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

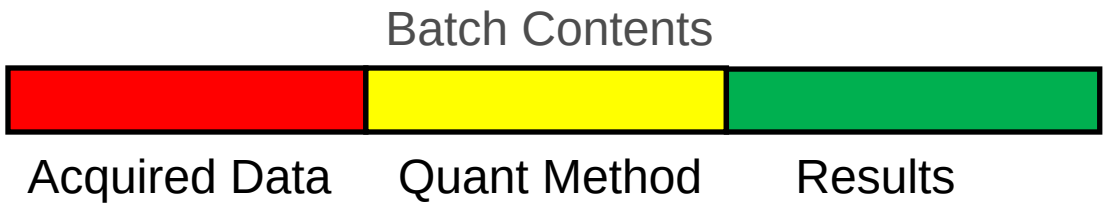
- Batch Definitions
- Three main views in MassHunter Quantitative Analysis
- Developing a quantitation method
  - Method Editor tasks
- Analyze the batch
- Outlier setup
- Advanced Tasks
  - Integration parameters
- Data review
- Generating a report, modifying graphic output

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

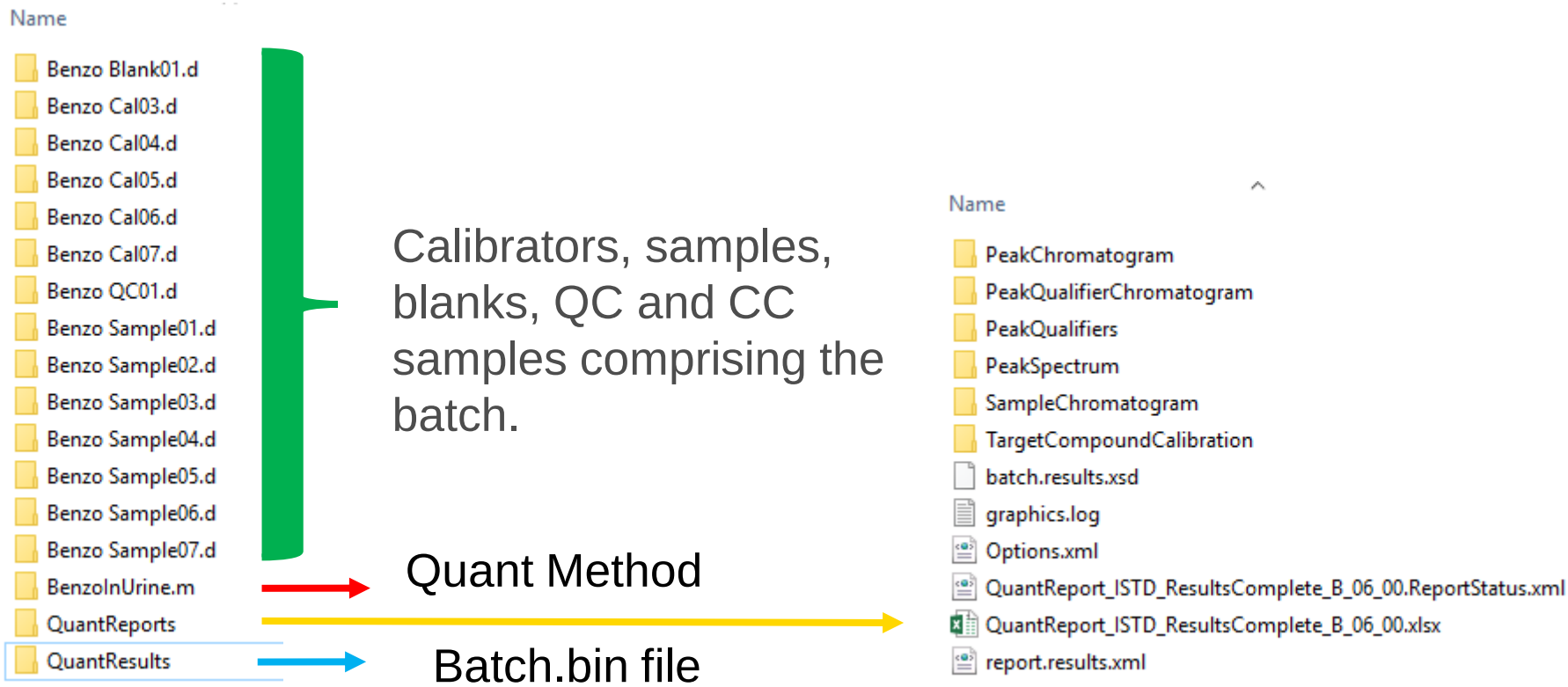
Use the icon applicable to the instrument and dataset for the application.

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

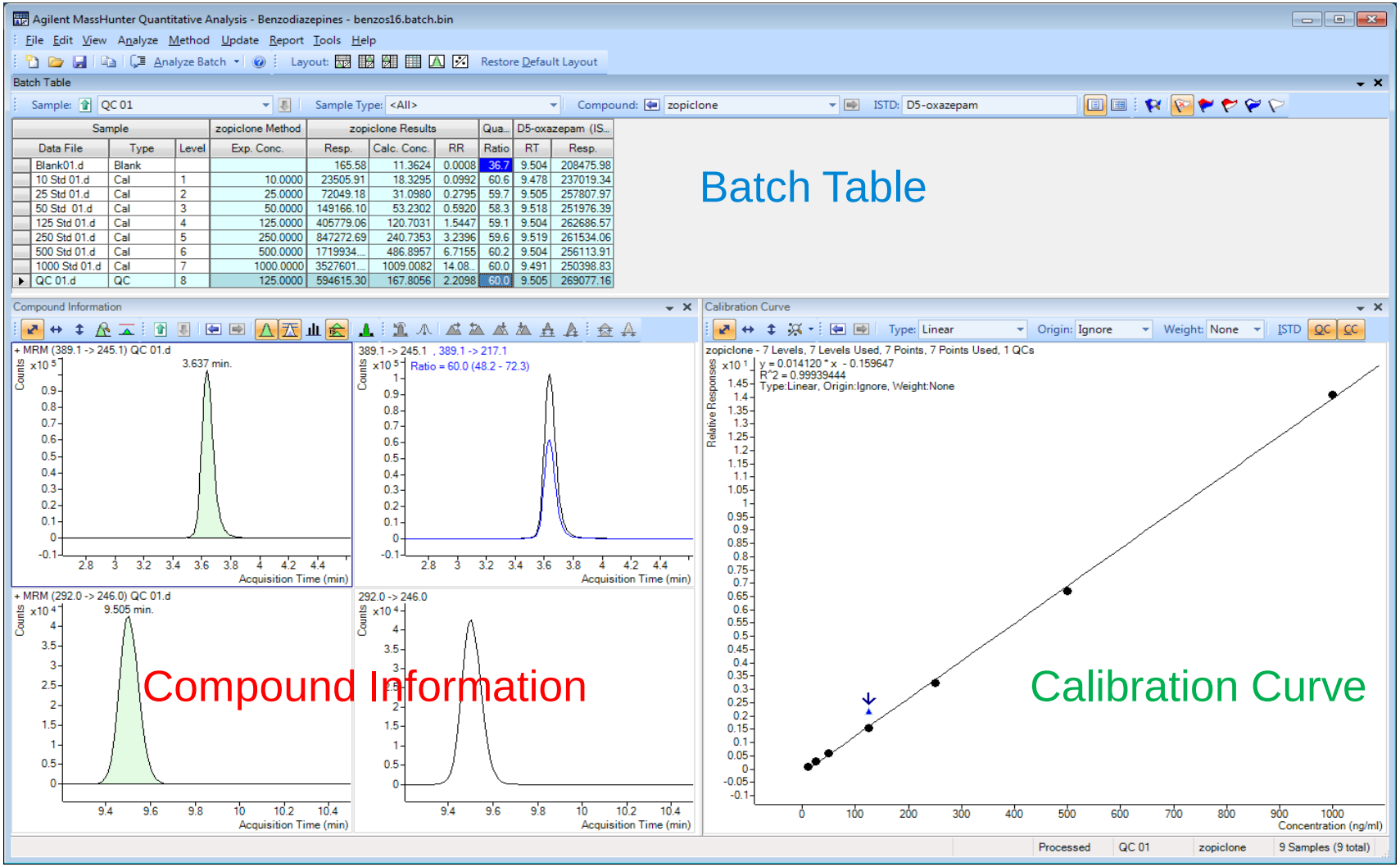
Four Basic Components to the Batch Directory



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

MassHunter Quantitative Software

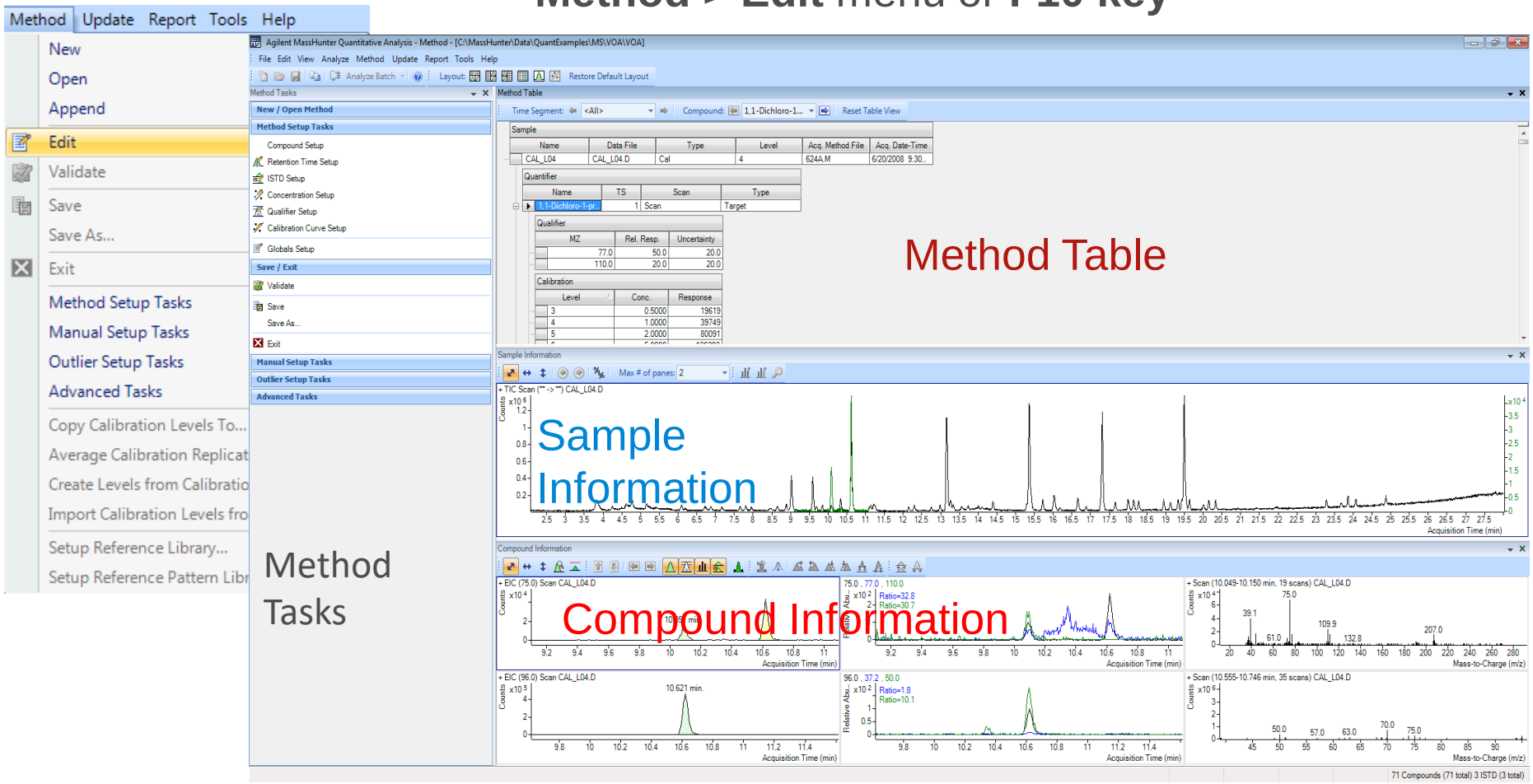
Batch-at-a-Glance View



MassHunter Quantitative Software

Method Editor View

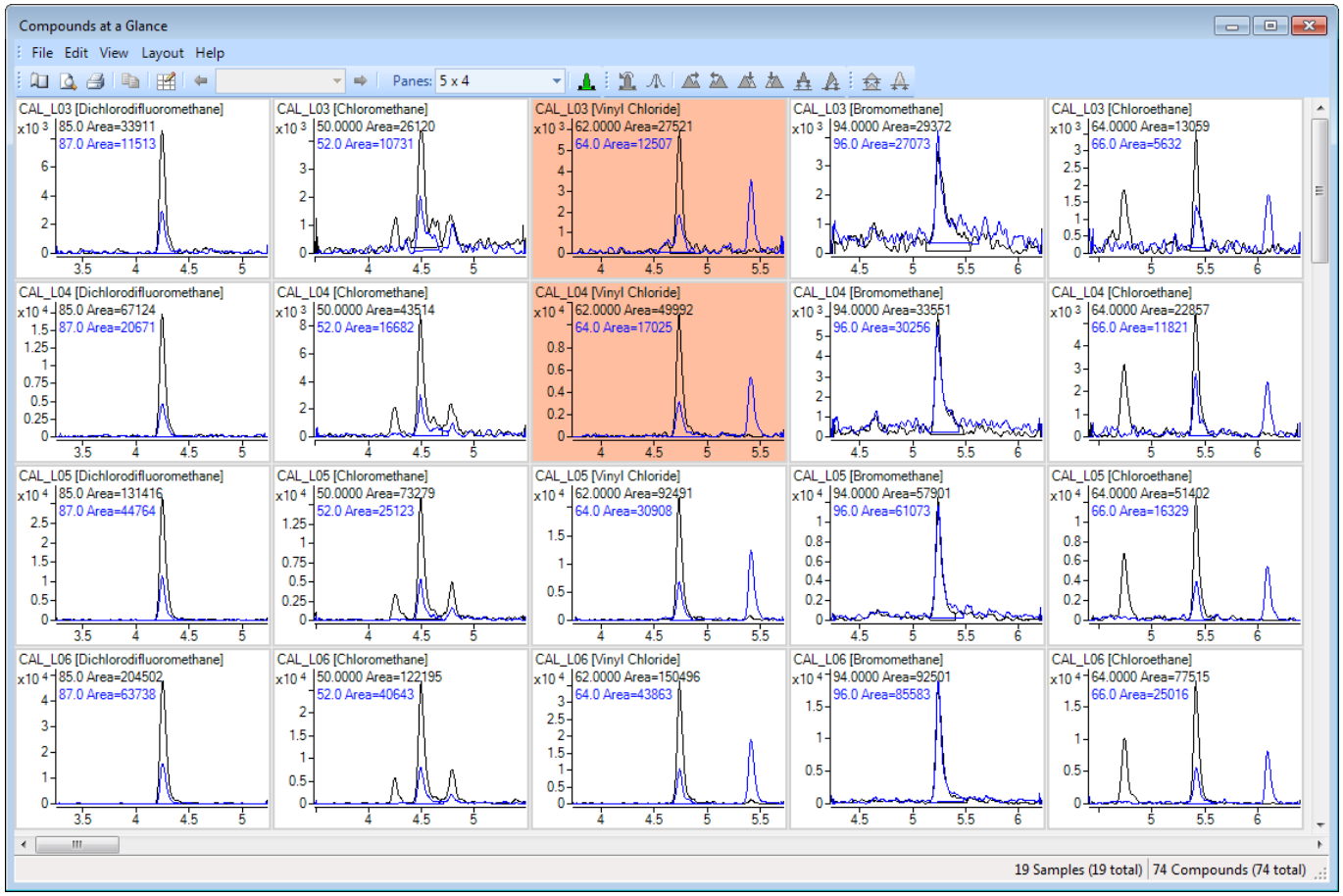
Method > Edit menu or **F10 key**



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.

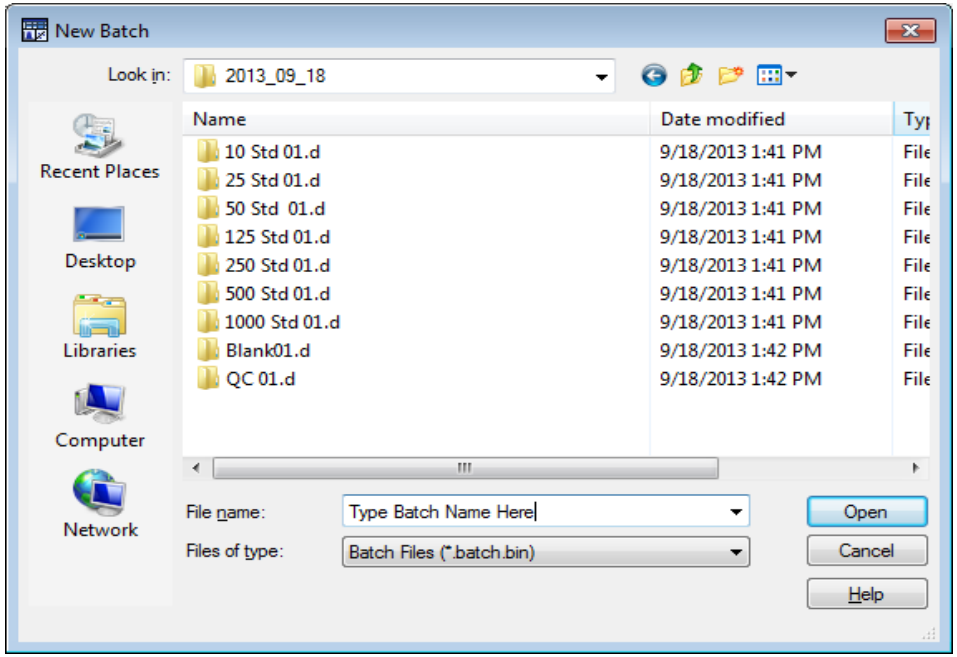
Tip: When in doubt, right-click to add columns or additional features.

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.

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…

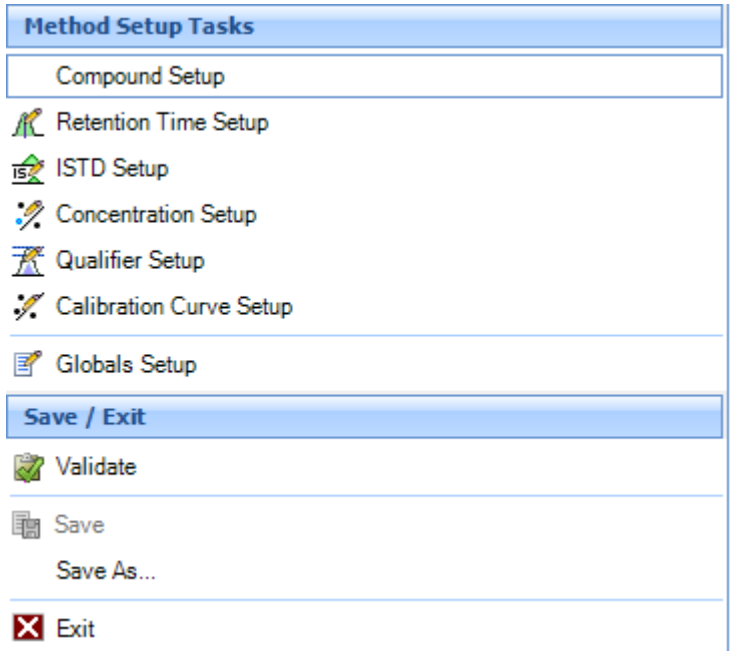
From CEF file generated in Qualitative Analysis.
From a small user generated library.

Tip: Avoid using Manual Setup

Editing a Quantitation Method

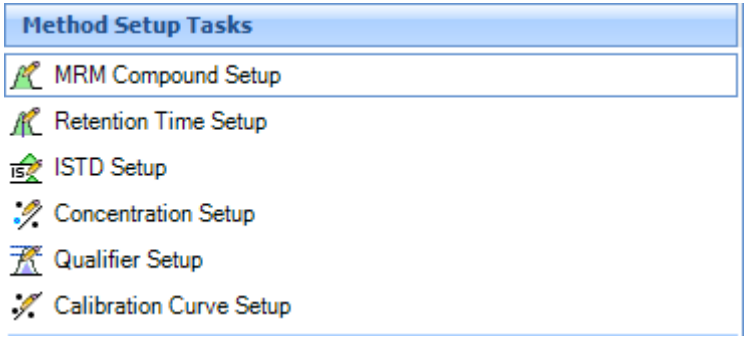
Step through Method Setup Tasks

Applies to SQ, TOF, QTOF.



In QQQ MRM Setup

Allows setup of transitions with precursor and product ions.



Method Editor

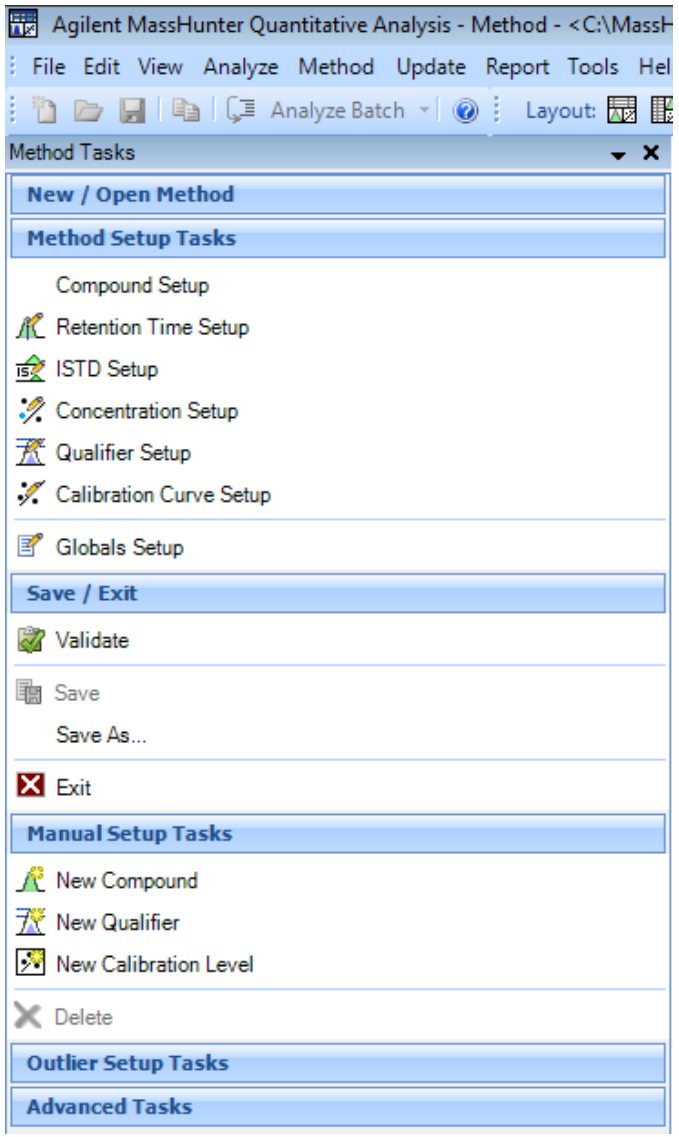
-Method Tasks

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'-Dibromooctafluorobiphenyl	1	Scan	ISTD	<None>	☑	0.4970	☐
Sulfotep	1	Scan	Target	4,4'-Dibromooctafluorobiphenyl	☐		☐
Phorate	1	Scan	Target	4,4'-Dibromooctafluorobiphenyl	☐		☐
BHC alpha isomer	1	Scan	Target	4,4'-Dibromooctafluorobiphenyl	☐		☐
Pentachloroanisole	1	Scan	Target	4,4'-Dibromooctafluorobiphenyl	☐		☐

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

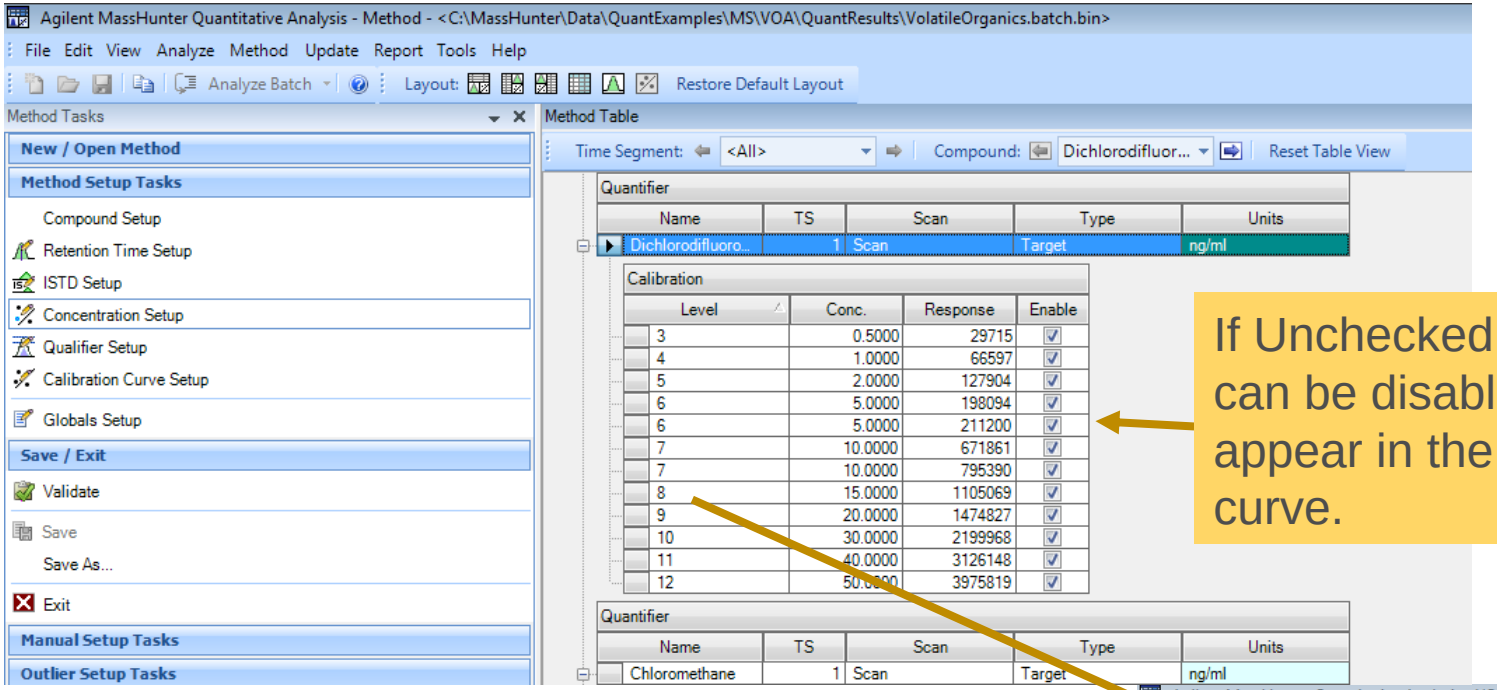
Time Reference Flag – only ISTD can be assigned as time reference compounds

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 a on a per sample basis.

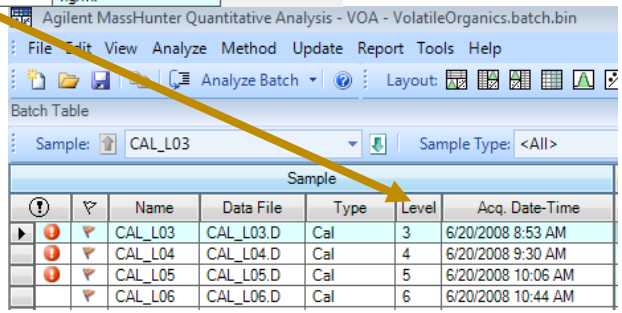
Editing a Quantitation Method for All Instruments

Concentration Setup

Defines the concentration of each compound in the standards.



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



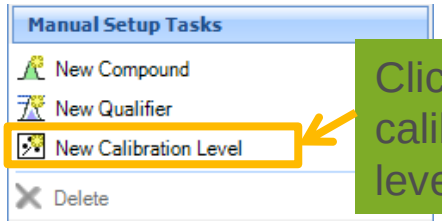
Level in Method must match Level in Batch table!

Editing a Quantitation Method for All Instruments

Concentration Setup

Calibration levels can be created manually or automatically.

Manual Setup



Click to add calibration levels.

Calibration

Level	Conc.	Response	Enable
10	30.0000	6482345	☑
11	40.0000	9154502	☑
12	50.0000	11963873	☑

Quantifier

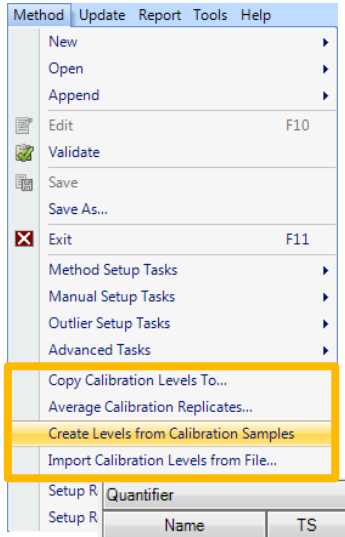
Name	TS	Scan	Type	Units
1,4-Dichloroben...	1	Scan	ISTD	ng/ml
n-Butylbenzene	1	Scan	Target	ng/ml

Calibration

Level	Conc.	Response	Enable
3	0.5000		☑
4	1.0000		☑
5	2.0000		☑
6	5.0000		☑

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!

Quantifier

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

Calibration

Level	Conc.	Response	Enable
3	0.5000		☑
4	1.0000		☑
5	2.0000		☑
6	5.0000		☑
7	10.0000		☑
8	10.0000		☑
9	10.0000		☑
10	10.0000		☑
11	10.0000		☑
12	10.0000		☑

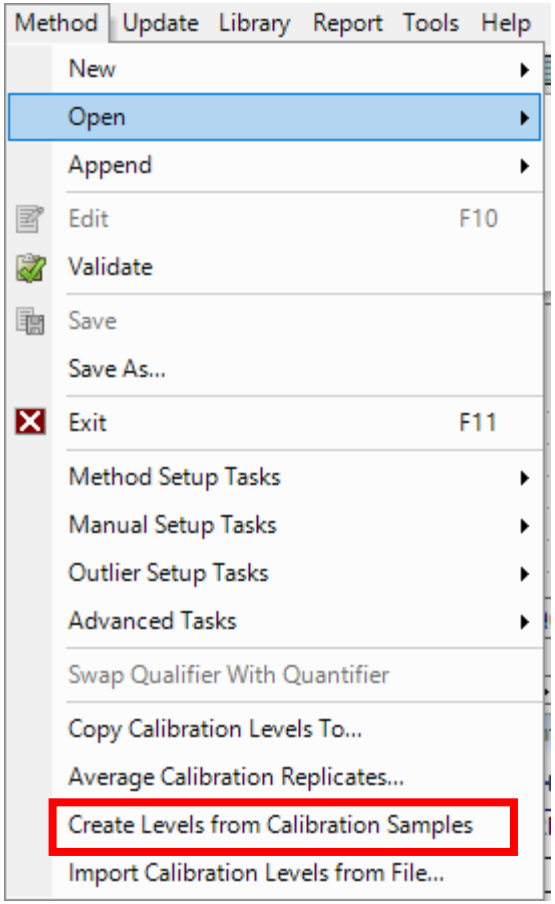
Creating a Quantitation Method for All Instruments

Concentration Setup – Create Levels from Calibration Samples

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

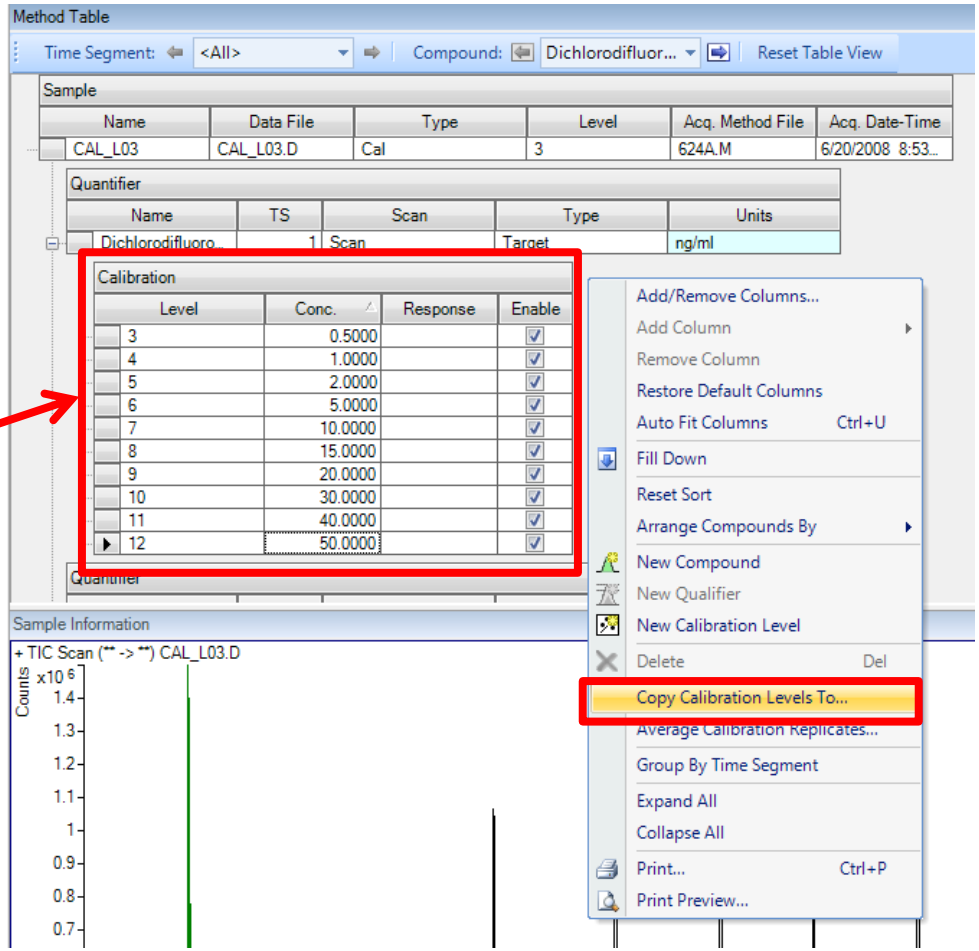
Name	Data File	Type	Level	Exp. Conc.
Benzo Cal03	Benzo Cal03.d	Cal	L1	25.0000
Benzo Cal04	Benzo Cal04.d	Cal	L2	50.0000
Benzo Cal05	Benzo Cal05.d	Cal	L3	125.0000
Benzo Cal06	Benzo Cal06.d	Cal	L4	250.0000
Benzo Cal07	Benzo Cal07.d	Cal	L5	500.0000
Benzo QC	Benzo QC01.d	QC	QC1	189.0000

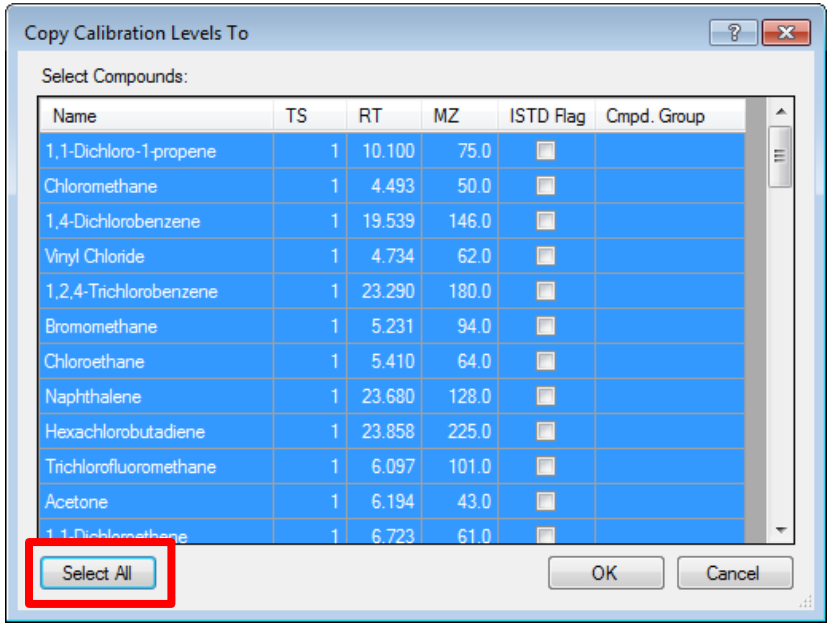
Then **Method > Edit** and then **Method > Create Levels from Calibration Sample.**



Editing a Quantitation Method for All Instruments

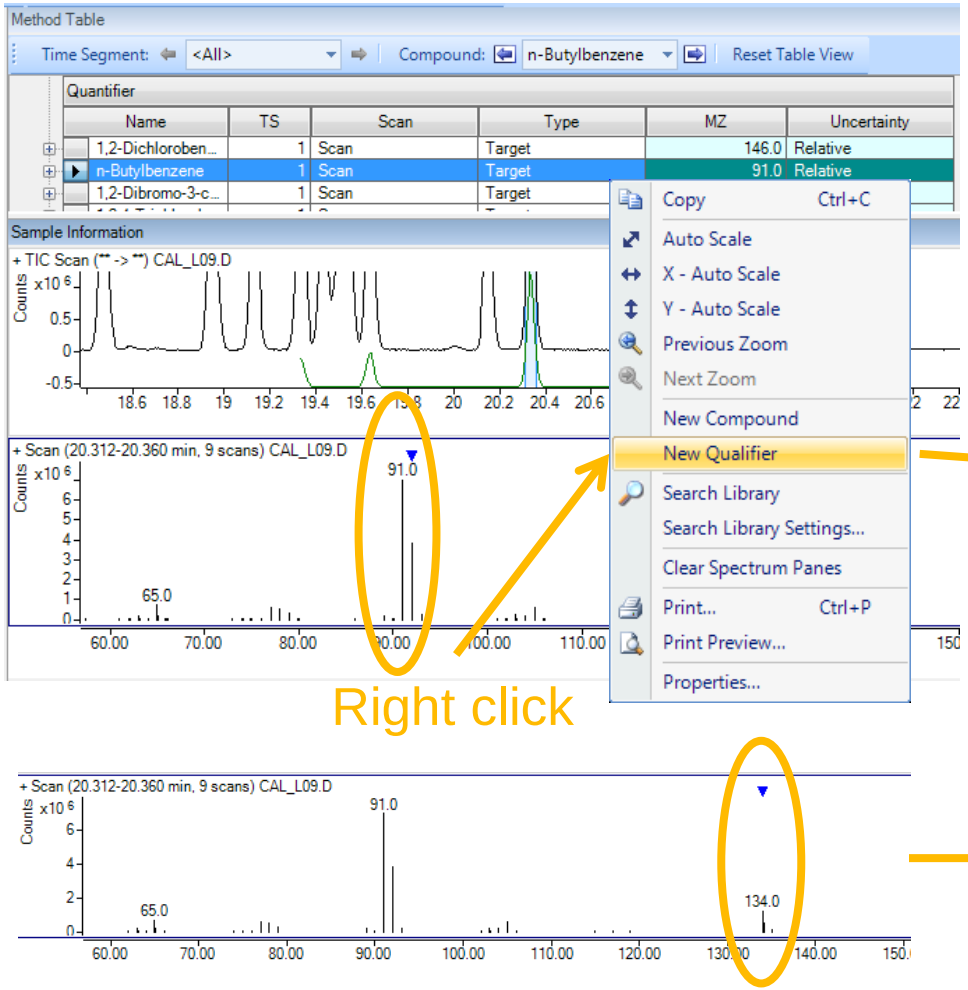
Concentration Setup





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

Editing a Quantitation Method for All Instruments
Qualifier Setup



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	

Quantifier

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

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	
134.0	25.4	20.0	

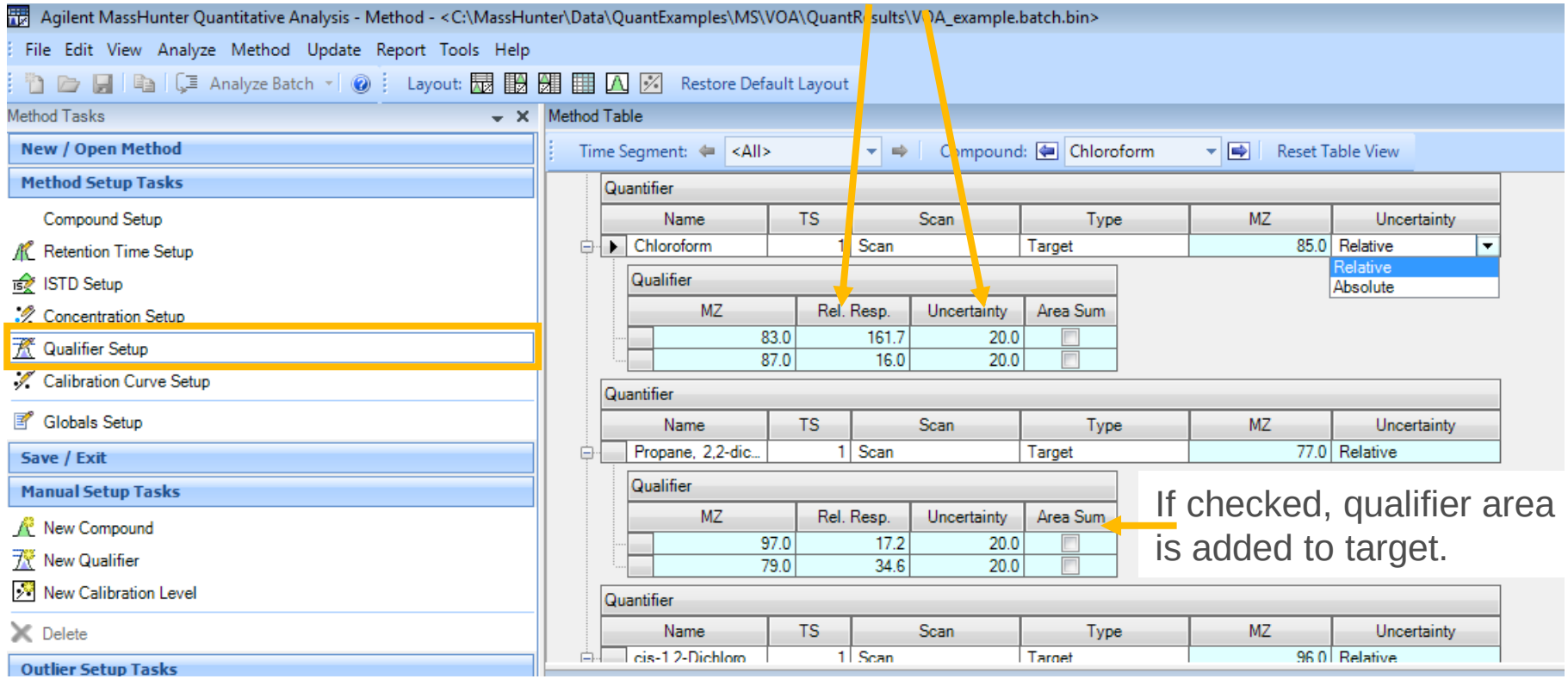
Quantifier

Name	TS	Scan	Type	MZ

Editing a Quantitation Method for All Instruments

Qualifier Setup

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



If checked, qualifier area is added to target.

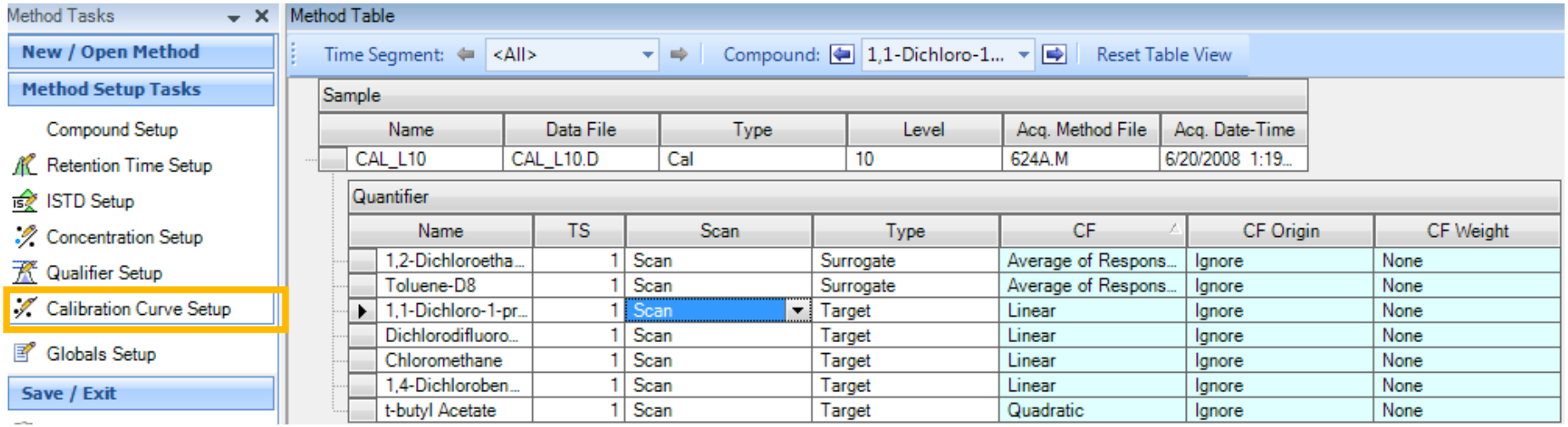
80% Relative Response with 20% Uncertainty

Absolute = 80 +/- 20 = range of 60-100

Relative = 80 +/-(80*20/100) = range of 74 - 96

Editing a Quantitation Method for All Instruments
Calibration Curve

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

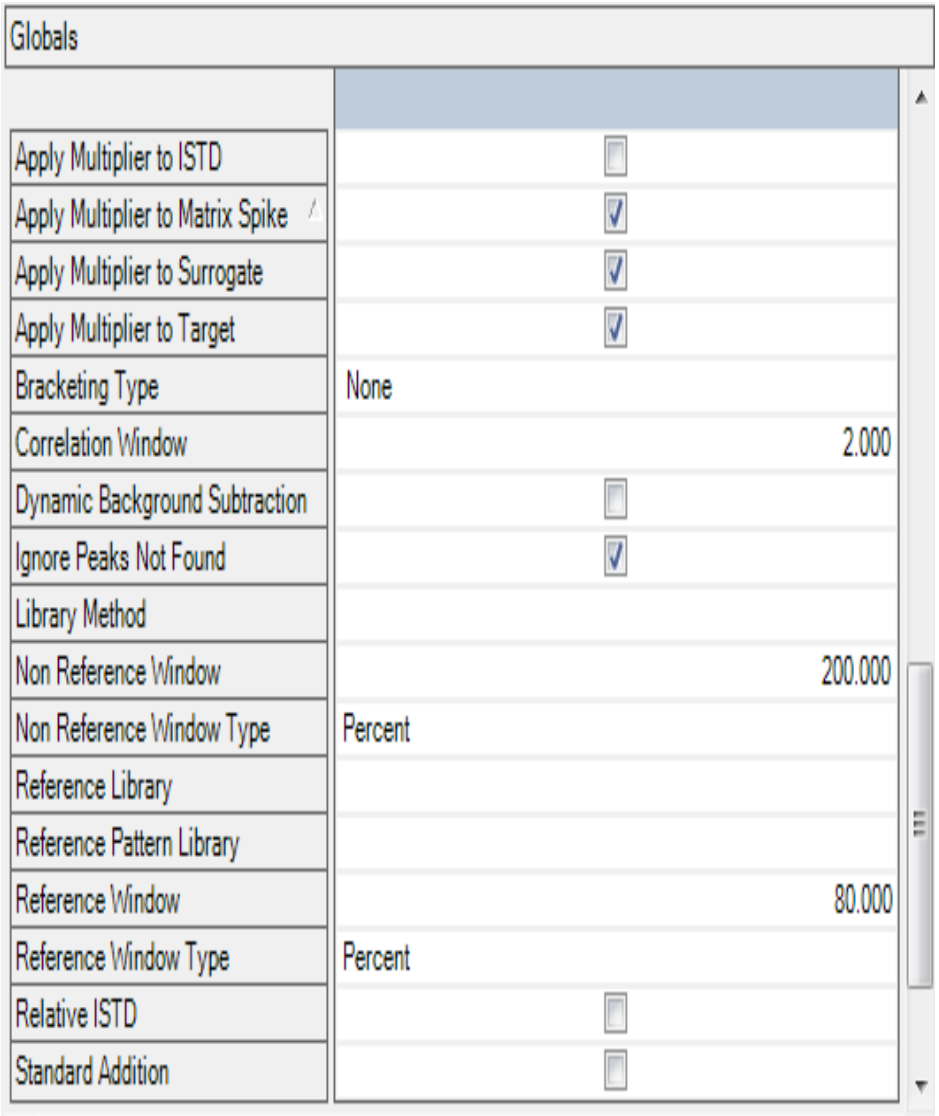


Curve Fit
- Linear.
- Quadratic.
- Power.
- 1st order ln.
- 2nd order ln.
- Average response factors.

Curve Fit Origin
- Ignore
- Include.
- Force.
- Blank offset.

Curve Fit Weight
- None (equal wt.)
- $1/x$, $1/x^2$
- $1/y$,$1/y^2$
- Log
- $1/SD^2$.

Editing a Quantitation Method for All Instruments
Globals Settings



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)

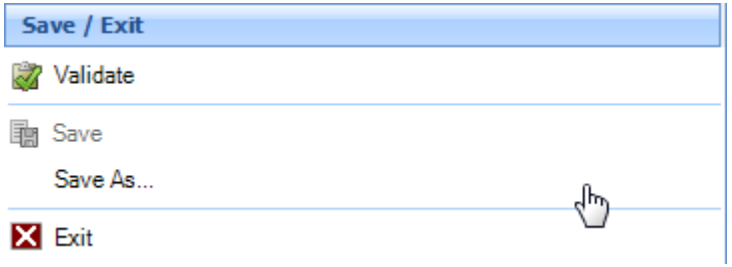
Peak identification within the extraction window

(ISTD with Time Reference Flag checked)

→ Semi quant relative to ISTD

→ Quantitate with Standard Addition

Editing a Quantitation Method for All Instruments
Validate

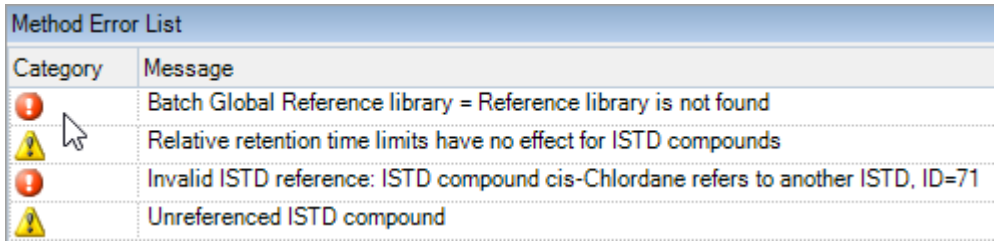


Save and Save As – A quant method can be saved and applied to multiple batches.

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

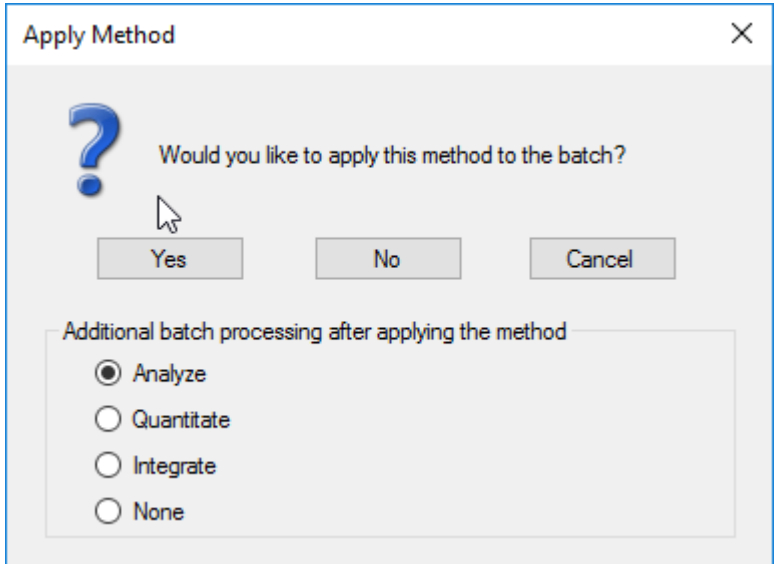
Red icon – Must be corrected

Yellow icon - Warning



Tip: Double click on the error.

Editing a Quantitation Method for All Instruments
Exit Method Editor and Apply Method



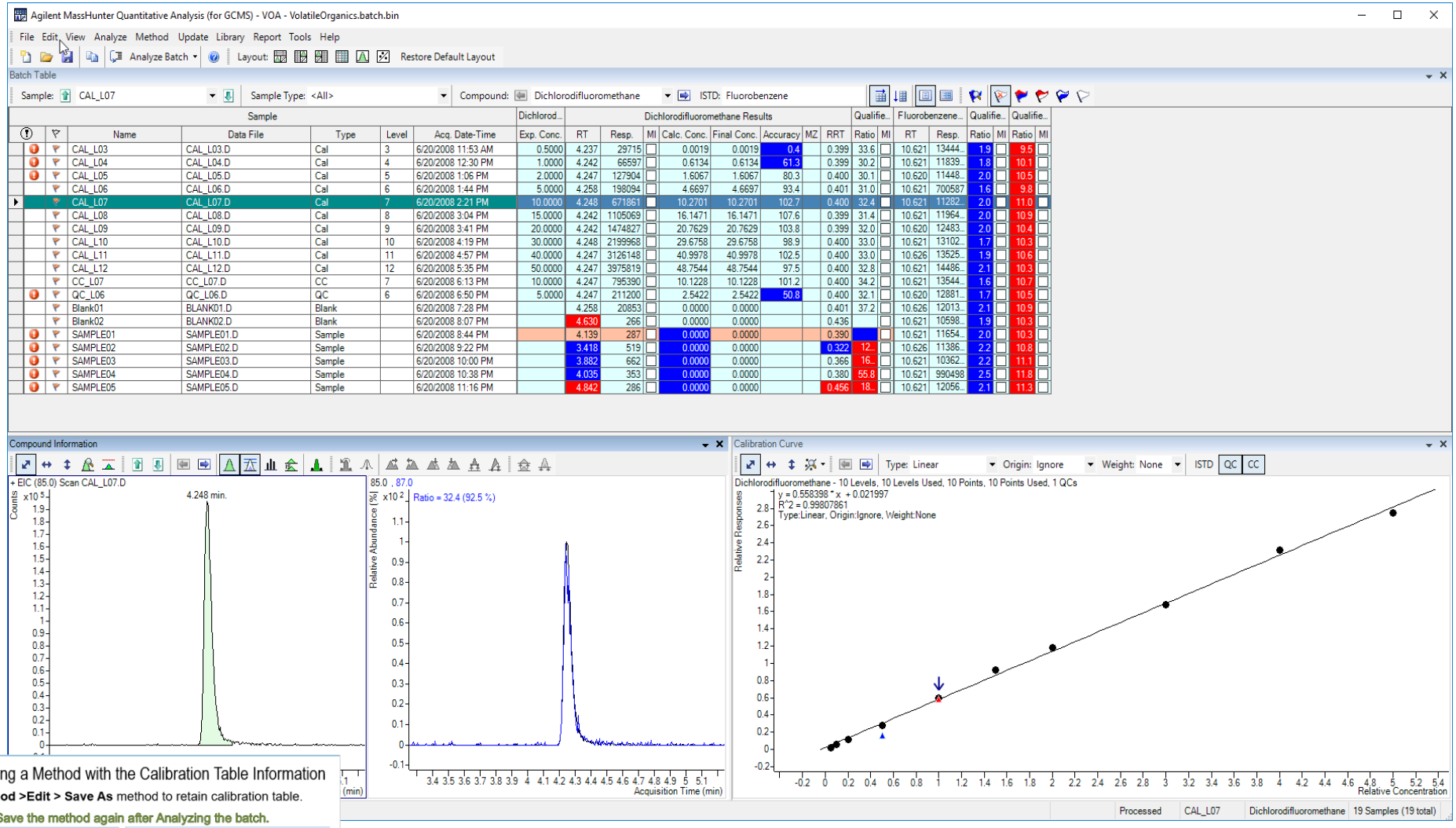
Analyze may (*) rebuild the calibration curve and then calculates analyte concentrations.

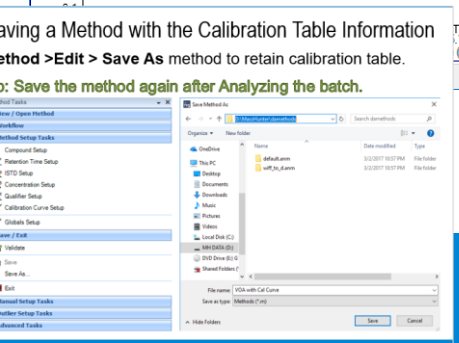
Quantitate does ***not*** rebuild the calibration curve but calculates concentrations based on the existing curve.

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

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

Analyzed Batch !!!



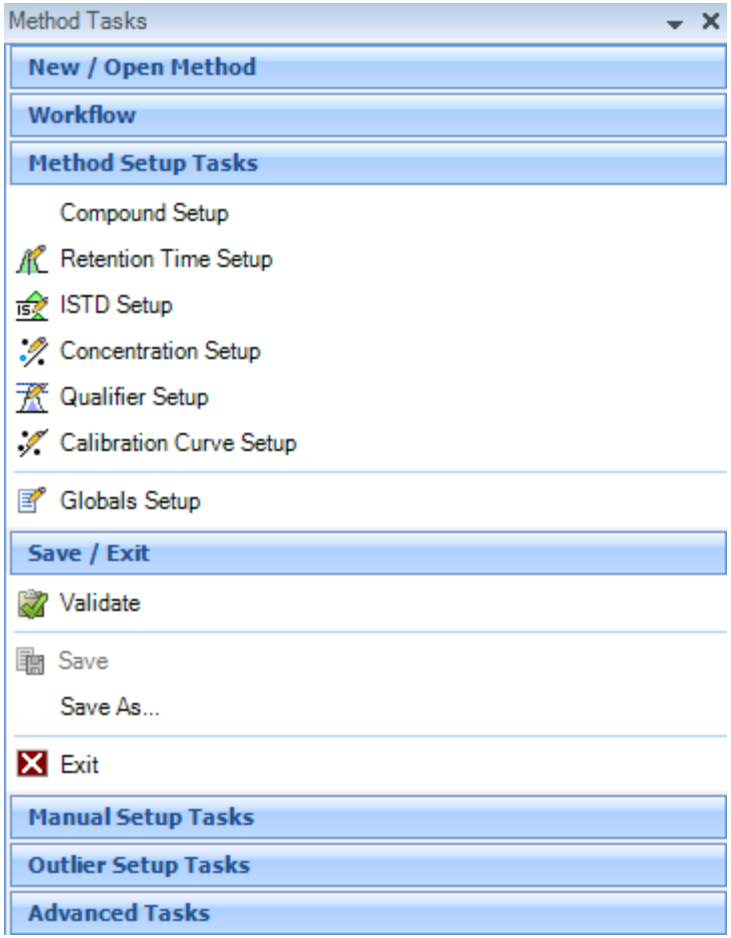


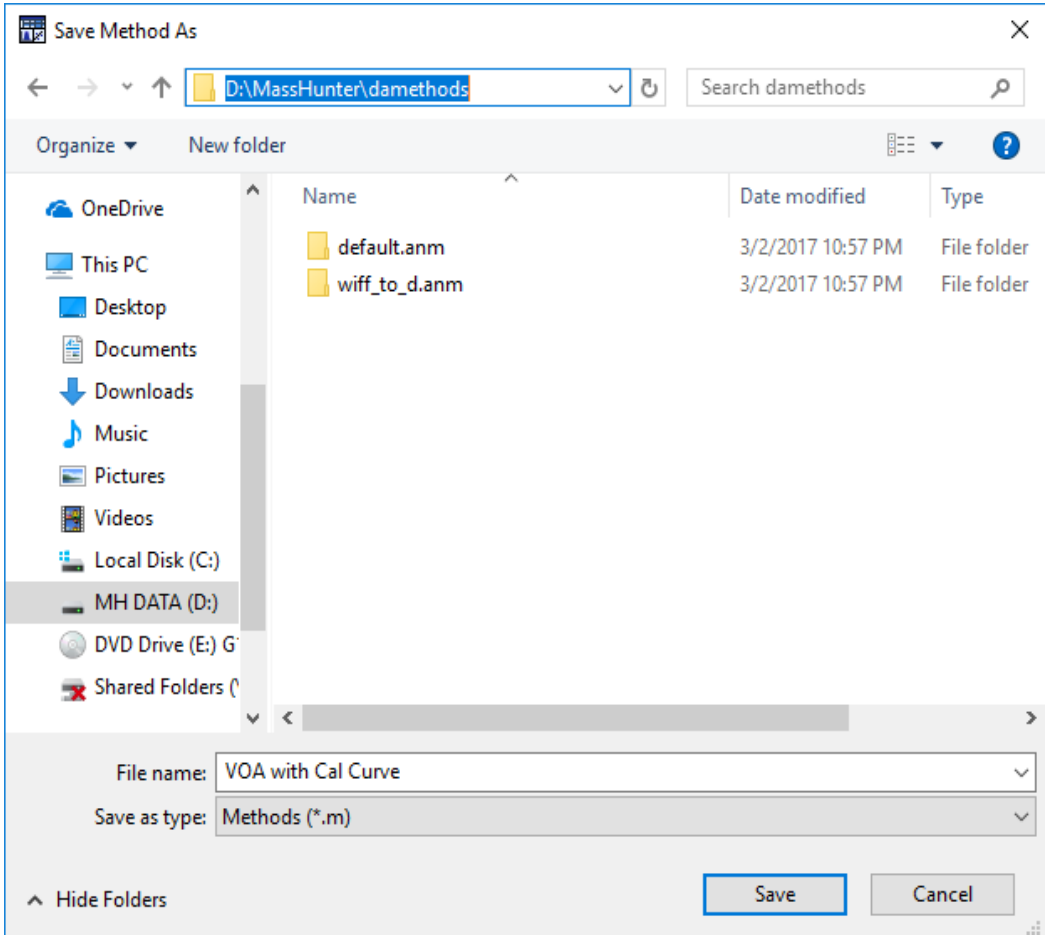
Methods can be used over and over.

Saving a Method with the Calibration Table Information

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

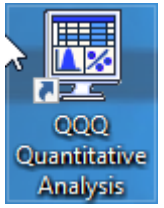
Tip: Save the method again after Analyzing the batch.





Editing a Quantitation Method for QQQ

Compound Setup



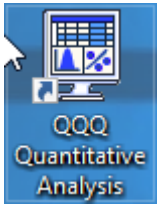
Name – compound name
TS – time segment usually 1 for scan data
may be many time segments for SIM and MRM data
Transition – Precursor ion →Product ion
Scan – MRM (Multiple Reaction Monitor)
Type – Target, ISTD, Surrogate or Matrix Spike
Precursor ion – mass of the ion
Product Ion – mass of the ion
RT – 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	☐

Editing a Quantitation Method for TOF
Mass Extraction Setup

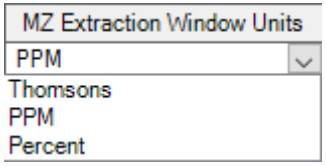
Method > Edit > Advanced Tasks > Mass Extraction Setup

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

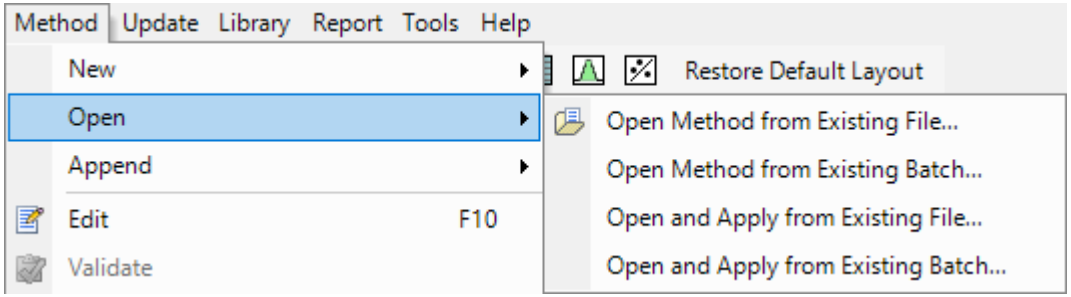
Name – Compound name
TS – time segments may be multiple
Transition – Precursor ion →Product ion scan
Scan – Product Ion
Type – Target, ISTD, Surrogate or Matrix Spike
Precursor Ion – mass of the ion
Product Ion – mass of the ion for the target ion to monitor
RT – retention time of compound of interest
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

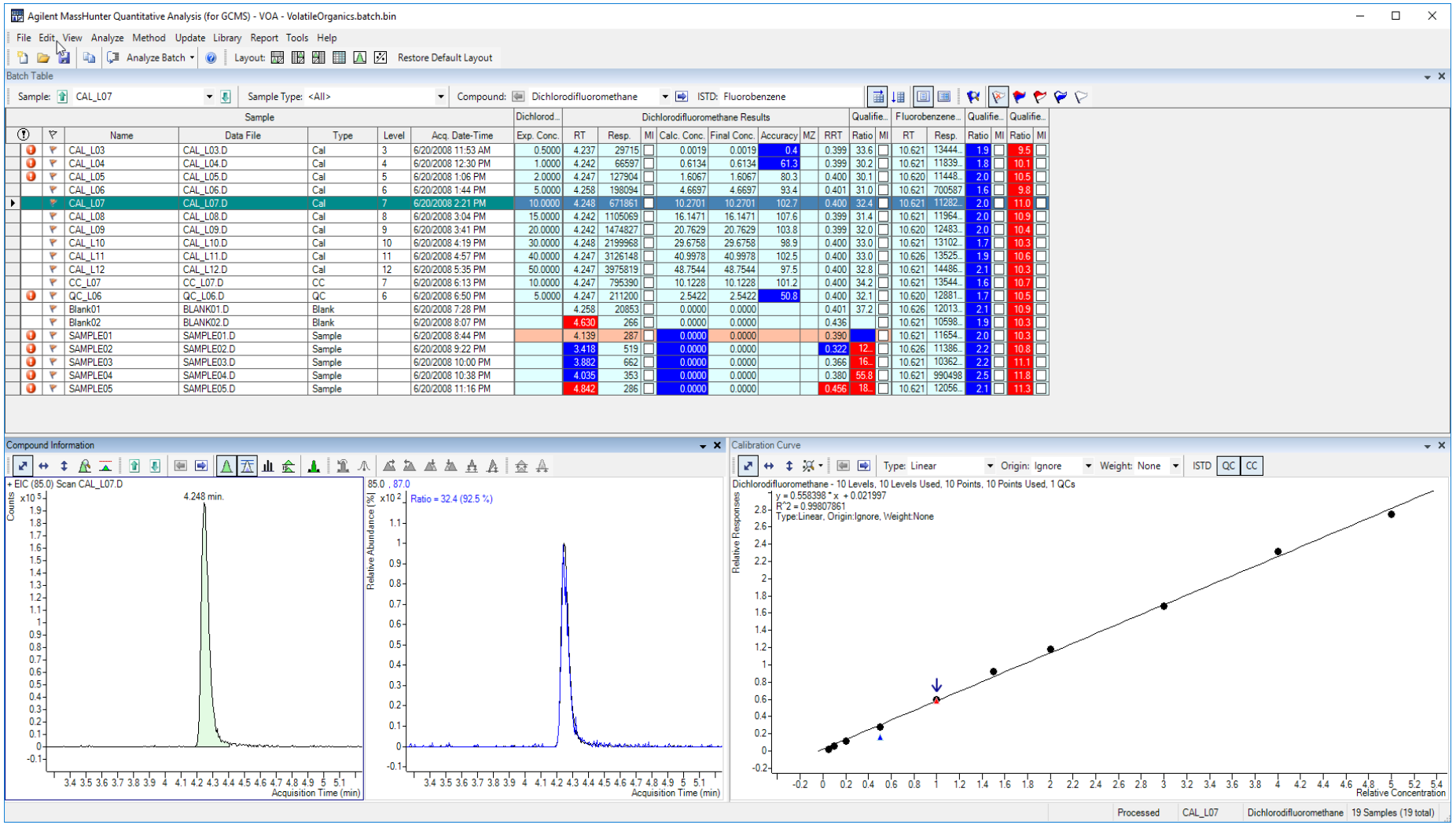
Method > Open from Existing File…
Method > Open from Existing Batch…

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.

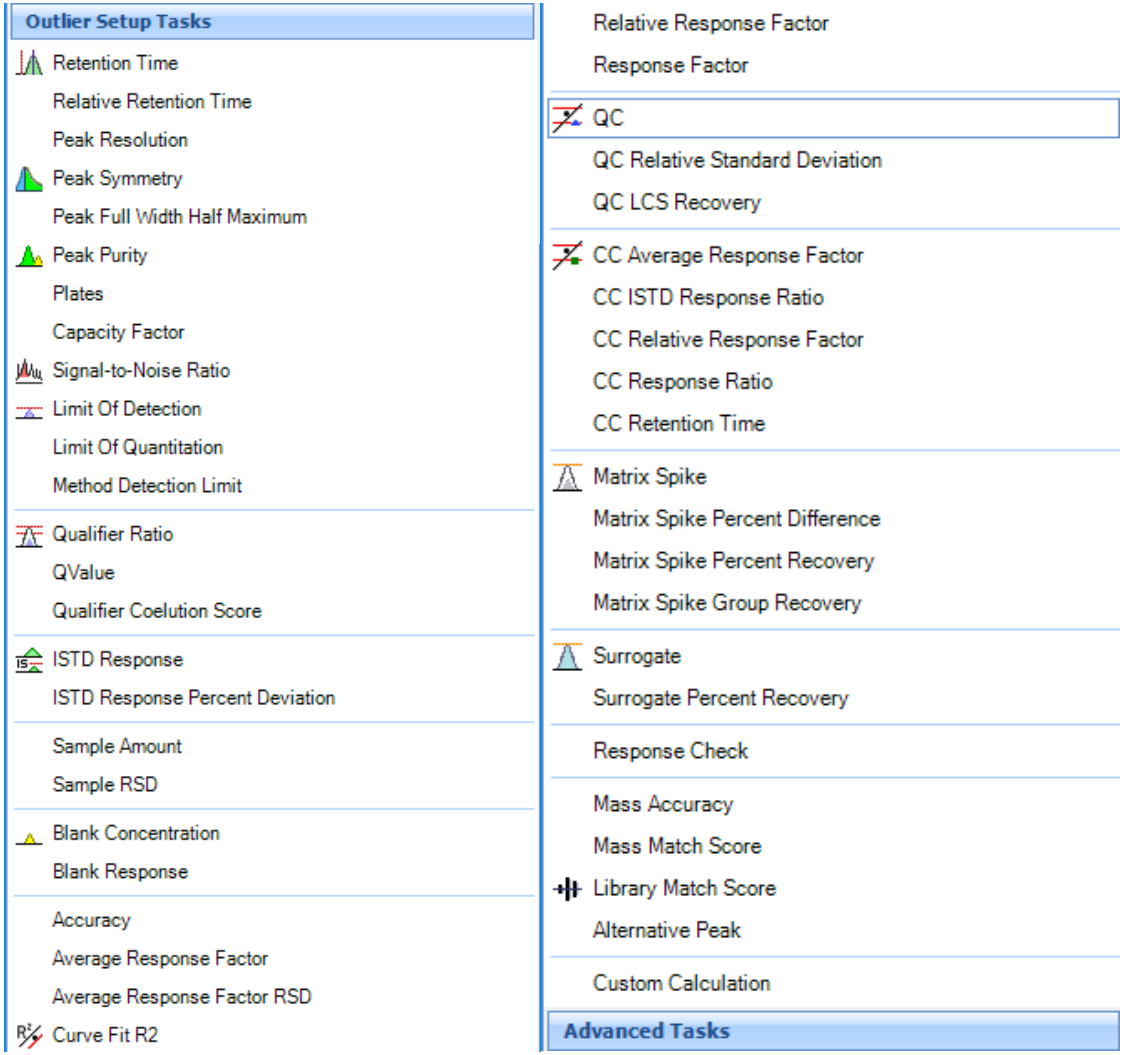
Outliers are used to perform automated quality checks.

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.



Outliers in Batch At a Glance

Icons on the toolbar

Select Outliers

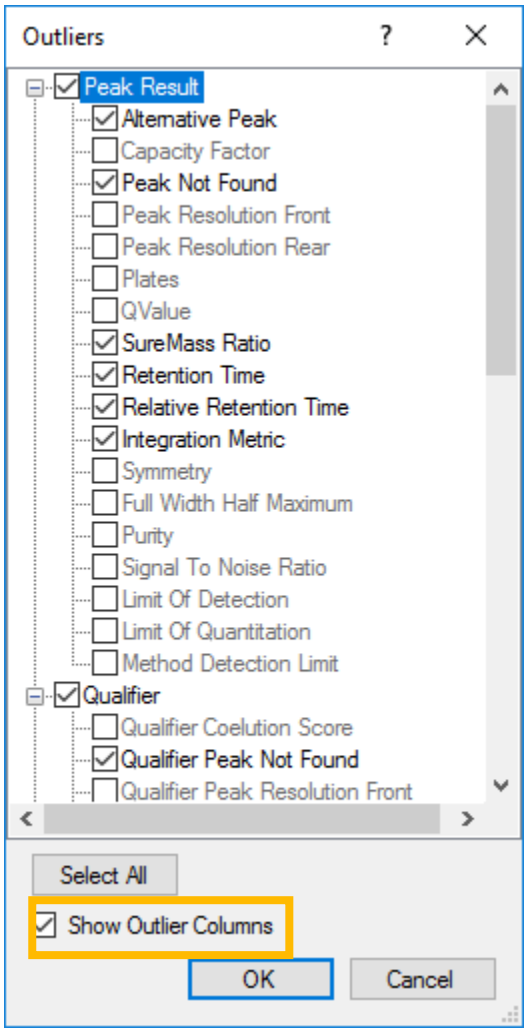
Turn off outlier filter

Display rows that have High/Low outliers

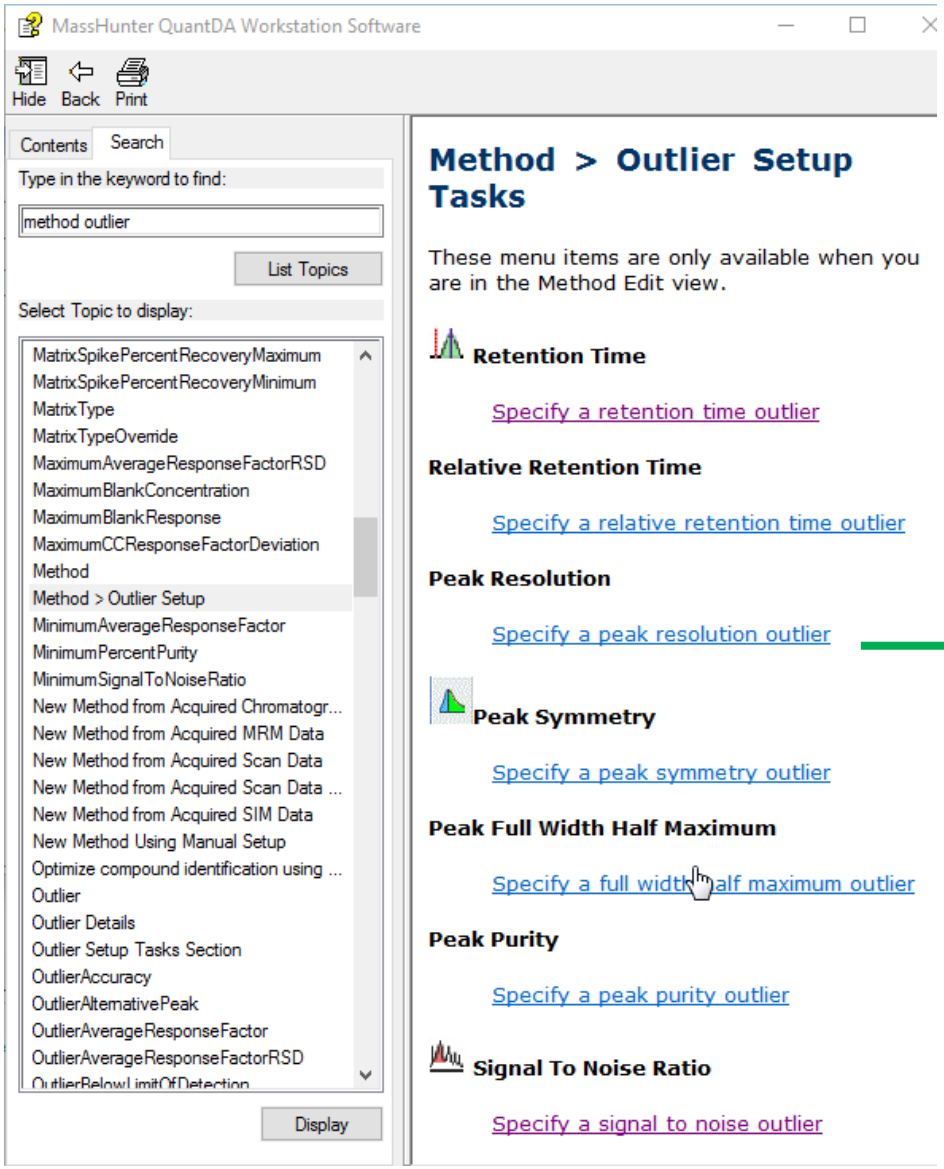
Display rows that have High outliers

Display rows that have Low outliers

Display rows that have no outliers



Outliers Help



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

ResolutionFront (ResolutionRear) < 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**

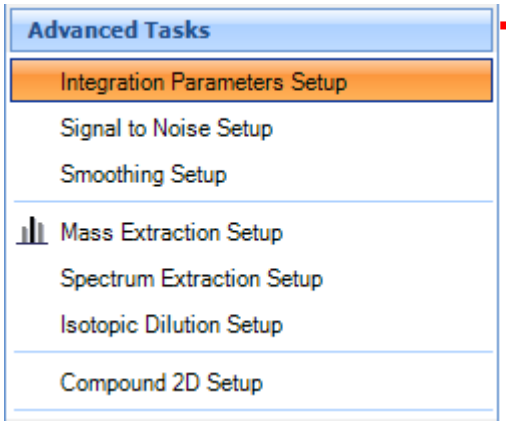
Quant Outliers

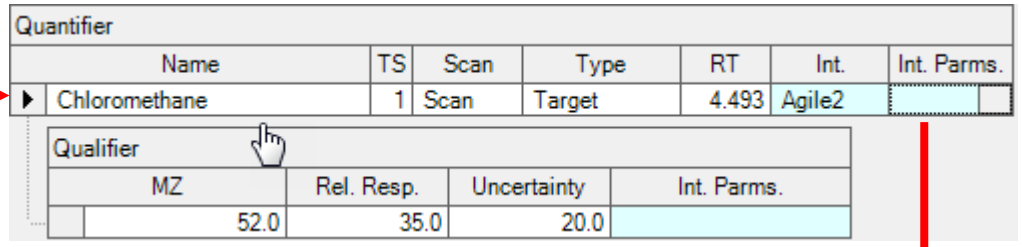
- Method Editor - Alternative Peak outlier (Advanced)
- Method Editor - Signal to Noise Ratio outlier (Advanced)
- Method Editor - Theoretical Plates outlier (Advanced)
- Method Editor - Peak Symmetry outlier (Advanced)
- Method Editor - Capacity outlier (Advanced)
- Method Editor - QValue outlier (Advanced)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

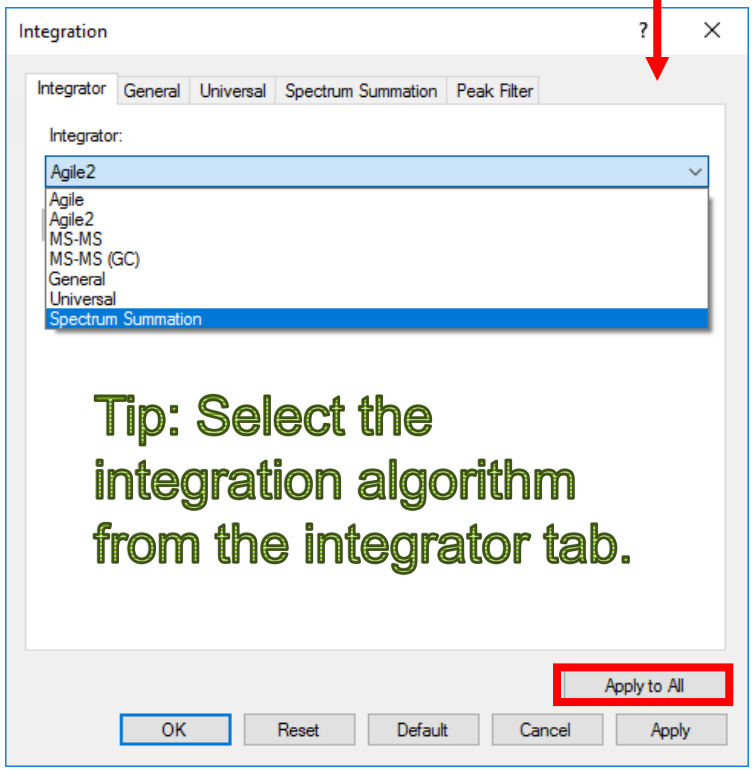
Editing a Quantitation Method

Advanced Tasks Integration Parameters

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







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, 3rd generation parameter less integrator
Better baselines, higher sensitivity to smaller peaks.

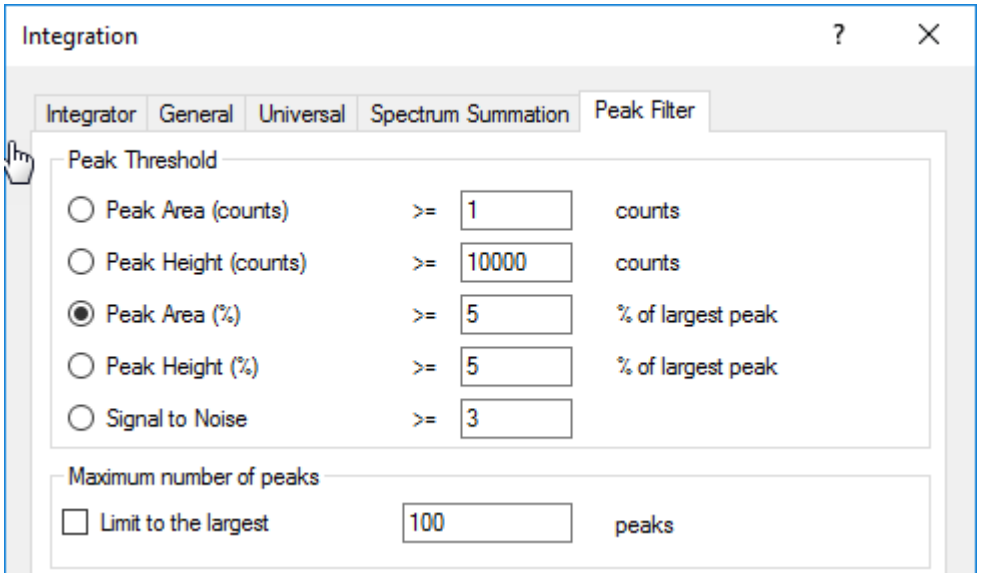
Agile

2nd generation parameter less integrator.

MS/MS and MS/MS (GC)

1st 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.

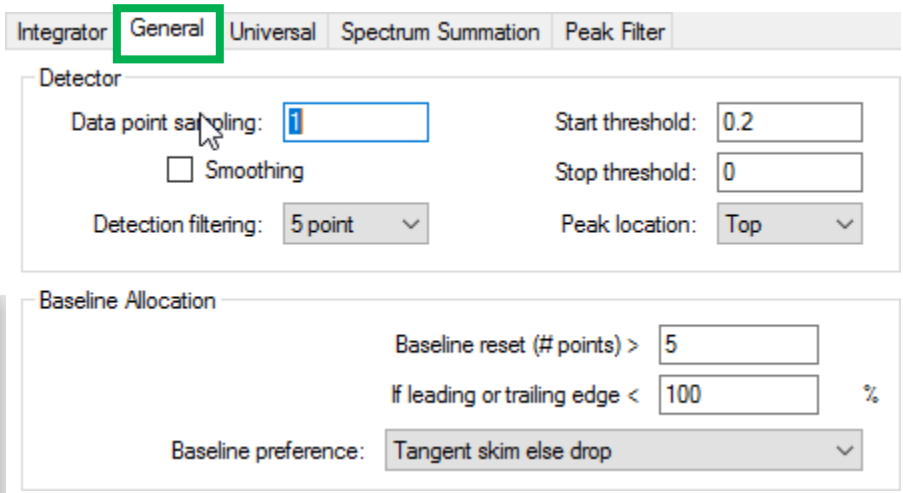


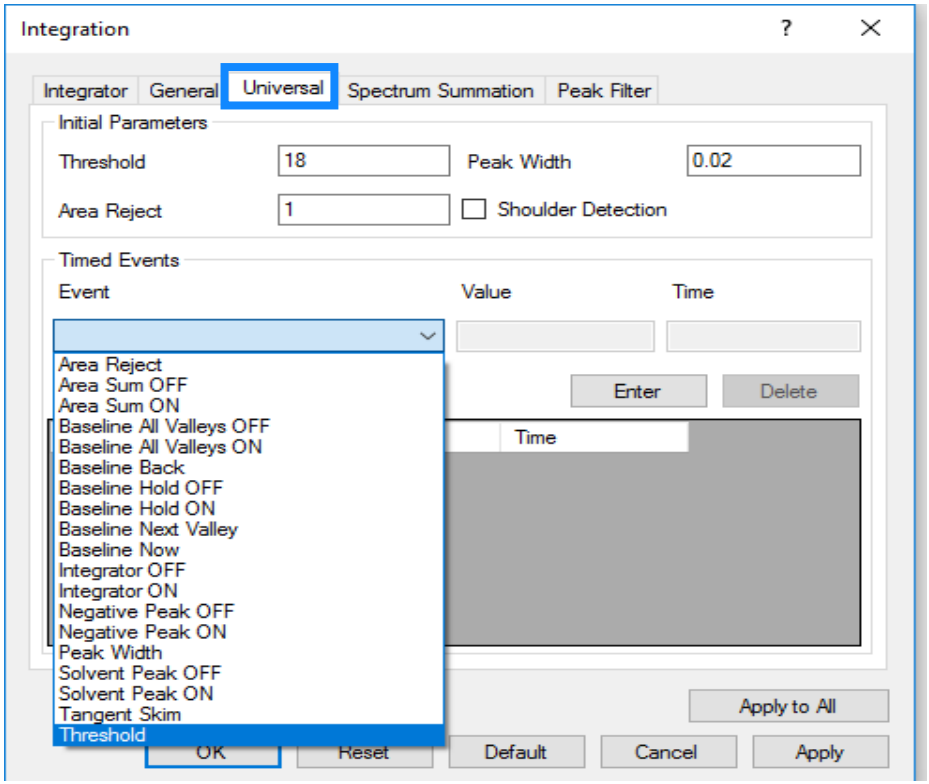
Editing a Quantitation Method
Integrator Parameters

General (RTE)

Familiar to MSD ChemStation users.

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





Universal

1st 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.

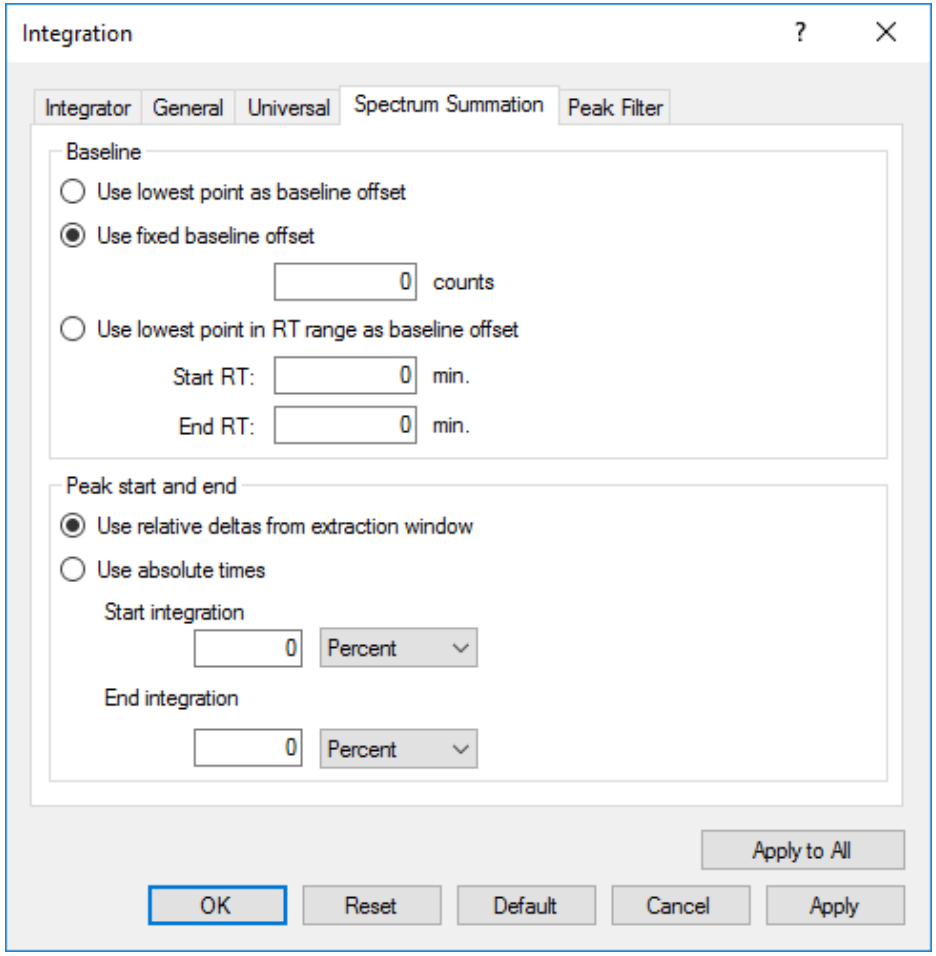
- PCB mixtures, TPH and GRO
- Fraction cut in hydrocarbons
- Flow injection analysis

Sums signal over a time range

Exclude signal below threshold

Always gives a horizontal baseline

RT reported as the center of the time range

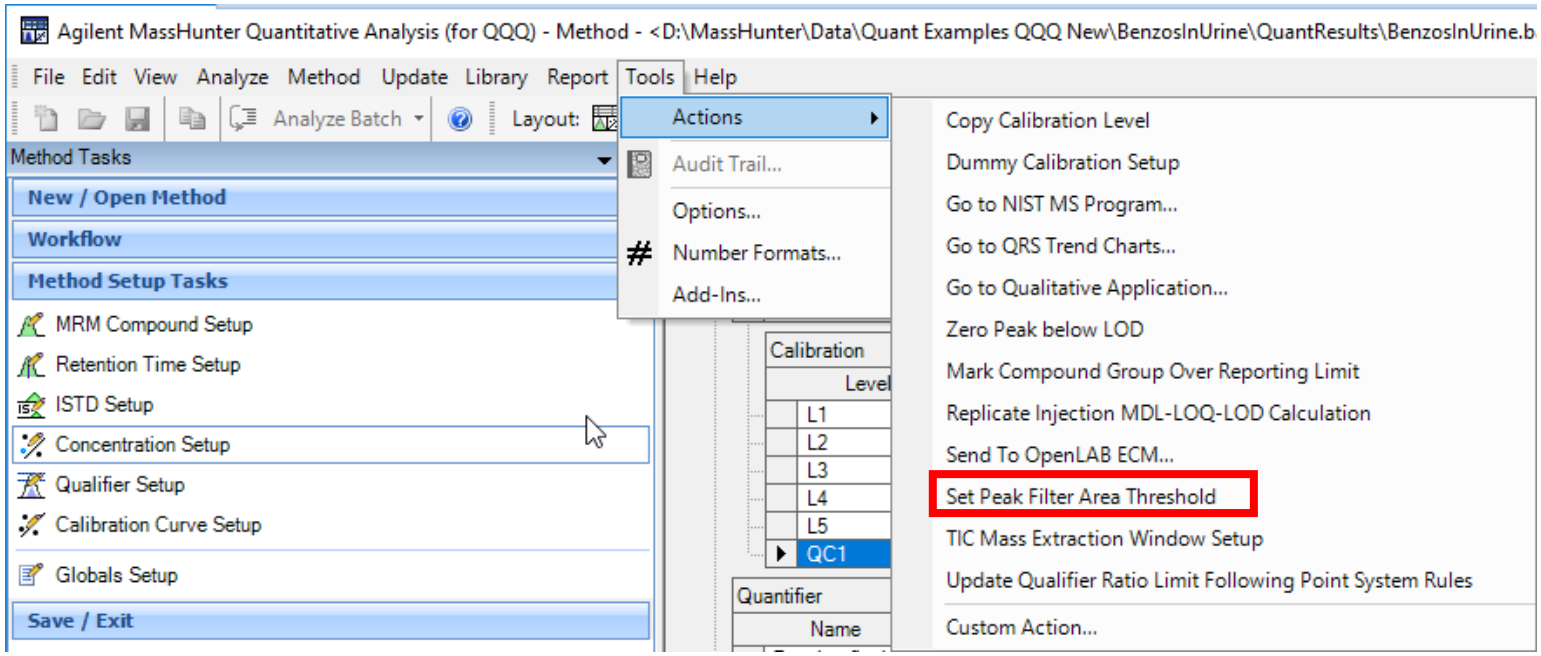


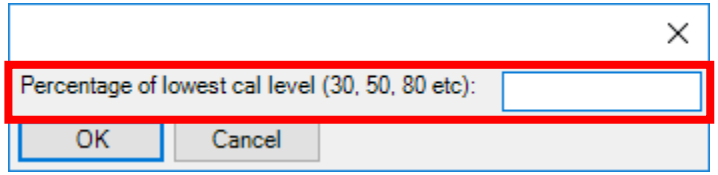
Editing a Quantitation Method

Setting an integration threshold

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

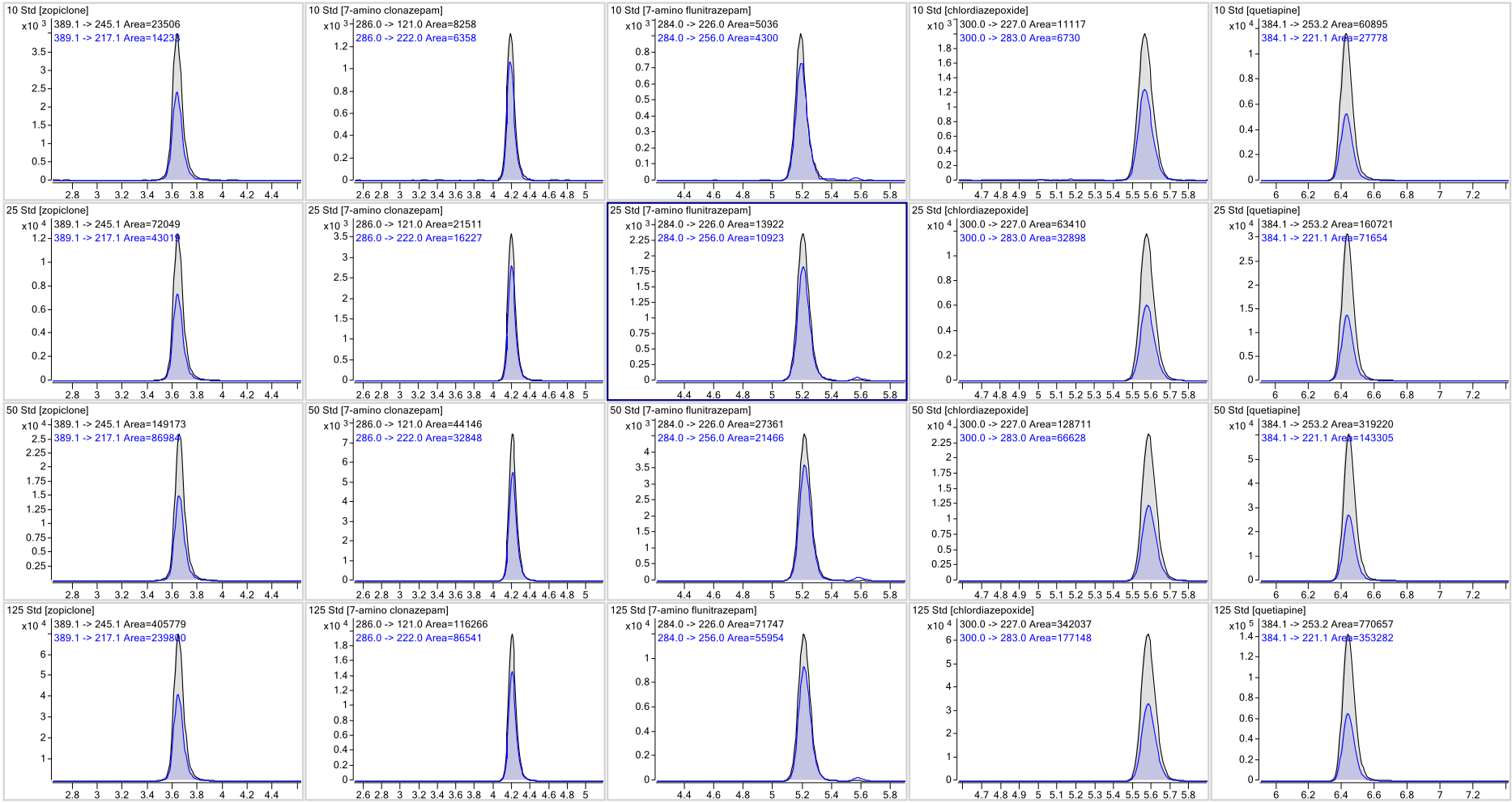
Choose any value as a percentage of lowest calibrator





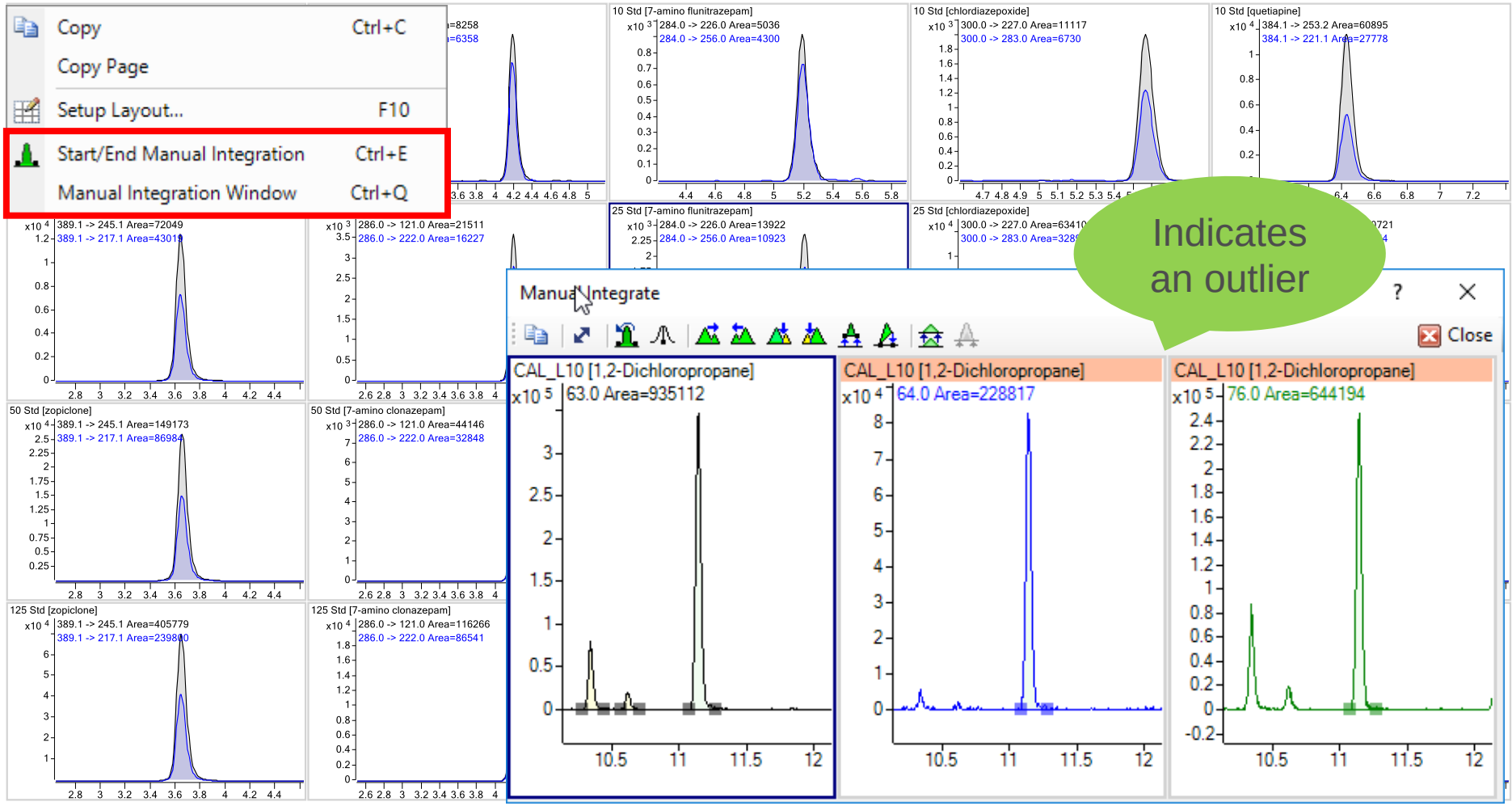
Compounds-at-a-Glance

View > Compounds-at-a-Glance…



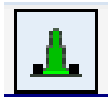
Compounds-at-a-Glance

Manual integration – right-click context menu or 

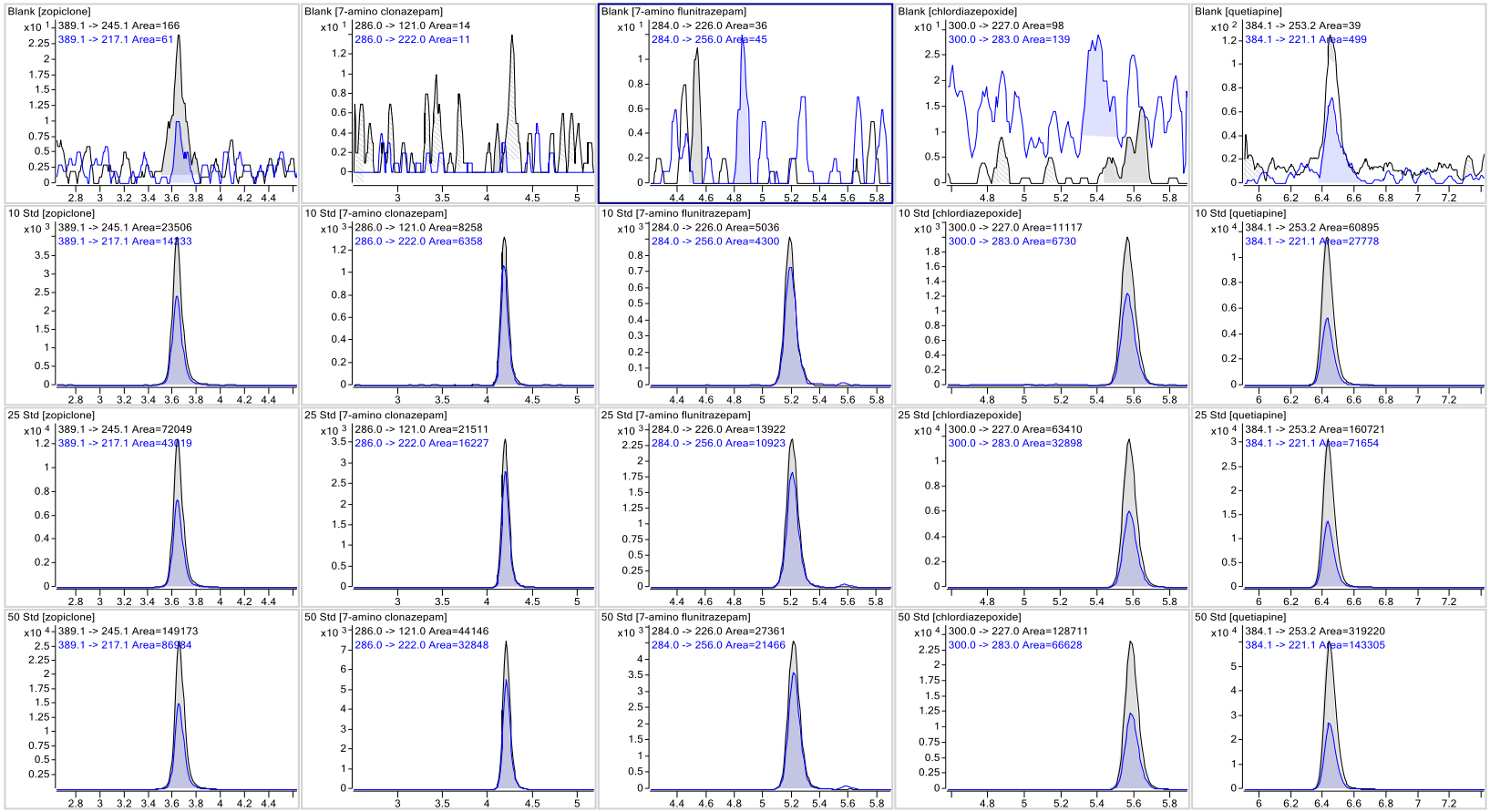


Compounds-at-a-Glance

Zero multiple peaks

Select manual integration icon 

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



Demo

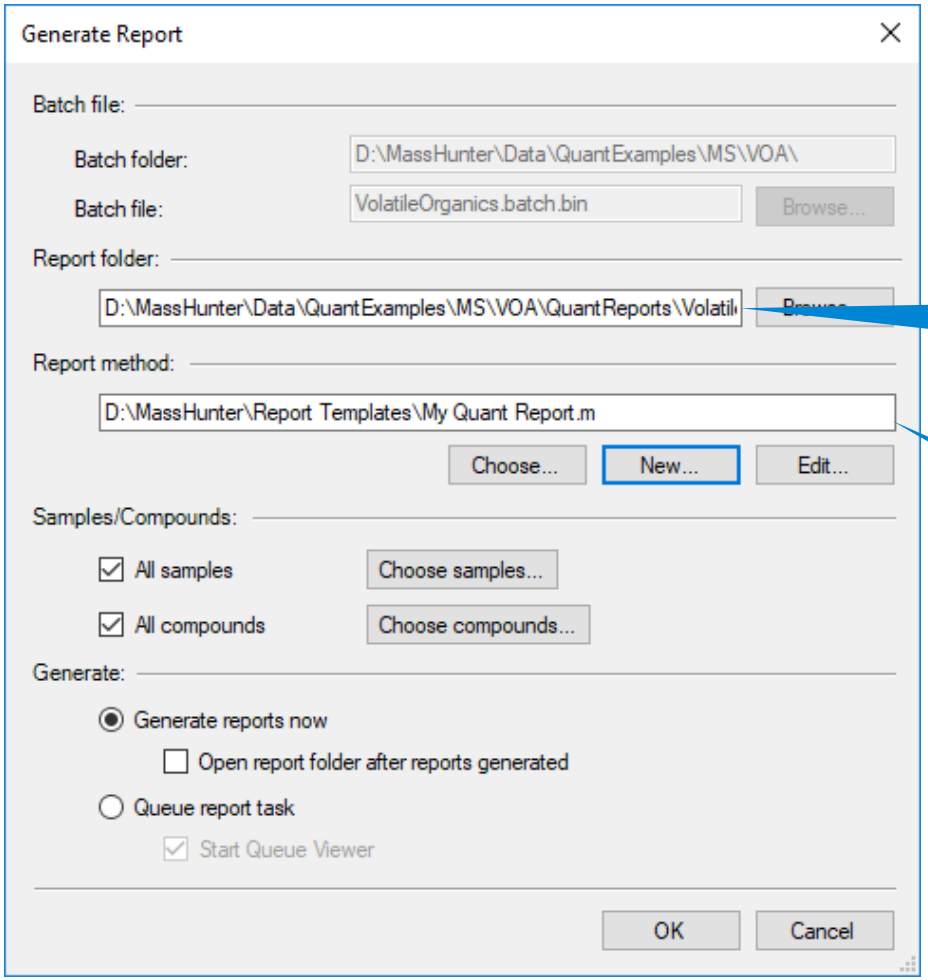
Let’s take a moment for questions on Compounds at a Glance

Up Next:

Reporting

Report Generation
Excel

Report > Generate



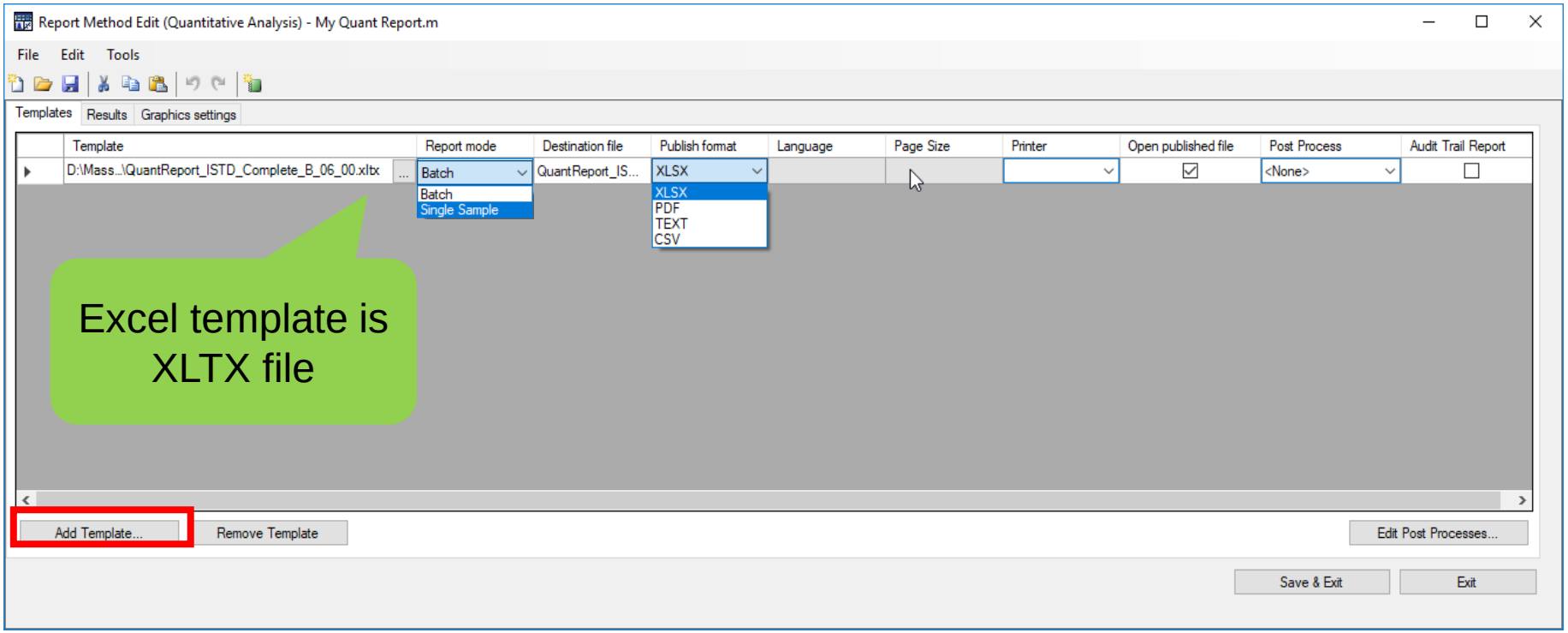
Report folder

Quant **Report Method**

Report Method Edit
Excel

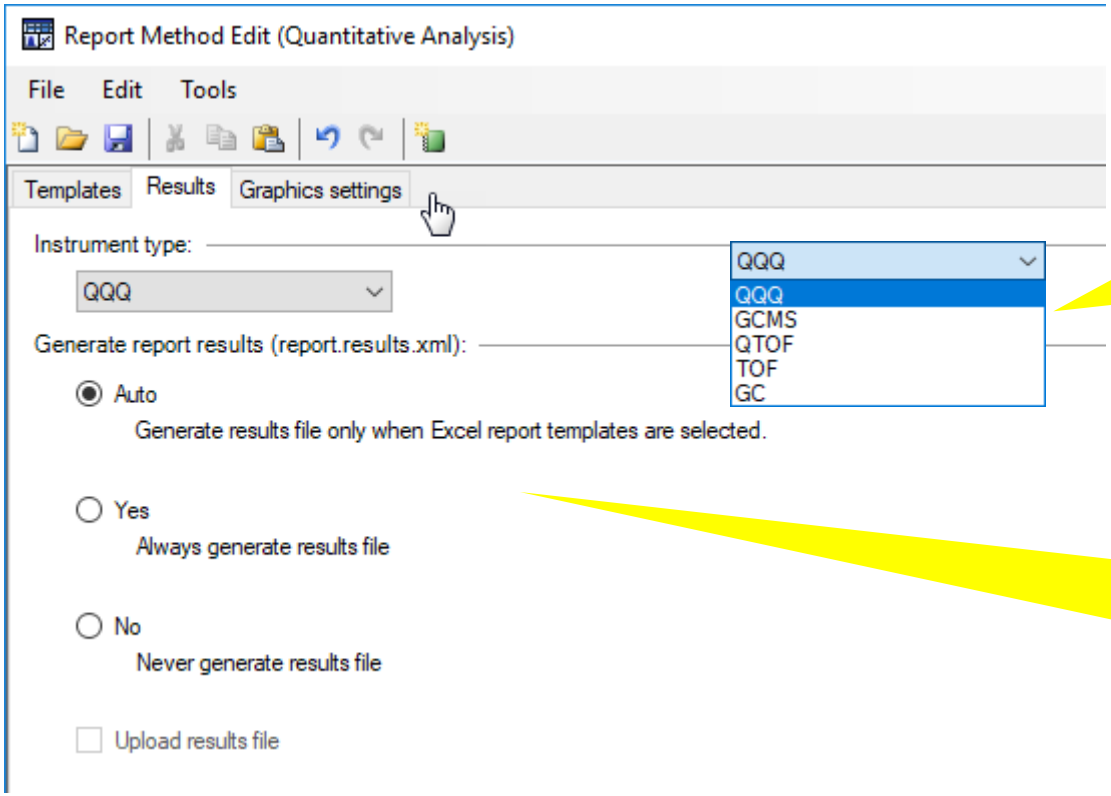
Report Mode – Batch or Single Sample.

Publish Format – XLSX, PDF, TEXT or CSV.



Report Method Edit
Excel

Results tab



Select the correct instrument type

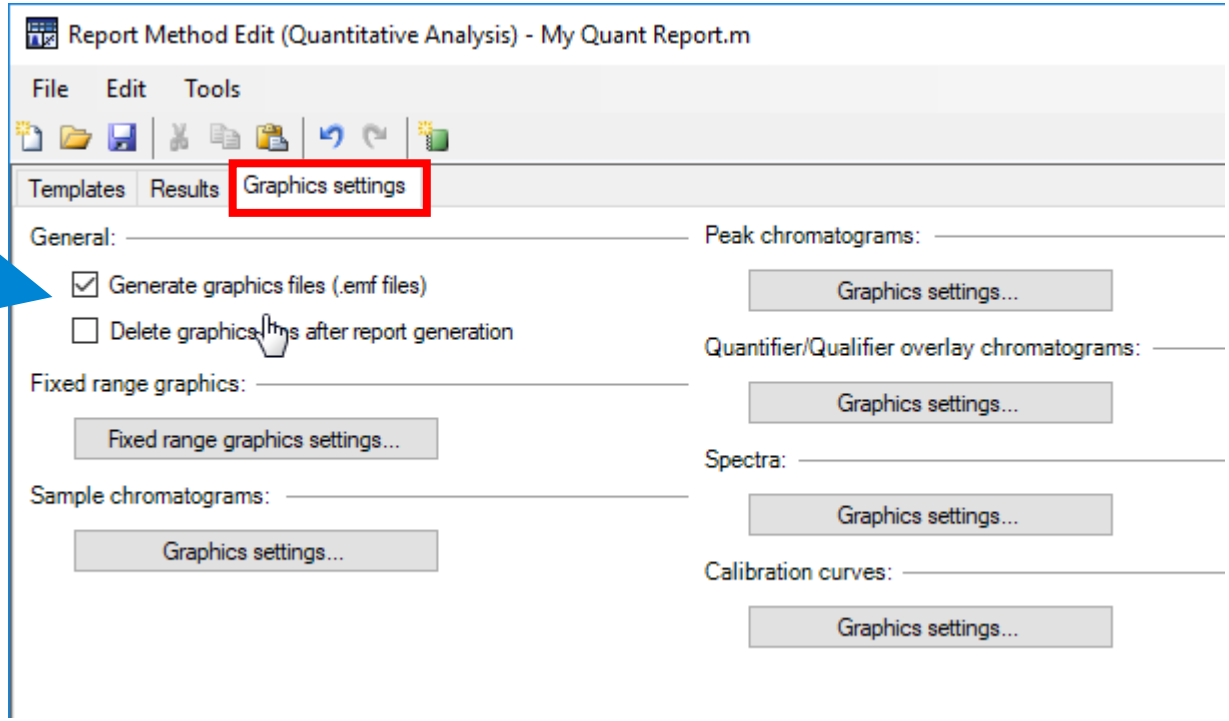
For Excel always select Auto or Yes

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.

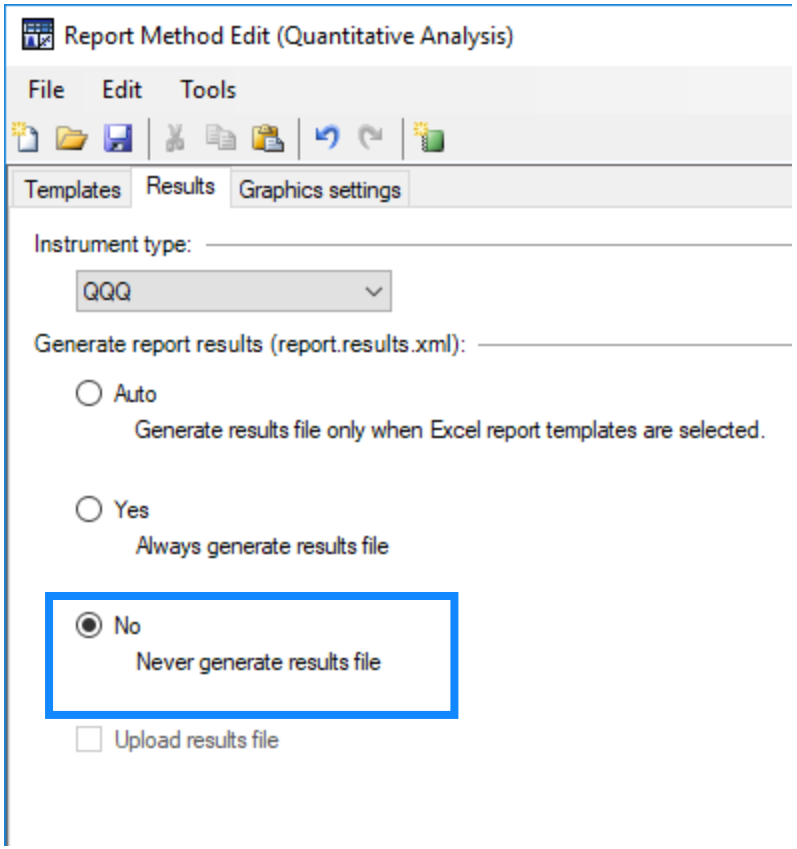
PDF reports are built on Python code and take the form of xml files.

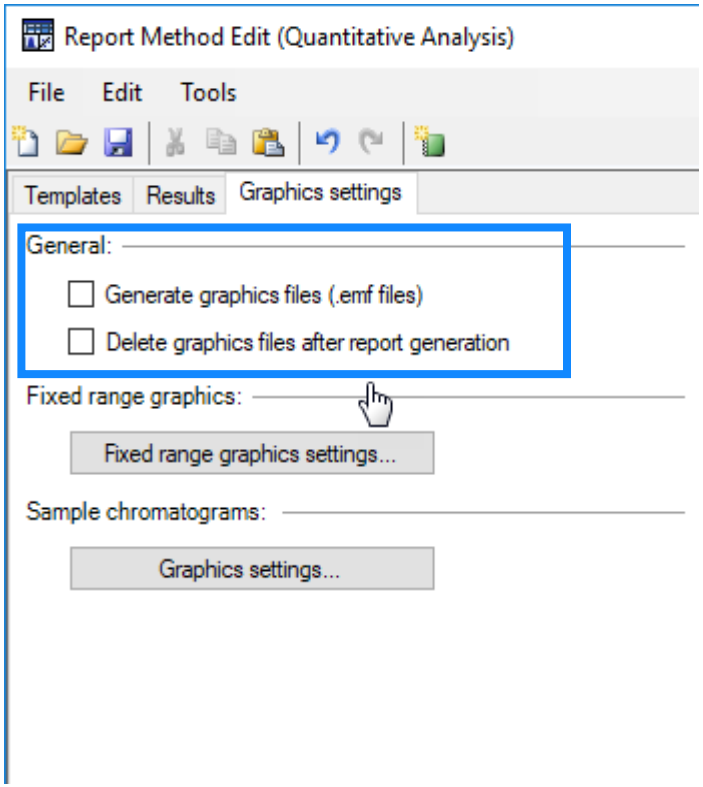
Only available Publish format is PDF.

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



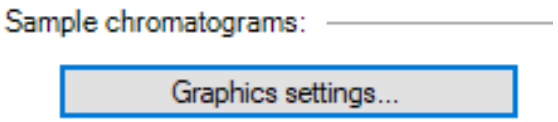


PDF Reporting will still generate graphics even when this checkbox is disabled.

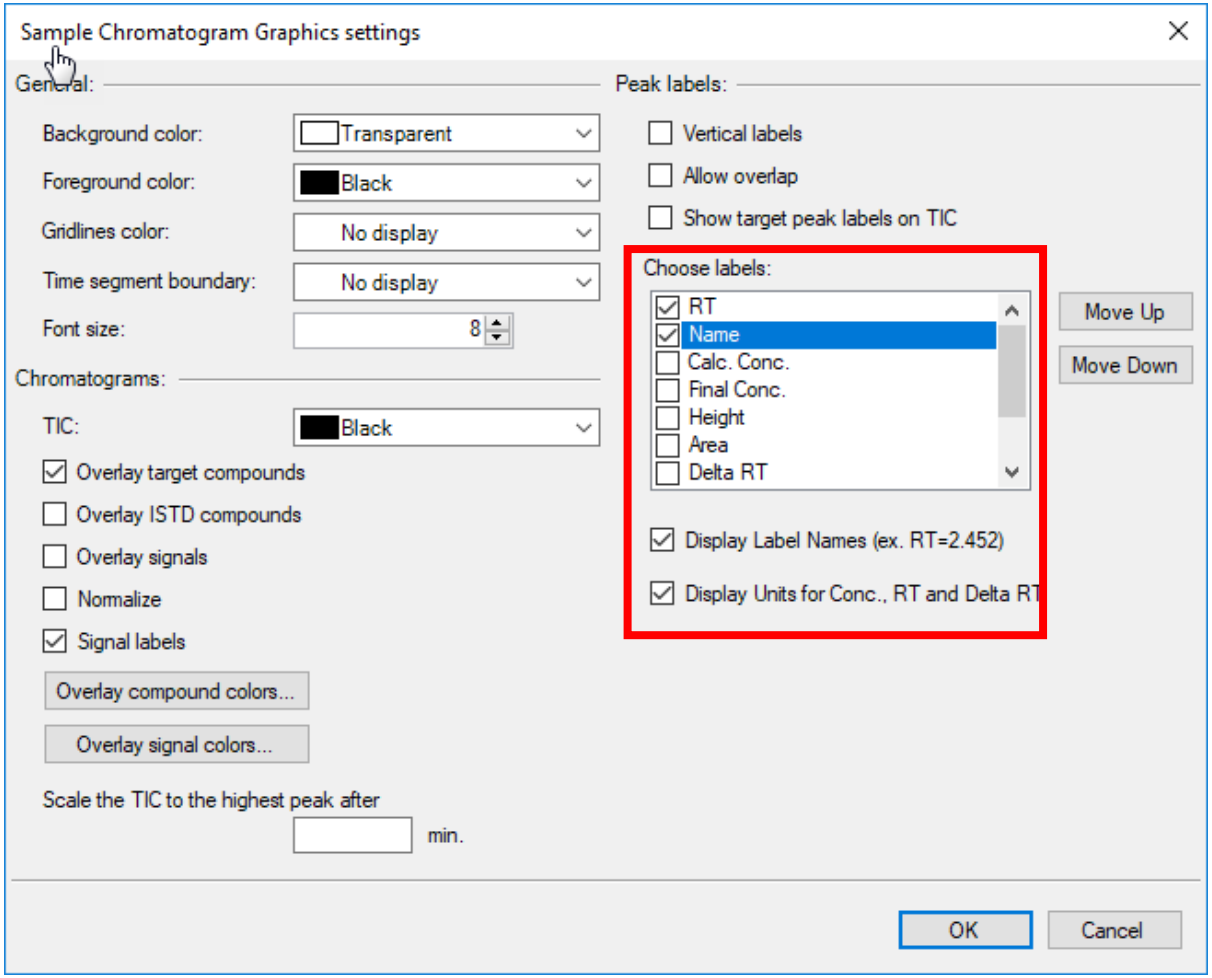
Report Method
Graphic Settings

Applies to Excel or PDF Reporting.

Label compound name on the TIC.

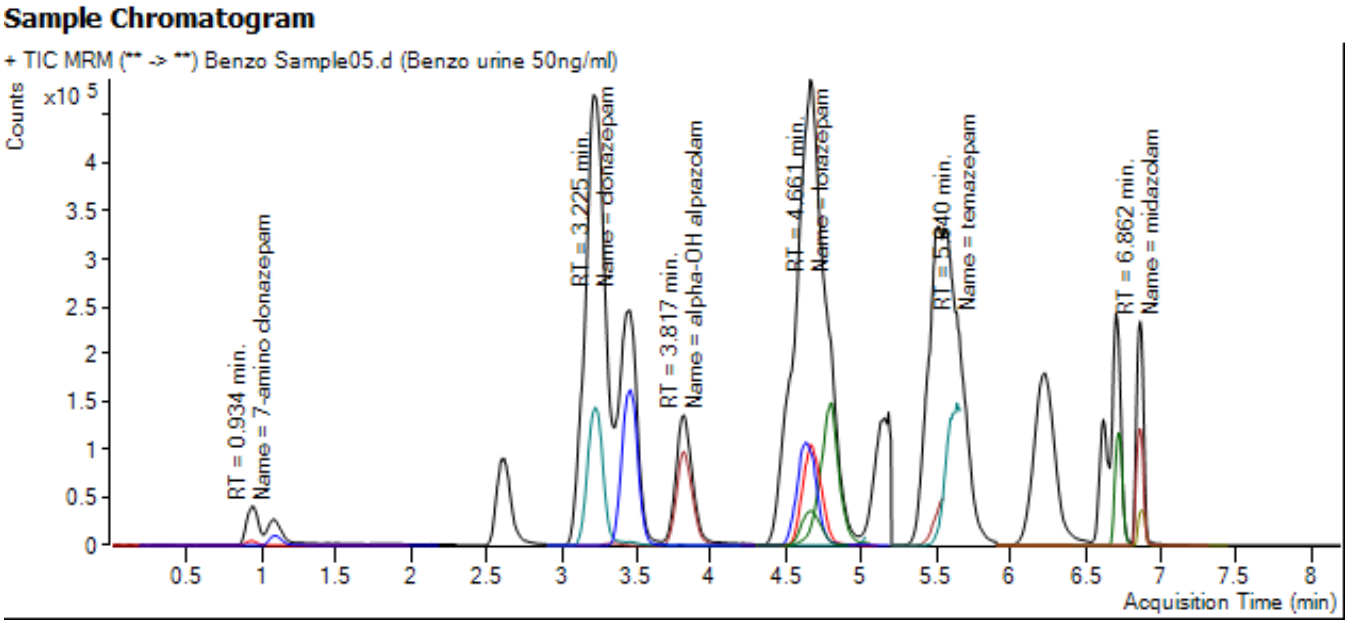


For 2D data such as GC/FID, check “overlay signals” to display the sample chromatogram.



Report Method
Example

TIC labeled with RT and Compound Name and Overlay Targets.



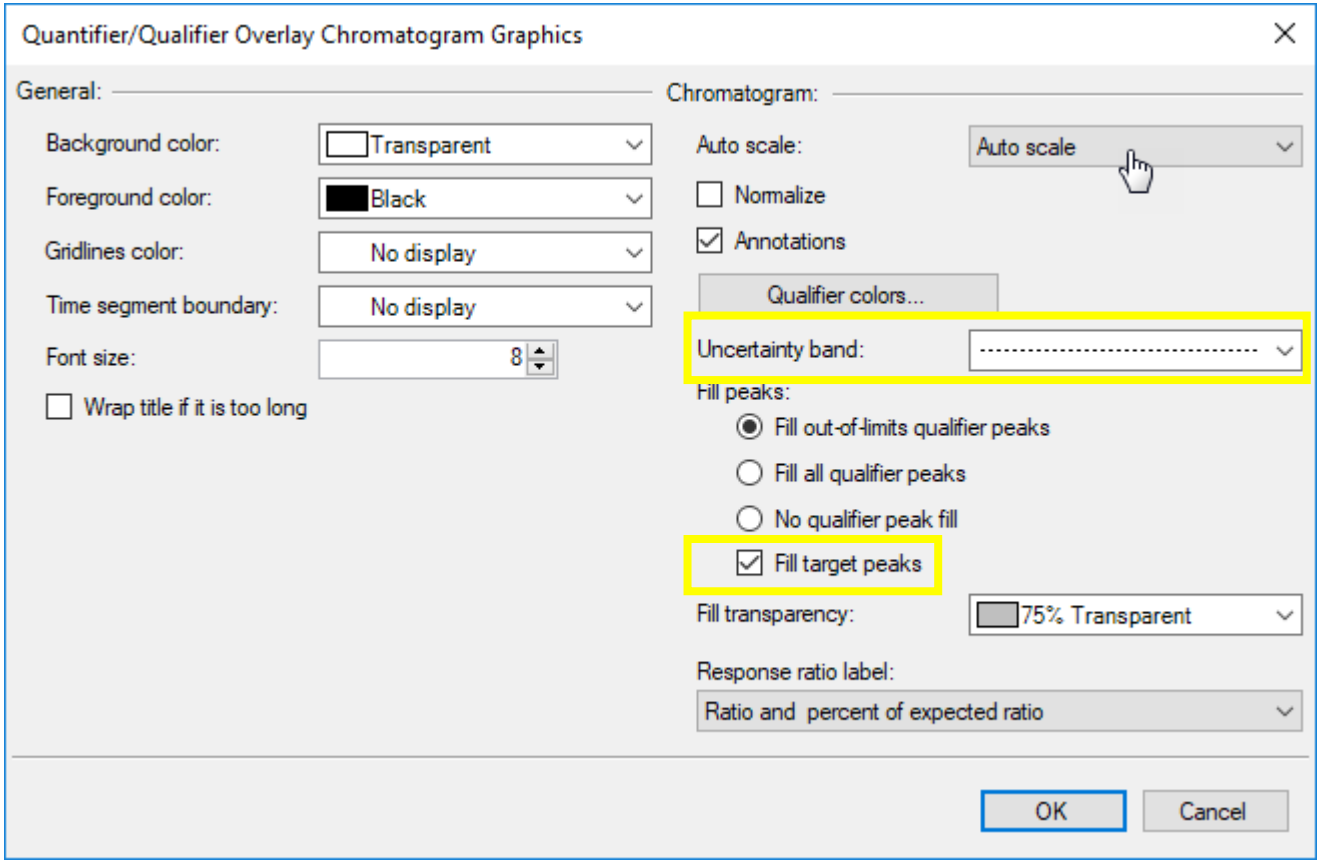
Report Method
Graphic Settings

Applies to Excel or PDF Reporting.

Normalize the qualifier ions.

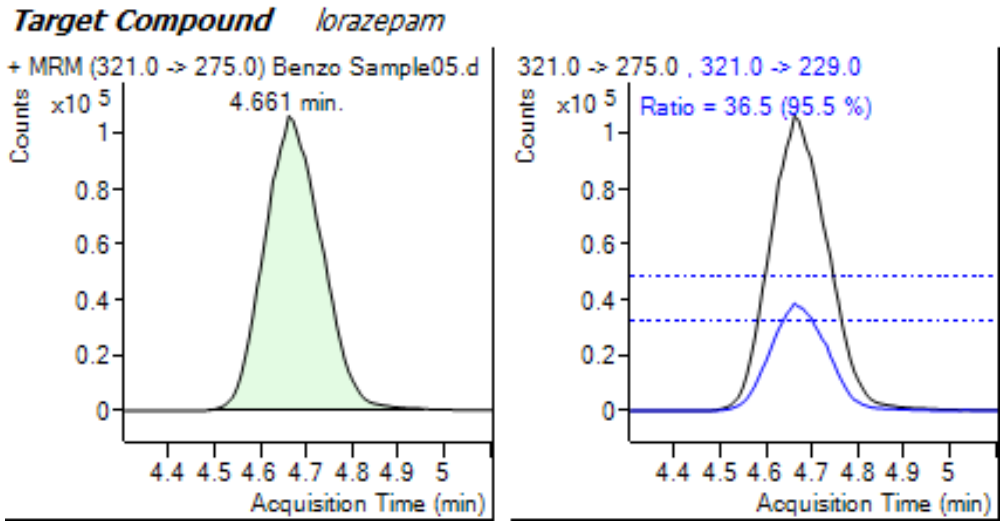
Quantifier/Qualifier overlay chromatograms

Graphics settings...



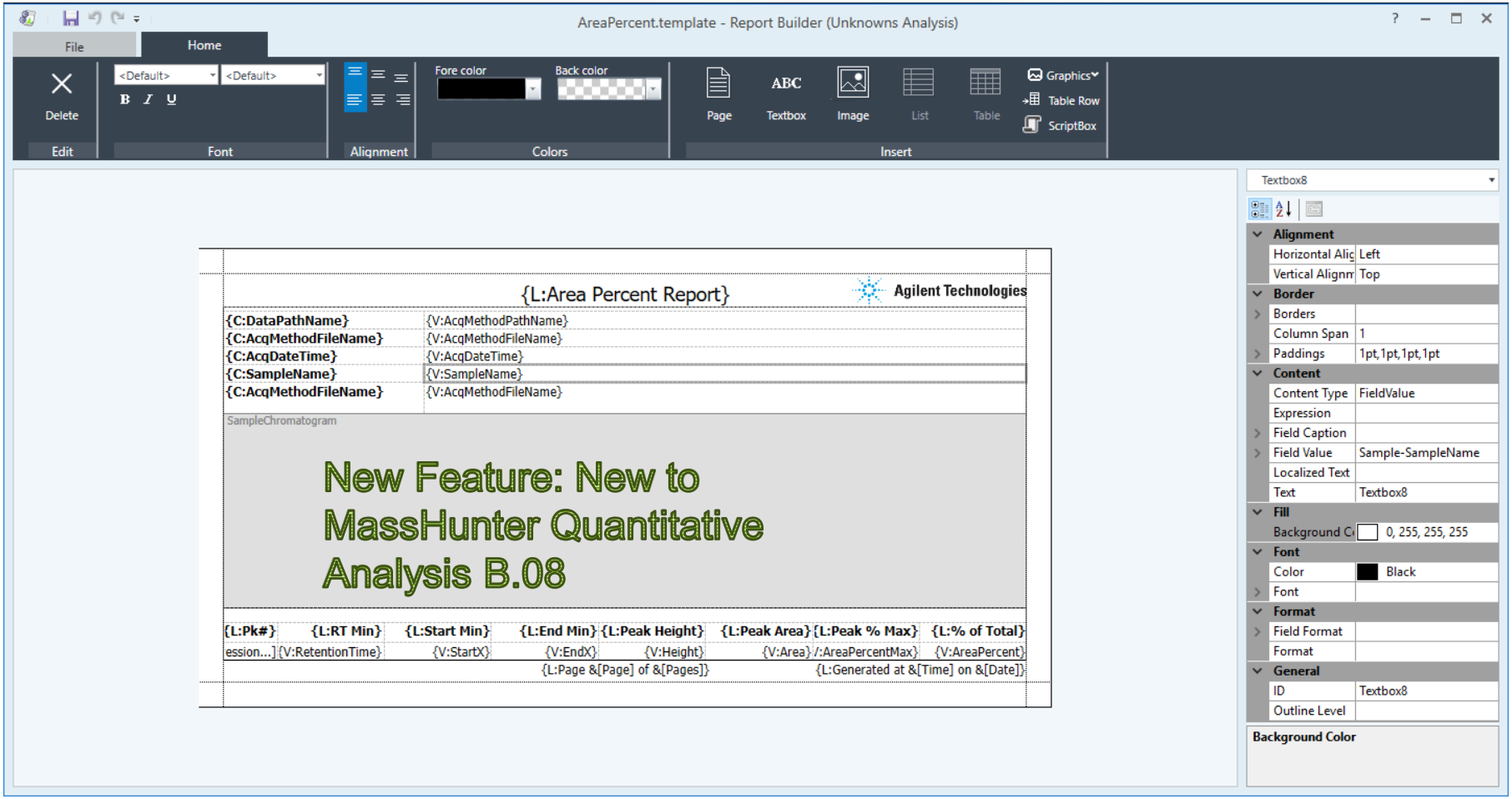
Report Method
Example

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



PDF Report Builder

Allows user to generate unique report styles



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

- PDF Report Builder overview (Starter) New!
- PDF Report Builder design flow (Advanced) New!
  - PDF Report Builder Design Architecture (Expert) New!
- PDF Report Builder - .csv to LIMs (Starter) New!
- PDF Report Builder - Add Columns Demo (Advanced) New!
- PDF Report Builder - Remove Columns Demo (Advanced) New!
- PDF Report Builder - Replace Columns Demo (Advanced) New!
- PDF Report Builder - Modify Graphics Demo (Advanced) New!
- 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.
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Agilent UNIVERSITY

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

Introduce new eLearning capabilities:

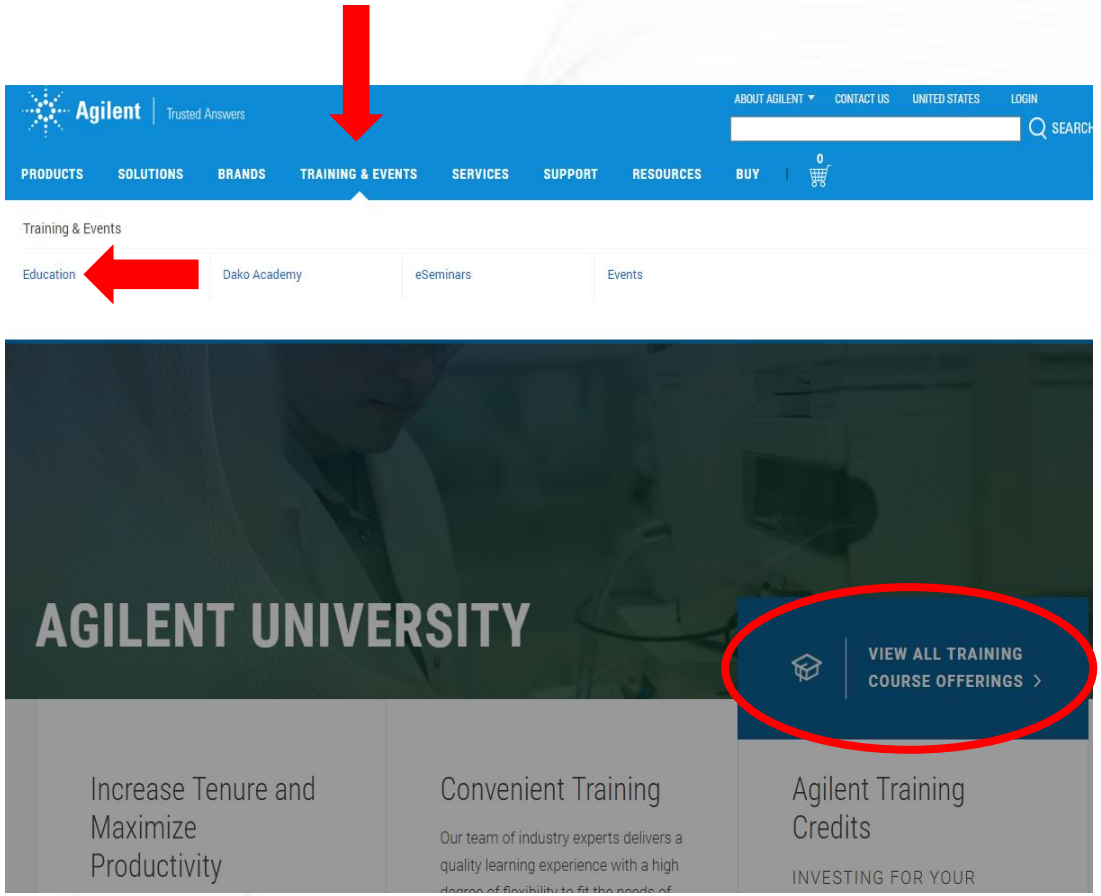
- Recorded and video-based learning
- Virtual online classes

Expanded portfolio:

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

Helping customers:

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



Questions on today's material…

Thank you for your attention.

MassHunter Quantitative Analysis

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