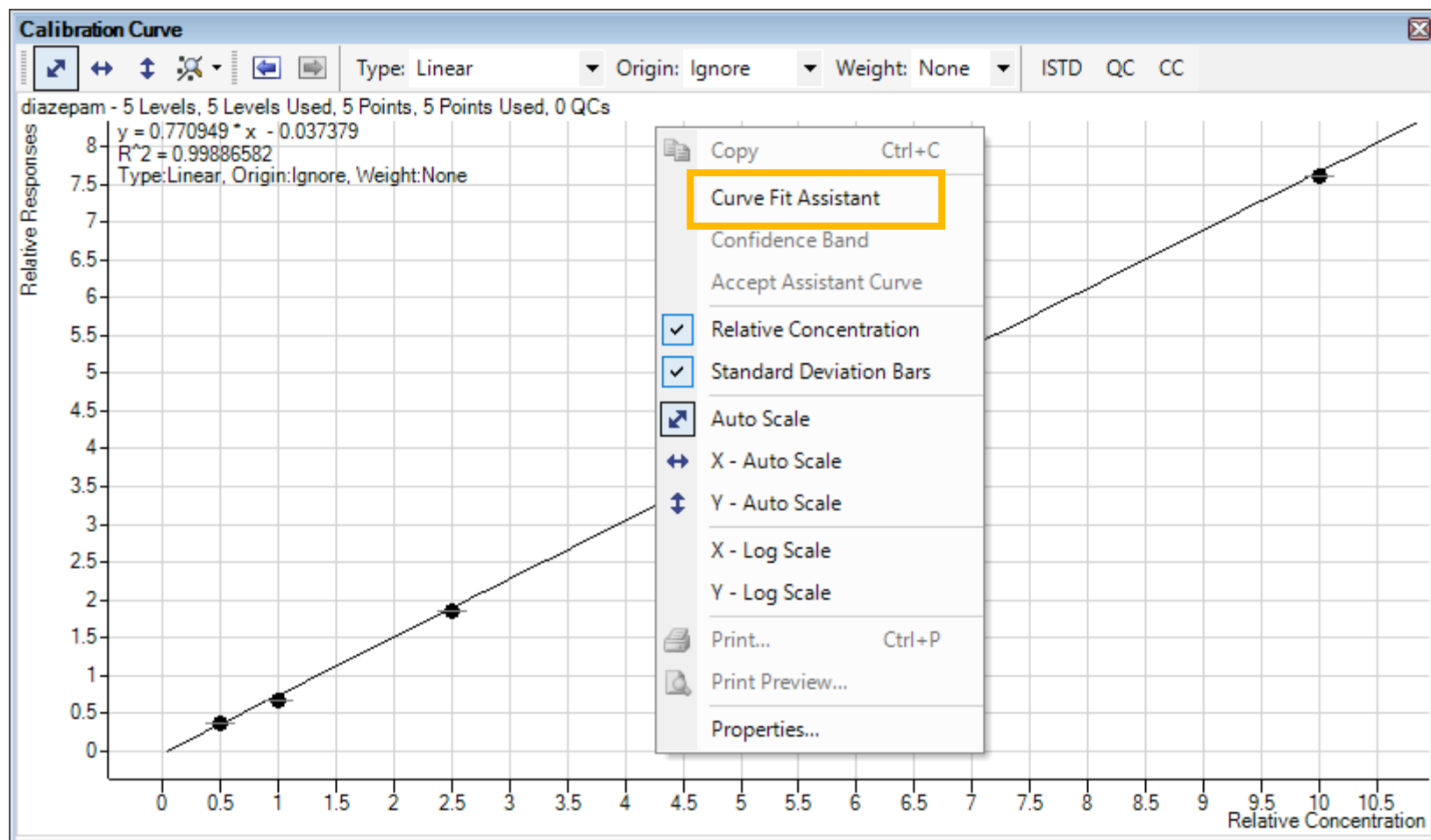


Click on **calibration point** once to disable and remove from curve.

Tip: After changing the curve always reanalyze the batch.



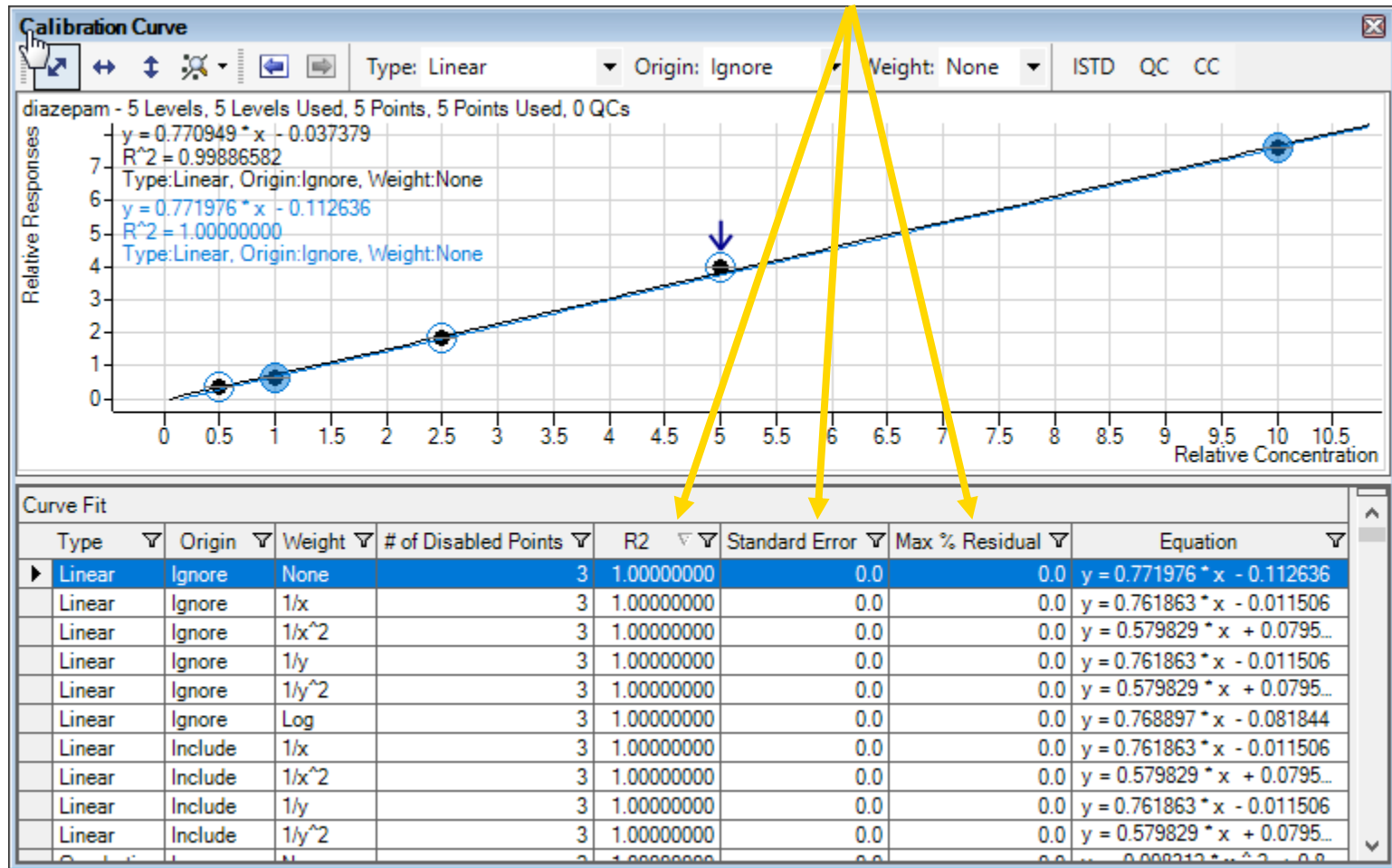
Curve Fit Assistant



Curve Fit Assistant

Sorting Columns

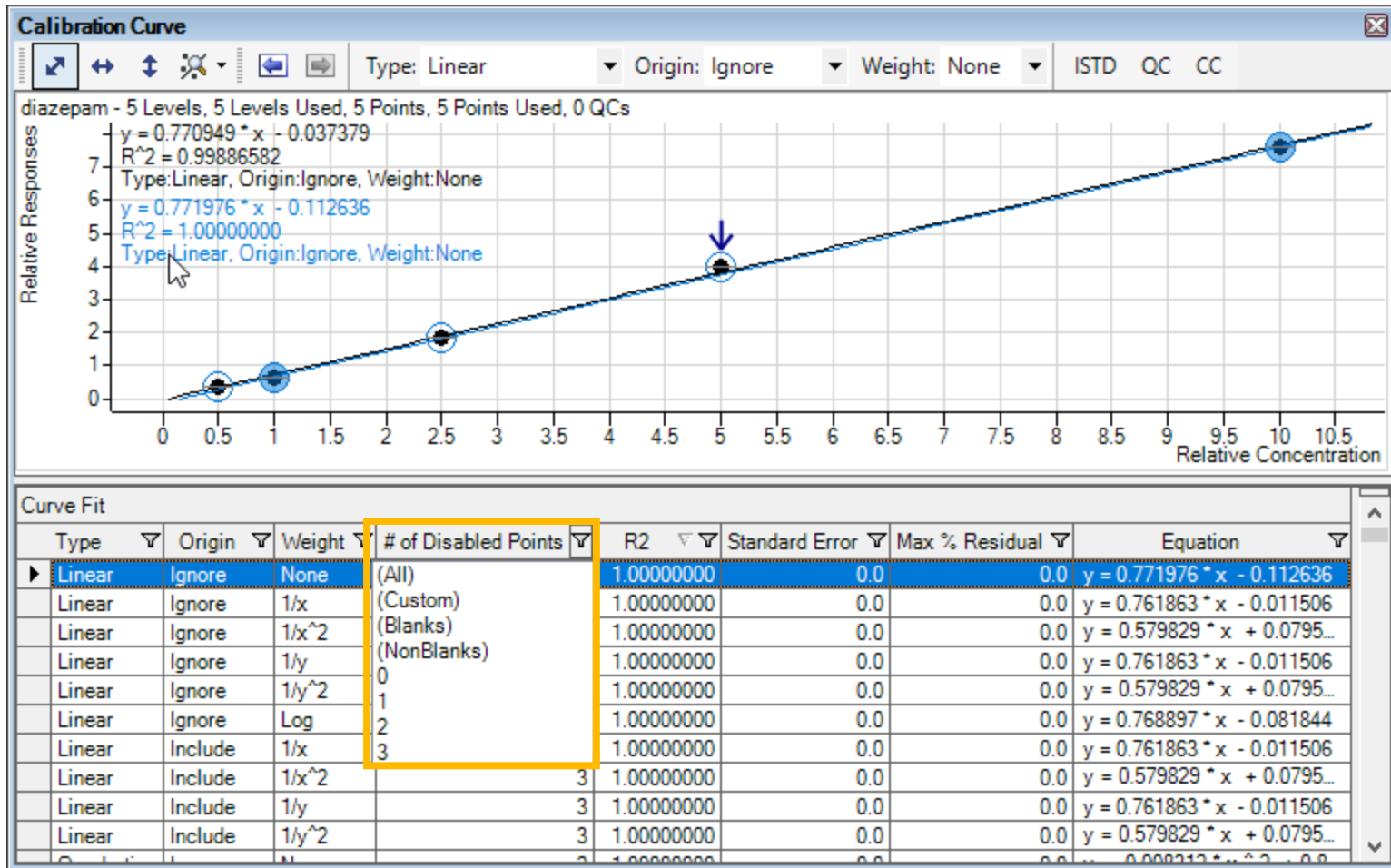
Best curve fit may be ranked using by R^2 , Standard Error, or Max % Residual.



Curve Fit Assistant calculates the mathematical curves.

Curve Fit Assistant

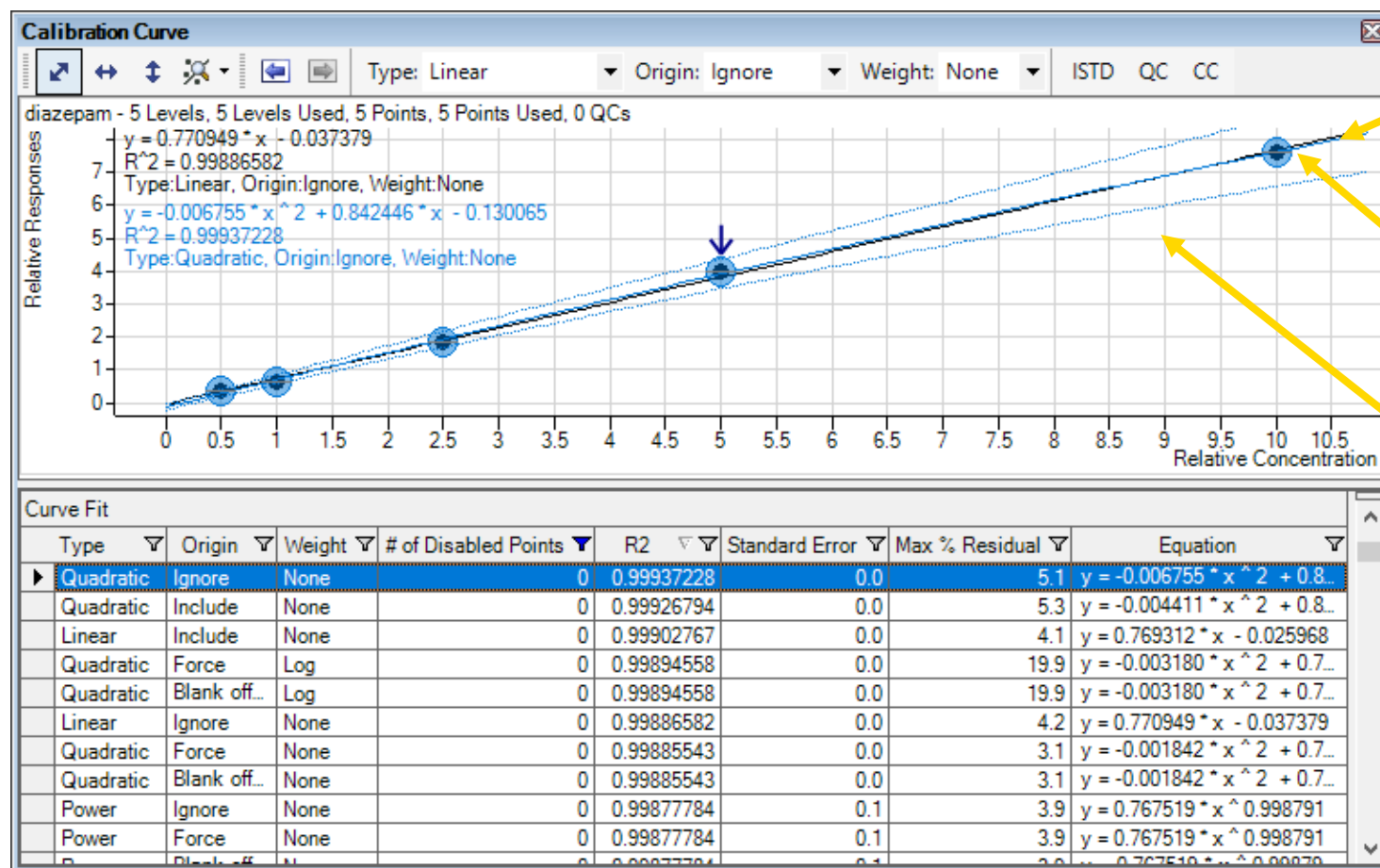
Disabled Points



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

Curve Fit Assistant

Confidence Band



Original Fit
(black)

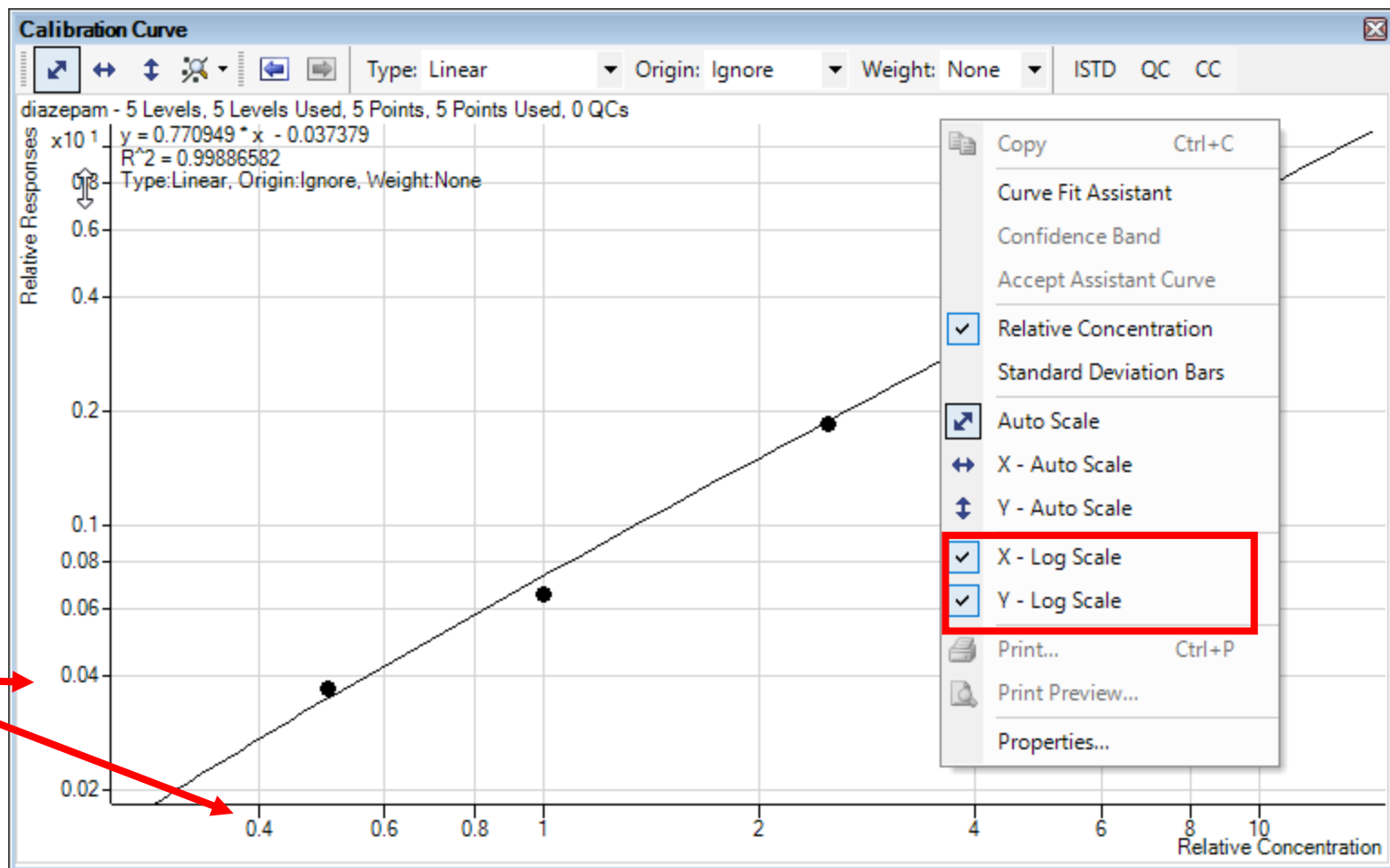
Best Fit
(blue)

Confidence
Band
(blue)



Calibration Curve

Log Log Plot



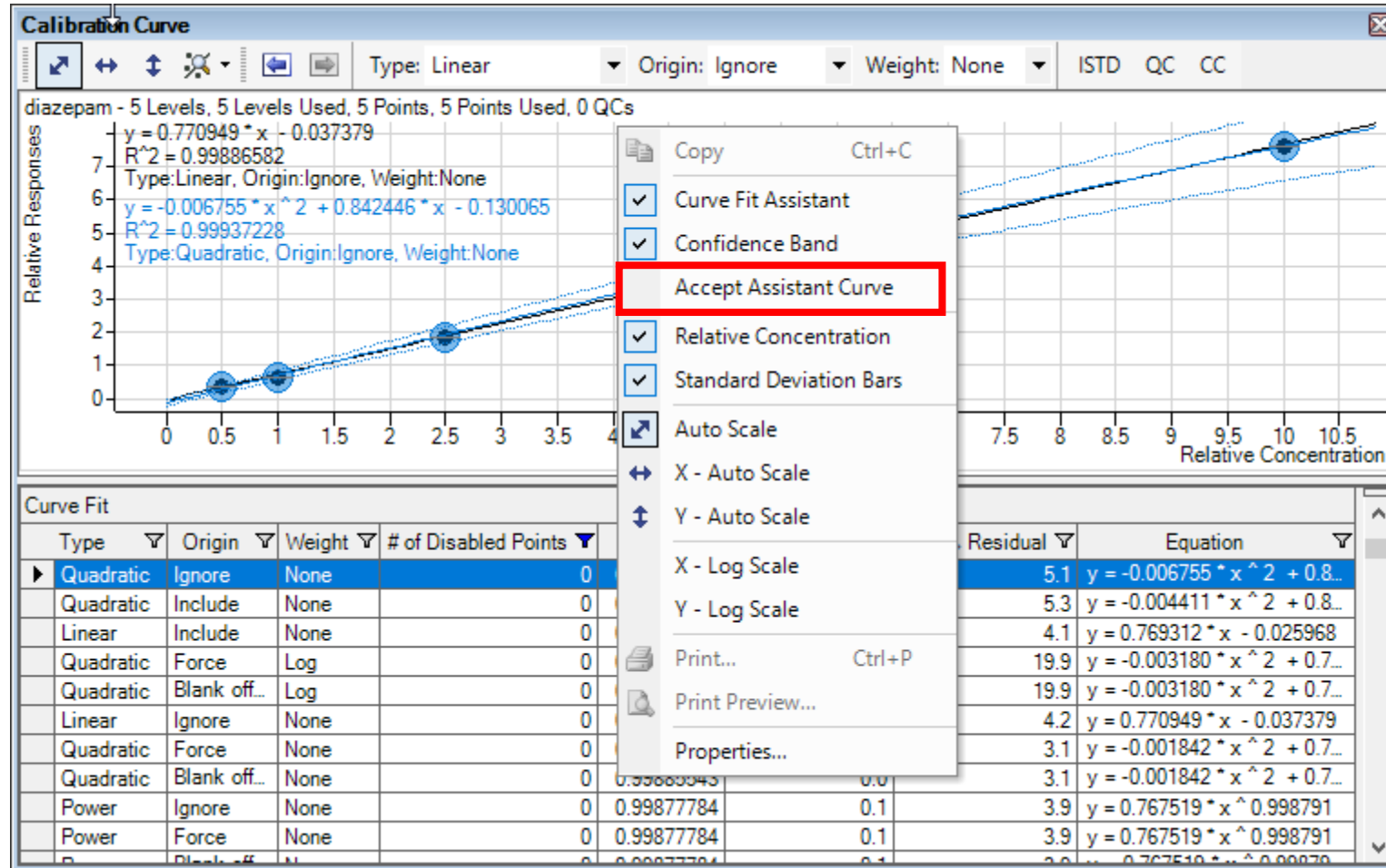
NEW FEATURE!



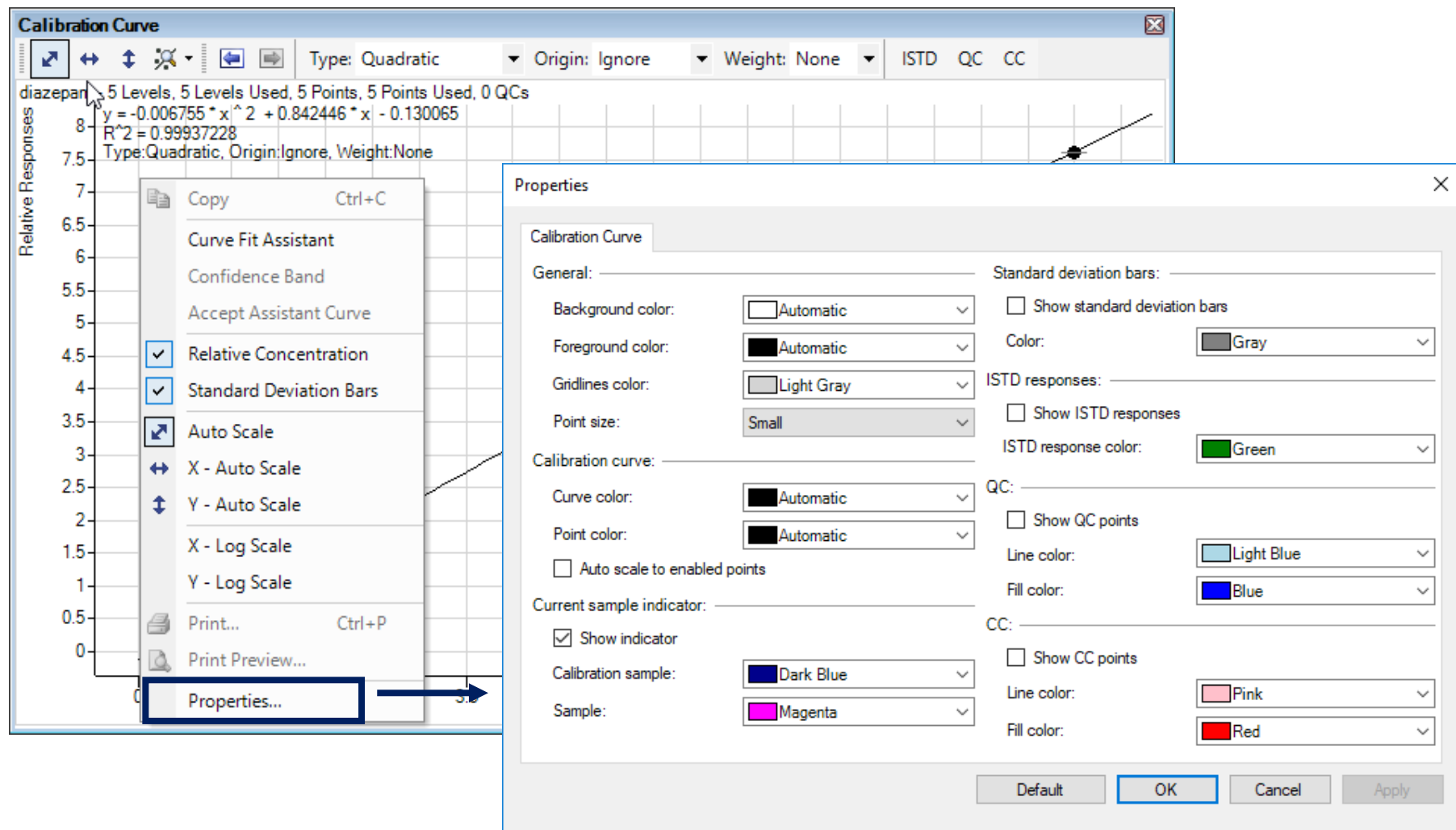
Agilent Technologies

Curve Fit Assistant

Accept Assistant Curve



Calibration Curve Properties



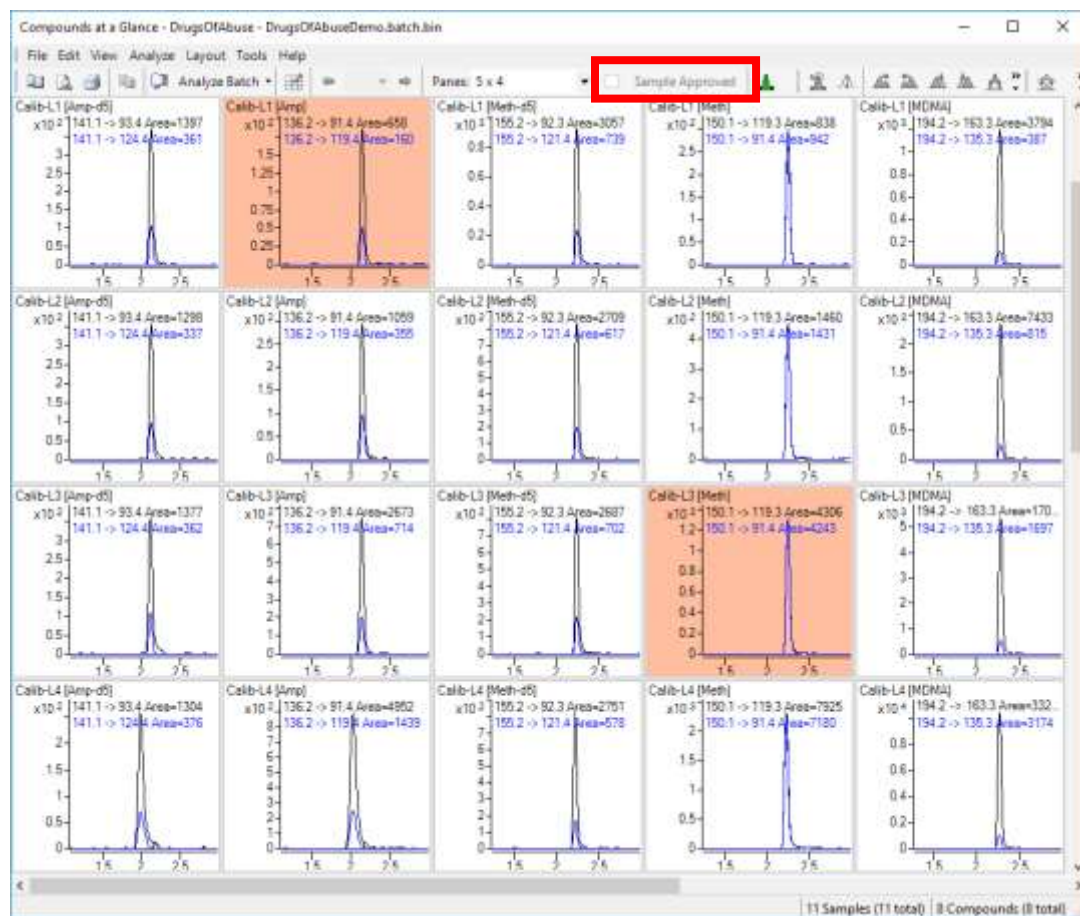


Let's take a moment
for questions on
Calibration Curve and
Curve Fit Assistant

Next up:
Compounds at a Glance

Compounds-at-a-Glance

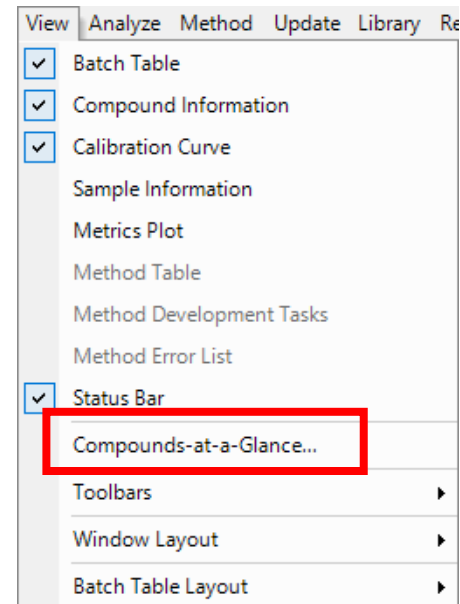
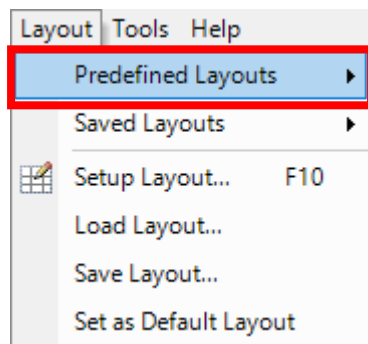
High throughput data review environment.
View compounds across multiple samples.
View all compounds within a sample.



Compounds-at-a-Glance

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

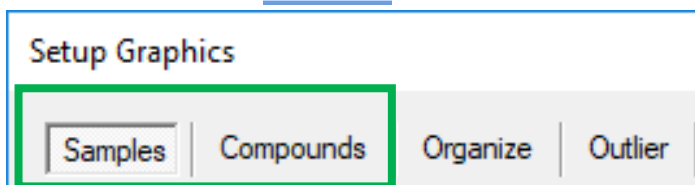
Choose **Layout > Predefined Layout**



Compounds-at-a-Glance

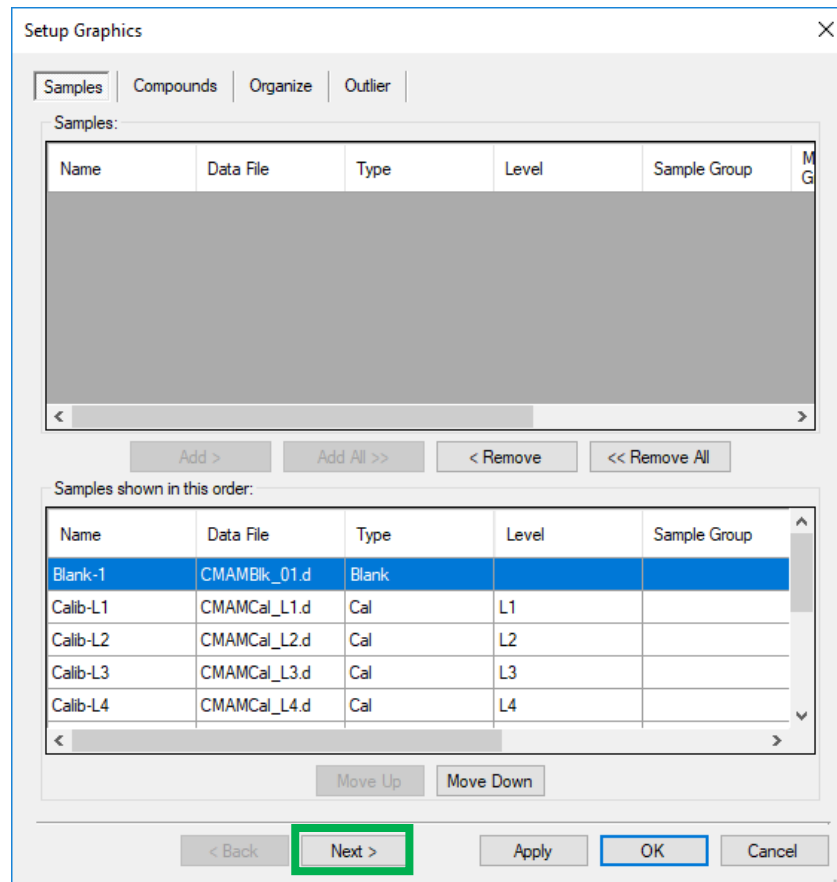
Setup Graphics Wizard

To customize select **Layout > Setup...**



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.



Compounds-at-a-Glance

Setup Graphics Wizard

The screenshot shows the 'Setup Graphics' dialog box with the 'Organize' tab selected. The 'Organize Rows by:' section has 'Samples' selected. The 'Overlay:' section has 'Qualifiers' selected. The 'Review Mode' section has 'None' selected. The 'Pane Dimension' is set to '5 x 4'. The 'Display Options' section has 'Baselines' checked. The 'Peak annotations...' button is visible at the bottom.

Setup Graphics

Samples | Compounds | **Organize** | Outlier

Organize Rows by:

- ☐ Compounds
- ☒ Samples

Overlay:

- ☐ None - target only
- ☐ None - target and qualifiers
- ☒ Qualifiers
- ☐ ISTD
- ☐ Matrix Spike
- ☐ Compound Groups
- ☐ Sample Groups
- ☐ Compounds
- ☐ Samples

Review Mode

- ☒ None
- ☐ Sample by Sample
- ☐ Compound by Compound
- ☐ Compound Group by Compound Group

Pane Dimension

5 x 4

Display Options

- ☐ Wrap Rows
- ☒ Baselines
- ☐ Fill Peaks
- ☐ Normalize
- ☐ Uncertainty Band

Peak annotations...

< Back | Next > | Apply | **OK** | Cancel

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

The screenshot shows the 'Display Options' section of the Setup Graphics Wizard. The options are: Wrap Rows (unchecked), Baselines (unchecked), Fill Peaks (unchecked), Normalize (unchecked), and Uncertainty Band (unchecked).

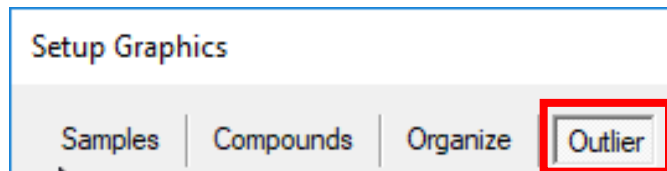
Display Options

- ☐ Wrap Rows
- ☐ Baselines
- ☐ Fill Peaks
- ☐ Normalize
- ☐ Uncertainty Band



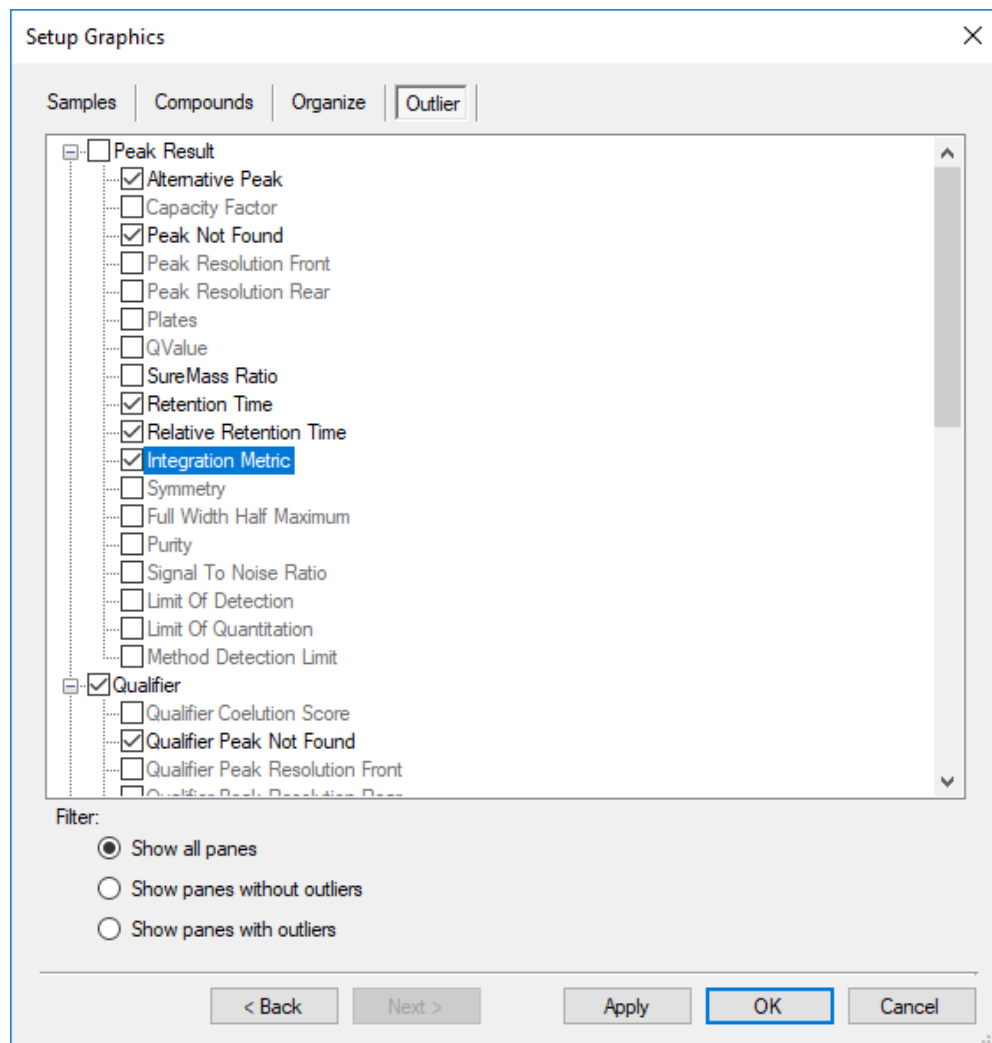
Compounds-at-a-Glance

Setup Graphics Wizard



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

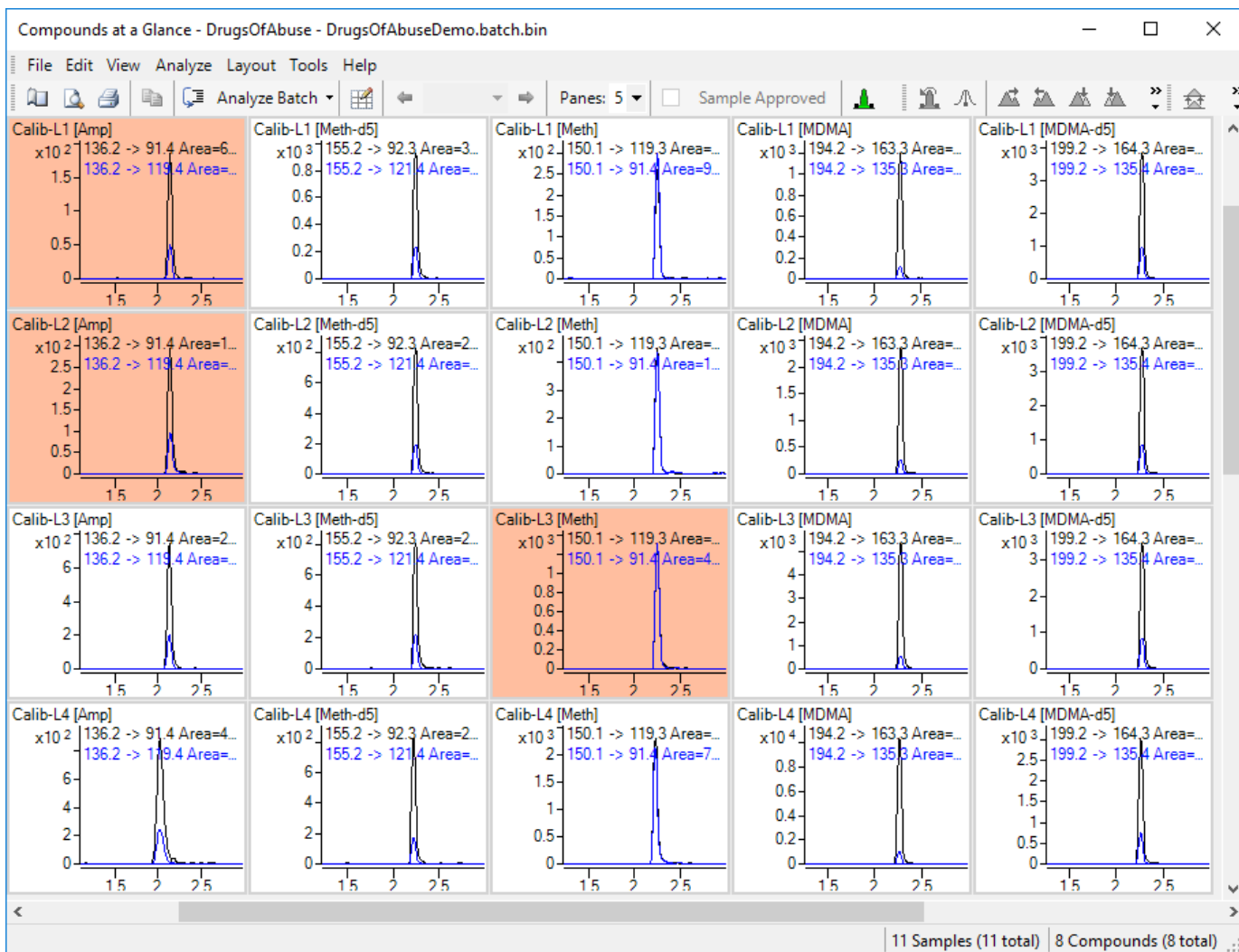
Outliers can also be filtered by
Panels without outliers
Panels with outliers



Compounds-at-a-Glance

Outliers

Outliers are highlighted in red.

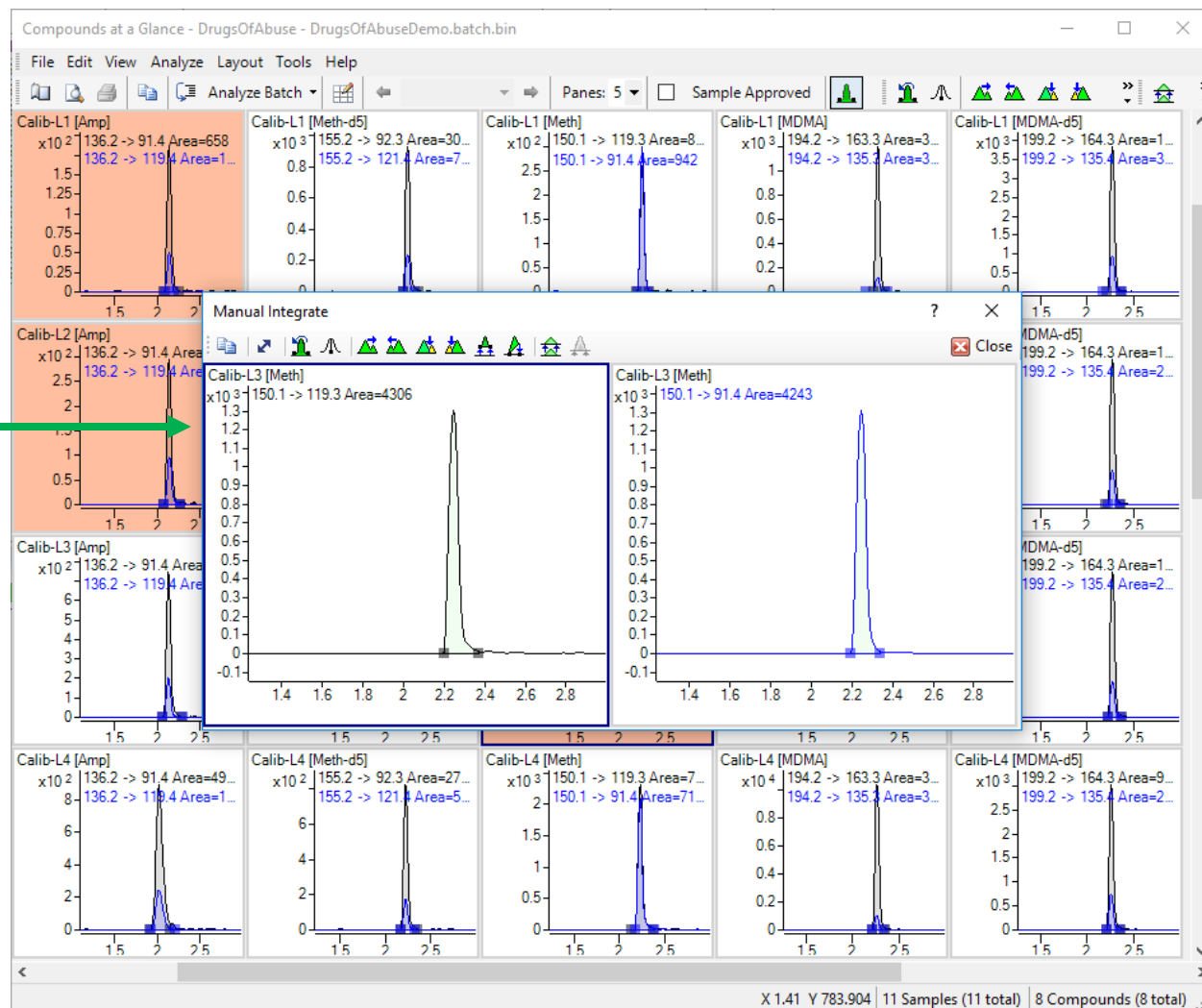


Compounds-at-a-Glance

Manual Integration Pop Up

Double click for
single pane
access.

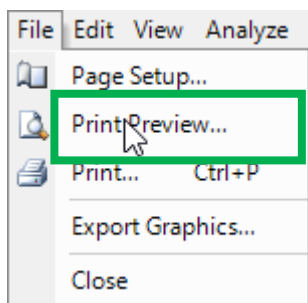
Can be accessed
without manual
integration being
activated.



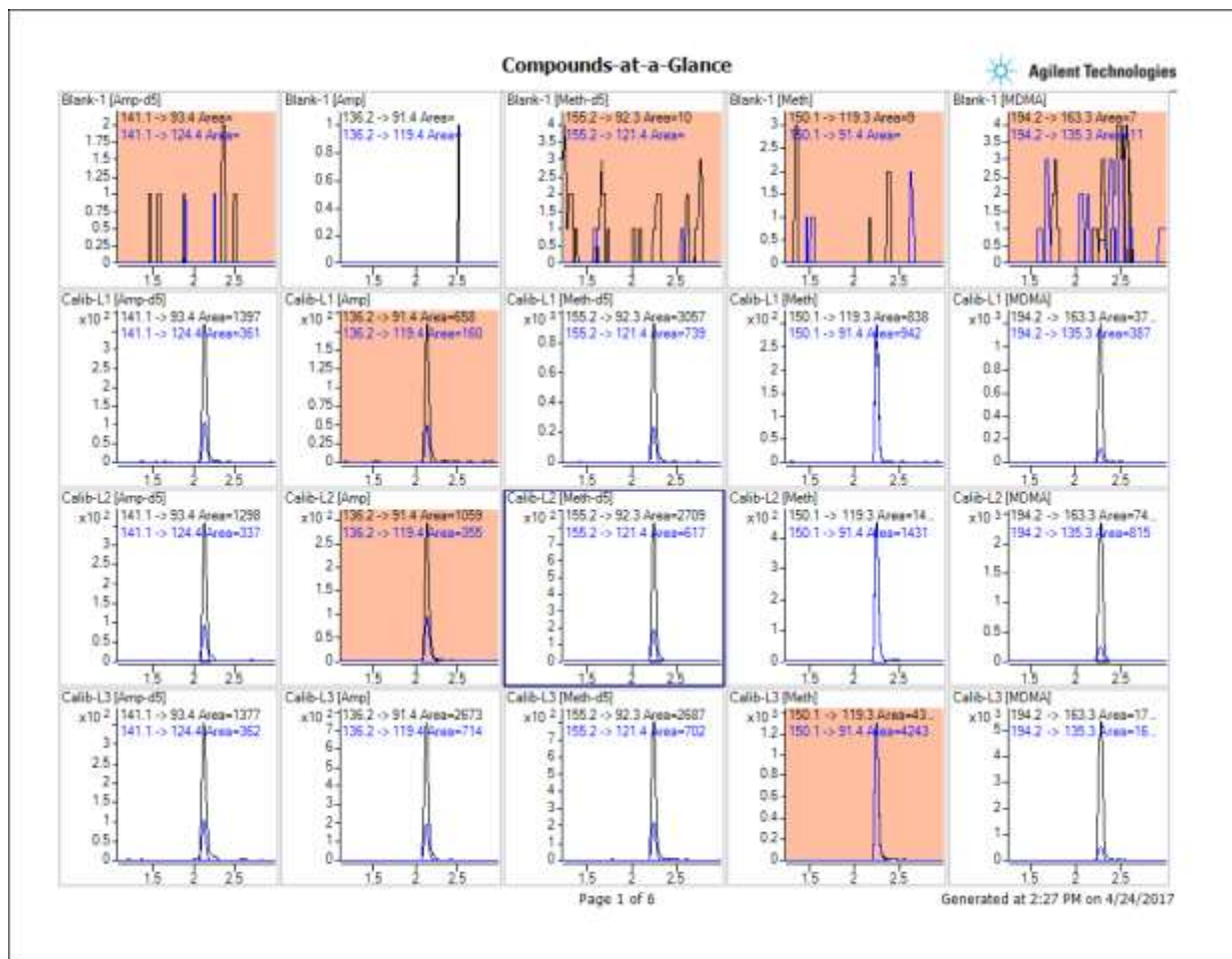
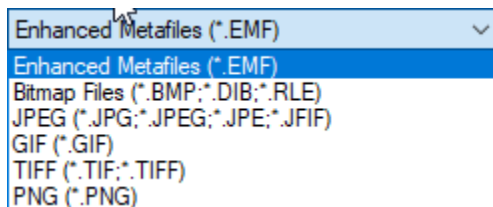
Compounds-at-a-Glance

Print Preview

Select **File > Print Preview** to create a chromatogram report.



Export Graphics
give a graphic
image in various
formats.



Compounds-at-a-Glance

Properties

From the
context menu
select
Properties

Properties

Compounds-at-a-Glance

General:

Background color:

Foreground color:

Gridlines color:

Outlier color:

Pane border:

Selected pane border:

Font size:

Chromatogram colors...

Chromatogram Colors

Colors:

- Black
- Blue
- Green
- Red
- Brown
- Magenta
- Yellow

Move Up

Move Down

Remove

Change

Insert

Default OK Cancel

Peaks:

☒ Baselines

☐ Normalize

☐ Uncertainty band

☒ Peak annotations...

Peak fill:

Fill alternate peaks when:

Retention Time:

Reference RT:

Recognition window:

Manual integration:

☒ Show baseline start/end boxes

Manual integration:

Max. # of panes:

Navigation:

☐ Synchronize Navigation

Peak Annotations

☒ Area

☐ Calc. Conc.

☐ Final Conc.

☐ RT

☐ Height

☐ Ratio

☐ Delta RT

☐ S/N

☐ Q. Computed

Move Up

Move Down

☒ Display annotation names (ex. RT=2.452)

☐ Display units for Conc., RT and Delta RT

Response ratio label:

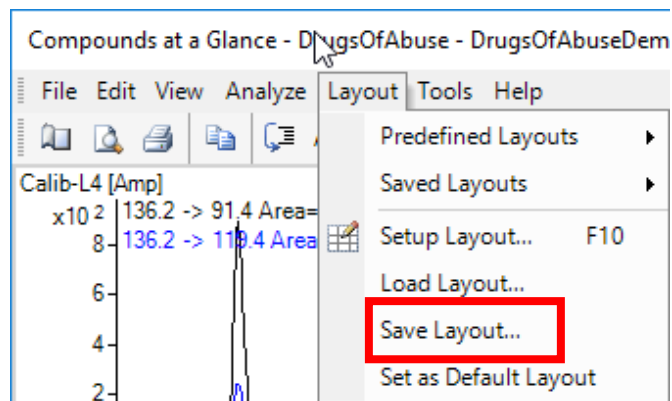
OK Cancel

Default OK Cancel Apply

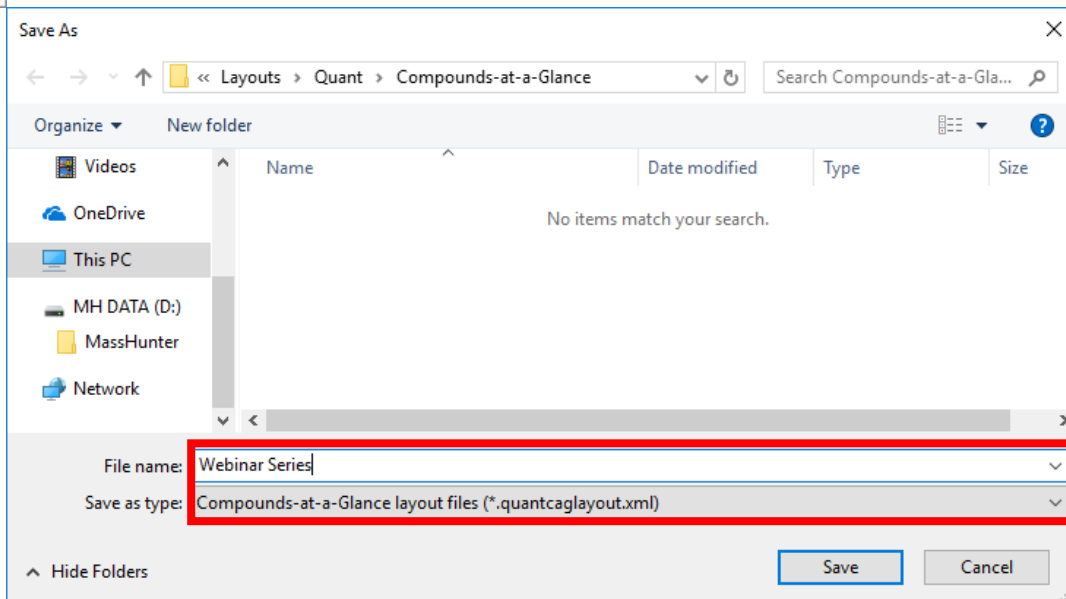


Compounds-at-a-Glance

Save Layout



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





Let's take a moment
for questions on
Compounds at a
Glance

Next up:
Global Settings

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	<input type="checkbox"/>
Apply Multiplier to Matrix Spike	<input checked="" type="checkbox"/>
Apply Multiplier to Surrogate	<input checked="" type="checkbox"/>
Apply Multiplier to Target	<input checked="" type="checkbox"/>
Bracketing Type	None
Correlation Window	2.000
Dynamic Background Subtraction	<input type="checkbox"/>
Ignore Peaks Not Found	<input checked="" type="checkbox"/>
Library Method	
Non Reference Window	200.000
Non Reference Window Type	Percent
Reference Library	
Reference Pattern Library	
Reference Window	80.000
Reference Window Type	Percent
Relative ISTD	<input type="checkbox"/>
Standard Addition	<input type="checkbox"/>



Apply Multiplier's

- None or Overlapped or Sample Group
- Associates target and qualifiers in min
- **Dynamic Background Subtraction**
- To avoid flagging target compounds that absent
- Part of unified method



Peak identification within the extraction window

- Spectral Reference Library (.reflibrary.xml)
- Spectral Pattern Reference Library (.reflibrary.xml)



Peak identification within the extraction window
(ISTD with Time Reference Flag checked)

- Semi quant relative to ISTD
- Quantitate with Standard Addition



Globals Settings

Calculated and Final Concentration

Sample			1,2,4-Trichlorobe...		1,2,4-Trichlorobenzene Results				
Type	Level	Dil.	Exp. Conc.	Units	RT	Resp.	MI	Calc. Conc.	Final Conc.
Sample		1.0		ng/ml	23.280	1138	<input type="checkbox"/>	0.6341	0.6341
Sample		1.0		ng/ml	24.071	2074	<input type="checkbox"/>	0.6581	0.6581
Sample		1.0		ng/ml	23.280	2272	<input type="checkbox"/>	0.6580	0.6580
Sample		1.0		ng/ml	23.280	5189	<input type="checkbox"/>	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

$$\text{Sample Amount Multiplier} = \text{TotalAmt}/\text{Amt}$$

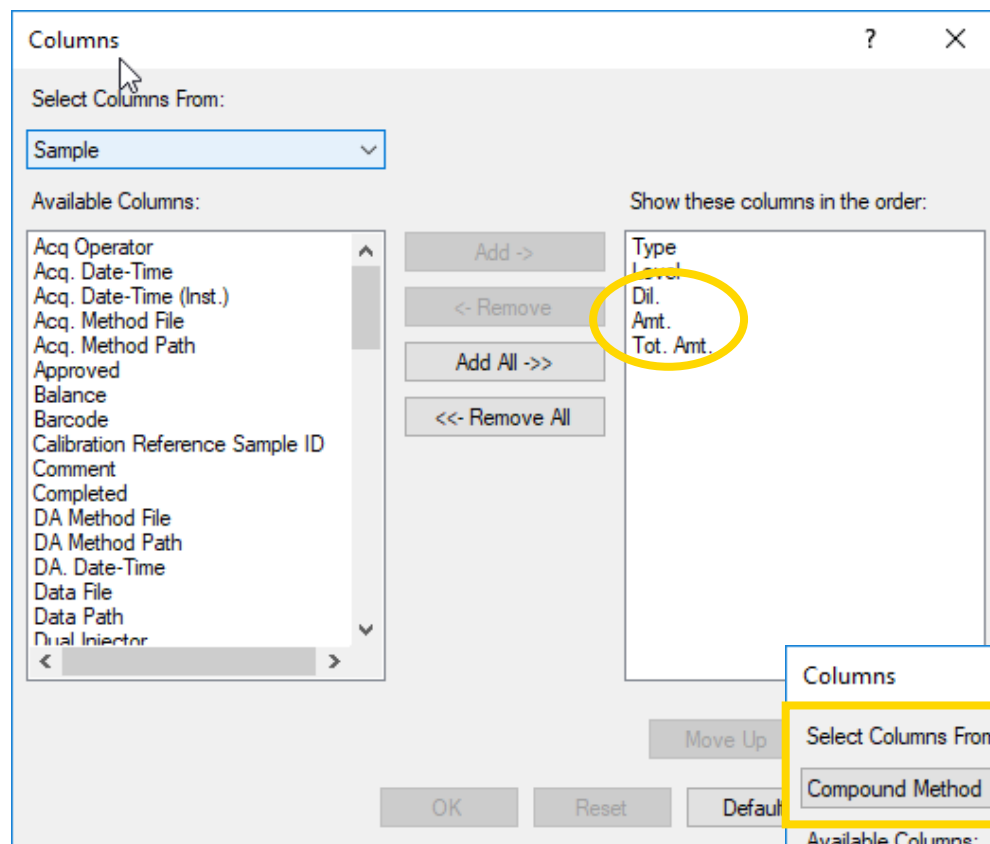
All three of the factors are columns in the Sample section of the Batch Table. By default, they are set to 1, either explicitly (Dil.) or implicitly (Amt. and Tot. Amt.)

Sample					1,2,4-Trichlorobe...	1,2,4-Trichlorobenzene Results					
Type	Level	Dil.	Amt.	Tot. Amt.	Exp. Conc.	Units	RT	Resp.	MI	Calc. Conc.	Final Conc.
Sample		1.0				ng/ml	23.280	1138	<input type="checkbox"/>	0.6341	0.6341
Sample		1.0				ng/ml	24.071	2074	<input type="checkbox"/>	0.6581	0.6581
Sample		1.0				ng/ml	23.280	2272	<input type="checkbox"/>	0.6580	0.6580
Sample		1.0				ng/ml	23.280	5189	<input type="checkbox"/>	0.6964	0.6964



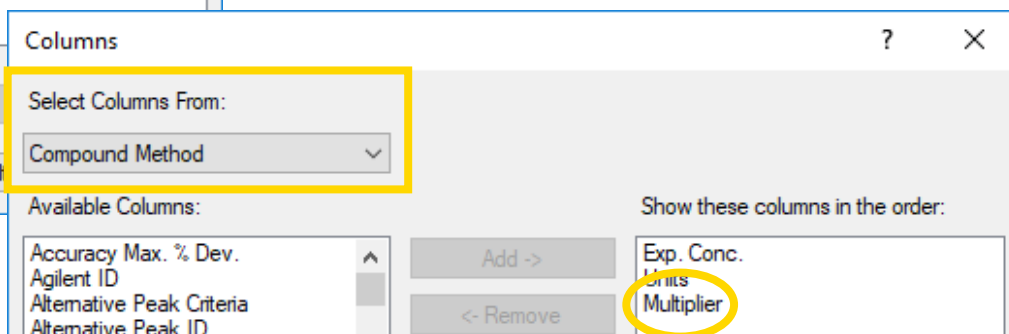
Globals Settings

Multiplier



The columns (Dil., Amt., TotalAmt, and Multiplier) must be added to the Batch Table.

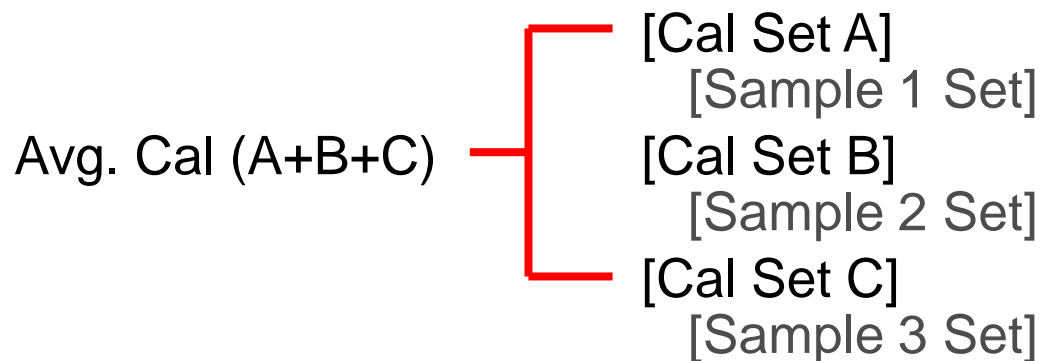
The Multiplier in the Compound Results represents the product applied to the compound.



Globals Settings

Bracketing type = None

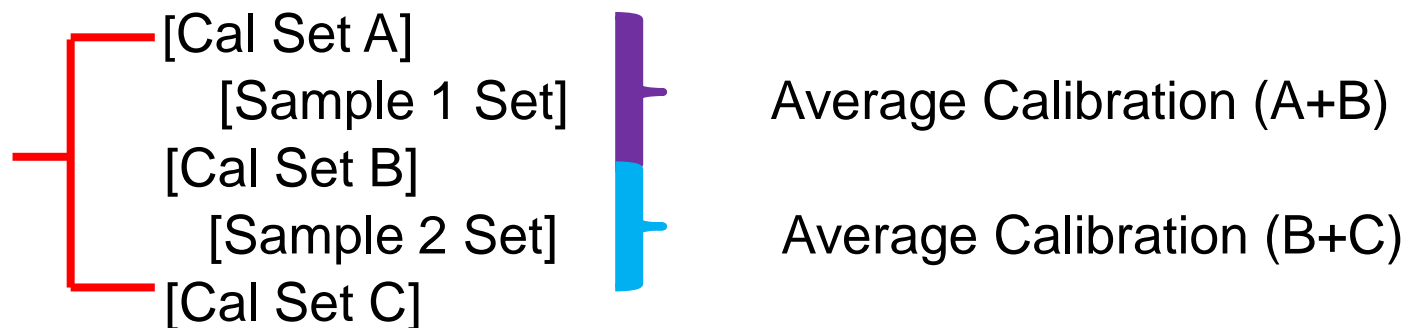
No (None) Bracketing allows the user to have sample(s) quantitated using the average of **all** the calibration standards in the batch without regard to order.



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.



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	

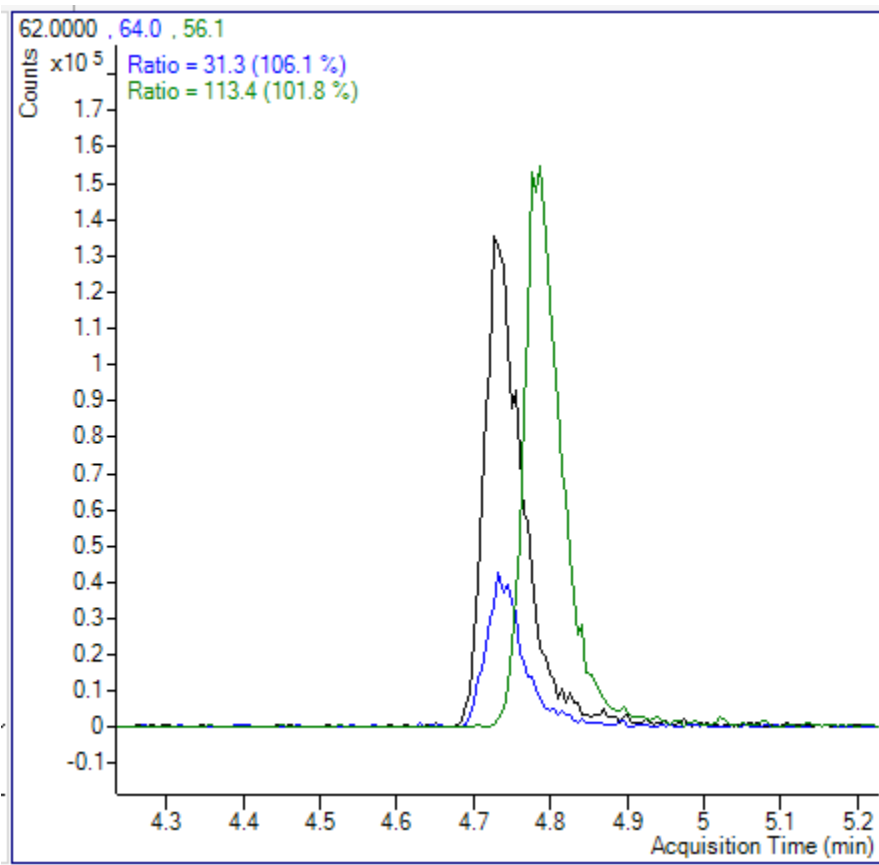
Added from Worklist or Batch Table.



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.

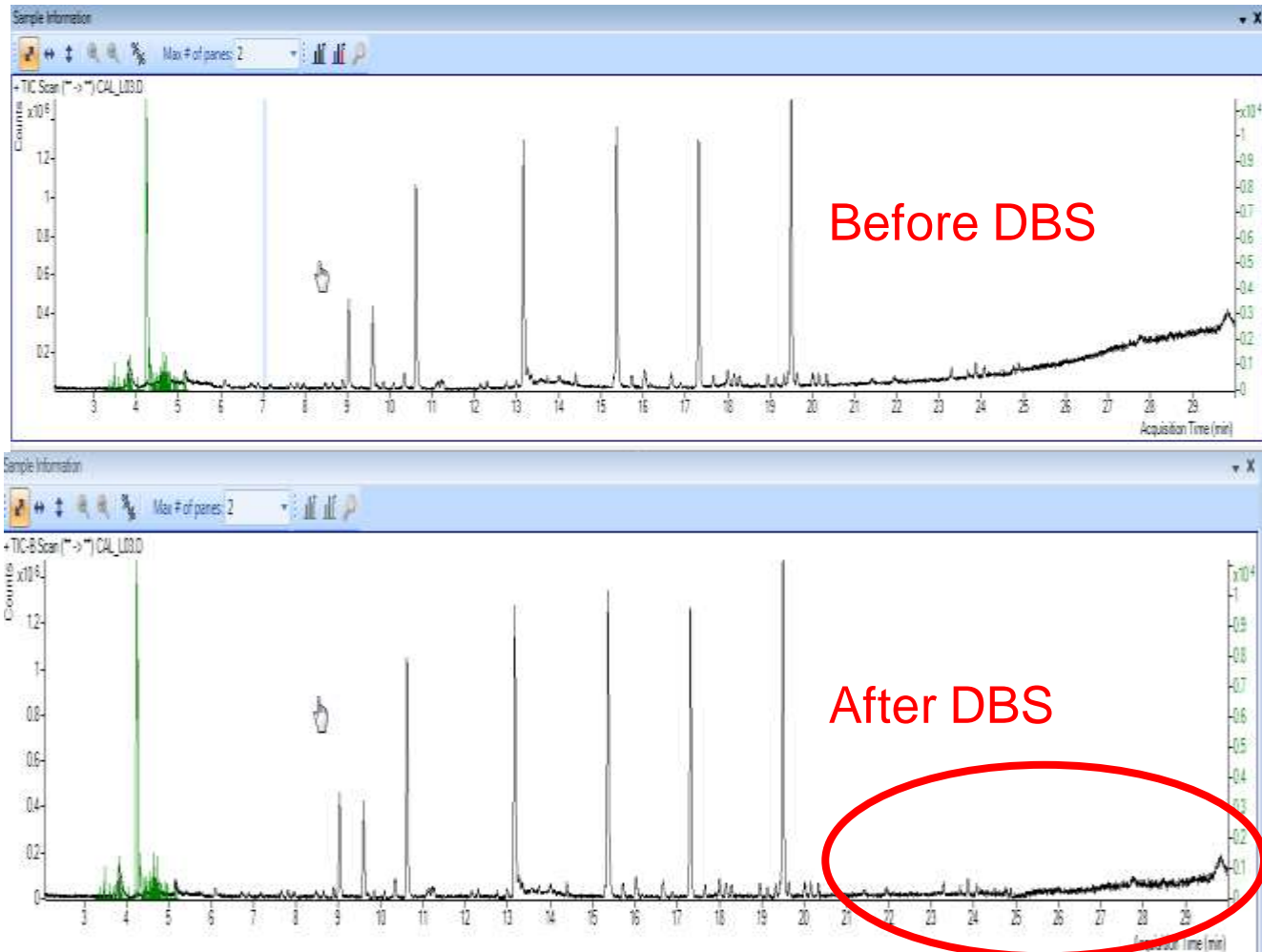
Typically 0.01 to 0.05 min (0.6 sec to 3 sec)



Globals Settings

Dynamic Background Subtraction

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



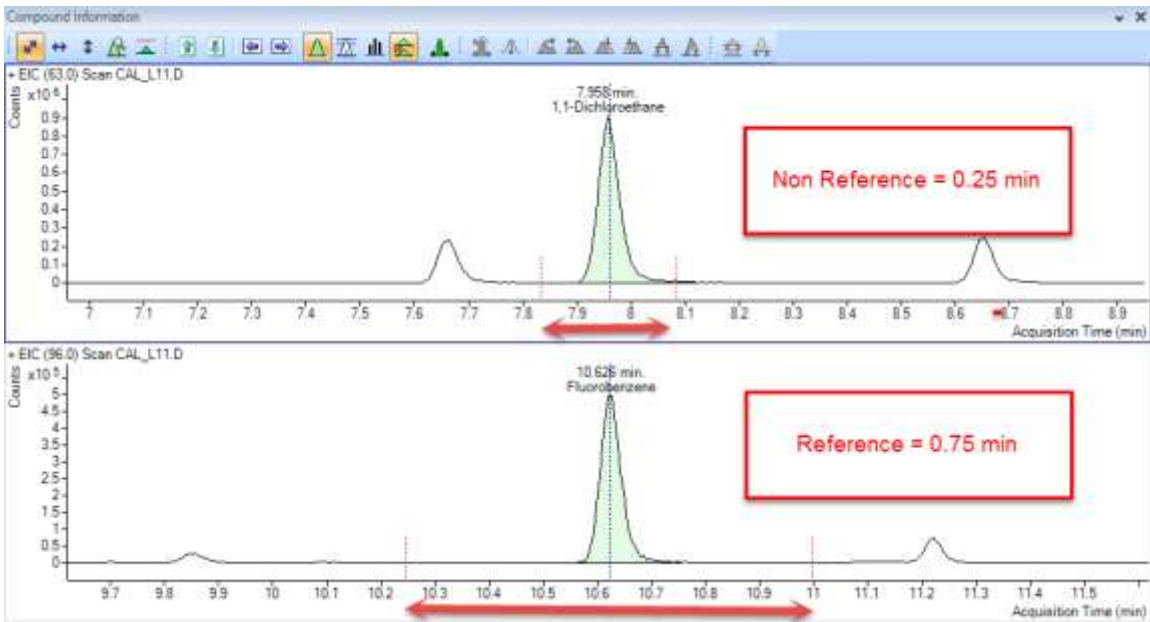
Globals Settings

Non Reference & Reference Window

Globals

Apply Multiplier to ISTD	<input type="checkbox"/>
Apply Multiplier to Matrix Spike	<input checked="" type="checkbox"/>
Apply Multiplier to Surrogate	<input checked="" type="checkbox"/>
Apply Multiplier to Target	<input checked="" type="checkbox"/>
Bracketing Type	None
CC Maximum Elapsed Time In Hours	0.000
Correlation Window	2.000
Dynamic Background Subtraction	<input type="checkbox"/>
Ignore Peaks Not Found	<input type="checkbox"/>
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	<input type="checkbox"/>
Standard Addition	<input type="checkbox"/>

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



Quantifier

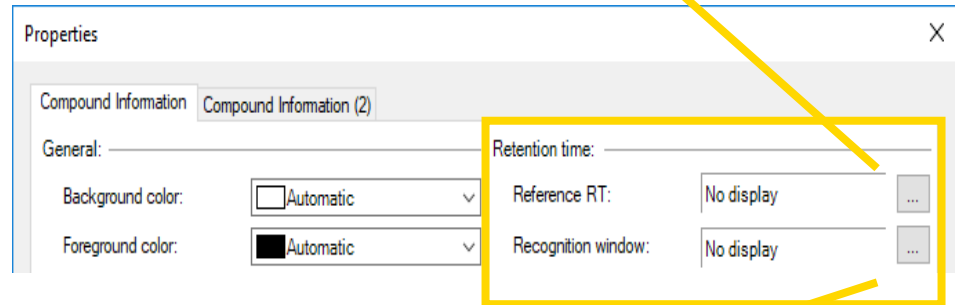
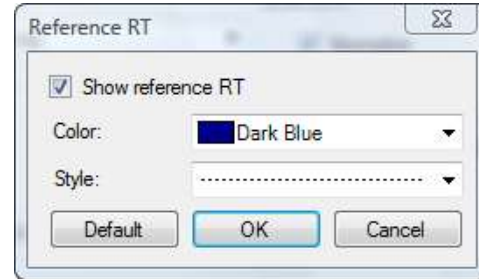
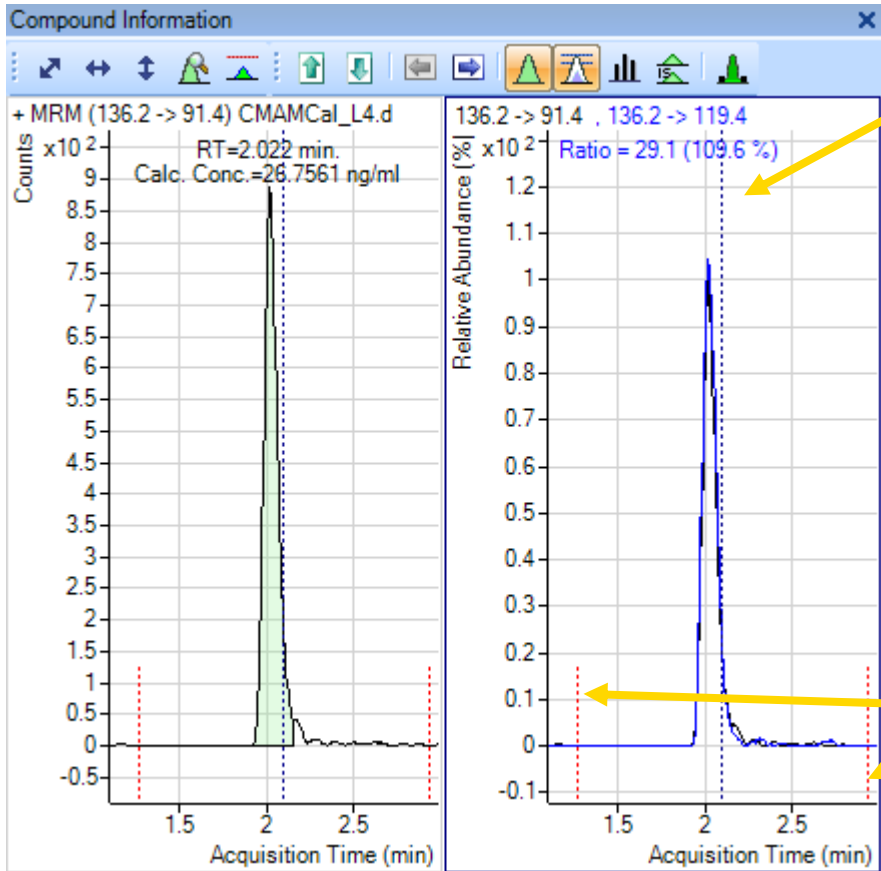
Name	TS	Scan	Type	ISTD Compound Name	ISTD Flag	ISTD Conc.	Time Reference Flag
Fluorobenzene	1	Scan	ISTD	<None>	<input checked="" type="checkbox"/>	10.0000	<input checked="" type="checkbox"/>
Chlorobenzene-d5	1	Scan	ISTD	<None>	<input checked="" type="checkbox"/>	10.0000	<input type="checkbox"/>
1,4-Dichlorobenzene-d4	1	Scan	ISTD	<None>	<input checked="" type="checkbox"/>	10.0000	<input type="checkbox"/>
1,2-Dichloroethane-d4	1	Scan	Surrogate	Fluorobenzene	<input type="checkbox"/>	10.0000	<input type="checkbox"/>
Toluene-D8	1	Scan	Surrogate	Chlorobenzene-d5	<input type="checkbox"/>	10.0000	<input type="checkbox"/>
1,1-Dichloro-1-propene	1	Scan	Target	Fluorobenzene	<input type="checkbox"/>	10.0000	<input type="checkbox"/>
Dichlorodifluoromethane	1	Scan	Target	Fluorobenzene	<input type="checkbox"/>	10.0000	<input type="checkbox"/>
Chloromethane	1	Scan	Tarotet	Fluorobenzene	<input type="checkbox"/>	10.0000	<input type="checkbox"/>

Reference = ISTD + Time Reference

Non Reference = Everything else

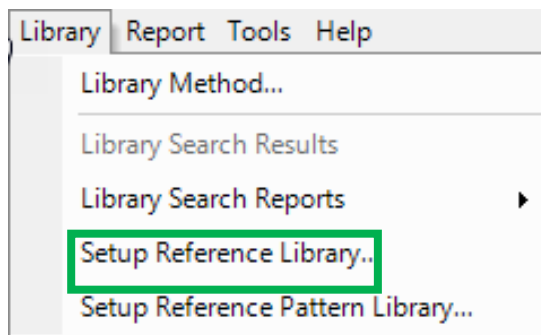
Option to Display Reference RT and Window Compound Information > Properties > Retention time

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



Globals Settings

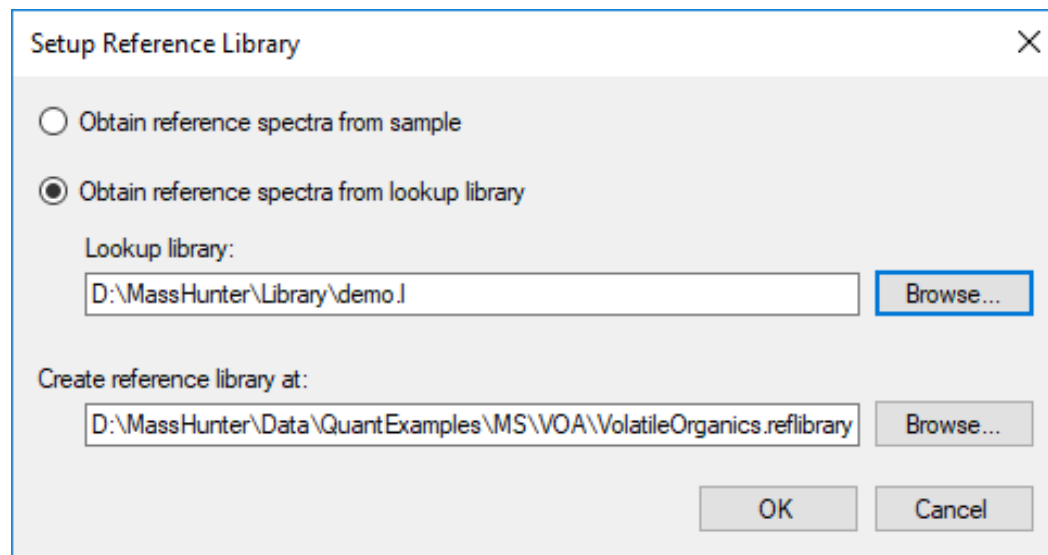
Reference Library



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.



Globals Settings

Reference Library

Vinyl Chloride Results					
RT	Resp.	MI	Calc. Conc.	Final Conc.	Library Match Score
4.739	17767	<input type="checkbox"/>	0.0574	0.0574	53.1
5.181	352	<input type="checkbox"/>	0.0000	0.0000	31.1
4.733	1072	<input type="checkbox"/>	0.0000	0.0000	35.1
4.646	1199	<input type="checkbox"/>	0.0000	0.0000	34.4
4.449	805	<input type="checkbox"/>	0.0000	0.0000	29.0
4.733	125882	<input type="checkbox"/>	2.2745	2.2745	59.0
4.739	21858	<input type="checkbox"/>	0.0938	0.0938	61.8
4.728	46684	<input type="checkbox"/>	0.6698	0.6698	72.8
4.722	89753	<input type="checkbox"/>	1.6307	1.6307	83.0

Properties

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

☐ No qualifier peak fill

☐ Fill target peaks

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

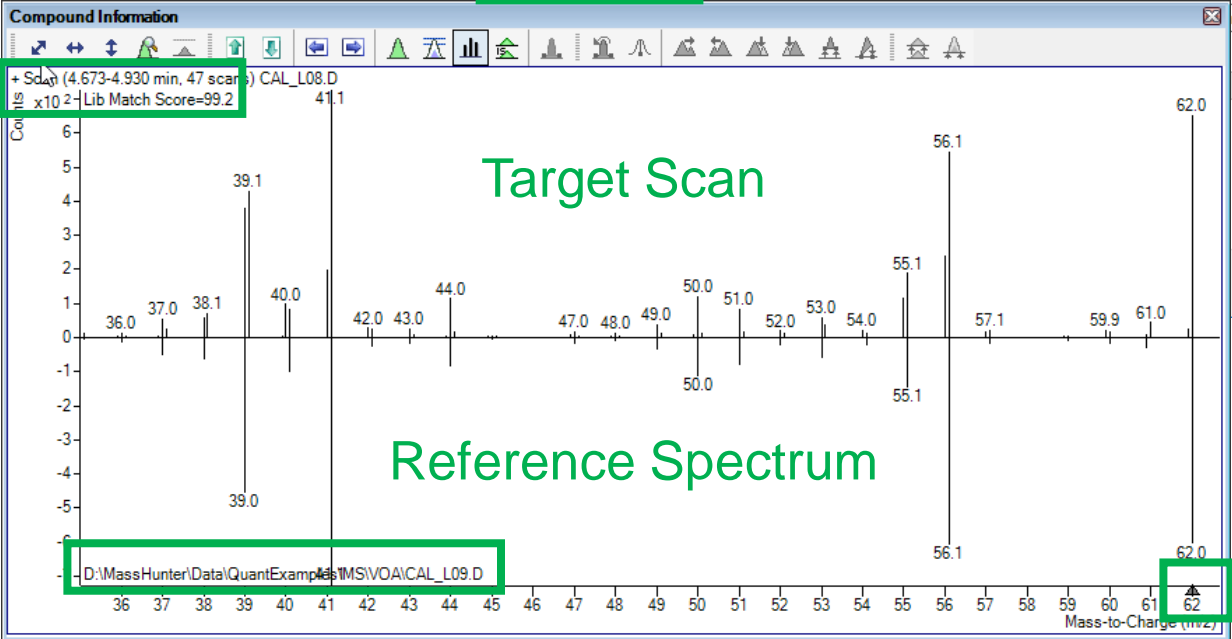
Max. # of panes per row: 3

Default

OK

Cancel

Apply



Library Match Score is column that can be added in the Batch Table.

Globals Settings

Relative ISTD

A method of semi quantitation.

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

$$[Phe] = \frac{\text{Intensity of Phe}}{\text{Intensity of } D_5Phe} \times [D_5Phe]$$

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

$$\frac{\text{Response}}{\text{ISTDResponse}} * \text{ISTDConcentration} * \text{ISTDRelativeMultiplier} = \text{CalculatedConcentration}$$



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 sample that is spiked 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	<input type="checkbox"/>
Apply Multiplier to Matrix Spike	<input checked="" type="checkbox"/>
Apply Multiplier to Surrogate	<input checked="" type="checkbox"/>
Apply Multiplier to Target	<input checked="" type="checkbox"/>
Bracketing Type	None
Correlation Window	2.000
Dynamic Background Subtraction	<input type="checkbox"/>
Ignore Peaks Not Found	<input type="checkbox"/>
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	<input type="checkbox"/>
Standard Addition	<input type="checkbox"/>

		Name	Type	Level
!		Sample 1	Sample	
!		Sample 1 Spike 1	Cal	L1
!		Sample 1 Spike 2	Cal	L2
!		Sample 2	Sample	
!		Sample 2 Spike 1	Cal	L1
!		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

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- **Customized On-Site Training** – Effective learning environment designed to achieve operational excellence and employee development without the need to travel.
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Upgraded customer experience:

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Introduce new eLearning capabilities:

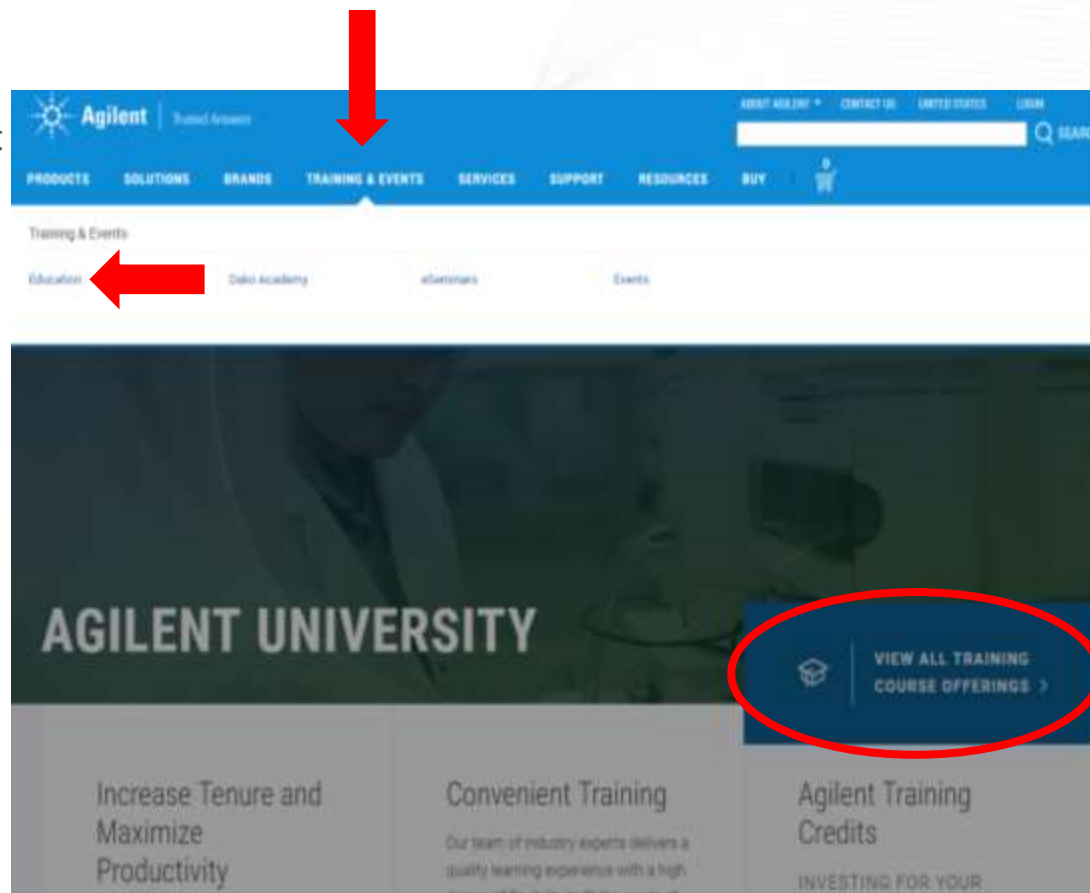
- Recorded and video-based learning
- Virtual online classes

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

Helping customers:

- Educate your employees on Agilent instruments and software
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Questions on today's material...

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