



# Agilent MassHunter Quantitative Data Analysis

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MassHunter Quantitation:  
Batch and Method Setup  
Outliers, Data Review,  
Reporting

# MassHunter Quantitative Analysis Software Review and Quant Method Optimization

## Topics

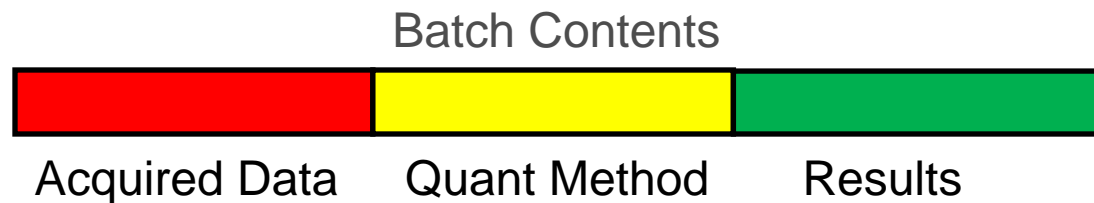
- Batch Definitions
- Three main views in MassHunter Quantitative Analysis
- Developing a quantitation method
  - Method Editor tasks
- Analyze the batch
- Outlier setup
- Advanced Tasks
  - Integration parameters
- Data review
- Generating a report, modifying graphic output

# Definitions

**Batch** - A set of data files that may include calibrators, samples, blanks, and QC samples. The data in the batch will be operated on by one method. The method and calculated results are contained in the batch.

**Quant Method** – A list of target compounds with quantifier and qualifier ions specified for each compound, retention times, ISTD info, calibrator concentrations, outliers, integration parameters, and much more.

**Results** – After the batch has been analyzed, results are generated and contained within the batch (xml file). These results are displayed in a tabular format in the Batch Table and graphically in either the Batch View or the Compounds at a Glance View.



# Definitions

**SQ** – Single quadrupole instrument low or unit mass resolution data. Can be scan data or SIM.

**QQQ** – Triple quadrupole or tandem quadrupole. Composed of a Q1, collision cell (Q2) and Q3. Usually acquired in multiple reaction monitor (MRM). MS/MS data.

**TOF** – Time of flight High resolution mode. Gives exact mass to 4 decimal places. Data acquired in scan mode.

**Q TOF** – Quadrupole combined with high resolution TOF. MS/MS data.

# MassHunter Quantitative Software

There are 15 possible Quantitative Analysis icons

Use the icon applicable to the instrument and dataset for the application.

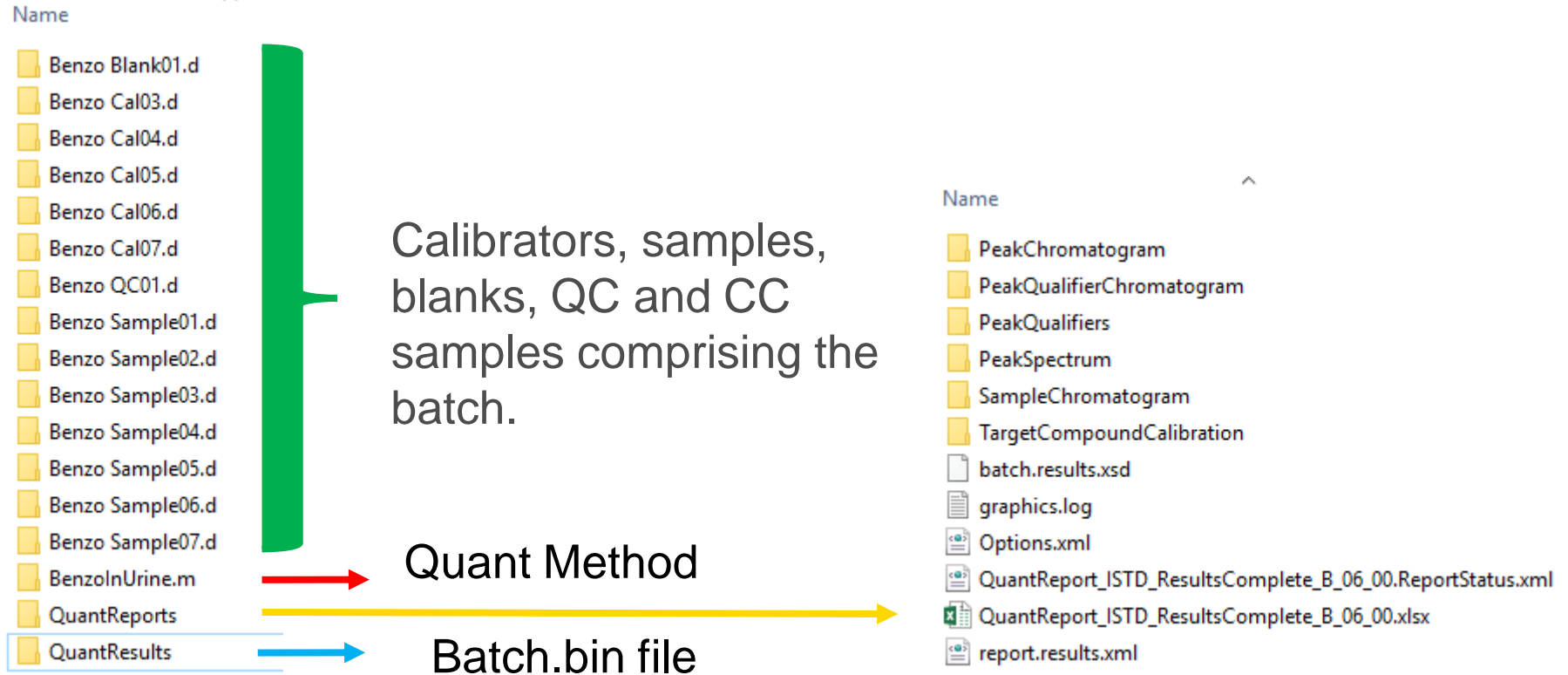
2D UV signals (UV only) can be processed with the GC icon or as part of an MS method.

Same core software different UI.



# Typical Data Folder Structure

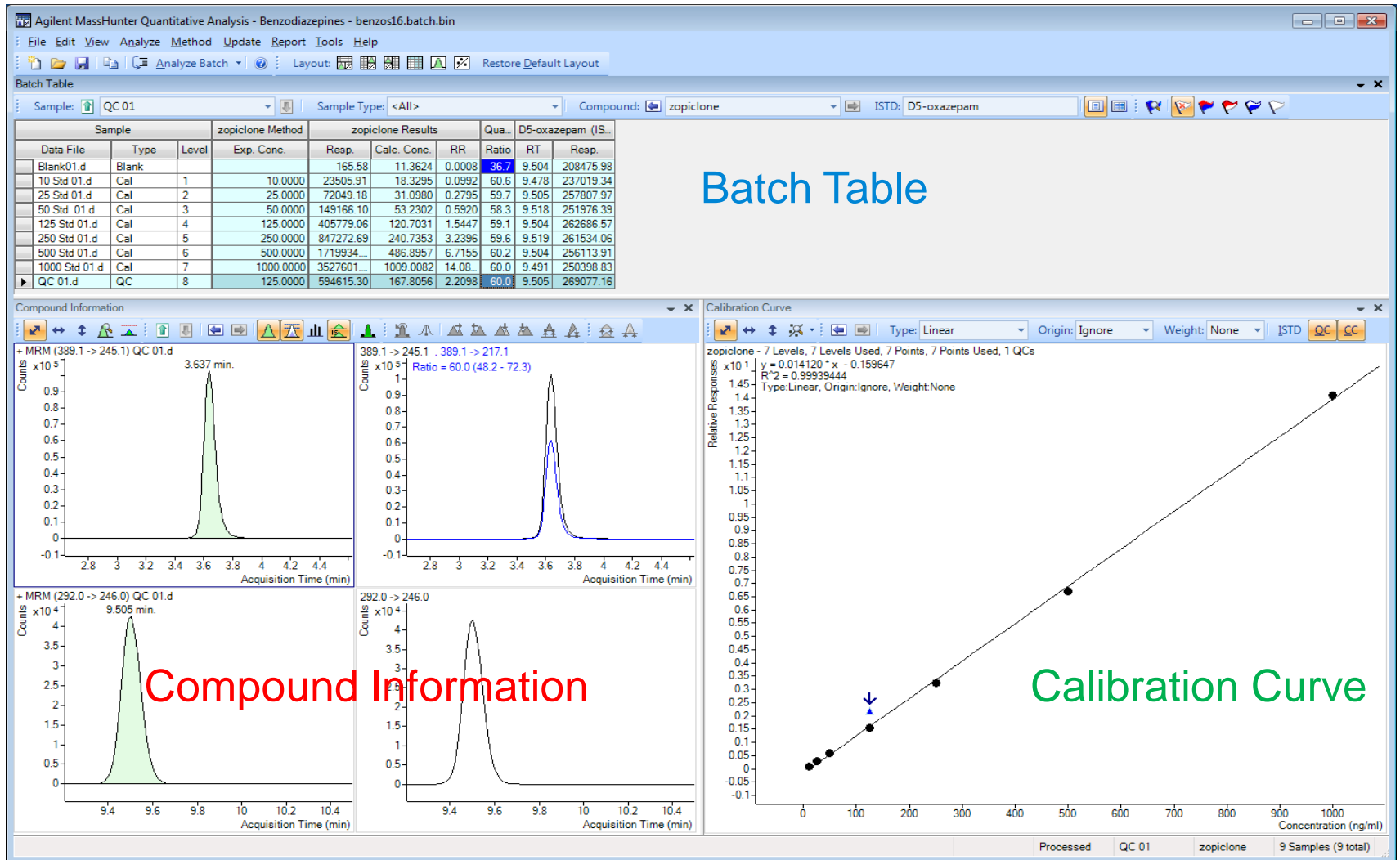
## Four Basic Components to the Batch Directory



Use the icon applicable to the instrument and dataset for the application.

# MassHunter Quantitative Software

## Batch-at-a-Glance View



# MassHunter Quantitative Software Method Editor View

Method > Edit menu or F10 key

The screenshot displays the MassHunter Method Editor interface. On the left is a 'Method Tasks' menu with options like 'New', 'Open', 'Append', 'Edit', 'Validate', 'Save', 'Save As...', 'Exit', and various setup tasks. The main window is titled 'Agilent MassHunter Quantitative Analysis - Method - [C:\MassHunter\Data\QuantExamples\MS\VOA\VOA]'. It features a 'Method Table' at the top, a 'Sample Information' panel with a Total Ion Chromatogram (TIC) plot, and a 'Compound Information' panel with several zoomed-in chromatograms.

**Method Table**

Name	Data File	Type	Level	Acq. Method File	Acq. Date-Time
CAL_L04	CAL_L04.D	Cal	4	624A.M	6/20/2008 9:30...

Name	TS	Scan	Type
1,1-Dichloro-1-pr...	1	Scan	Target

MZ	Rel. Resp.	Uncertainty
77.0	50.0	20.0
110.0	20.0	20.0

Level	Conc.	Response
3	0.5000	19619
4	1.0000	39749
5	2.0000	80091
7		

**Sample Information**

TIC Scan (→) CAL\_L04.D

**Compound Information**

EIC (75.0) Scan CAL\_L04.D

75.0, 77.0, 110.0

Ratio=32.8

Ratio=30.7

Scan (10.049-10.150 min, 19 scans) CAL\_L04.D

39.1, 61.0, 75.0, 109.9, 132.8, 207.0

EIC (96.0) Scan CAL\_L04.D

10.621 min.

96.0, 37.2, 50.0

Ratio=1.8

Ratio=10.1

Scan (10.555-10.746 min, 35 scans) CAL\_L04.D

50.0, 57.0, 63.0, 70.0, 75.0

71 Compounds (71 total) 3 ISTD (3 total)

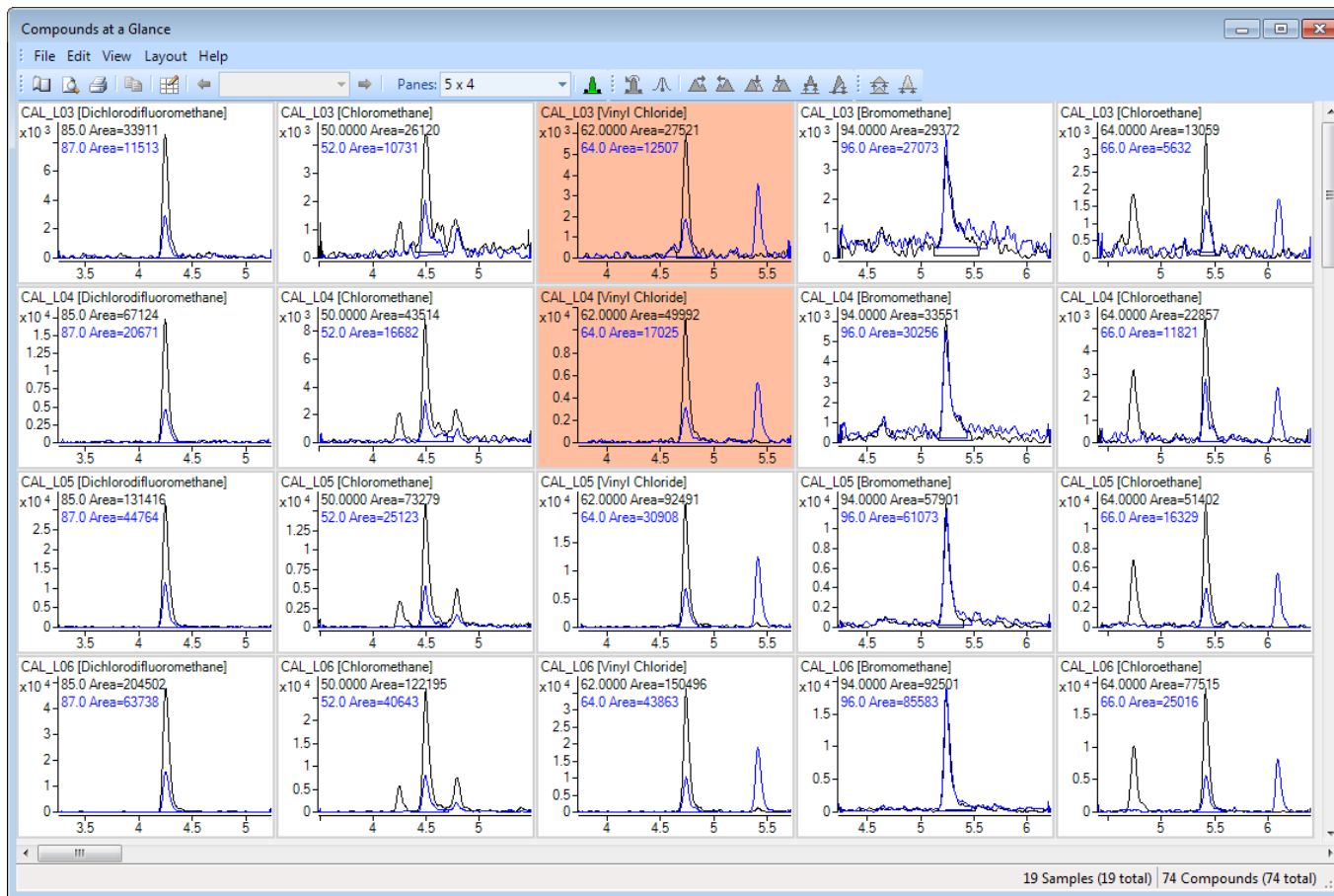
Tip: Only one data file is seen in Method Editor – choose a calibrator.



# MassHunter Quantitative Software

## Compounds at a Glance

View > Compounds-at-a-Glance



# Important MassHunter Quant Concepts and Rules

## Batch Setup

A Batch is a file which contains all the Quant results from a set of data files and the Quant method used.

All the data files in a Batch must reside in a single directory, so put them all together before creating a New Batch.

**Tip: Acquire the data in a unique directory.**

Create the Batch name within the batch directory.

Using the single batch concept allows for easy archiving and retrieving of data.

All information about the batch is stored in the QuantResults\batch.bin file

# Important MassHunter Quant Concepts and Rules: Quant Methods

The most common method problem: Calibration/QC level names in Batch and Quant method do not match, e.g.

- Method: levels are 1,2,3,4,5
- Batch: levels are L1,L2,L3,L4,L5

Second most common problem: a hidden column in the Method with a key parameter, e.g. Ion Polarity if method created manually.

Many Quant parameters can be applied to multiple compounds with the Fill Down feature or Apply to All button.

**Tip: When in doubt, right-click to add columns or additional features.**

# Creating a Batch for Processing

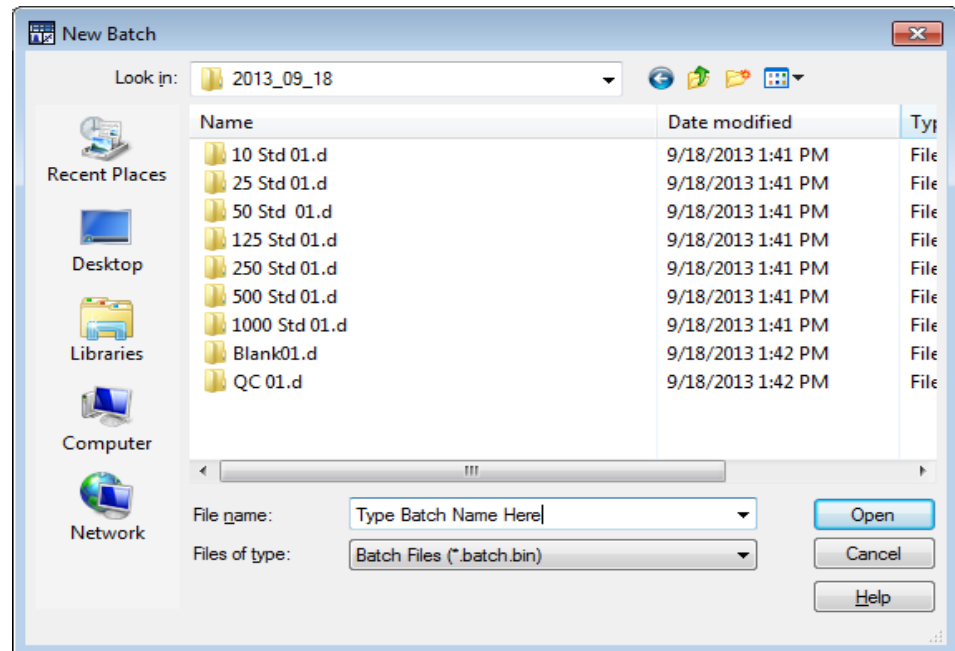
## Batch-at-a-Glance

1) **File > New Batch...**

2) Create the batch in the directory in which the data files reside

3) **Add Samples**

4) **Tip: Highlight or select a high to mid range calibrator before editing the method.**



5) **Method > Open Method from Existing File...**

**Or Method > Open Method from Existing Batch...**

## Short Demo



Let's take a moment for questions on batch definitions and setting up a batch.

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Up Next:

Setting up a quantitation method.

# Creating a Quantitation Method for SQ

## Method > New

### **New Method from Acquired SIM Data...**

Only available from MS Quantitative Analysis icon.  
Available in QQQ but not as useful.

### **New Method from Acquired Scan Data... (with Library Search)**

Use Library Method to identify and create compounds.  
Clean up unwanted compounds.  
Edit ions choices (Selected ions may not be the “best” ions).

### **New Method from Acquired Chromatographic Data...**

Used for 2D Data (UV, FID, ECD, etc.).  
Gives only Compound\_1, etc. based on RT.

### **New Method using Manual Setup**

Manually enter compound data (RT, concentration, masses, etc.).  
Can be tedious for large number of compounds.

### **New Method from File...**

From CEF file generated in Qualitative Analysis.  
From a small user generated library.









**Tip: Avoid using Manual Setup**






# Editing a Quantitation Method

Step through Method Setup Tasks  
Applies to SQ, TOF, QTOF.



In QQQ MRM Setup  
Allows setup of transitions with precursor  
and product ions.

Method Setup Tasks	
Compound Setup	
	Retention Time Setup
	ISTD Setup
	Concentration Setup
	Qualifier Setup
	Calibration Curve Setup
Globals Setup	
Save / Exit	
	Validate
	Save
	Save As...
	Exit

Method Setup Tasks	
MRM Compound Setup	
	Retention Time Setup
	ISTD Setup
	Concentration Setup
	Qualifier Setup
	Calibration Curve Setup

# Method Editor

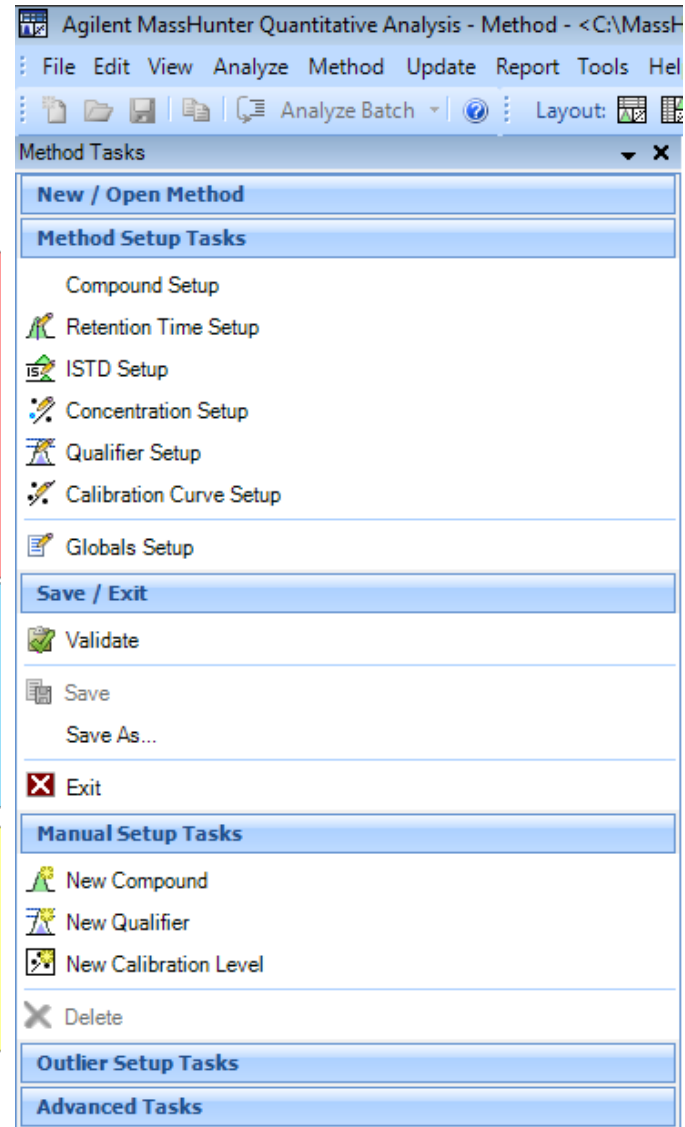
## -Method Tasks

Method Tasks organizes the method actions and parameters into related sections.

Main method editing functions.

Validate content, save and apply Quant method.

Use when you cannot add compounds or qualifiers automatically.





# Editing a Quantitation Method for SQ Compound Setup

**Name** – compound name

**TS** – time segment usually 1 for scan data  
may be many time segments for SIM and MRM data

**Type** – Target, ISTD, Surrogate or Matrix Spike

**MZ** – mass of target or quantifier ion

**RT** – retention time of compound of interest

**Ion Polarity** – may be Positive, Negative, Unassigned or Both  
- in most applications, it will be positive

**Criteria** – Close RT, Close RT with Qualifiers, Greatest Response or  
Greatest Q- value

Quantifier							
Name	TS	Scan	Type	MZ	RT	Ion Polarity	Criteria
BHC beta isomer	1	Scan	Target	219.0	14.327	Positive	Close RT
BHC delta isomer	1	Scan	Target	181.0	15.693	Positive	Close RT
Disulfoton	1	Scan	Target	88.0	15.688	Positive	Close RT
▶ Methyl parathion	1	Scan	Target	263.0	17.726	Positive	Close RT

# Editing a Quantitation Method for All Instruments

## Retention Time Setup

**RT** – retention time of compound of interest

**Left RT Delta** – represents the left side of the EIC window around the expected retention time.

**Right RT Delta** - represents the right side of the EIC window around the expected retention time

**RT Delta Units** – typically in minutes.

Quantifier							
Name	TS	Scan	Type	RT	Left RT Delta	Right RT Delta	RT Delta Units
▶ BHC beta isomer	1	Scan	Target	14.327	0.164	0.164	Minutes
BHC delta isomer	1	Scan	Target	15.693	0.164	0.164	Minutes
Disulfoton	1	Scan	Target	15.688	0.164	0.164	Minutes
Methyl parathion	1	Scan	Target	17.726	0.164	0.164	Minutes
Endosulfan (alph...	1	Scan	Target	23.619	0.164	0.164	Minutes

# Editing a Quantitation Method for All Instruments

Quantifier								
Name	TS	Scan	Type	ISTD Compound Name	ISTD Flag	ISTD Conc.	Time Reference Flag	
4,4'-Dibromooctfluorobiphenyl	1	Scan	ISTD	<None>	<input checked="" type="checkbox"/>	0.4970	<input type="checkbox"/>	
Sulfotep	1	Scan	Target	4,4'-Dibromooctfluorobiphenyl	<input type="checkbox"/>		<input type="checkbox"/>	
Phorate	1	Scan	Target	4,4'-Dibromooctfluorobiphenyl	<input type="checkbox"/>		<input type="checkbox"/>	
BHC alpha isomer	1	Scan	Target	4,4'-Dibromooctfluorobiphenyl	<input type="checkbox"/>		<input type="checkbox"/>	
▶ Pentachloroanisole	1	Scan	Target	4,4'-Dibromooctfluorobiphenyl	<input type="checkbox"/>		<input type="checkbox"/>	

## ISTD Setup

Defines the ISTD and associates each ISTD with one or more target compounds.

Multiple ISTDs can be assigned in a method.

**ISTD - Flag** Toggle this flag on for all ISTDs

**Type** - Compounds assigned as an ISTD become available

**ISTD - Compound Name** Establishes concentration levels

**ISTD Conc.** – a concentration must assigned for each ISTD

**Time Reference Flag** – only ISTD can be assigned as time reference compounds

A Time Reference ISTD adjusts the RT of all target compounds related to a given ISTD due to slight RT shifting due to extraneous factors such as matrix effects. This is done on a per sample basis.

# Editing a Quantitation Method for All Instruments Concentration Setup

Defines the concentration of each compound in the standards.

Agilent MassHunter Quantitative Analysis - Method - <C:\MassHunter\Data\QuantExamples\MS\VOA\QuantResults\VolatileOrganics.batch.bin>

File Edit View Analyze Method Update Report Tools Help

Analyze Batch Layout: Restore Default Layout

Method Tasks

- New / Open Method
- Method Setup Tasks
  - Compound Setup
  - Retention Time Setup
  - ISTD Setup
  - Concentration Setup
  - Qualifier Setup
  - Calibration Curve Setup
  - Globals Setup
- Save / Exit
  - Validate
  - Save
  - Save As...
  - Exit
- Manual Setup Tasks
- Outlier Setup Tasks

Method Table

Time Segment: <All> Compound: Dichlorodifluoro... Reset Table View

Quantifier				
Name	TS	Scan	Type	Units
Dichlorodifluoro...	1	Scan	Target	ng/ml

Calibration			
Level	Conc.	Response	Enable
3	0.5000	29715	<input checked="" type="checkbox"/>
4	1.0000	66597	<input checked="" type="checkbox"/>
5	2.0000	127904	<input checked="" type="checkbox"/>
6	5.0000	198094	<input checked="" type="checkbox"/>
6	5.0000	211200	<input checked="" type="checkbox"/>
7	10.0000	671861	<input checked="" type="checkbox"/>
7	10.0000	795390	<input checked="" type="checkbox"/>
8	15.0000	1105069	<input checked="" type="checkbox"/>
9	20.0000	1474827	<input checked="" type="checkbox"/>
10	30.0000	2199968	<input checked="" type="checkbox"/>
11	40.0000	3126148	<input checked="" type="checkbox"/>
12	50.0000	3975819	<input checked="" type="checkbox"/>

If Unchecked a level can be disabled and not appear in the calibration curve.

Batch Table

Sample: CAL\_L03 Sample Type: <All>

Sample					
Name	Data File	Type	Level	Acq. Date-Time	
CAL_L03	CAL_L03.D	Cal	3	6/20/2008 8:53 AM	
CAL_L04	CAL_L04.D	Cal	4	6/20/2008 9:30 AM	
CAL_L05	CAL_L05.D	Cal	5	6/20/2008 10:06 AM	
CAL_L06	CAL_L06.D	Cal	6	6/20/2008 10:44 AM	

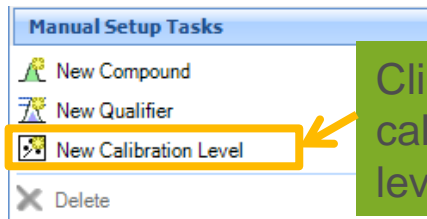
Level in Method must match Level in Batch table!

# Editing a Quantitation Method for All Instruments

## Concentration Setup

Calibration levels can be created manually or automatically.

### Manual Setup



Click to add calibration levels.

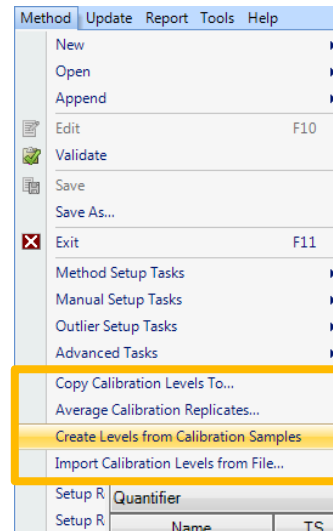
Level	Conc.	Response	Enable
10	30.0000	6482345	<input checked="" type="checkbox"/>
11	40.0000	9154502	<input checked="" type="checkbox"/>
12	50.0000	11963873	<input checked="" type="checkbox"/>

Name	TS	Scan	Type	Units
1,4-Dichloroben...	1	Scan	ISTD	ng/ml
n-Butylbenzene	1	Scan	Target	ng/ml

Level	Conc.	Response	Enable
3	0.5000		<input checked="" type="checkbox"/>
4	1.0000		<input checked="" type="checkbox"/>
5	2.0000		<input checked="" type="checkbox"/>
6	5.0000		<input checked="" type="checkbox"/>
			<input checked="" type="checkbox"/>
			<input checked="" type="checkbox"/>
			<input checked="" type="checkbox"/>
			<input checked="" type="checkbox"/>
			<input checked="" type="checkbox"/>
			<input checked="" type="checkbox"/>

Fill in levels and associated concentrations

### Setup Levels from Calibrators, QCs & CCs in Batch



Level IDs are filled in from the Calibrators, QCs & CCs in the batch. Concentrations must be updated!

Name	TS	Scan	Type	Units
Vinyl Chloride	1	Scan	Target	ng/ml

Level	Conc.	Response	Enable
3	0.5000		<input checked="" type="checkbox"/>
4	1.0000		<input checked="" type="checkbox"/>
5	2.0000		<input checked="" type="checkbox"/>
6	5.0000		<input checked="" type="checkbox"/>
7	10.0000		<input checked="" type="checkbox"/>
8	10.0000		<input checked="" type="checkbox"/>
9	10.0000		<input checked="" type="checkbox"/>
10	10.0000		<input checked="" type="checkbox"/>
11	10.0000		<input checked="" type="checkbox"/>
12	10.0000		<input checked="" type="checkbox"/>

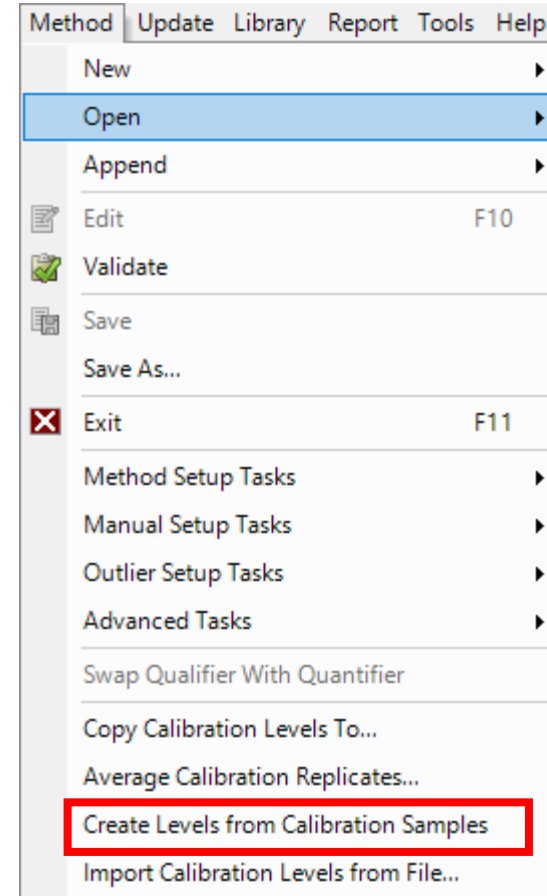
# Creating a Quantitation Method for All Instruments

## Concentration Setup – Create Levels from Calibration Samples

Tip: Fill in the Type, Level and Exp. Conc. columns in the Batch Table

Name	Data File	Type	Level	Exp. Conc.
Benzo Cal03	Benzo Cal03.d	Cal	L1	25.0000
Benzo Cal04	Benzo Cal04.d	Cal	L2	50.0000
Benzo Cal05	Benzo Cal05.d	Cal	L3	125.0000
Benzo Cal06	Benzo Cal06.d	Cal	L4	250.0000
Benzo Cal07	Benzo Cal07.d	Cal	L5	500.0000
Benzo QC	Benzo QC01.d	QC	QC1	189.0000

Then **Method > Edit** and then **Method > Create Levels from Calibration Sample**.



# Editing a Quantitation Method for All Instruments

## Concentration Setup

Method Table

Time Segment: <All> Compound: Dichlorodifluor... Reset Table View

Name	Data File	Type	Level	Acq. Method File	Acq. Date-Time
CAL_L03	CAL_L03.D	Cal	3	624A.M	6/20/2008 8:53...

Quantifier

Name	TS	Scan	Type	Units
Dichlorodifluoro	1	Scan	Target	ng/ml

Calibration

Level	Conc.	Response	Enable
3	0.5000		<input checked="" type="checkbox"/>
4	1.0000		<input checked="" type="checkbox"/>
5	2.0000		<input checked="" type="checkbox"/>
6	5.0000		<input checked="" type="checkbox"/>
7	10.0000		<input checked="" type="checkbox"/>
8	15.0000		<input checked="" type="checkbox"/>
9	20.0000		<input checked="" type="checkbox"/>
10	30.0000		<input checked="" type="checkbox"/>
11	40.0000		<input checked="" type="checkbox"/>
12	50.0000		<input checked="" type="checkbox"/>

Sample Information

+ TIC Scan (\*\* -> \*\*) CAL\_L03.D

Counts x10<sup>6</sup>

1.4  
1.3  
1.2  
1.1  
1  
0.9  
0.8  
0.7

Copy Calibration Levels To...

Copy Calibration Levels To

Select Compounds:

Name	TS	RT	MZ	ISTD Flag	Cmpd. Group
1,1-Dichloro-1-propene	1	10.100	75.0	<input type="checkbox"/>	
Chloromethane	1	4.493	50.0	<input type="checkbox"/>	
1,4-Dichlorobenzene	1	19.539	146.0	<input type="checkbox"/>	
Vinyl Chloride	1	4.734	62.0	<input type="checkbox"/>	
1,2,4-Trichlorobenzene	1	23.290	180.0	<input type="checkbox"/>	
Bromomethane	1	5.231	94.0	<input type="checkbox"/>	
Chloroethane	1	5.410	64.0	<input type="checkbox"/>	
Naphthalene	1	23.680	128.0	<input type="checkbox"/>	
Hexachlorobutadiene	1	23.858	225.0	<input type="checkbox"/>	
Trichlorofluoromethane	1	6.097	101.0	<input type="checkbox"/>	
Acetone	1	6.194	43.0	<input type="checkbox"/>	
1,1-Dichloroethane	1	6.723	61.0	<input type="checkbox"/>	

Select All

OK Cancel

If concentrations are the same, they can be copied to the other compounds.

# Editing a Quantitation Method for All Instruments

## Qualifier Setup

Method Table

Time Segment: <All> Compound: n-Butylbenzene Reset Table View

Quantifier					
Name	TS	Scan	Type	MZ	Uncertainty
1,2-Dichloroben...	1	Scan	Target	146.0	Relative
n-Butylbenzene	1	Scan	Target	91.0	Relative
1,2-Dibromo-3-c...	1	Scan	Target		

Sample Information

+ TIC Scan (\*\* -> \*\*) CAL\_L09.D

+ Scan (20.312-20.360 min, 9 scans) CAL\_L09.D

Right click

- Copy Ctrl+C
- Auto Scale
- X - Auto Scale
- Y - Auto Scale
- Previous Zoom
- Next Zoom
- New Compound
- New Qualifier**
- Search Library
- Search Library Settings...
- Clear Spectrum Panes
- Print... Ctrl+P
- Print Preview...
- Properties...

Qualifier may be added interactively

Quantifier

Name	TS	Scan	Type	MZ
1,2-Dichloroben...	1	Scan	Target	146.0
n-Butylbenzene	1	Scan	Target	91.0

Qualifier

MZ	Rel. Resp.	Uncertainty	Area Sum
92.0	54.4	20.0	<input type="checkbox"/>

Quantifier

Name	TS	Scan	Type	MZ
1,2-Dibromo-3-c...	1	Scan	Target	157.0

+ Scan (20.312-20.360 min, 9 scans) CAL\_L09.D

Quantifier

Name	TS	Scan	Type	MZ
1,2-Dichloroben...	1	Scan	Target	146.0
n-Butylbenzene	1	Scan	Target	91.0

Qualifier

MZ	Rel. Resp.	Uncertainty	Area Sum
92.0	54.4	20.0	<input type="checkbox"/>
134.0	25.4	20.0	<input type="checkbox"/>

Quantifier

Name	TS	Scan	Type	MZ
1,2-Dibromo-3-c...	1	Scan	Target	157.0



# Editing a Quantitation Method for All Instruments

## Qualifier Setup

Expected Qualifier Ion response as Percentage of Quant Ion, and Percentage Uncertainty.

Method Table

Time Segment: <All> Compound: Chloroform

Qualifier					
Name	TS	Scan	Type	MZ	Uncertainty
Chloroform	1	Scan	Target	85.0	Relative
Qualifier					
MZ	Rel. Resp.	Uncertainty	Area Sum		
83.0	161.7	20.0	<input type="checkbox"/>		
87.0	16.0	20.0	<input type="checkbox"/>		
Qualifier					
Name	TS	Scan	Type	MZ	Uncertainty
Propane, 2,2-dic...	1	Scan	Target	77.0	Relative
Qualifier					
MZ	Rel. Resp.	Uncertainty	Area Sum		
97.0	17.2	20.0	<input type="checkbox"/>		
79.0	34.6	20.0	<input type="checkbox"/>		
Qualifier					
Name	TS	Scan	Type	MZ	Uncertainty
cis-1,2-Dichloro...	1	Scan	Target	96.0	Relative

If checked, qualifier area is added to target.

80% Relative Response with 20% Uncertainty

Absolute =  $80 \pm 20 = \text{range of } 60-100$

Relative =  $80 \pm (80 \cdot 20 / 100) = \text{range of } 74 - 96$

# Editing a Quantitation Method for All Instruments

## Calibration Curve

Note: Calibration Curve not available for viewing until batch is analyzed.

The screenshot shows the 'Method Table' window with the following data:

Sample						
Name	Data File	Type	Level	Acq. Method File	Acq. Date-Time	
CAL_L10	CAL_L10.D	Cal	10	624A.M	6/20/2008 1:19...	

Quantifier							
Name	TS	Scan	Type	CF	CF Origin	CF Weight	
1,2-Dichloroetha...	1	Scan	Surrogate	Average of Respons...	Ignore	None	
Toluene-D8	1	Scan	Surrogate	Average of Respons...	Ignore	None	
▶ 1,1-Dichloro-1-pr...	1	Scan	Target	Linear	Ignore	None	
Dichlorodifluoro...	1	Scan	Target	Linear	Ignore	None	
Chloromethane	1	Scan	Target	Linear	Ignore	None	
1,4-Dichloroben...	1	Scan	Target	Linear	Ignore	None	
t-butyl Acetate	1	Scan	Target	Quadratic	Ignore	None	

### Curve Fit

- Linear.
- Quadratic.
- Power.
- 1<sup>st</sup> order In.
- 2<sup>nd</sup> order In.
- Average response factors.

### Curve Fit Origin

- Ignore
- Include.
- Force.
- Blank offset.

### Curve Fit Weight

- None (equal wt.)
- 1/x, 1/x<sup>2</sup>
- 1/y, 1/y<sup>2</sup>
- Log
- 1/SD<sup>2</sup>.

# Editing a Quantitation Method for All Instruments

## 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"/>

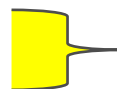


### Apply Multiplier's

- None or Overlapped or Sample Group
- Associates target and qualifiers in min
- [Dynamic Background Subtraction Video](#)
- 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)

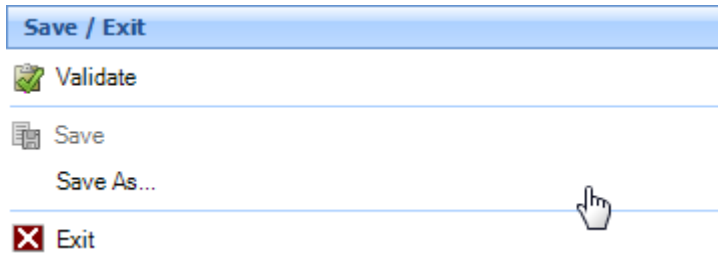


- Peak identification within the extraction window (ISTD with Time Reference Flag checked)
- Semi quant relative to ISTD
- Quantitate with Standard Addition



# Editing a Quantitation Method for All Instruments

## Validate

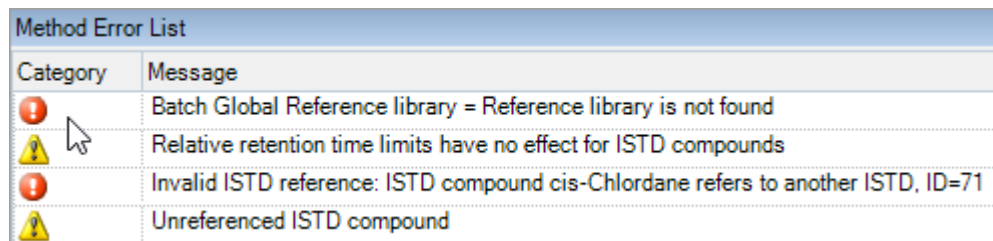






Save and Save As – A quant method can be saved and applied to multiple batches.

**Tip: The calibration table is saved within the method.\***

Red icon – Must be corrected

Yellow icon - Warning

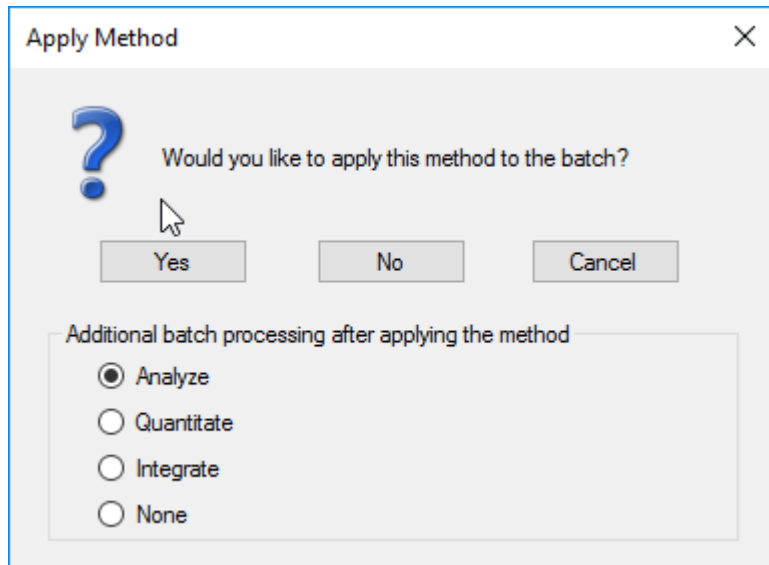


Category	Message
	Batch Global Reference library = Reference library is not found
	Relative retention time limits have no effect for ISTD compounds
	Invalid ISTD reference: ISTD compound cis-Chlordane refers to another ISTD, ID=71
	Unreferenced ISTD compound

**Tip: Double click on the error.**

# Editing a Quantitation Method for All Instruments

## Exit Method Editor and Apply Method



\* **New Feature: B.07.00 and later – Calibration Curve is cleared IF batch contains any Cals.**

**Analyze** may (\*) rebuild the calibration curve and then calculates analyte concentrations.

**Quantitate** does *not* rebuild the calibration curve but calculates concentrations based on the existing curve.

**Integrate** simply calculates the response for compounds in the batch. It does not use the calibration curve nor obtain final concentrations.

# Analyzed Batch !!!

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

File Edit View Analyze Method Update Library Report Tools Help

Analyze Batch Layout: Restore Default Layout

Batch Table

Sample: CAL\_L07 Sample Type: <All> Compound: Dichlorodifluoromethane ISTD: Fluorobenzene

Sample				Dichlorodifluoromethane Results										Qualif..		Fluorobenzene...		Qualif..		Qualif..	
Name	Data File	Type	Level	Acq. Date-Time	Exp. Conc.	RT	Resp.	MI	Calc. Conc.	Final Conc.	Accuracy	MZ	RRT	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		0.0019	0.0019	0.4	0.399	33.6		10.621	13444	1.9		9.5		
CAL_L04	CAL_L04.D	Cal	4	6/20/2008 12:30 PM	1.0000	4.242	66597		0.6134	0.6134	61.3	0.399	30.2		10.621	11839	1.8		10.1		
CAL_L05	CAL_L05.D	Cal	5	6/20/2008 1:06 PM	2.0000	4.247	127904		1.6067	1.6067	80.3	0.400	30.1		10.620	11448	2.0		10.6		
CAL_L06	CAL_L06.D	Cal	6	6/20/2008 1:44 PM	5.0000	4.258	198094		4.6697	4.6697	93.4	0.401	31.0		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		10.2701	10.2701	102.7	0.400	32.4		10.621	11282	2.0		11.0		
CAL_L08	CAL_L08.D	Cal	8	6/20/2008 3:04 PM	15.0000	4.242	1105069		16.1471	16.1471	107.6	0.399	31.4		10.621	11964	2.0		10.9		
CAL_L09	CAL_L09.D	Cal	9	6/20/2008 3:41 PM	20.0000	4.242	1474827		20.7629	20.7629	103.8	0.399	32.0		10.620	12483	2.0		10.4		
CAL_L10	CAL_L10.D	Cal	10	6/20/2008 4:19 PM	30.0000	4.248	2199968		29.6758	29.6758	98.9	0.400	33.0		10.621	13102	1.7		10.3		
CAL_L11	CAL_L11.D	Cal	11	6/20/2008 4:57 PM	40.0000	4.247	3126148		40.9978	40.9978	102.5	0.400	33.0		10.626	13525	1.9		10.6		
CAL_L12	CAL_L12.D	Cal	12	6/20/2008 5:35 PM	50.0000	4.247	3975819		48.7544	48.7544	97.5	0.400	32.8		10.621	14486	2.1		10.3		
CC_L07	CC_L07.D	CC	7	6/20/2008 6:13 PM	10.0000	4.247	795390		10.1228	10.1228	101.2	0.400	34.2		10.621	13544	1.6		10.7		
QC_L05	QC_L05.D	QC	6	6/20/2008 6:50 PM	5.0000	4.247	211200		2.5422	2.5422	50.8	0.400	32.1		10.620	12881	1.7		10.5		
Blank01	BLANK01.D	Blank		6/20/2008 7:28 PM	0.0000	4.258	20853		0.0000	0.0000		0.401	37.2		10.626	12013	2.1		10.9		
Blank02	BLANK02.D	Blank		6/20/2008 8:07 PM	0.0000	4.630	266		0.0000	0.0000		0.436			10.621	10598	1.9		10.3		
SAMPLE01	SAMPLE01.D	Sample		6/20/2008 8:44 PM	0.0000	4.139	287		0.0000	0.0000		0.390			10.621	11654	2.0		10.3		
SAMPLE02	SAMPLE02.D	Sample		6/20/2008 9:22 PM	0.0000	3.418	519		0.0000	0.0000		0.322	12.		10.626	11386	2.2		10.8		
SAMPLE03	SAMPLE03.D	Sample		6/20/2008 10:00 PM	0.0000	3.882	662		0.0000	0.0000		0.366	16.		10.621	10362	2.2		11.1		
SAMPLE04	SAMPLE04.D	Sample		6/20/2008 10:38 PM	0.0000	4.035	353		0.0000	0.0000		0.380	55.8		10.621	990498	2.5		11.8		
SAMPLE05	SAMPLE05.D	Sample		6/20/2008 11:16 PM	0.0000	4.842	286		0.0000	0.0000		0.456	18.		10.621	12056	2.1		11.3		

Compound Information

EIC (85.0) Scan CAL\_L07.D

85.0 .870  
Ratio = 32.4 (92.5 %)

Calibration Curve

Dichlorodifluoromethane - 10 Levels, 10 Levels Used, 10 Points, 10 Points Used, 1 QCs

Type: Linear Origin: Ignore Weight: None ISTD: QC CC

Relative Responses

$y = 0.558398 * x + 0.021997$   
 $R^2 = 0.99807851$   
 Type: Linear, Origin: Ignore, Weight: None

Processed CAL\_L07 Dichlorodifluoromethane 19 Samples (19 total)

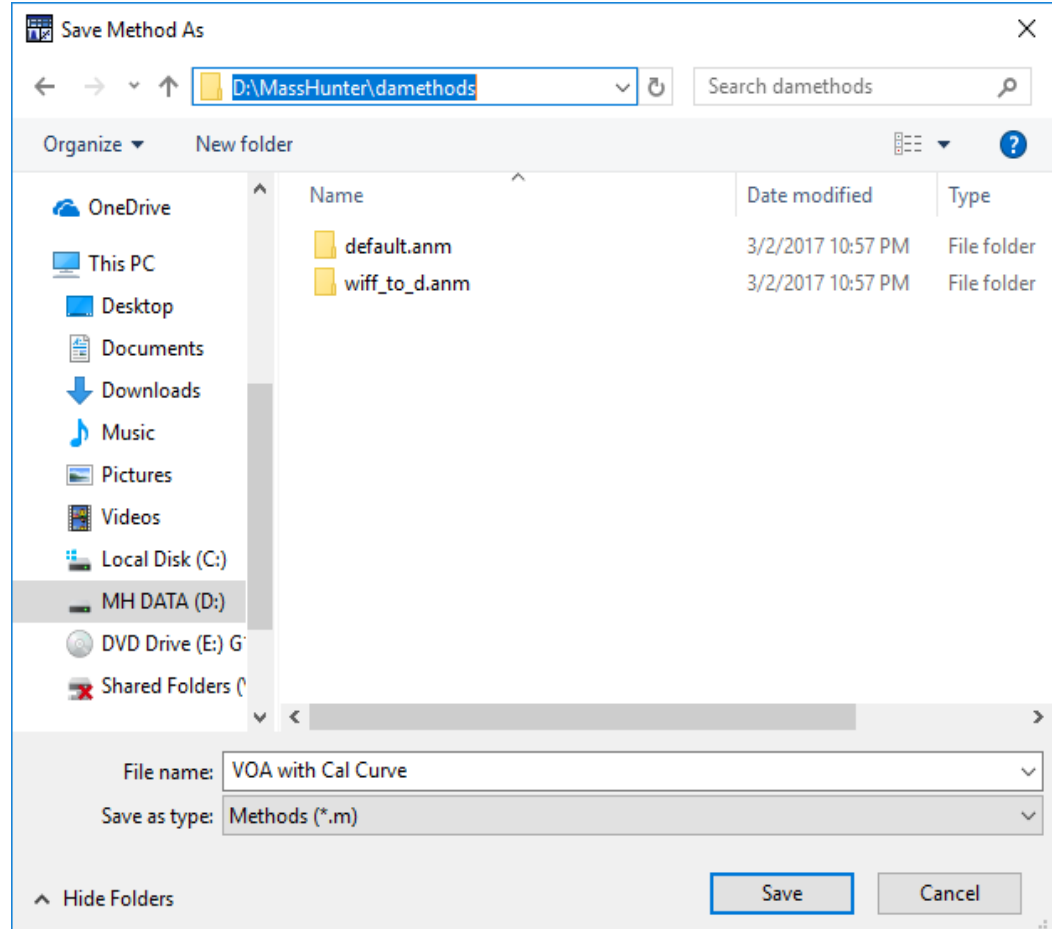
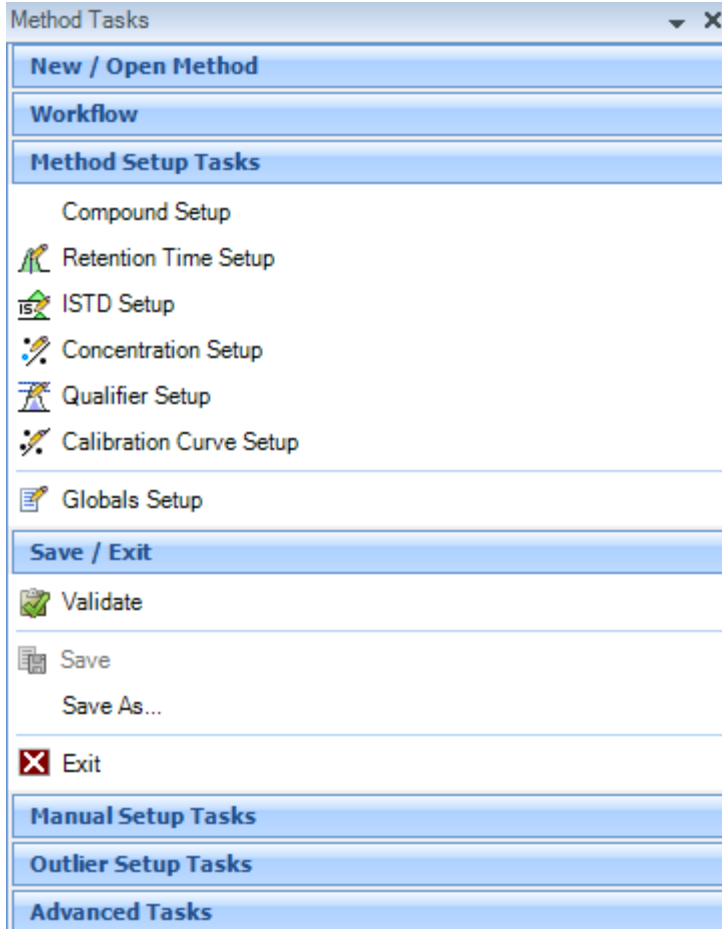
Saving a Method with the Calibration Table Information  
 Method > Edit > Save As method to retain calibration table.  
 Note: Save the method again after Analyzing the batch.

Methods can be used over and over.

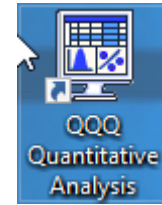
# Saving a Method with the Calibration Table Information

**Method > Edit > Save As** method to retain calibration table.

**Tip: Save the method again after Analyzing the batch.**



# Editing a Quantitation Method for QQQ Compound Setup



**Name** – compound name

**TS** – time segment usually 1 for scan data

may be many time segments for SIM and MRM data

**Transition** – Precursor ion → Product ion

**Scan** – MRM (Multiple Reaction Monitor)

**Type** – Target, ISTD, Surrogate or Matrix Spike

**Precursor ion** – mass of the ion

**Product Ion** – mass of the ion

**RT** – retention time of compound of interest

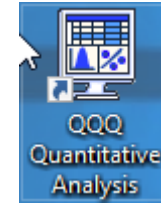
**Ion Polarity** – may be Positive, Negative, Unassigned or Both  
- in most applications, it will be positive

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

Quantifier								
Name	TS	Transition	Scan	Type	Precursor Ion	Product Ion	RT	Ion Polarity
7-amino clonazepam	1	286.0 -> 121.0	MRM	Target	286.0	121.0	0.983	Positive
7-amino flunitrazepam	1	284.0 -> 226.0	MRM	Target	284.0	226.0	1.181	Positive
D4-7-amino clonazepam	1	290.0 -> 226.0	MRM	ISTD	290.0	226.0	0.973	Positive
zopiclone	2	389.1 -> 245.1	MRM	Target	389.1	245.1	2.471	Positive



# Editing a Quantitation Method for QQQ Qualifier Setup



**Precursor Ion** – mass of the ion

**Product Ion** – mass of the ion

**Transition** – Precursor ion → Product ion

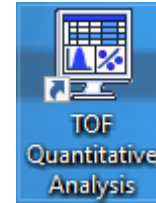
**Relative Response** – ratio of Qualifier to Quantifier

**Uncertainty** – amount of variation of the relative response

**Area Sum** – summation of qualifier area to the target area.

Quantifier								
Name	TS /	Transition	Scan	Type	Precursor Ion	Product Ion	Uncertainty	
clonazepam	3	316.0 -> 270.0	MRM	Target	316.0	270.0	Relative	
Qualifier								
Precursor Ion	Product Ion	Transition	Rel. Resp.	Uncertainty	Area Sum			
316.0	214.0	316.0 -> 214.0	23.0	20.0	<input type="checkbox"/>			

# Editing a Quantitation Method for TOF Mass Extraction Setup

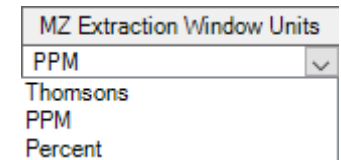


## Method > Edit > Advanced Tasks > Mass Extraction Setup

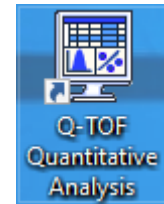
Allows for a mass range for the extraction of the accurate mass (MZ).

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



# 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

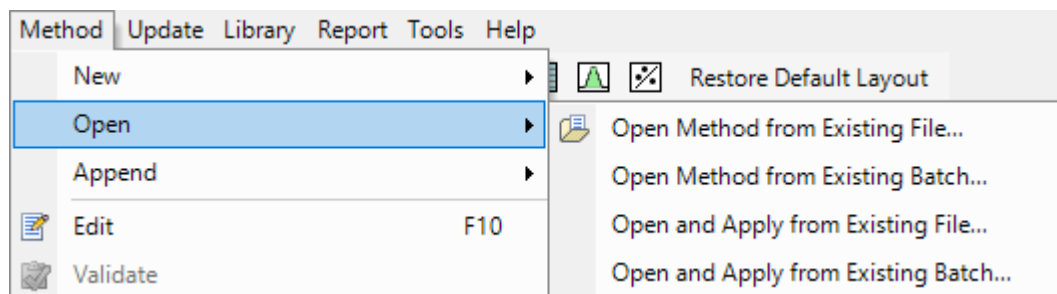
**Tip:** Enter the Precursor Ion and the Product Ion—Transition auto populates.

# Using an Existing Method

**Method > Open from Existing File...**

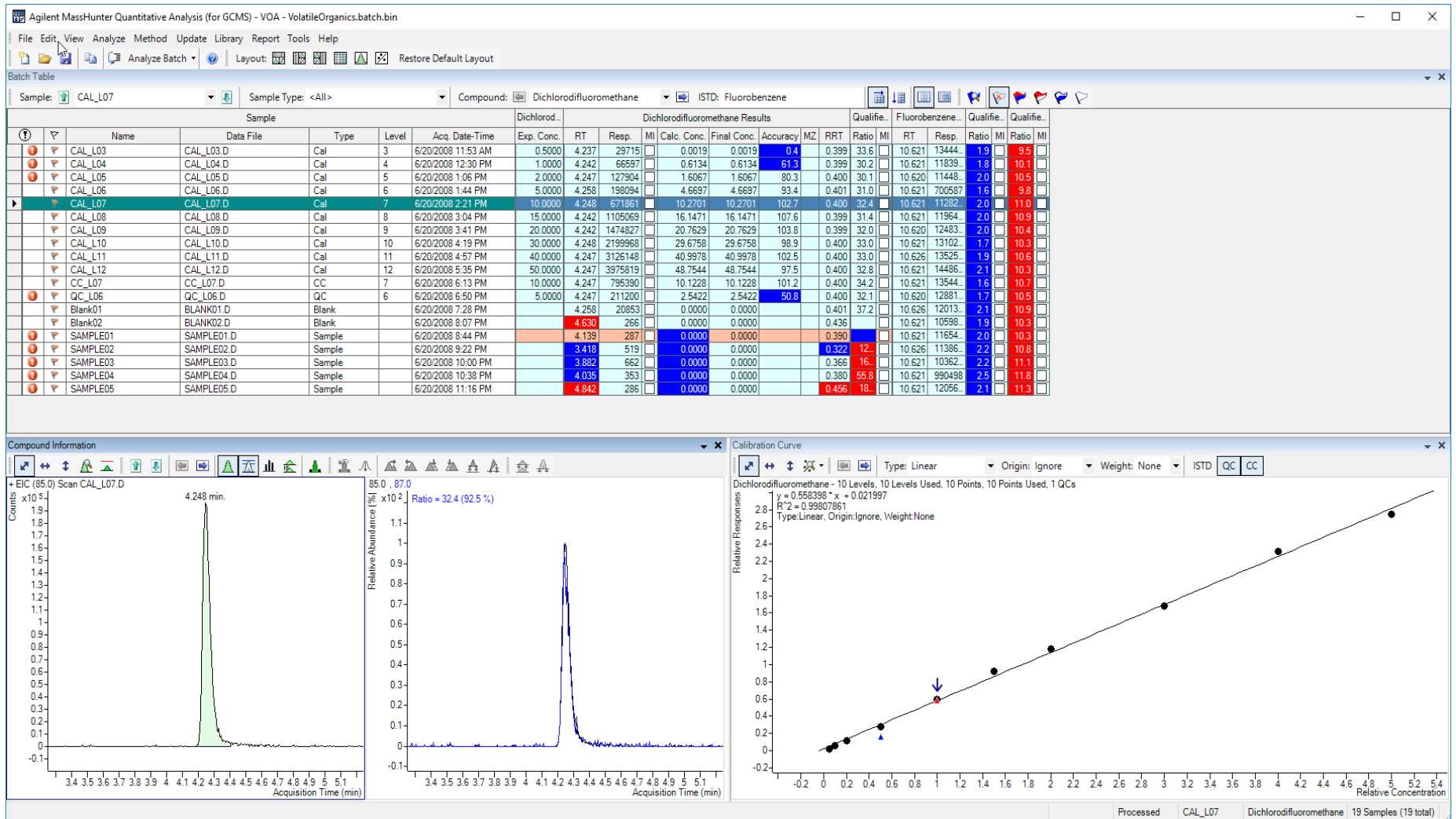
**Method > Open from Existing Batch...**

The quantitation database is saved in the method and in the batch file and can be recalled from either location.



Opening and applying method from existing file or batch does not automatically enter the Method Editor—stays at the Batch Table.

# Analyzed Batch !!!



Once developed, Methods can be used over and over.

Demo



Let's take a moment  
for questions on  
setting up a  
quantitation method  
and Method Editor.

Up Next:  
Outlier Tasks

# Outlier Setup Tasks

Outliers are setup in the Method Editor and are part of quant method.

Outliers are used to perform automated quality checks.

Aids in data review by highlighting problem areas.

Increases confidence in data integrity by applying outliers.

Greater than 45 outliers are available.

Can create Custom Calculations.

Outlier Setup Tasks	
Retention Time	Relative Response Factor
Relative Retention Time	Response Factor
Peak Resolution	<input type="checkbox"/> QC
Peak Symmetry	QC Relative Standard Deviation
Peak Full Width Half Maximum	QC LCS Recovery
Peak Purity	<input checked="" type="checkbox"/> CC Average Response Factor
Plates	CC ISTD Response Ratio
Capacity Factor	CC Relative Response Factor
Signal-to-Noise Ratio	CC Response Ratio
<input checked="" type="checkbox"/> Limit Of Detection	CC Retention Time
Limit Of Quantitation	<input checked="" type="checkbox"/> Matrix Spike
Method Detection Limit	Matrix Spike Percent Difference
<input checked="" type="checkbox"/> Qualifier Ratio	Matrix Spike Percent Recovery
QValue	Matrix Spike Group Recovery
Qualifier Coelution Score	<input checked="" type="checkbox"/> Surrogate
ISTD Response	Surrogate Percent Recovery
ISTD Response Percent Deviation	Response Check
Sample Amount	Mass Accuracy
Sample RSD	Mass Match Score
Blank Concentration	<input checked="" type="checkbox"/> Library Match Score
Blank Response	Alternative Peak
Accuracy	Custom Calculation
Average Response Factor	
Average Response Factor RSD	
<input checked="" type="checkbox"/> Curve Fit R2	

# Outliers in Batch At a Glance



Icons on the toolbar



Select Outliers



Turn off outlier filter



Display rows that have High/Low outliers



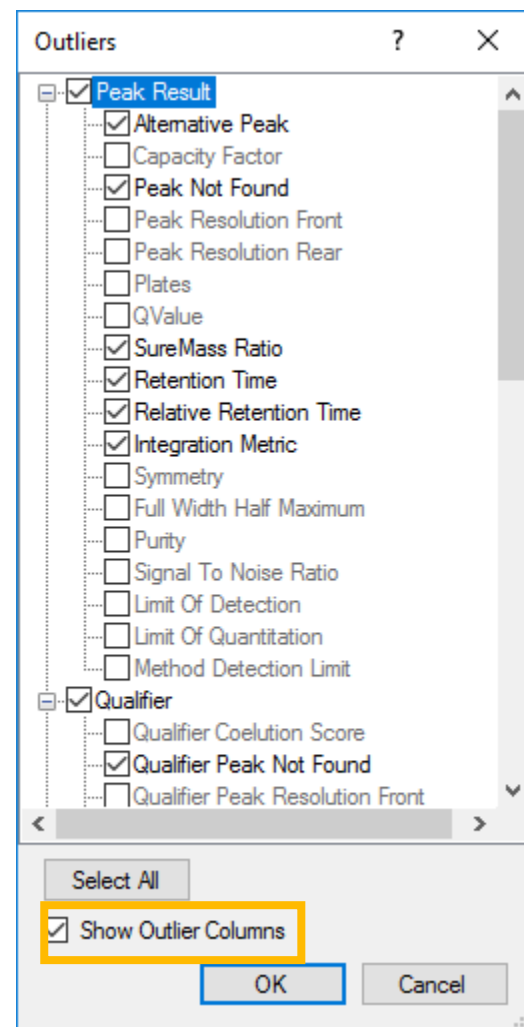
Display rows that have High outliers



Display rows that have Low outliers



Display rows that have no outliers





# Outliers Help

MassHunter QuantDA Workstation Software

Hide Back Print

Contents Search

Type in the keyword to find:

method outlier

List Topics

Select Topic to display:

- MatrixSpikePercentRecoveryMaximum
- MatrixSpikePercentRecoveryMinimum
- MatrixType
- MatrixTypeOverride
- MaximumAverageResponseFactorRSD
- MaximumBlankConcentration
- MaximumBlankResponse
- MaximumCCResponseFactorDeviation
- Method
- Method > Outlier Setup
- MinimumAverageResponseFactor
- MinimumPercentPurity
- MinimumSignalToNoiseRatio
- New Method from Acquired Chromatogr...
- New Method from Acquired MRM Data
- New Method from Acquired Scan Data
- New Method from Acquired Scan Data ...
- New Method from Acquired SIM Data
- New Method Using Manual Setup
- Optimize compound identification using ...
- Outlier
- Outlier Details
- Outlier Setup Tasks Section
- OutlierAccuracy
- OutlierAlternativePeak
- OutlierAverageResponseFactor
- OutlierAverageResponseFactorRSD
- OutlierBelowLimitOfDetection

Display

## Method > Outlier Setup Tasks

These menu items are only available when you are in the Method Edit view.

### Retention Time

[Specify a retention time outlier](#)

### Relative Retention Time

[Specify a relative retention time outlier](#)

### Peak Resolution

[Specify a peak resolution outlier](#)

### Peak Symmetry

[Specify a peak symmetry outlier](#)

### Peak Full Width Half Maximum

[Specify a full width half maximum outlier](#)

### Peak Purity

[Specify a peak purity outlier](#)

### Signal To Noise Ratio

[Specify a signal to noise outlier](#)

## Specify a peak resolution outlier

This outlier metric is a measure of how well two neighboring peaks are separated. This outlier applies to the primary peaks of all compound types and all sample types.

This outlier metric is determined by comparing the calculated resolution value of the primary peak against a user-defined limit ResolutionLimit. The peak resolution outlier applies to target, qualifiers, and internal standard results.

To set the limit for the peak resolution:

1. From the Method Task window, select **Outlier Setup Tasks > Peak Resolution** to display the Quantifier Method Table with the Resolution Limit column highlighted.
2. Enter the value in the Resolution Limit column for the first compound.
3. Enter the values for the other compounds.

The outlier is set to **Low** if

$$\text{ResolutionFront (ResolutionRear)} < \text{ResolutionLimit}$$

# Outliers Videos

Many Outliers have videos associated on the topic



## Advanced User Videos

The following Agilent MassHunter Quantitative Analysis advanced video demonstrations are available on your installation DVD in the Supplemental > Videos > Quant folder. Open the outline.htm for a table of contents that organizes and links you to the videos.

## What's new in Quant B.08.00

Quant videos are located on the Desktop (if installed)

Quant B.08 DVD 2 of 3 in  
**MassHunter > Videos > Quant**

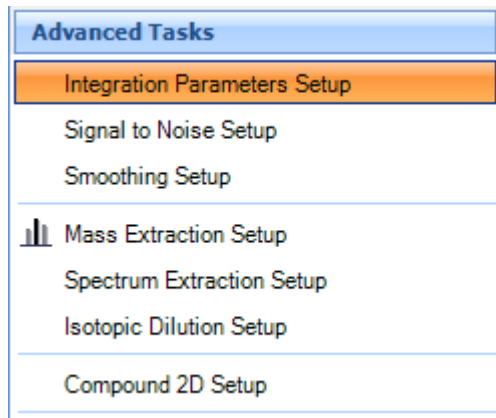
### Quant Outliers

- Method Editor - Alternative Peak outlier (Advanced)
- Method Editor - Signal to Noise Ratio outlier (Advanced)
- Method Editor - Theoretical Plates outlier (Advanced)
- Method Editor - Peak Symmetry outlier (Advanced)
- Method Editor - Capacity outlier (Advanced)
- Method Editor - QValue outlier (Advanced)
- Method Editor - MatrixType outlier (Advanced)

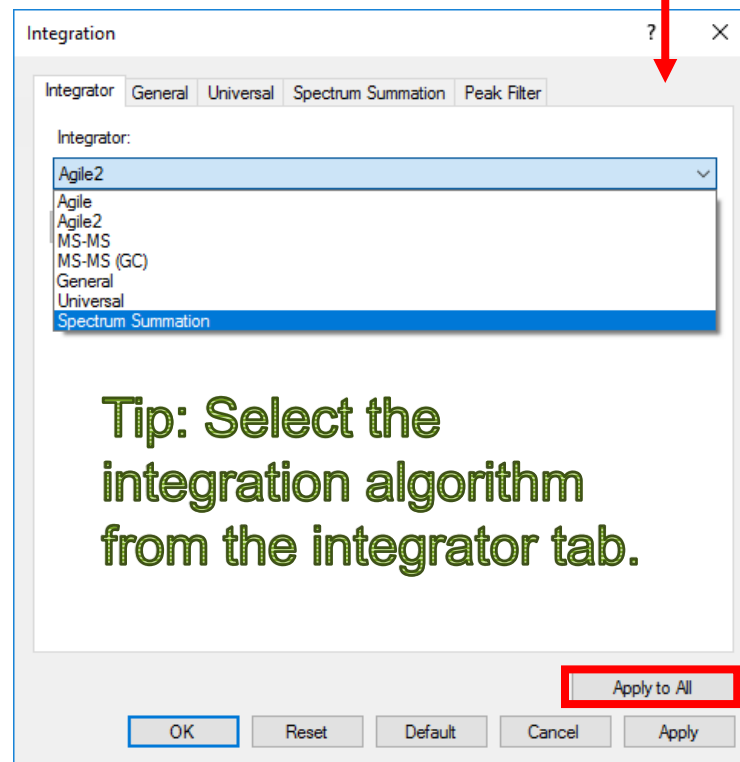
# Editing a Quantitation Method

## Advanced Tasks Integration Parameters

Accessed via **Method > Edit > Advanced Tasks > Integration Parameters Setup**



Quantifier							
Name	TS	Scan	Type	RT	Int.	Int. Params.	
Chloromethane	1	Scan	Target	4.493	Agile2		
Qualifier							
MZ	Rel. Resp.	Uncertainty	Int. Params.				
52.0	35.0	20.0					



Each compound can have a unique set of integration parameters.

Each qualifier can have unique parameters or same as target ion.

Integration parameters can be applied to ALL compounds.

# Editing a Quantitation Method

## Integrator Parameters

### Agile2

Default Integrator, 3<sup>rd</sup> generation parameter less integrator  
Better baselines, higher sensitivity to smaller peaks.

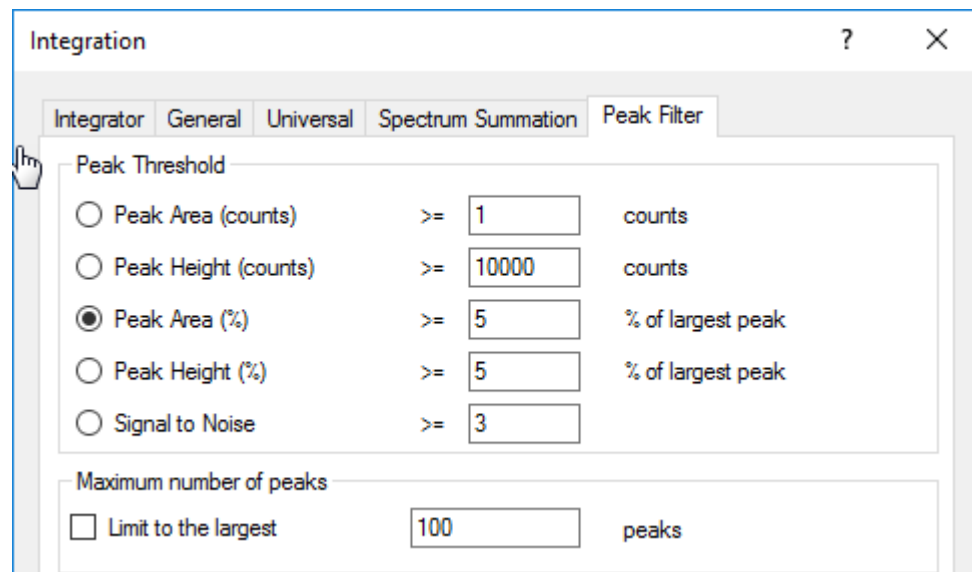
### Agile

2<sup>nd</sup> generation parameter less integrator.

### MS/MS and MS/MS (GC)

1<sup>st</sup> generation parameter less integrator intended for MS/MS systems, not recommended for SQ. Originally required 64 data points.

All parameter less algorithms have Peak Filter tab.



The screenshot shows the 'Integration' window with the 'Peak Filter' tab selected. The window has a title bar with a question mark and a close button. Below the title bar are five tabs: 'Integrator', 'General', 'Universal', 'Spectrum Summation', and 'Peak Filter'. The 'Peak Filter' tab is active and contains the following settings:

Parameter	Operator	Value	Unit
<input type="radio"/> Peak Area (counts)	>=	1	counts
<input type="radio"/> Peak Height (counts)	>=	10000	counts
<input checked="" type="radio"/> Peak Area (%)	>=	5	% of largest peak
<input type="radio"/> Peak Height (%)	>=	5	% of largest peak
<input type="radio"/> Signal to Noise	>=	3	

Below the 'Peak Threshold' section is the 'Maximum number of peaks' section:

<input type="checkbox"/> Limit to the largest	100	peaks
---	-----	-------

# Editing a Quantitation Method

## Integrator Parameters

### General (RTE)

Familiar to MSD ChemStation users.

Areas in Universal are 10 time smaller than seen in ChemStation.

Integrator Parameters

Initial Parameters

Threshold: 18 Peak Width: 0.02

Area Reject: 1  Shoulder Detection

Timed Events

Event	Value	Time
Area Reject		
Area Sum OFF		
Area Sum ON		
Baseline All Valleys OFF		
Baseline All Valleys ON		
Baseline Back		
Baseline Hold OFF		
Baseline Hold ON		
Baseline Next Valley		
Baseline Now		
Integrator OFF		
Integrator ON		
Negative Peak OFF		
Negative Peak ON		
Peak Width		
Solvent Peak OFF		
Solvent Peak ON		
Tangent Skim		
Threshold		

Buttons: OK, Reset, Default, Cancel, Apply

Integrator Parameters

Detector

Data point sampling: 1

Smoothing

Detection filtering: 5 point

Start threshold: 0.2

Stop threshold: 0

Peak location: Top

Baseline Allocation

Baseline reset (# points) > 5

If leading or trailing edge < 100 %

Baseline preference: Tangent skim else drop

### Universal

1<sup>st</sup> generation ChemStation integrator.

Familiar to MSD ChemStation users.

Significant number of timed events.

# Editing a Quantitation Method

## Integrator Parameters

### Spectrum Summation

Integrator designed for situations where compounds are poorly separated or peak shape is highly irregular.

PCB mixtures, TPH and GRO  
Fraction cut in hydrocarbons  
Flow injection analysis

Sums signal over a time range

Exclude signal below threshold

Always gives a horizontal baseline

RT reported as the center of the time range

The screenshot shows the 'Integration' dialog box with the 'Spectrum Summation' tab selected. The 'Baseline' section has three radio button options: 'Use lowest point as baseline offset', 'Use fixed baseline offset' (which is selected), and 'Use lowest point in RT range as baseline offset'. Below the selected option is a text input field containing '0' followed by the unit 'counts'. The 'Use lowest point in RT range as baseline offset' option has two sub-inputs: 'Start RT: 0 min.' and 'End RT: 0 min.'. The 'Peak start and end' section has two radio button options: 'Use relative deltas from extraction window' (selected) and 'Use absolute times'. Below the selected option are two rows of input fields: 'Start integration' with a text input '0' and a dropdown menu set to 'Percent', and 'End integration' with a text input '0' and a dropdown menu set to 'Percent'. At the bottom of the dialog are buttons for 'Apply to All', 'OK', 'Reset', 'Default', 'Cancel', and 'Apply'.

# Editing a Quantitation Method

## Setting an integration threshold

**Method > Edit then Tools > Actions > Set Peak Filter Area Threshold**

Choose any value as a percentage of lowest calibrator

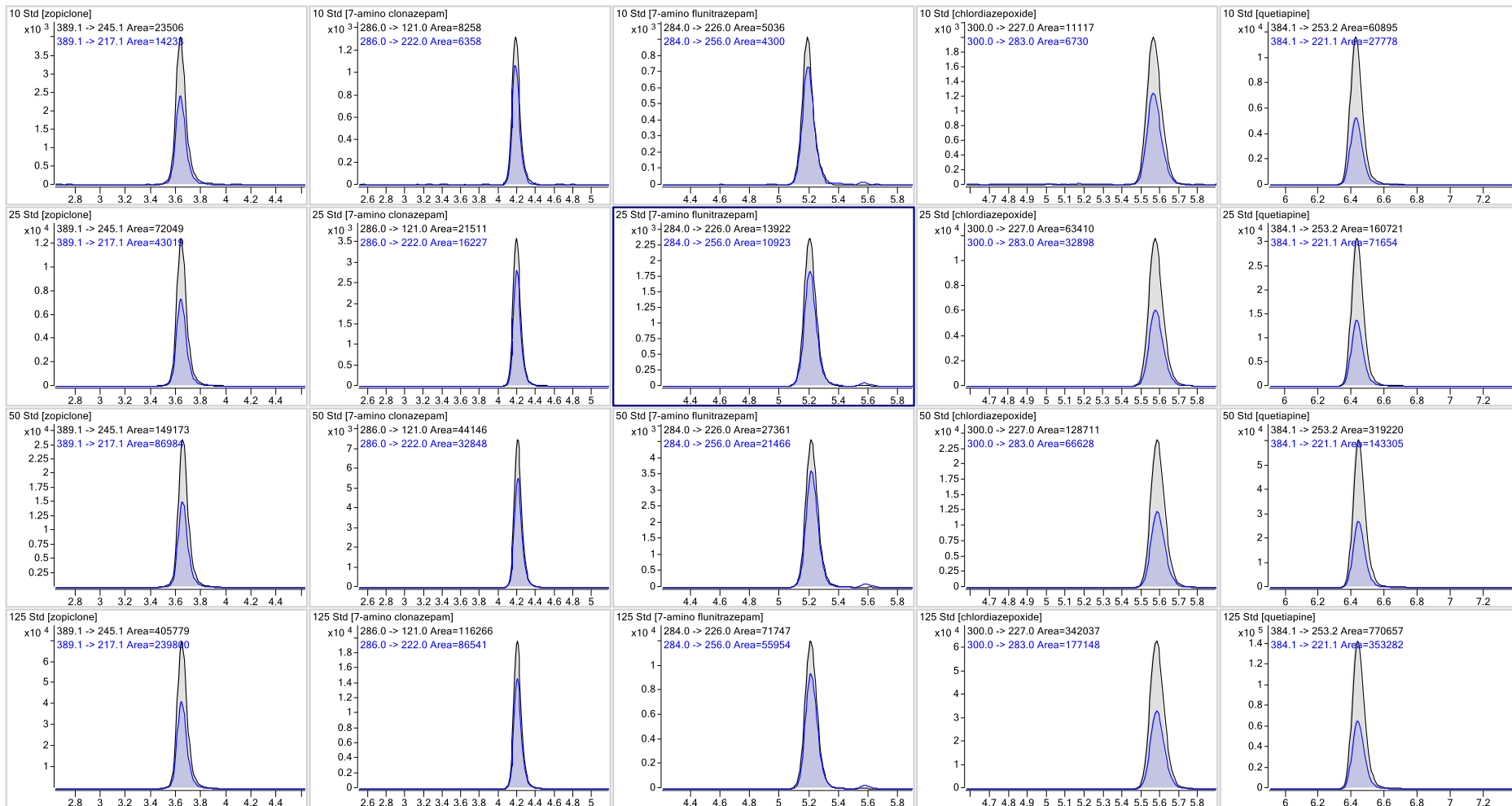
The screenshot shows the Agilent MassHunter Quantitative Analysis (for QQQ) interface. The 'Tools' menu is open, and the 'Actions' sub-menu is displayed. The 'Set Peak Filter Area Threshold' option is highlighted with a red box. The background shows the 'Method Setup Tasks' pane with 'Concentration Setup' selected, and a 'Calibration' table with levels L1 through L5, where 'QC1' is selected.

Level
L1
L2
L3
L4
L5
QC1

The dialog box is titled 'Set Peak Filter Area Threshold'. It contains a text input field with the label 'Percentage of lowest cal level (30, 50, 80 etc):'. The input field is highlighted with a red box. Below the input field are 'OK' and 'Cancel' buttons.

# Compounds-at-a-Glance

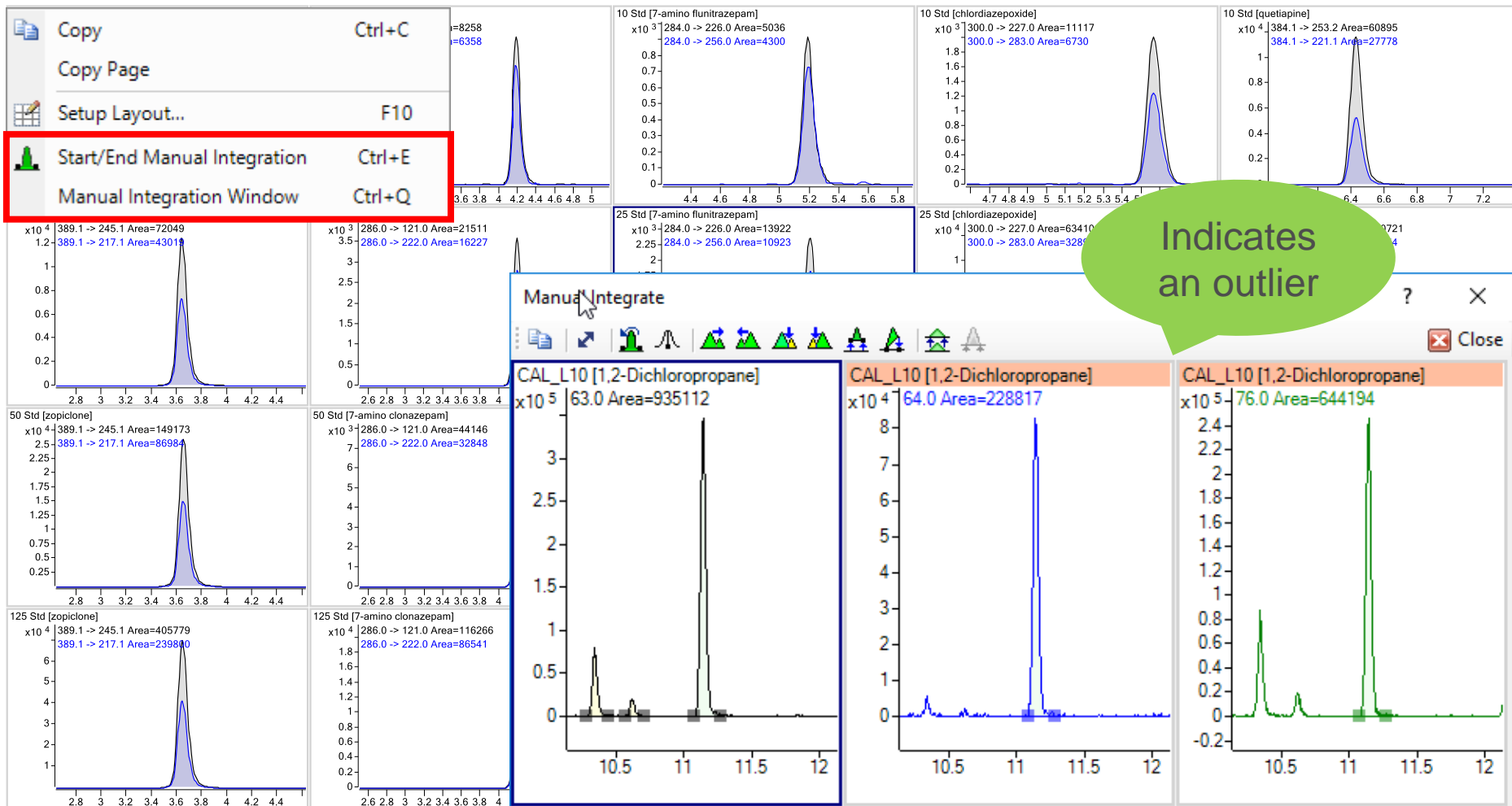
## View > Compounds-at-a-Glance...





# Compounds-at-a-Glance

Manual integration – right-click context menu or 



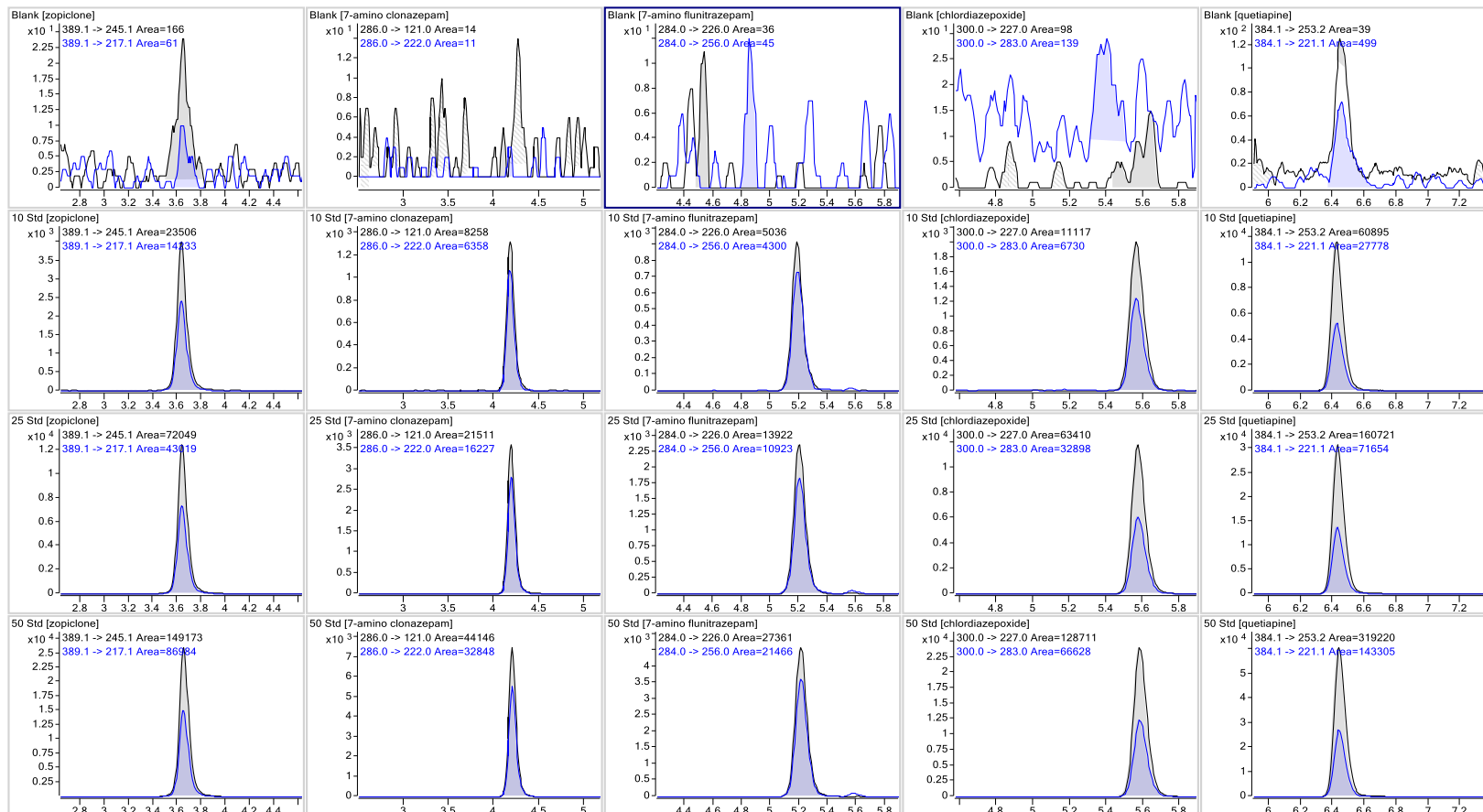
# Compounds-at-a-Glance

## Zero multiple peaks

Select manual integration icon



Hold down CTRL key, click multiple peaks, click the zero peak icon.



Demo



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

---

Up Next:  
Reporting

# Report Generation Excel

Report > Generate

Generate Report

Batch file:

Batch folder: D:\MassHunter\Data\QuantExamples\MS\VOA\  
Batch file: VolatileOrganics.batch.bin Browse...

Report folder: D:\MassHunter\Data\QuantExamples\MS\VOA\QuantReports\Volatilil Browse...

Report method: D:\MassHunter\Report Templates\My Quant Report.m  
Choose... New... Edit...

Samples/Compounds:

All samples Choose samples...  
 All compounds Choose compounds...

Generate:

Generate reports now  
 Open report folder after reports generated  
 Queue report task  
 Start Queue Viewer

OK Cancel

Report folder

Quant Report  
Method

# Report Method Edit Excel

**Report Mode** – Batch or Single Sample.

**Publish Format** – XLSX, PDF, TEXT or CSV.

Report Method Edit (Quantitative Analysis) - My Quant Report.m

File Edit Tools

Templates Results Graphics settings

Template	Report mode	Destination file	Publish format	Language	Page Size	Printer	Open published file	Post Process	Audit Trail Report
D:\Mass...\QuantReport_ISTD_Complete_B_06_00.xlsx	Batch	QuantReport_IS...	XLSX				<input checked="" type="checkbox"/>	<None>	<input type="checkbox"/>

Excel template is XLTX file

Add Template... Remove Template Edit Post Processes... Save & Exit Exit

# Report Method Edit Excel

## Results tab

Report Method Edit (Quantitative Analysis)

File Edit Tools

Templates Results Graphics settings

Instrument type: QQQ

Generate report results (report.results.xml):

- Auto  
Generate results file only when Excel report templates are selected.
- Yes  
Always generate results file
- No  
Never generate results file
- Upload results file

Instrument type options: QQQ, QQQ, GCMS, QTOF, TOF, GC

Select the correct  
instrument type

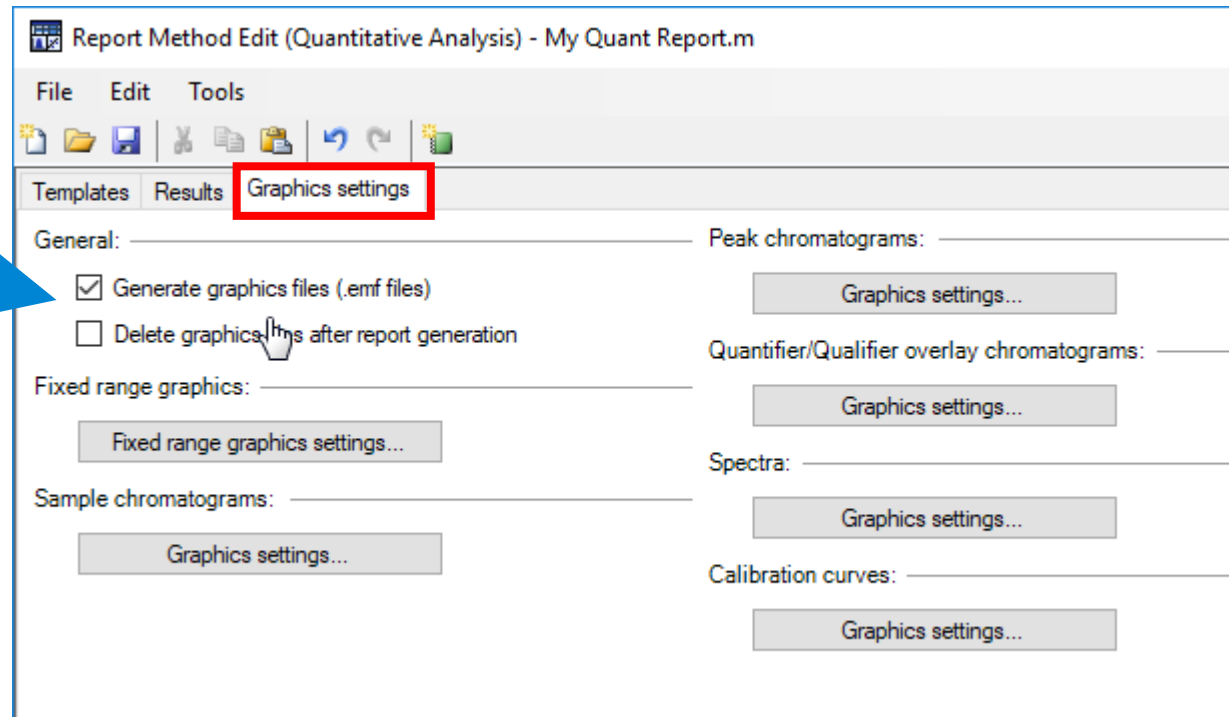
For Excel always select  
Auto or Yes

# Report Method Edit Excel

## Graphic Settings tab.

Allows customization of the graphics output.

Always generate the graphics if the file contains graphic output.



# Report Method Edit

## PDF Reporting

PDF Reports are located D:\MassHunter\Report Templates\Quant\PDF-Reporting folder.

Run much faster for large batches.

PDF reports are built on Python code and take the form of xml files.

Only available Publish format is PDF.

On the **Results** tab, there is no need to generate the results file.

On the **Graphic Settings** tab, there is no need to Generate graphics files.



# Report Method Edit

## PDF Reporting

Report Method Edit (Quantitative Analysis)

File Edit Tools

Templates Results Graphics settings

Instrument type: \_\_\_\_\_

QQQ

Generate report results (report.results.xml): \_\_\_\_\_

Auto  
Generate results file only when Excel report templates are selected.

Yes  
Always generate results file

No  
Never generate results file

Upload results file

Report Method Edit (Quantitative Analysis)

File Edit Tools

Templates Results Graphics settings

General: \_\_\_\_\_

Generate graphics files (.emf files)

Delete graphics files after report generation

Fixed range graphics: \_\_\_\_\_

Fixed range graphics settings...

Sample chromatograms: \_\_\_\_\_

Graphics settings...

PDF Reporting will still generate graphics even when this checkbox is disabled.

# Report Method Graphic Settings

Applies to Excel or PDF Reporting.

Label compound name on the TIC.

Sample chromatograms: \_\_\_\_\_

Graphics settings...

For 2D data such as GC/FID, check “overlay signals” to display the sample chromatogram.

Sample Chromatogram Graphics settings

General:

Background color:  Transparent

Foreground color:  Black

Gridlines color:  No display

Time segment boundary:  No display

Font size: 8

Chromatograms:

TIC:  Black

Overlay target compounds

Overlay ISTD compounds

Overlay signals

Normalize

Signal labels

Overlay compound colors...

Overlay signal colors...

Scale the TIC to the highest peak after  min.

Peak labels:

Vertical labels

Allow overlap

Show target peak labels on TIC

Choose labels:

- RT
- Name
- Calc. Conc.
- Final Conc.
- Height
- Area
- Delta RT

Display Label Names (ex. RT=2.452)

Display Units for Conc., RT and Delta RT

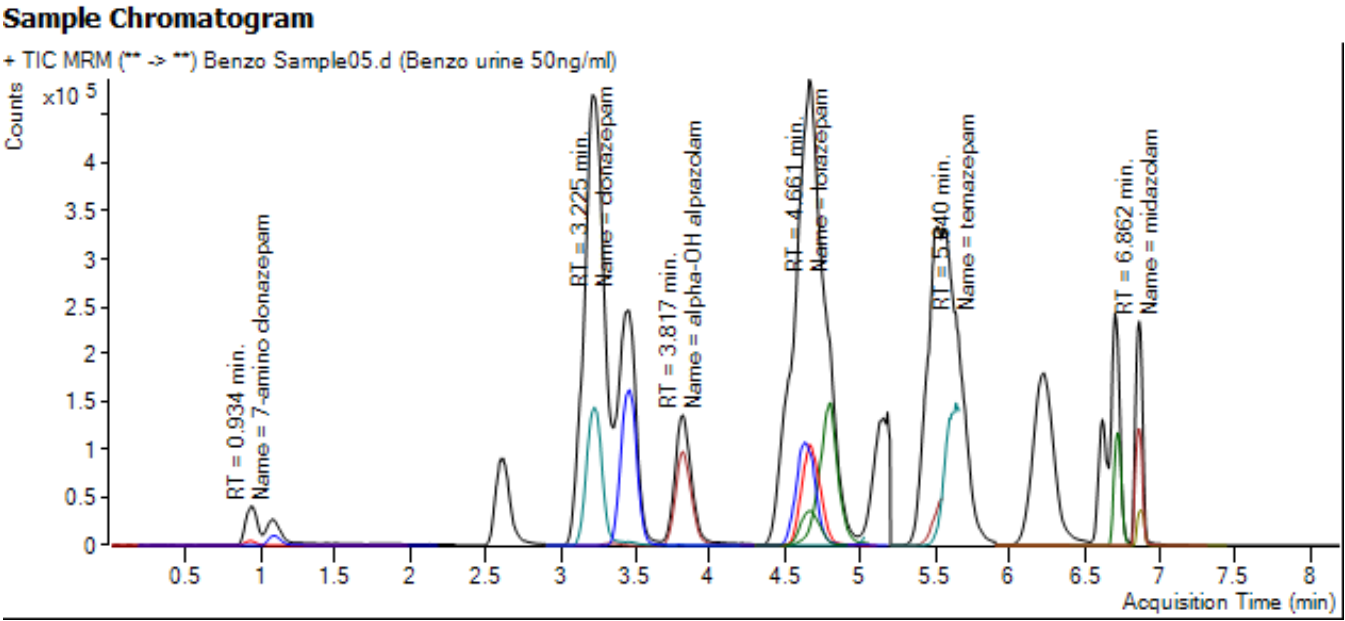
Move Up

Move Down

OK Cancel

# Report Method Example

TIC labeled with RT and Compound Name and Overlay Targets.



# Report Method Graphic Settings

Applies to Excel or PDF Reporting.  
Normalize the qualifier ions.

Quantifier/Qualifier overlay chromatograms

Graphics settings...

Quantifier/Qualifier Overlay Chromatogram Graphics

General:

Background color:  Transparent

Foreground color:  Black

Gridlines color: No display

Time segment boundary: No display

Font size: 8

Wrap title if it is too long

Chromatogram:

Auto scale: Auto scale

Normalize

Annotations

Qualifier colors...

Uncertainty band: .....

Hill peaks:

Fill out-of-limits qualifier peaks

Fill all qualifier peaks

No qualifier peak fill

Fill target peaks

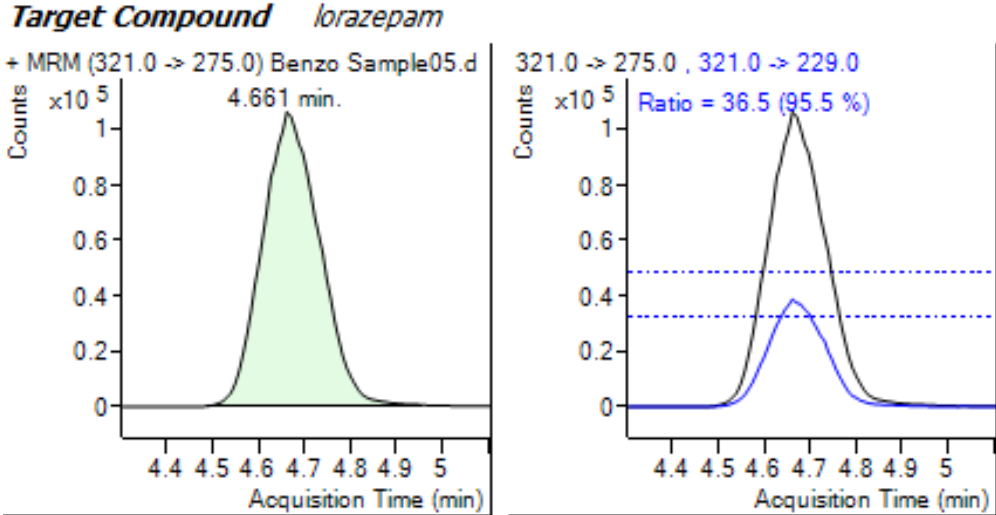
Fill transparency: 75% Transparent

Response ratio label: Ratio and percent of expected ratio

OK Cancel

# Report Method Example

Example of Target ion shaded green and qualifiers with uncertainty band.



# PDF Report Builder

## Allows user to generate unique report styles

The screenshot displays the 'AreaPercent.template - Report Builder (Unknowns Analysis)' application. The interface includes a ribbon with 'File' and 'Home' tabs, and a main workspace showing a report template. The template contains a header with the title '{L:Area Percent Report}' and the Agilent Technologies logo. Below the header is a table with columns for various report fields, including DataPathName, AcqMethodFileName, AcqDateTime, and SampleName. A large text box in the center of the report reads 'New Feature: New to MassHunter Quantitative Analysis B.08'. At the bottom of the report is a table with columns for peak identification and retention times, and a footer with page and date information.

On the right side of the interface is a 'Properties' panel for 'Textbox8'. The panel includes sections for:

- Alignment:** Horizontal Alignment (Left), Vertical Alignment (Top)
- Border:** Borders, Column Span (1), Paddings (1pt, 1pt, 1pt, 1pt)
- Content:** Content Type (FieldValue), Expression, Field Caption, Field Value (Sample-SampleName), Localized Text, Text (Textbox8)
- Fill:** Background Color (0, 255, 255, 255)
- Font:** Color (Black), Font
- Format:** Field Format, Format
- General:** ID (Textbox8), Outline Level

At the bottom of the Properties panel is a 'Background Color' section.

Allows user to customize report styles.

# PDF Report Builder

Relatively simple to learn and use.  
Uses a GUI to layout report items.  
Property based customization.  
12 Quant templates are available.  
Report Builder Familiarization guide.  
A number of videos are available.

## PDF Report Builder – Report customization

- o [PDF Report Builder overview](#) (Starter) *New!*
- o [PDF Report Builder design flow](#) (Advanced) *New!*
  - [PDF Report Builder Design Architecture](#) (Expert) *New!*
- o [PDF Report Builder - .csv to LIMS](#) (Starter) *New!*
- o [PDF Report Builder - Add Columns Demo](#) (Advanced) *New!*
- o [PDF Report Builder - Remove Columns Demo](#) (Advanced) *New!*
- o [PDF Report Builder - Replace Columns Demo](#) (Advanced) *New!*
- o [PDF Report Builder - Modify Graphics Demo](#) (Advanced) *New!*
- o [PDF Report Builder - Configure Graphics Demo](#) (Advanced) *New!*

# 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



# Introducing Agilent University

## 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

The screenshot shows the Agilent University website. A red arrow points to the 'TRAINING & EVENTS' menu item in the top navigation bar. Below this, a sub-menu is visible with 'Education' highlighted by another red arrow. In the main content area, the text 'AGILENT UNIVERSITY' is displayed over a background image. A red circle highlights a button labeled 'VIEW ALL TRAINING COURSE OFFERINGS >' with a graduation cap icon. Below this, three columns of text describe benefits: 'Increase Tenure and Maximize Productivity', 'Convenient Training' (with a sub-point: 'Our team of industry experts delivers a quality learning experience with a high degree of flexibility to fit the needs of...'), and 'Agilent Training Credits' (with a sub-point: 'INVESTING FOR YOUR...').

# Questions on today's material...

## Thank you for your attention.



MassHunter Quantitative Analysis

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