

Quant-My-Way Unknowns Analysis

MassHunter Quantitative Analysis Webinar Series

Howard Sanford

Stephen Harnos

With Tom Barrett & Matt Leyden & Kevin Costalunga

Quant-My-Way

MassHunter Quantitative Analysis B.09.00

Custom Desktop icons.



Agilent MassHunter Workstation

MassHunter Installer

Configure

Choose compliance type: Standard Workflow

No compliance support features will be installed.

Choose desktop icons: Quant-My-Way Classic UI

More Options...

Back Next Cancel

Quantitative Analysis B.09.00 (Build 9.0.640.0) © Agilent Technologies, Inc. 2017

Desktop Icons

Quantitative Analysis	Application		
	Standard	Drug Analysis	Environmental Analysis
MS (single quadrupole)	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
QQQ (triple quadrupole)	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
TOF (time-of-flight)	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
Q-TOF (quadrupole time-of-flight)	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
GC	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>

Unknowns Analysis

Unknowns Analysis

Pre-Configured Flavors

Vanilla

OK Cancel

Desktop Icons

Quantitative Analysis	Application		
	Standard	Drug Analysis	Environmental Analysis
MS (single quadrupole)	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
QQQ (triple quadrupole)	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
TOF (time-of-flight)	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
Q-TOF (quadrupole time-of-flight)	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
GC	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>

Unknowns Analysis

Unknowns Analysis

OK Cancel

Setup during installation.

Quant-My-Way

MassHunter Quantitative Analysis B.09.00

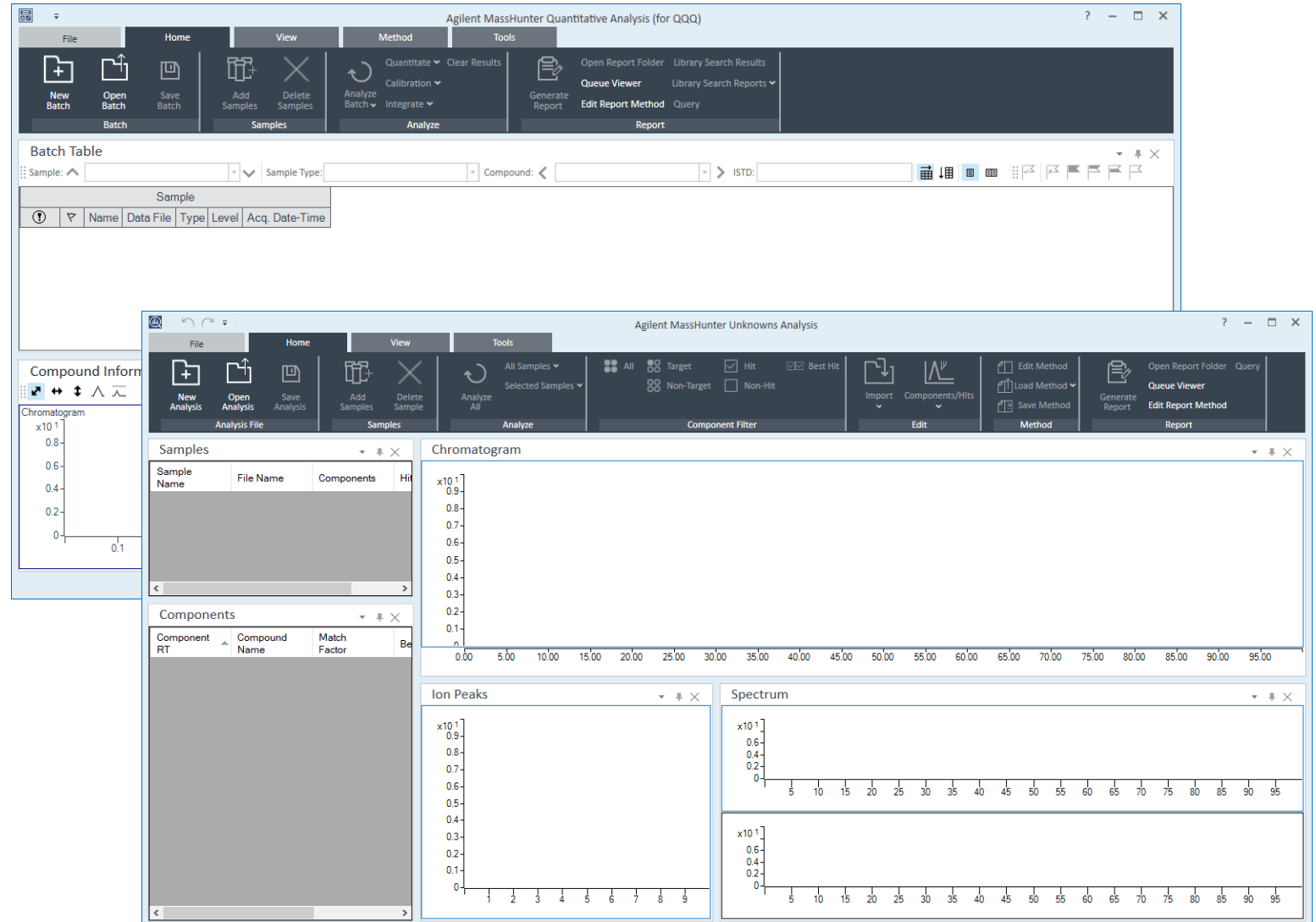
Preconfigured Quantitative and Unknowns Analysis Layouts.

Tools to

- Customize various layouts.
- Save the layouts.
- Share the layouts on other computers.

Customize Display for only relevant tools and menu items.

“OpenLab like” appearance with tabs and ribbons.



Classic UI

The screenshot displays the classic MassHunter interface. At the top, the 'Batch Table' shows a list of samples including Benzo Cal05, Benzo Sample02, and various urine samples. Below this, a detailed table lists results for 7-amino clonazepam, 7-amino flunitrazepam, zopiclone, clonazepam, flunitrazepam, and alpha-OH alprazolam. The bottom section features 'Compound Information' with chromatograms for peak 0.983 min and a 'Calibration Curve' showing a linear relationship between relative response and relative concentration.

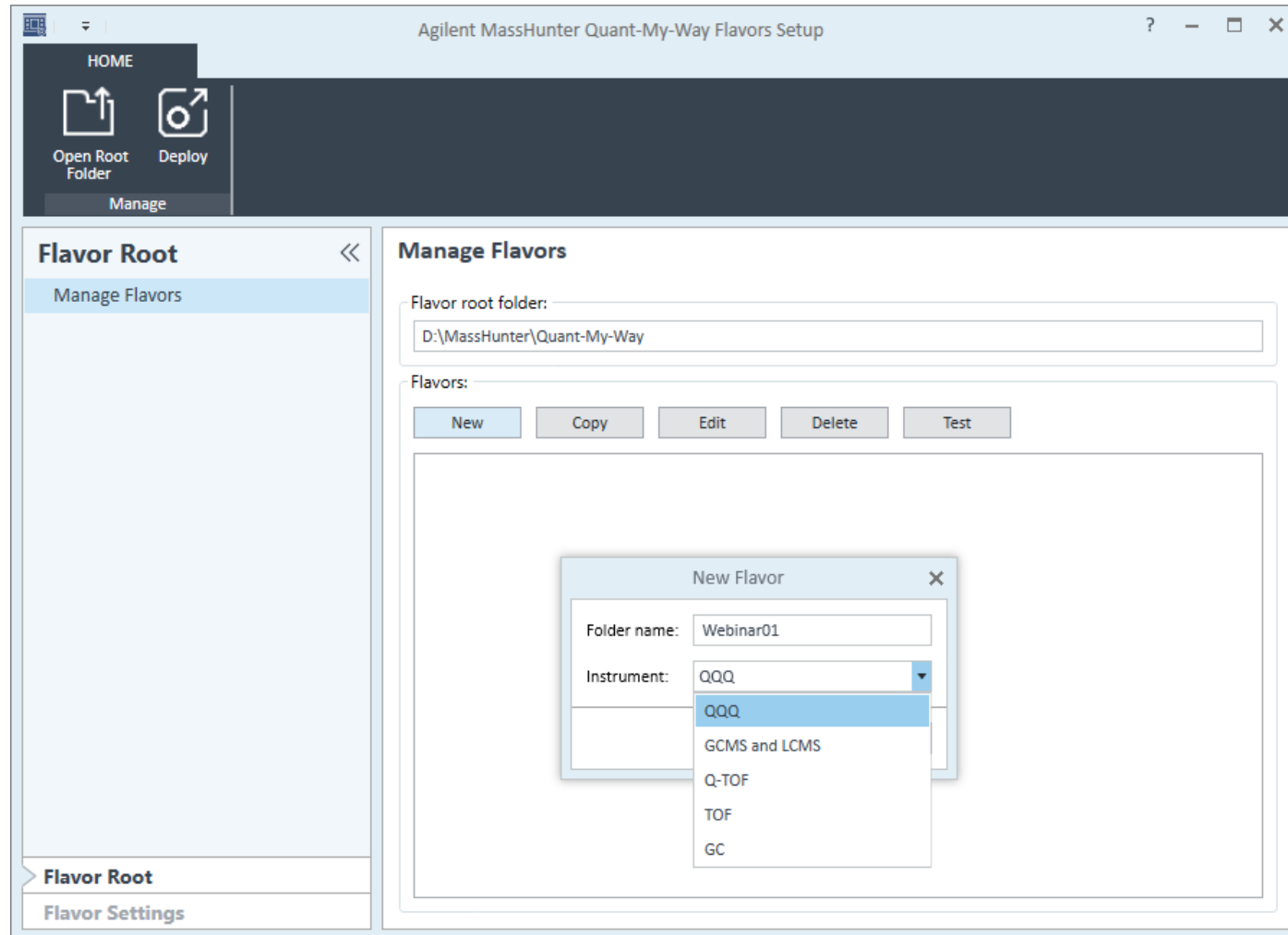
Quant-My-Way

The screenshot displays the Quant-My-Way MassHunter interface. The 'Batch Table' is more compact and highlights the 7-amino clonazepam results. The 'Compound Information' section shows chromatograms for peak 0.983 min and a 'Calibration Curve' with a linear fit equation: $y = 0.022152 \cdot x^2 + 1.255500 \cdot x - 0.087941$ and $R^2 = 0.99981912$.

Identical information → different appearance.

Quant-My-Way

Create and Manage Flavors



Click on Quant-My-Way Flavors Setup. Installed from **Start > Agilent MassHunter Quantitative Analysis > Quant-My-Way Flavors Setup.**

Select the Root Folder.

Click New and create a new Flavor for a given instrument type

- or -

Select an existing Flavor name.

Click Edit.....

Quant-My-Way

Edit the Flavor

Step through the various settings.

- General Settings
- Batch Table Settings
- Column Settings

Modify as desired.

- Change AcqDate Time variable → Webinar Time

Save Settings.

Step back to Flavor Root

Test

Agilent MassHunter Quant-My-Way Flavors Setup - Webinar01

HOME

Reload Settings Reset to Default Save Settings

General Settings

Agilent MassHunter Quant-My-Way Flavors Setup - Webinar01

HOME

Reload Settings Reset to Default Save Settings

Batch Table Settings

Agilent MassHunter Quant-My-Way Flavors Setup - Webinar01

HOME

Reload Settings Reset to Default Save Settings

Column Labels

Flavor Settings

- General Settings
- Batch Table Settings
- Column Labels
- Ribbon Settings
- Sample Types
- Outliers

Flavor Root

Flavor Settings

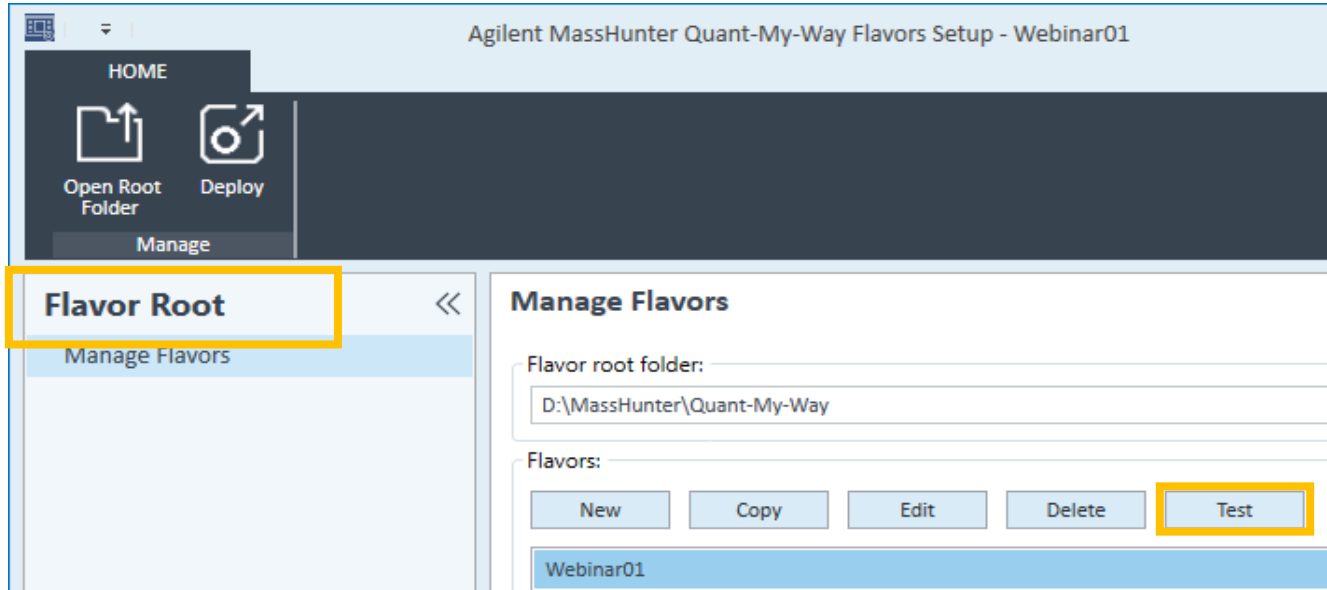
Column Labels

Table: Sample Language: <Default>

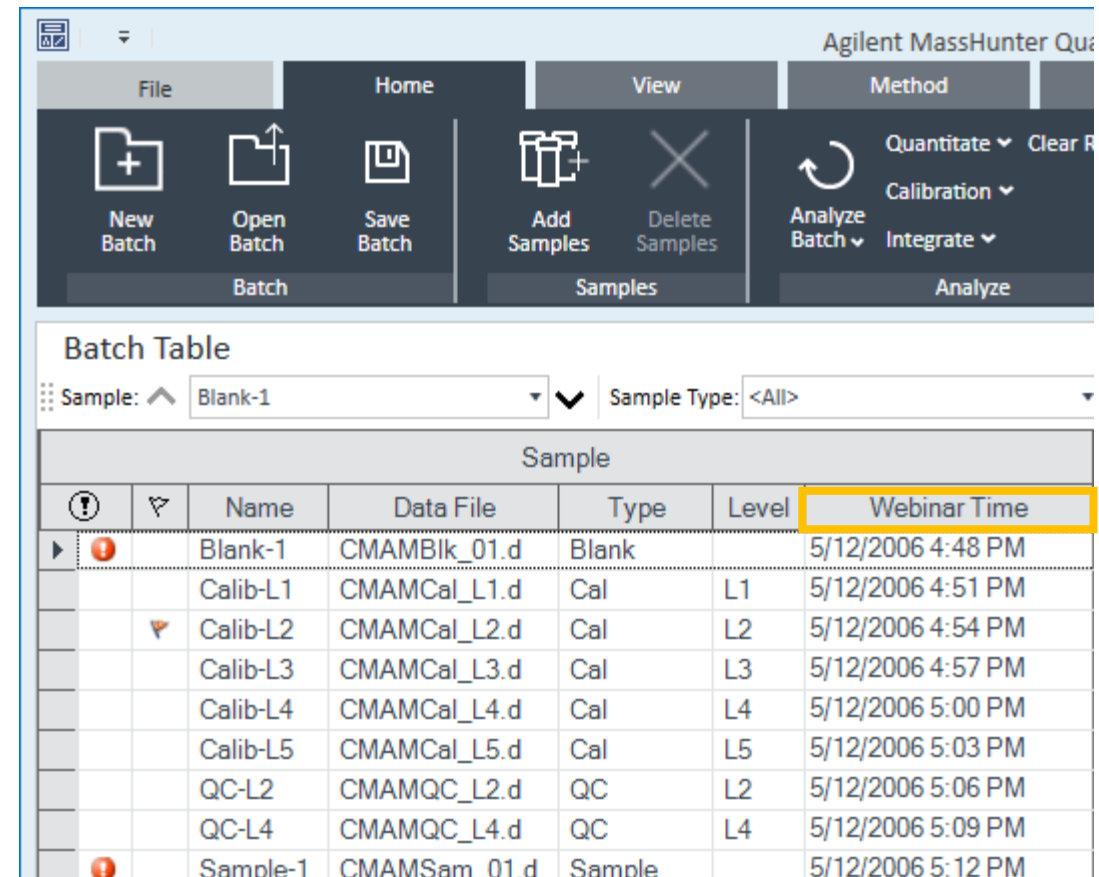
Column name	Visible	Column label
BatchID	<input type="checkbox"/>	Batch ID
SampleID	<input type="checkbox"/>	Sample ID
AcqDateTime	<input checked="" type="checkbox"/>	Webinar Time
AcqDateTimeLocal	<input checked="" type="checkbox"/>	Acq. Date-Time (Inst.)
AcqMethodFileName	<input checked="" type="checkbox"/>	Acq. Method File
AcqMethodPathName	<input checked="" type="checkbox"/>	Acq. Method Path
AcqOperator	<input checked="" type="checkbox"/>	Acq Operator
BalanceOverride	<input checked="" type="checkbox"/>	Balance
Barcode	<input checked="" type="checkbox"/>	Barcode
CalibrationReferenceSampleID	<input checked="" type="checkbox"/>	Calibration Reference Sample ID
Comment	<input checked="" type="checkbox"/>	Comment
Completed	<input checked="" type="checkbox"/>	Completed
DADateTime	<input checked="" type="checkbox"/>	DA. Date-Time
DAMethodFileName	<input checked="" type="checkbox"/>	DA Method File
DAMethodPathName	<input checked="" type="checkbox"/>	DA Method Path
DataFileName	<input checked="" type="checkbox"/>	Data File
DataPathName	<input checked="" type="checkbox"/>	Data Path

Quant-My-Way

Test the Flavor



Tip: Quant remembers the last configuration -> Restore User Settings.



Test the new flavor.

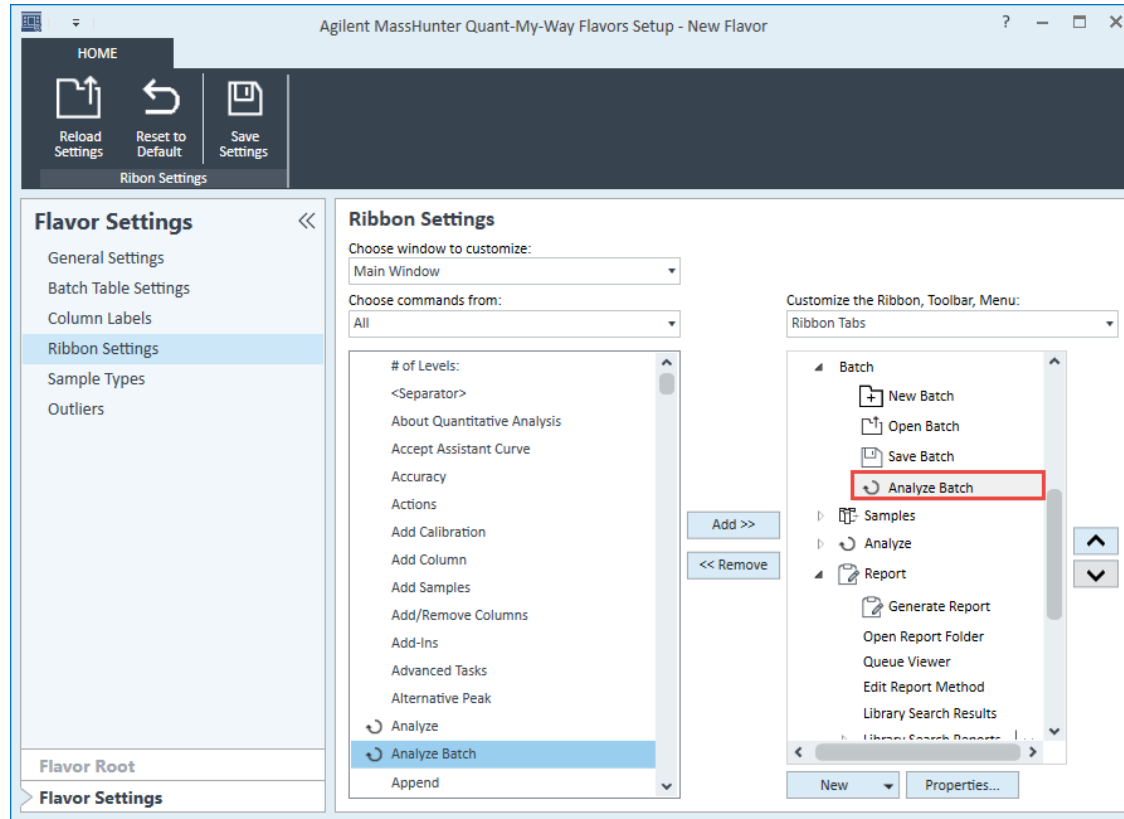
Automatically opens Quant-My-Way.

New label is present.

Tip: Test at each step of the way.

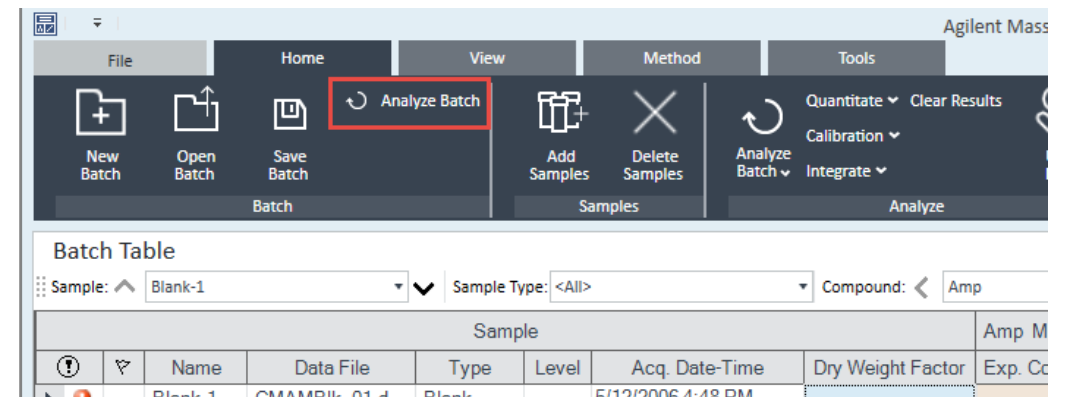
Quant-My-Way

Ribbon Layout



Easy access to frequently used items and features.

Remove unneeded or unused features to reduce clutter.



Quant-My-Way

Help Files

Classic UI

Agilent MassHunter Quantitative Analysis (for QQQ) - BenzosinUrine - BenzosinUrine.batch.bin

Batch Table

Sample	Name	Data File	Type	Level	Acq. Date-Time	7-amino clonazepam Results	7-amino flunitrazepam Resu...	zopiclone Results	clonazepam Results	flunitrazepam Results	alpha-OH alprazolam Results	triazolam	
						RT	Final Conc.	Accuracy	RT	Final Conc.	Accuracy	RT	Final C
Benzo Sample02	Benzo Sample02.d	Sample	2/23/2007 12:54 AM			0.887			3.186	2.9670			
Benzo urine 10ng/ml	Benzo Sample03.d	Sample	2/23/2007 1:08 AM			0.925	1.079		3.218	11.7224	3.446	12.1931	
Benzo urine 25ng/ml	Benzo Sample04.d	Sample	2/23/2007 1:22 AM			0.944	1.088		3.241	45.3633	3.461	43.2947	
Benzo urine 50ng/ml	Benzo Sample05.d	Sample	2/23/2007 1:35 AM			0.954	1.088		3.225	51.7133	3.461	48.3588	
Benzo urine 100ng/ml	Benzo Sample06.d	Sample	2/23/2007 1:49 AM			0.934	1.093		3.217	108.5878	3.469	95.4249	
Benzo urine pc 25ng/ml	Benzo Sample07.d	Sample	2/23/2007 2:03 AM			0.930	1.088		3.225	24.1696	3.446	25.3891	
Blank01	Benzo Blank01.d	Blank	3/8/2007 1:40 PM							3.310	5.0454		
Benzo Cal03	Benzo Cal03.d	Cal	L1	3/8/2007 1:50 PM		0.983	24.8024	99.5	1.172	25.2816	101.1	2.485	25.3066
Benzo Cal04	Benzo Cal04.d	Cal	L2	3/8/2007 2:00 PM		0.983	50.7888	101.6	1.177	48.1202	96.2	2.468	48.2252
Benzo Cal05	Benzo Cal05.d	Cal	L3	3/8/2007 2:11 PM		0.983	123.6924	99.0	1.177	132.6900	106.2	2.465	128.9238
Benzo Cal06	Benzo Cal06.d	Cal	L4	3/8/2007 2:21 PM		0.983	249.3775	99.8	1.181	243.2411	97.3	2.471	250.6659
Benzo Cal07	Benzo Cal07.d	Cal	L5	3/8/2007 2:31 PM		0.983	501.3506	100.3	1.181	502.1731	100.4	2.471	497.2698
Benzo QC	Benzo QC01.d	QC	QC1	3/8/2007 2:51 PM		0.983	183.4225	81.2	1.181	34.8793	94.9	3.196	91.9207
Benzo Sample01	Benzo Sample01.d	Sample	3/8/2007 3:01 PM			0.670	9.8132		2.465	11.3119		3.574	5.2123

MassHunter Quantitative Analysis Help

Getting Started | Quantitative Analysis | Method Development | Outliers | Reports | Reference

What's New
Demonstration videos
Read the Familiarization Guide more...

Analyze a batch
Create or modify the batch table
Integrate a batch, sample, or compound more...

Open a method
Create a new method
Edit a method more...

Outliers details
Outliers enabled by default
Display outlier monitored columns in the batch table more...

Generate a report
Generate a TIC Report
Create a report method more...

Basic Software Tasks
Batch table columns
Method table columns more...

Compound Information

MRM (286.0 -> 121.0) Benzo Cal05.d
0.983 min.

MRM (0.925-1.117) Benzo Cal05.d
Ratio = 83.1 (100.7%)

Processed Benzo Cal05 7-amino clonazepam 14 Samples (14 total) DESKTOP-976FDV\Ice

Quant-My-Way

Agilent MassHunter Quantitative Analysis (for QQQ) - BenzosinUrine - BenzosinUrine.batch.bin

Batch Table

Sample	Name	Data File	Type	Level	Acq. Date-Time	7-amino clonazepam Results	7-amino flunitrazepam Res...	zopiclone Results	clonazepam Results	Accuracy	
						RT	Final Conc.	Accuracy	RT	Final Conc.	Accuracy
Benzo Sample02	Benzo Sample02.d	Sample	2/23/2007 12:...			0.887			3.186	2.9670	
Benzo urine 10ng/ml	Benzo Sample03.d	Sample	2/23/2007 1:0...			0.925	1.079		3.218	11.7224	3.446
Benzo urine 25ng/ml	Benzo Sample04.d	Sample	2/23/2007 1:2...			0.944	1.088		3.241	45.3633	3.461
Benzo urine 50ng/ml	Benzo Sample05.d	Sample	2/23/2007 1:3...			0.934	1.088		3.225	51.7133	3.461
Benzo urine 100ng/ml	Benzo Sample06.d	Sample	2/23/2007 1:4...			0.934	1.093		3.217	108.5878	3.466
Blank01	Benzo Blank01.d	Blank	3/8/2007								
Benzo Cal03	Benzo Cal03.d	Cal	L1	3/8/2007							

MassHunter Quantitative Analysis Help

Getting Started | Quantitative Analysis | Method Development | Outliers | Reports | Reference

What's New
Demonstration Videos
Read the Familiarization Guide more...

Analyze a batch
Create or modify the batch table
Integrate a batch, sample, or compound more...

Open a method
Create a new method
Create a new method more...

Outliers details
Outliers enabled by default
Display outlier monitored columns in the batch table more...

Generate a report
Generate a TIC Report
Create a report method more...

Basic Software Tasks
Batch table columns
Method table columns more...

Compound Information

MRM (286.0 -> 121.0) Benzo Cal05.d
0.983 min.

MRM (0.925-1.117) Benzo Cal05.d
Ratio = 83.1 (100.7%)

Contain same help topics.
Slightly different navigation.
Help activated with F1 key.



Supplemental\MassHunter\Manuals\Quant

Name

- Quant-My-Way - Agile Iterative Development - Starter.mp4
- Quant-My-Way - Batch Table Settings - Demo - Advanced.mp4
- Quant-My-Way - Column Labels - Demo - Advanced.mp4
- Quant-My-Way - Compounds-at-a-Glance Demo - Starter.mp4
- Quant-My-Way - Custom Button.mp4
- Quant-My-Way - Deploy Flavors - Advanced.mp4
- Quant-My-Way - Flavors Setup steps - Starter.mp4
- Quant-My-Way - General Settings - Demo - Advanced.mp4
- Quant-My-Way - Introduction - Starter.mp4
- Quant-My-Way - Less is More - Starter.mp4
- Quant-My-Way - Outliers - Demo - Advanced.mp4
- Quant-My-Way - Ribbon Settings - Compounds-at-a-Glance.mp4
- Quant-My-Way - Ribbon Settings - Main Window - Batch Table - Toolbar+Context Menu - Advanced.mp4
- Quant-My-Way - Ribbon Settings - Main Window - Calibration Curve - Toolbar+Context Menu - Advanced.mp4
- Quant-My-Way - Ribbon Settings - Main Window - Compound Info - Toolbar+Context Menu - Advanced.mp4
- Quant-My-Way - Ribbon Settings - Main Window - MethodTable - Toolbar+Context Menu - Advanced.mp4
- Quant-My-Way - Ribbon Settings - Main Window - Others - Toolbar+Context Menu - Advanced.mp4
- Quant-My-Way - Ribbon Settings - Main Window - Ribbon Tabs - Advanced.mp4
- Quant-My-Way - Ribbon Settings - Main Window - Sample Info - Toolbar+Context Menu - Advanced.mp4
- Quant-My-Way - Ribbon Settings introduction - Advanced.mp4
- Quant-My-Way - Sample Types - Demo - Advanced.mp4

Supplemental\MassHunter\Videos\Quant

Quant-My-Way



Time for a demo

Next up:
Unknowns Analysis

Unknowns Analysis

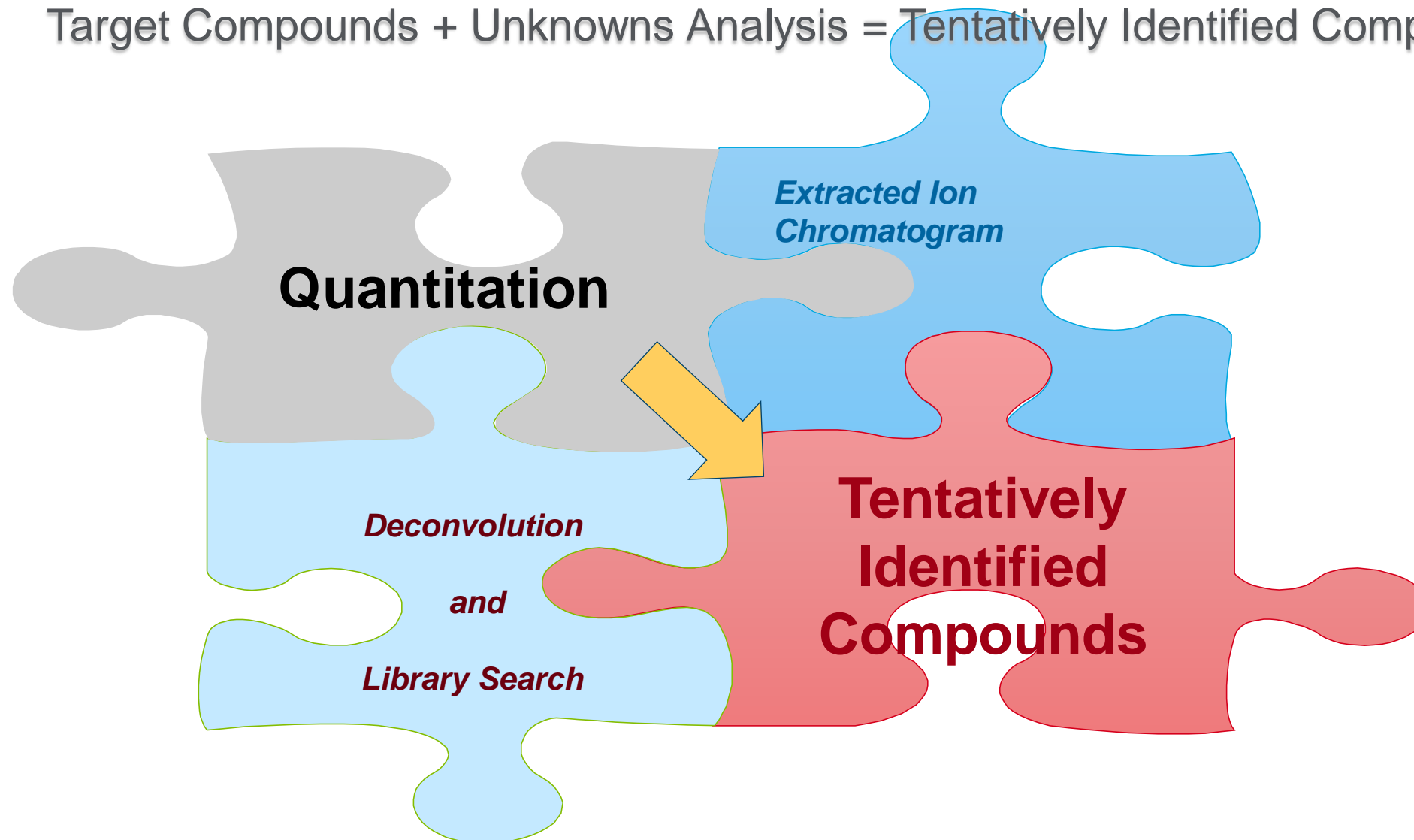
Overview

Tentatively Identified Compounds

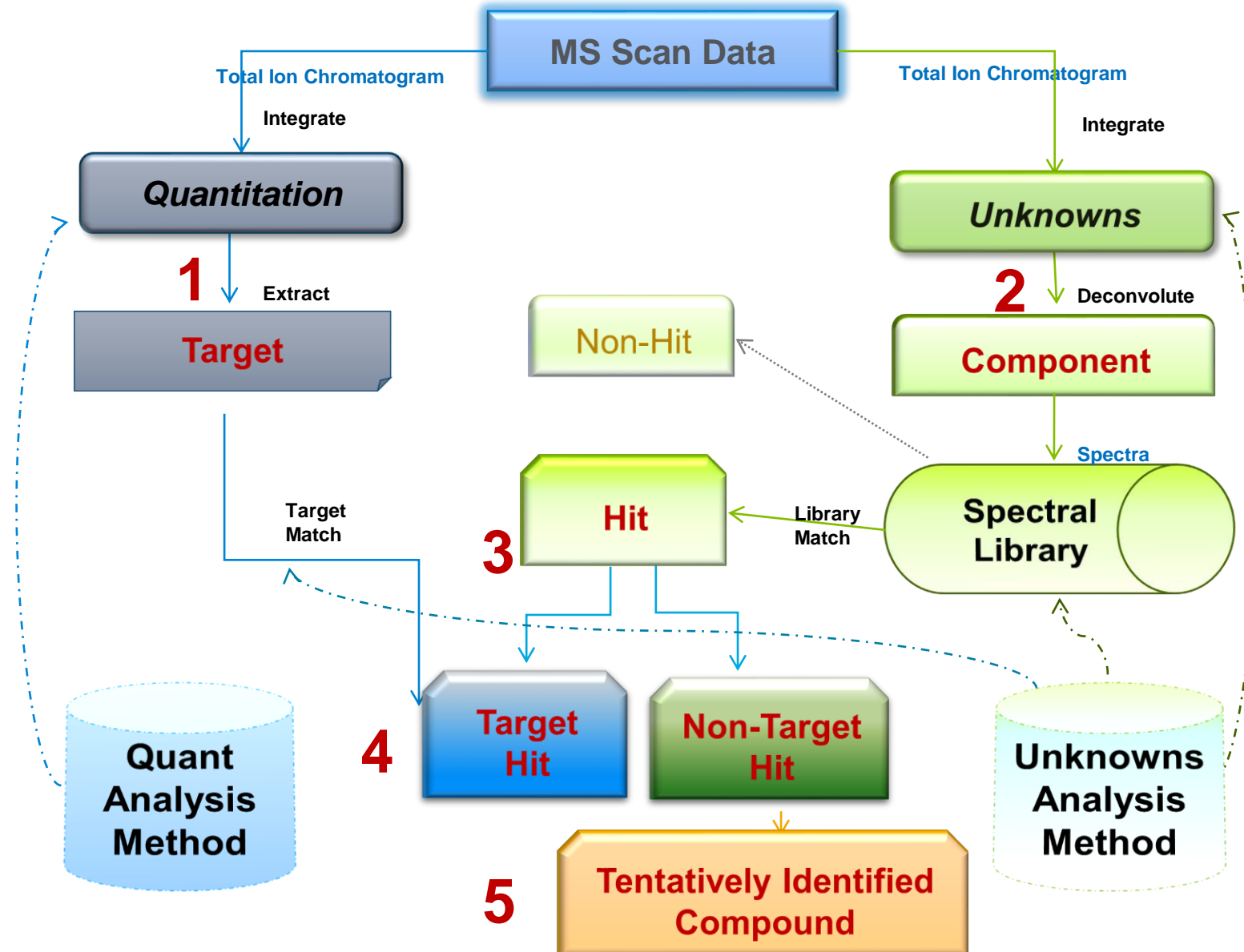
- Method Parameters
 - Peak Detection
 - Library Search
 - Compound Identification
 - Target Match (semi quantitation)
 - Blank Subtraction
- Component Review
- Screening
 - Minimal Sample Prep
 - Fast Chromatography
 - Component found \Rightarrow Confirmation
- Report Generation
 - PDF Report Builder
 - Queries

Overview of Unknowns Analysis

Target Compounds + Unknowns Analysis = Tentatively Identified Compounds



Quantitative Analysis & Unknowns Analysis Workflow

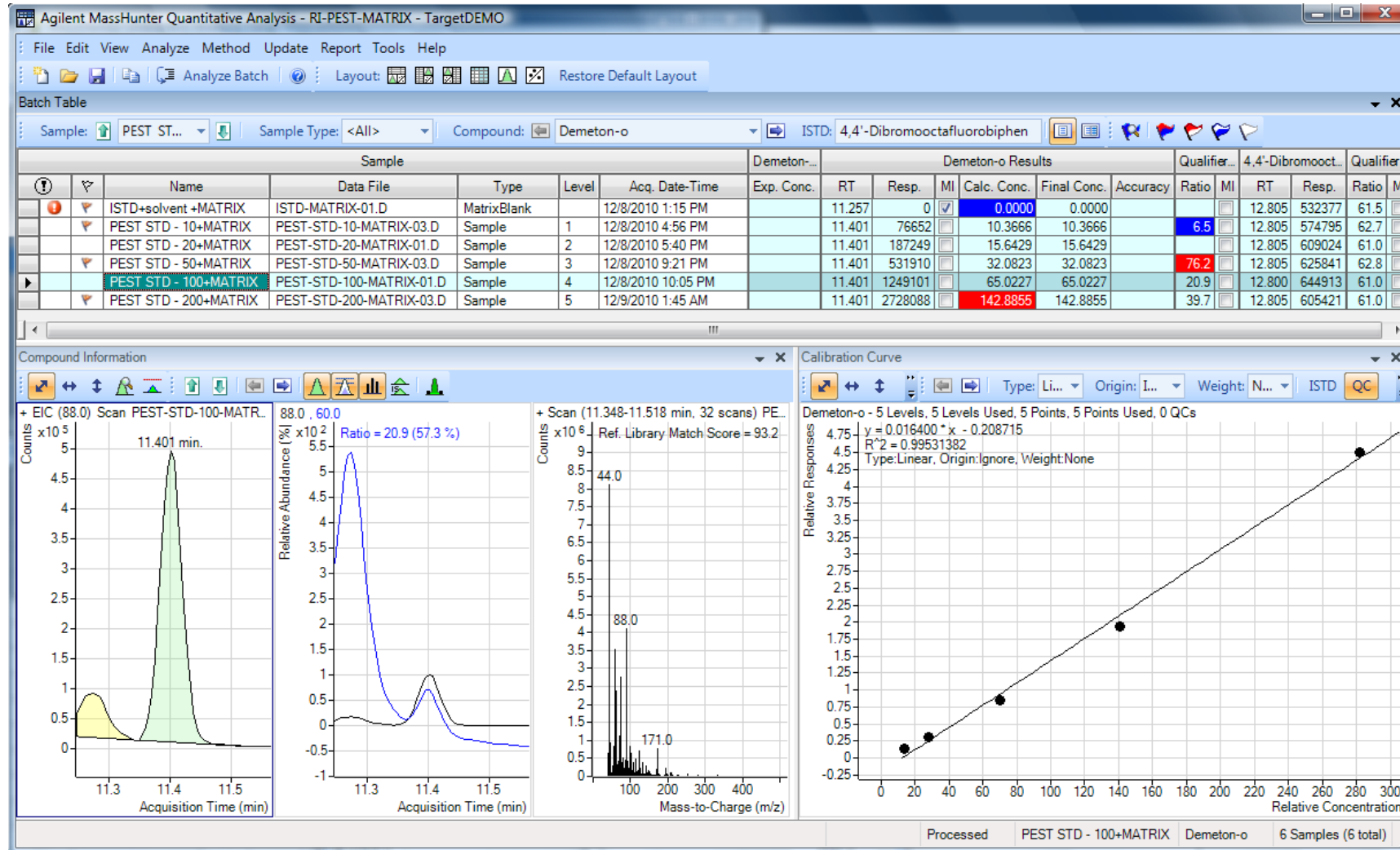


Tentatively Identified Compounds

- Process the batch of samples in Quantitative Analysis
- Start Unknowns Analysis
- Edit an Unknowns Analysis Method
 - Peak Detection
 - Library Search
 - Compound Identification
 - Target Match (semi quantitation)
 - Blank Subtraction
- Component Review
 - Review component and library spectrum
 - View ion peak shapes vs. component peak shape vs. TIC
 - Run Queries for custom review
- Report Generation
 - PDF Report Builder

Process Batch with Quantitative Analysis

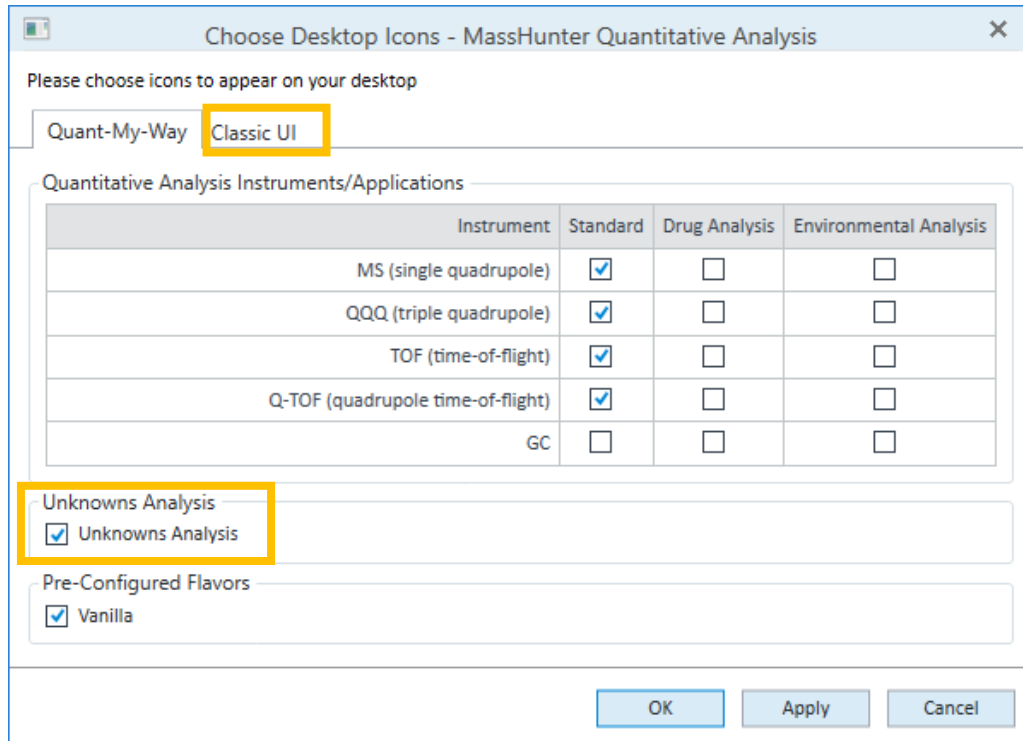
Information from the batch file (batch.bin) is used in Unknowns Analysis.



Unknowns Analysis Startup

Loaded as part of MassHunter Quantitative Analysis.

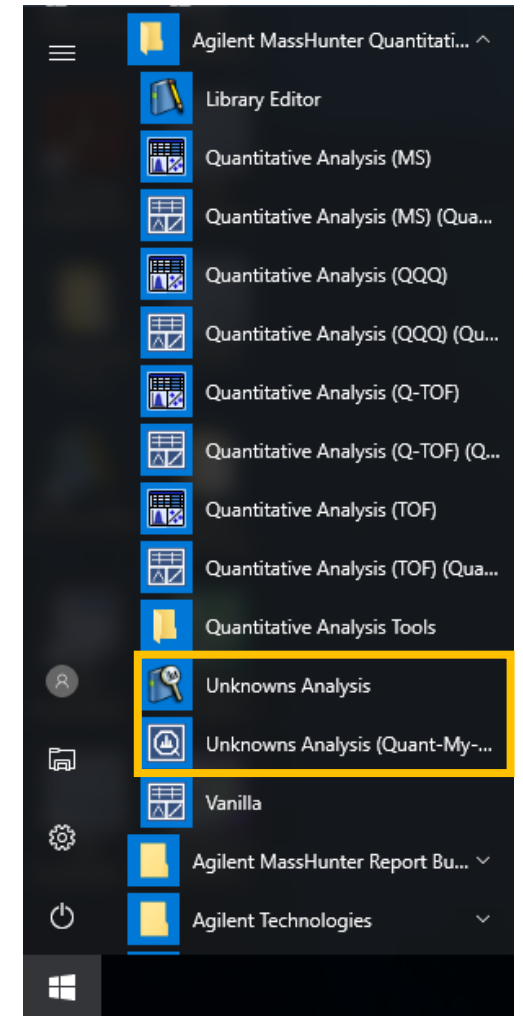
As of Quant B.09.00 it will not be displayed in the Start menu unless it is enabled using the Choose Desktop Icons utility.



Unknowns
Analysis



Unknowns
Analysis
(Quant-My-
-Way)

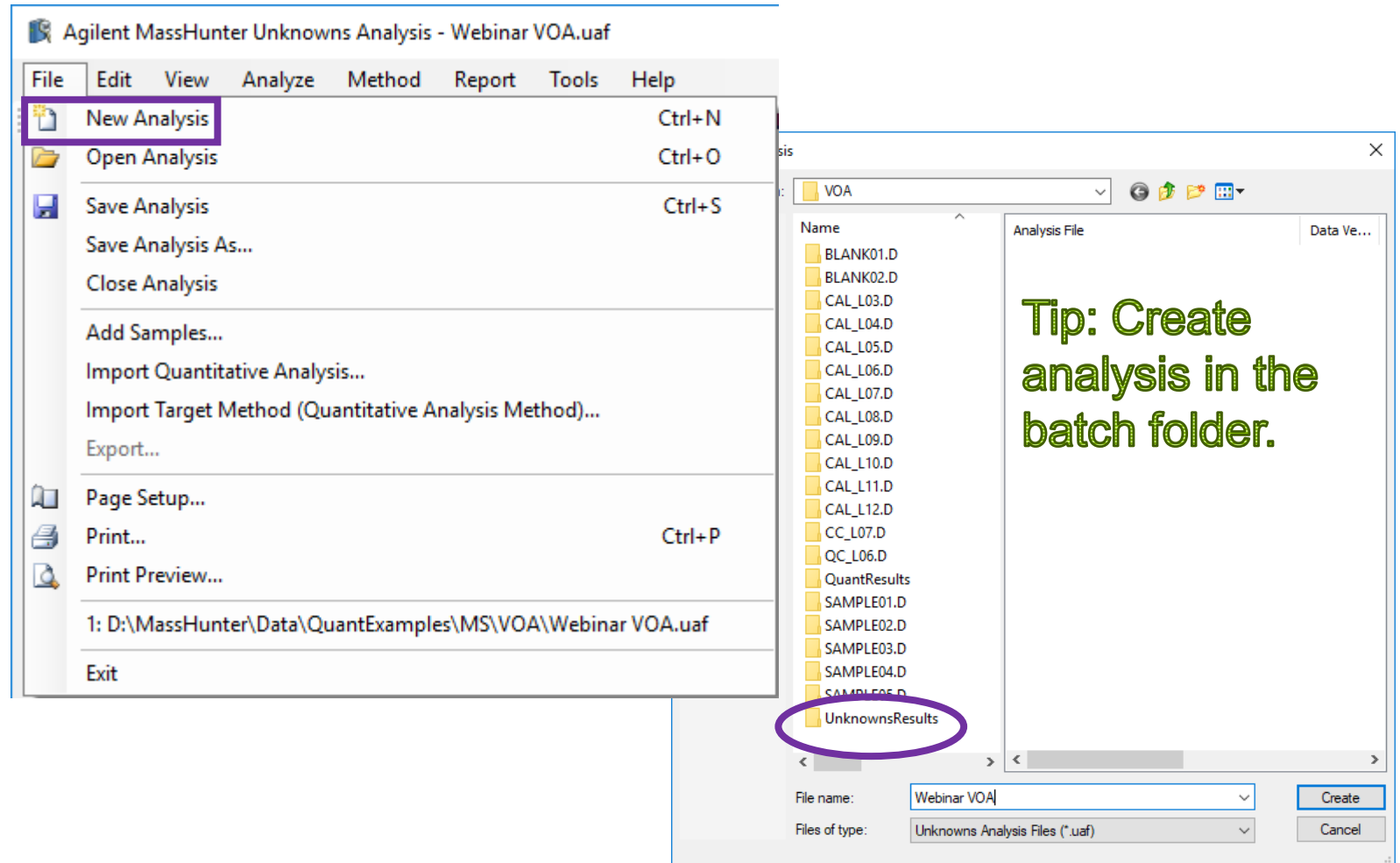


Setting Up an Analysis

New Analysis

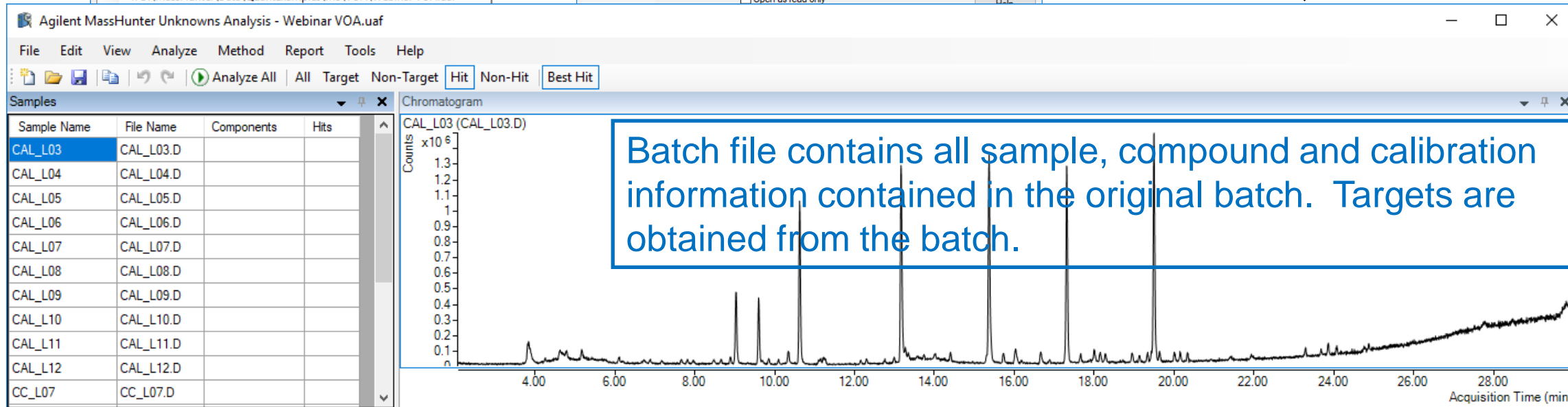
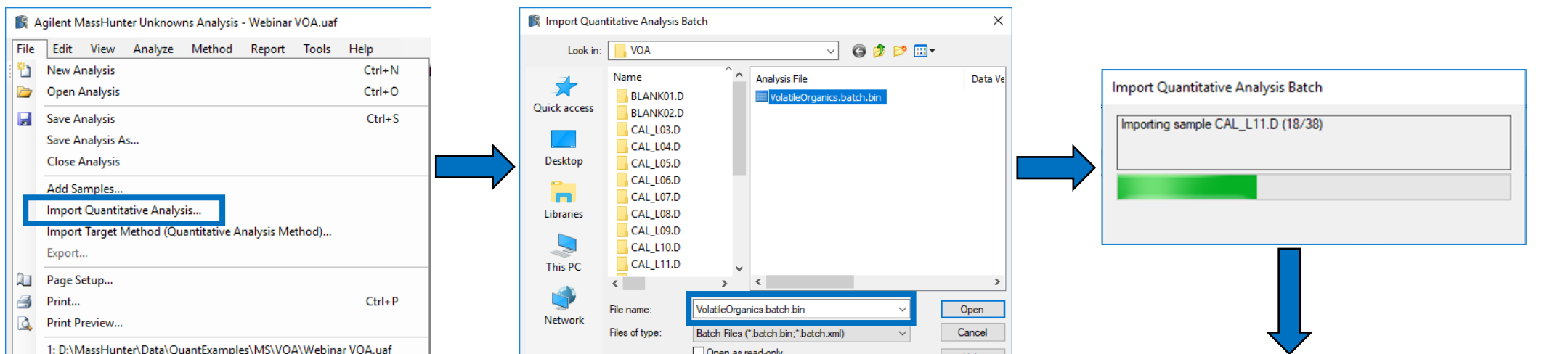
Unknowns Analysis file (.uaf) contains information on

- Quantitative Analysis batch (.batch.bin or .batch.xml)
- Unknowns Analysis Method (.uamethod.xml)
- Sample list (typically from Quantitative Analysis batch)
- Results
 - Components with any identity information.
- Component is the “compound” found in Unknowns Analysis.



Setting Up an Analysis

Import Quantitative Analysis Batch



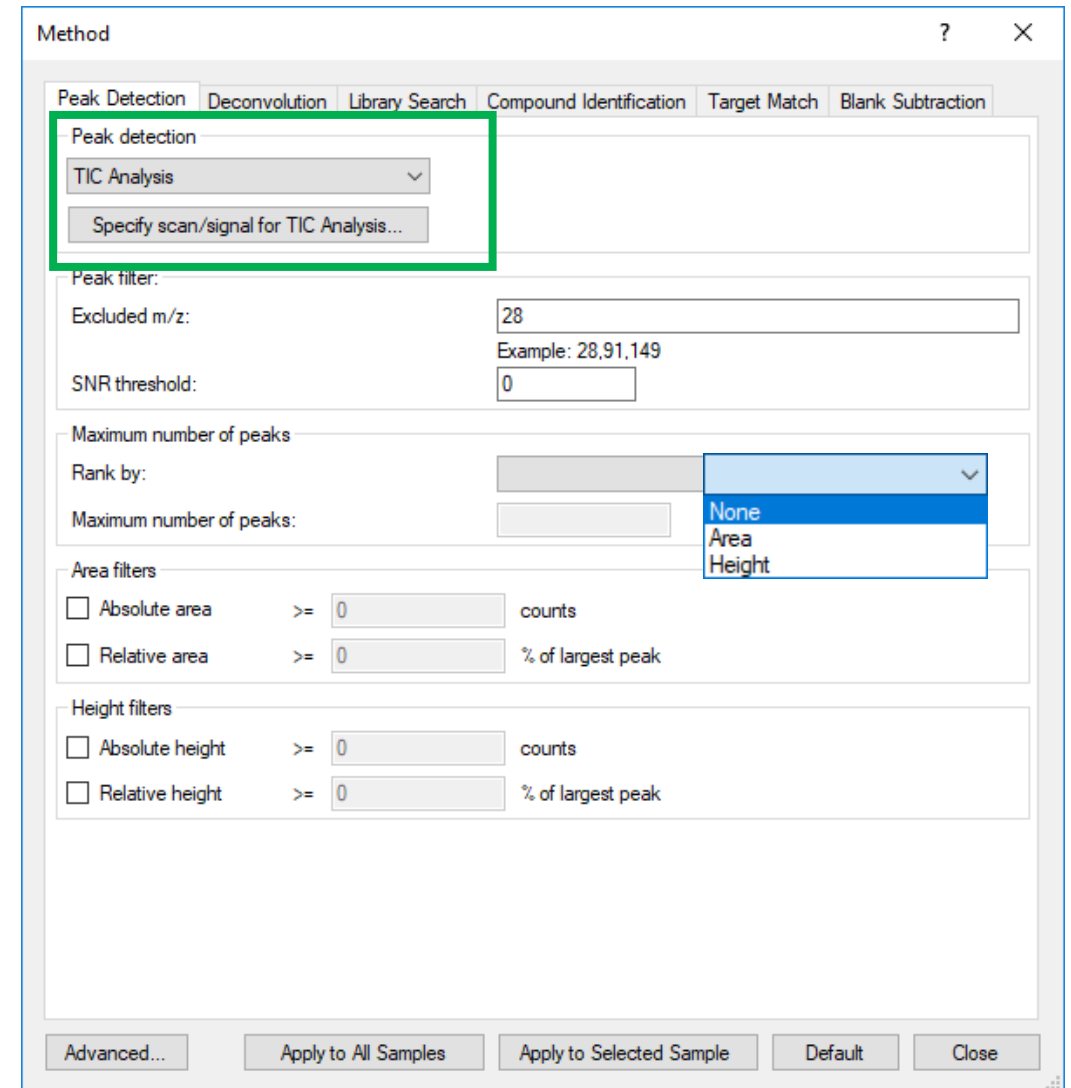
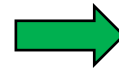
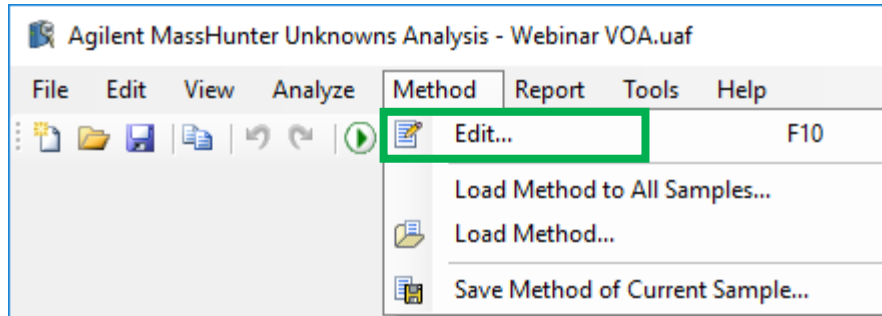
Unknowns Analysis



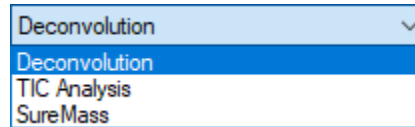
Time for a demo

Next up:
Unknowns Analysis Methods

Edit Method Peak Detection



Choose Peak Detection Parameters



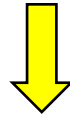
- TIC Analysis locates components by integration.
- Deconvolution locates components using parameters.
- SureMass applicable only to GC QTOF data.
 - Feature Extraction algorithm.
- Can also set Peak Filter parameters based on SNR, area or height.

Edit Method Peak Detection

Peak detection

TIC Analysis

Specify scan/signal for TIC Analysis...



Scan/Signal for TIC Analysis

MS

Signal

Signal type: All Scan Types

Signal instance:

Signal name:

OK Cancel

Scan/Signal for TIC Analysis

MS

Signal

Signal type: DAD

Signal instance: 1

Signal name: A

OK Cancel

Scan/Signal for TIC Analysis

MS

Signal

Signal type: FID

Signal instance: 1

Signal name: A

OK Cancel

MS

Can focus on various scan types.

UV

Can select various DAD signals.

GC

Can look at various GC signals.

Tip: TIC Analysis uses an integration algorithm.

Edit Method

Deconvolution

Method

Peak Detection Deconvolution Library Search Compound Identification Target Match Blank Subtraction

Resolution:

RT window size factor: 25,50,100,200

Extraction window:

Left m/z delta: 0.3

Right m/z delta: 0.7

m/z delta units: AMU

Use integer m/z values

Component shape:

Use base peak shape

Sharpness threshold: 25 %

Ion peaks:

Min # of ion peaks: 3

Max # of ion peak shapes to store: 10

Tip: Start with the default parameters and a small representative batch.

Advanced... Apply to All Samples Apply to Selected Sample Default Close

Deconvolution Parameters

- RT window size factor → Key parameter that controls the grouping of EIC peaks into components.
 - Larger value ⇒ fewer components.
 - Equivalent to RT window in AMDIS, but unitless.
- Extraction window → Allowable mass drift.
 - More applicable to high resolution data.
 - Low resolution data can use integer m/z values.
- Use integer m/z values → Evaluates both rounded (integer) and unrounded m/z values when extracting EICs.
 - Almost always doubles number of components.
- Component shape → Matches the EIC peak shape across the component.
- Ion Peaks → controls the number of mass spectral peaks (depends on data EI, CI, ESI, APCI, etc.).

Edit Method Library Search

The screenshot shows the 'Method' dialog box with the 'Library Search' tab selected. The 'Libraries' section contains two entries: 'D:\MassHunter\Library\NIST17.L' and 'D:\MassHunter\Data\QuantExamples\MS\VOA\VolatileOrganics.reflibrary.xml'. The 'Search criteria' section has 'Pre-search type' set to 'None' (with a dropdown menu open showing 'None', 'Normal', and 'Fast'), and 'Adjust S' checked. The 'Forward-Reverse Search' section has 'Pure Weight Factor' set to '0.7'. The 'Match factor' section has 'Use RT Match' unchecked, 'RT penalty function' set to 'Gaussian' (with 'RT range' at 6 and 'Standard deviation' at 6), and 'RT mismatch penalty' set to 'Multiplicative' (with 'Max RT penalty' at 20). The 'RT calibration file' field is empty. At the bottom, there are buttons for 'Advanced...', 'Apply to All Samples', 'Apply to Selected Sample', 'Default', and 'Close'.

Library Search Parameters

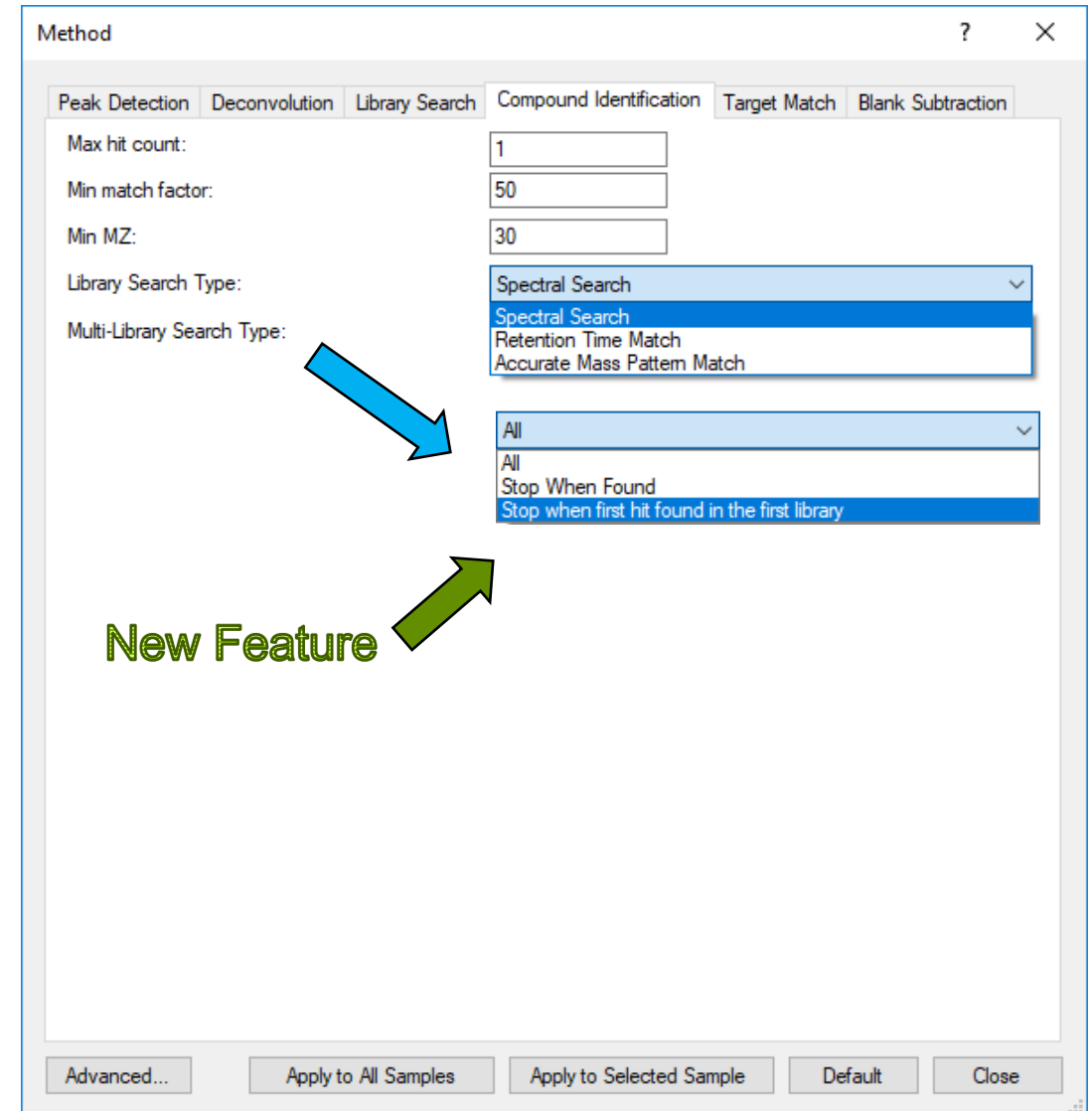
- Libraries → Multiple Libraries can be searched.
 - Search ordered can be changed.
 - Library can be opened and viewed in Library Editor.
- Search Criteria **Tip: Recommended → Normal**
 - None ⇒ no preliminary search.
 - Normal ⇒ Screens entire library ⇒ 50-100 times faster.
 - Fast ⇒ Uses an index for potential candidates. ⇒ 100-1000 faster
- Forward-Reverse-Search Pure Weight Factor **New Feature**
- Match Factor
 - Uses retention times from library or retention indices (RT calibration file needed).
- Can set different parameters for different libraries.
 - Including different Match factor parameters, RT and RI libraries

Edit Method

Compound Identification

Compound Identification Parameters

- Max hit count \Rightarrow number of library matches to save.
- Min match factor
- Min MZ \Rightarrow Important factor
 - Set to minimum scan ranges
 - avoids penalties for low masses that may be in library but not is spectrum.
- Library Search Type
 - Spectral Search used dot product search.
 - Retention Time Match \Rightarrow for GC, LC 2D data.
 - Accurate Mass Pattern Match \Rightarrow Isotopic pattern match for TOF only.
- Multi-Library Search Type
 - stop when first hit found in the first library.
 - put a user generated library first.



Edit Method

Target Match

Target Match Parameters

- Target requirements \Rightarrow Filters the quant method compound (target) list.
 - Final/target concentration > 0
 - Qualifier ions found
 - Qualifier ratios in specified ratio
- Hit ion match criteria \Rightarrow Filters the components list.
 - Target ion > 0
 - Target ion found and/or Qualifier ion(s) found.
 - Qualifier ions in specified ratios.
- Hit RT match criteria \Rightarrow component within Quant RT window
- Additional target hit match
 - must be present in quant method and match library.

The screenshot shows the 'Method' dialog box with the 'Target Match' tab selected. The dialog has a title bar with a question mark and a close button. Below the title bar are several tabs: 'Peak Detection', 'Deconvolution', 'Library Search', 'Compound Identification', 'Target Match', and 'Blank Subtraction'. The 'Target Match' tab contains the following sections:

- Target requirements:**
 - Final concentration
 - Target response
 - Qualifier ion(s)
 - Qualifier ion ratios
- Hit ion match criteria:**
 - Target ion
 - Qualifier ion(s)
 - Qualifier ion ratios
- Hit RT match criteria:**
 - Within target RT window
- Additional target hit match:**
 - Use compound name
 - Use CAS#
- Estimation response factor:**
 - Estimation:
 - Manual response factor:

At the bottom of the dialog are five buttons: 'Advanced...', 'Apply to All Samples', 'Apply to Selected Sample', 'Default', and 'Close'.

Edit Method

Target Match –Semi Quantitation

Target Match Parameters

- Estimation response factor \Rightarrow Method of semi quantitation.
 - Based on response factors from Quantitative Analysis.
 - Calculates the estimated concentration based on value chosen.
 - A manual response factor can be chosen for semi quantitation of the components.

Method

Peak Detection Deconvolution Library Search Compound Identification Target Match Blank Subtraction

Target requirements:

Final concentration Qualifier ion(s)

Target response Qualifier ion ratios

Hit ion match criteria:

Target ion Qualifier ion(s)

Qualifier ion ratios

Hit RT match criteria:

Within target RT window

Additional target hit match:

Use compound name Use CAS#

Estimation response factor:

Estimation:

No estimation

Average RF of all targets

Average RF of closest target

Average RF of all ISTDs

RF of closest target's ISTD

RF of closest ISTD

Relative ISTD Estimation

Manual RF

No estimation

Advanced... Apply to All Samples Apply to Selected Sample Default Close

Edit Method

Blank Subtraction

Blank Subtraction Parameters

- Perform Blank Subtraction
 - assumes a blank is present in sample list
 - annotates blank subtracted from sample
- Retention Time Window => allows for RT variation between blank and sample
 - No retention time window active => sample and blank must have 'same' retention time to be subtracted.
 - FWHM when checked the blank peak must be within the specified multiple of the sample peaks Full Width at Half Maximum.
 - Minutes when active, blank peak must be specified minutes to the sample.
- Peak Threshold
 - Blank peaks will not be subtracted from sample peaks unless the Component Area/Estimated Concentration exceeds the specified percentage of the samples.

Method

Peak Detection Deconvolution Library Search Compound Identification Target Match Blank Subtraction

Perform Blank Subtraction

Retention Time Window

No retention time window

FWHM

5 times

Minutes

0.05 min.

3 – 6 seconds

Peak Threshold

Component Area

Sample <= 100 % of Blank
(Example: 100)

Component Area
None
Component Area
Estimated Concentration

Advanced... Apply to All Samples Apply to Selected Sample Default Close

Edit Method

Advanced Parameters

Method

Deconvolution Library Search Compound Identification Target Match Blank Subtraction Auxiliary

Sample	File Name	Sample Group	Algorithm	Integrator	EIC Peak Threshold	EIC SNR Threshold	Excluded MZs	Left MZ Delta	Right MZ Delta	MZ Delta Units	Window Size Factor	Use Integer MZ Values	Min # of Peaks	Max # of ion peak shapes to store
CAL_L03	CAL_L03.D		TIC Analysis	Agile 2	0.00	0.00	28	0.3	0.7	AMU	25.0	<input checked="" type="checkbox"/>	3	10
CAL_L03	CAL_L03.D		Deconvolution TIC Analysis	Agile 2	0.00	0.00	28	0.3	0.7	AMU Percent	50.0	<input checked="" type="checkbox"/>	3	10
CAL_L03	CAL_L03.D		Target Deconvolu SureMass	Agile 2	0.00	0.00	28	0.3	0.7	PPM AMU	100.0	<input checked="" type="checkbox"/>	3	10
CAL_L03	CAL_L03.D		TIC Analysis	Agile 2	0.00	0.00	28	0.3	0.7	AMU	200.0	<input checked="" type="checkbox"/>	3	10
CAL_L04	CAL_L04.D		TIC Analysis	Agile 2	0.00	0.00	28	0.3	0.7	AMU	25.0	<input checked="" type="checkbox"/>	3	10
CAL_L04	CAL_L04.D		TIC Analysis	Agile 2	0.00	0.00	28	0.3	0.7	AMU	50.0	<input checked="" type="checkbox"/>	3	10
CAL_L04	CAL_L04.D		TIC Analysis	Agile 2	0.00	0.00	28	0.3	0.7	AMU	100.0	<input checked="" type="checkbox"/>	3	10
CAL_L04	CAL_L04.D		TIC Analysis	Agile 2	0.00	0.00	28	0.3	0.7	AMU	200.0	<input checked="" type="checkbox"/>	3	10
CAL_L05	CAL_L05.D		TIC Analysis	Agile 2	0.00	0.00	28	0.3	0.7	AMU	25.0	<input checked="" type="checkbox"/>	3	10
CAL_L05	CAL_L05.D		TIC Analysis	Agile 2	0.00	0.00	28	0.3	0.7	AMU	50.0	<input checked="" type="checkbox"/>	3	10

Standard... Apply Default OK Cancel

Method

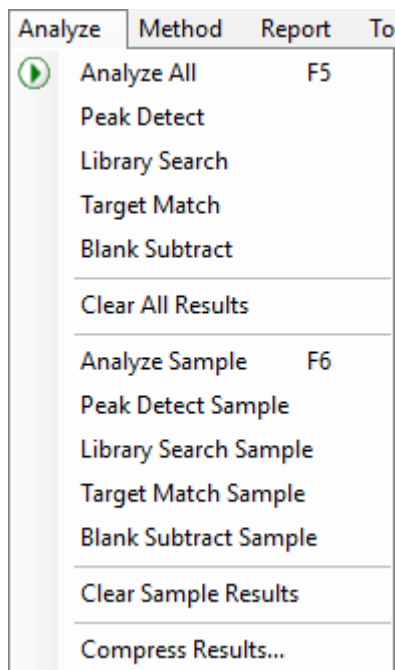
Deconvolution Library Search Compound Identification Target Match Blank Subtraction Auxiliary

Sample Name	File Name	Sample Group	Library File	Library Path	Library Type	Pre-search Enabled	Pre-search Type	NIST Compatibility	Pure Weight	Search	RT Calibration	RT Match Factor Type	RT Max Penalty
CAL_L03	CAL_L03.D		VolatileOrg...fiibrary.xml	D:\MassHunter\Data\QuantExempl...VOA	XML	<input checked="" type="checkbox"/>	Normal	<input checked="" type="checkbox"/>	0.7000	2		None	20.0000
CAL_L03	CAL_L03.D		NIST17.L	D:\MassHunter\Library	XML	<input type="checkbox"/>		<input checked="" type="checkbox"/>	0.7000	0		None	20.0000
CAL_L04	CAL_L04.D		VolatileOrg...fiibrary.xml	D:\MassHunter\Data\QuantExempl...VOA	Binary	<input checked="" type="checkbox"/>	Normal	<input checked="" type="checkbox"/>	0.7000	2		None	20.0000
CAL_L04	CAL_L04.D		NIST17.L	D:\MassHunter\Library	Compressed PCDL	<input type="checkbox"/>	Normal	<input checked="" type="checkbox"/>	0.7000	0		None	20.0000
CAL_L05	CAL_L05.D		VolatileOrg...fiibrary.xml	D:\MassHunter\Data\QuantExempl...VOA	XML	<input checked="" type="checkbox"/>		<input checked="" type="checkbox"/>	0.7000	2		None	20.0000
CAL_L05	CAL_L05.D		NIST17.L	D:\MassHunter\Library	Compressed	<input type="checkbox"/>	Normal	<input checked="" type="checkbox"/>	0.7000	0		None	20.0000
CAL_L06	CAL_L06.D		VolatileOrg...fiibrary.xml	D:\MassHunter\Data\QuantExempl...VOA	XML	<input checked="" type="checkbox"/>	Fast	<input checked="" type="checkbox"/>	0.7000	2		Gaussian Trapezoidal	20.0000
CAL_L06	CAL_L06.D		NIST17.L	D:\MassHunter\Library	Compressed	<input type="checkbox"/>		<input checked="" type="checkbox"/>	0.7000	0		None	20.0000
CAL_L07	CAL_L07.D		VolatileOrg...fiibrary.xml	D:\MassHunter\Data\QuantExempl...VOA	XML	<input checked="" type="checkbox"/>	Normal	<input checked="" type="checkbox"/>	0.7000	2		None	20.0000
CAL_L07	CAL_L07.D		NIST17.L	D:\MassHunter\Library	Compressed	<input type="checkbox"/>		<input checked="" type="checkbox"/>	0.7000	0		None	20.0000

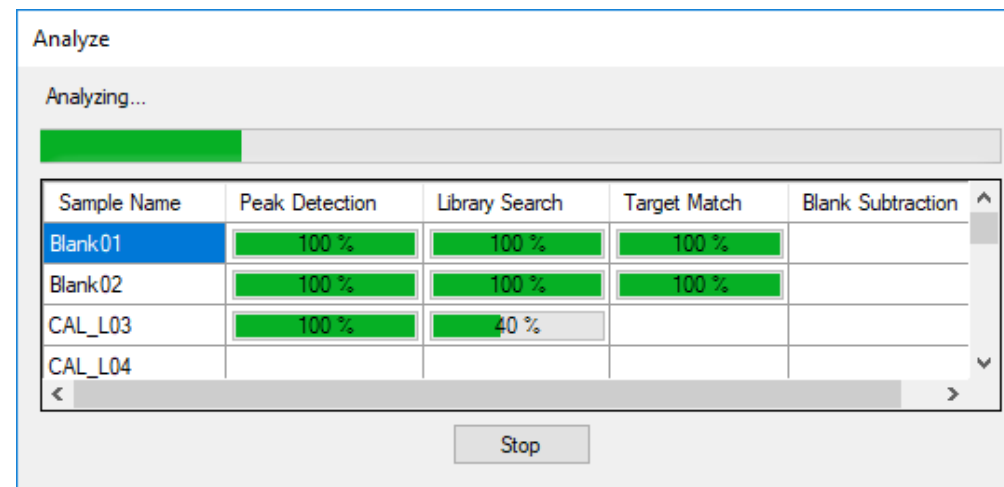
Standard... Apply Default OK Cancel

Analyze

Analyze All

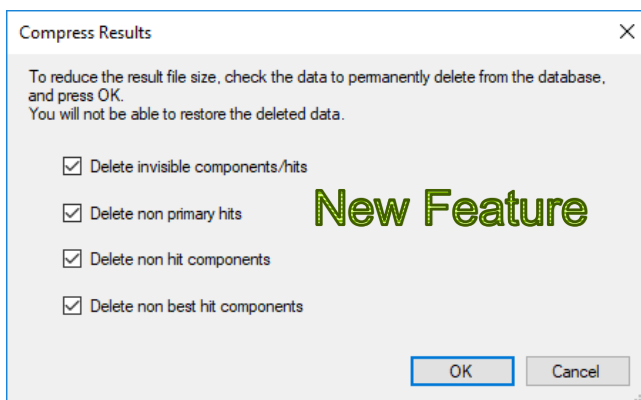


Clicking **Analyze All** causes each sample to be fully processed. This step can take several minutes.

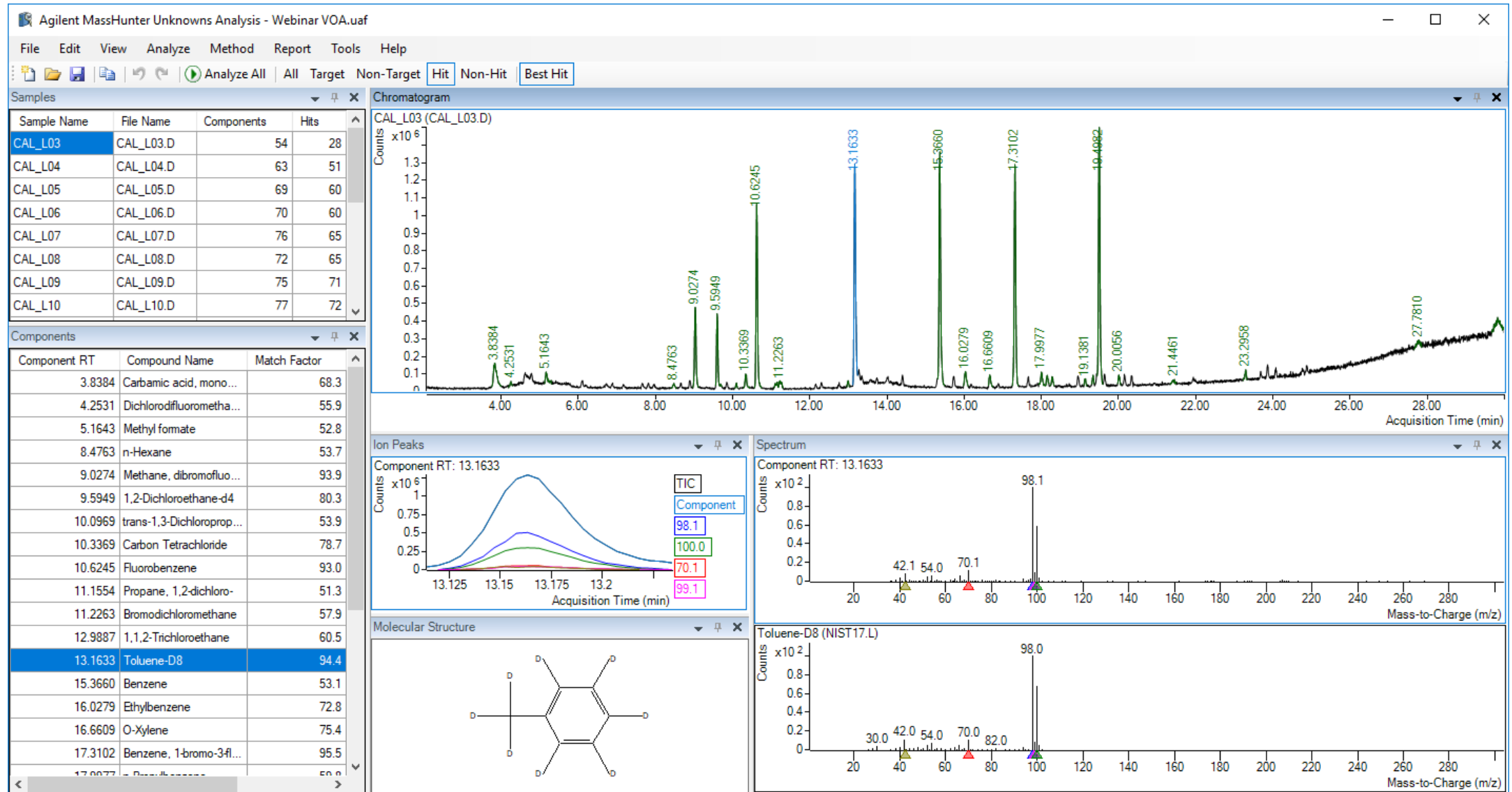


Analysis Messages		
Type	Target	Message
i	Sample Blank01	Deconvolution process has been already performed before. Skipping deconvolution process.
i	Sample Blank02	Deconvolution process has been already performed before. Skipping deconvolution process.
i	Sample CAL_L03	Deconvolution process has been already performed before. Skipping deconvolution process.
i	Sample CAL_L04	Deconvolution process has been already performed before. Skipping deconvolution process.
i	Sample Blank01	This sample is one of the blank sample types. Skipping blank subtraction process.
i	Sample Blank02	This sample is one of the blank sample types. Skipping blank subtraction process.

Analysis Messages provide guidance with information and errors.



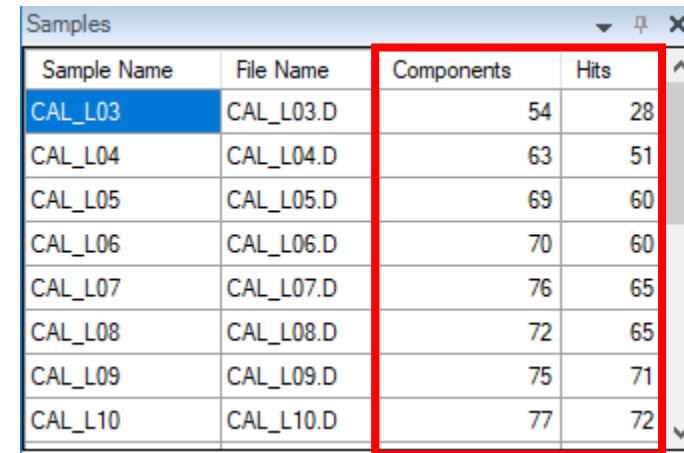
Component Review



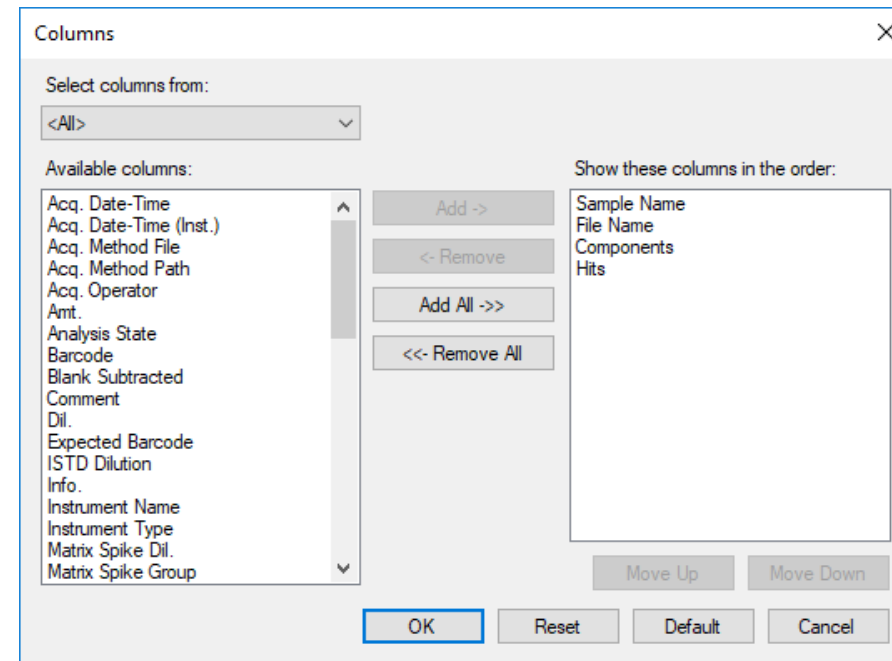
Component Review

Sample Table

- Sample table gives summary information on number of components found and number of library matches.
- Used to navigate between samples.
- Samples can be removed or added as needed.
- Additional sample info accessible by Add/Remove Columns.
- Numerous parameters are available in the tables.



Sample Name	File Name	Components	Hits
CAL_L03	CAL_L03.D	54	28
CAL_L04	CAL_L04.D	63	51
CAL_L05	CAL_L05.D	69	60
CAL_L06	CAL_L06.D	70	60
CAL_L07	CAL_L07.D	76	65
CAL_L08	CAL_L08.D	72	65
CAL_L09	CAL_L09.D	75	71
CAL_L10	CAL_L10.D	77	72



Columns

Select columns from:
<All>

Available columns:

- Acq. Date-Time
- Acq. Date-Time (Inst.)
- Acq. Method File
- Acq. Method Path
- Acq. Operator
- Amt.
- Analysis State
- Barcode
- Blank Subtracted
- Comment
- Dil.
- Expected Barcode
- ISTD Dilution
- Info.
- Instrument Name
- Instrument Type
- Matrix Spike Dil.
- Matrix Spike Group

Show these columns in the order:

- Sample Name
- File Name
- Components
- Hits

Buttons: Add ->, <- Remove, Add All ->>, <<- Remove All, Move Up, Move Down, OK, Reset, Default, Cancel

Component Review

Components Table

- Displays components and associated data.
- Extensive number of data columns.

Sample Name	Component RT	Compound Name	Formula	Match Factor	Best Hit	CAS#	Estimated Conc.	Base Peak Area	Area %	Area % Max.	Algorithm
CAL_L08	3.8275	(2-Aziridinylethyl)amine	C4H10N2	50.5	<input checked="" type="checkbox"/>	4025-37-0	9.003	554638.2	0.259	4.98	TIC Analysis
CAL_L08	4.2476	Dichlorodifluoromethane	CCl2F2	94.6	<input checked="" type="checkbox"/>	75-71-8	24.39	965394.4	0.700	13.48	TIC Analysis
CAL_L08	4.4931	Chloromethane	CH3Cl	73.7	<input checked="" type="checkbox"/>	74-87-3					
CAL_L08	4.7823	1-Propene, 2-methyl-	C4H8	89.4	<input checked="" type="checkbox"/>	115-11-7					
CAL_L08	5.2352	Methane, bromo-	CH3Br	88.4	<input checked="" type="checkbox"/>	74-83-9					
CAL_L08	5.4044	Ethyl Chloride	C2H5Cl	81.7	<input checked="" type="checkbox"/>	75-00-3					
CAL_L08	6.0973	Trichloromonofluoromethane	CCl3F	95.0	<input checked="" type="checkbox"/>	75-69-4					

Add/Remove Columns...

Copy

Delete Hits Del

Restore All Hits

Export...

→

<All>

<All>

Sample

Component

Model Peak Ion

Base Peak

Library Hit

Deconvolution Method

Library Search Method

Target Compound (from Quant)

Target Peak (from Quant)

→

Columns

Select columns from:

<All>

Available columns:

- Accurate Mass Tolerance
- Acq. Date-Time
- Acq. Date-Time (Inst.)
- Acq. Method File
- Acq. Method Path
- Acq. Operator
- Amt.
- Analysis State
- Area Filter Absolute
- Area Filter Relative
- Barcode
- Base Peak Custom Calc.
- Base Peak Deconvoluted Area
- Base Peak Deconvoluted Height
- Base Peak End X
- Base Peak FWHM
- Base Peak Height
- Base Peak MZ

Show these columns in the order:

- Sample Name
- Component RT
- Compound Name
- Formula
- Match Factor
- Best Hit
- CAS#
- Estimated Conc.
- Base Peak Area
- Area %
- Area % Max.
- Algorithm

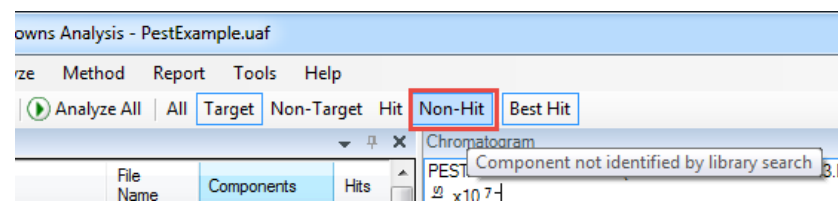
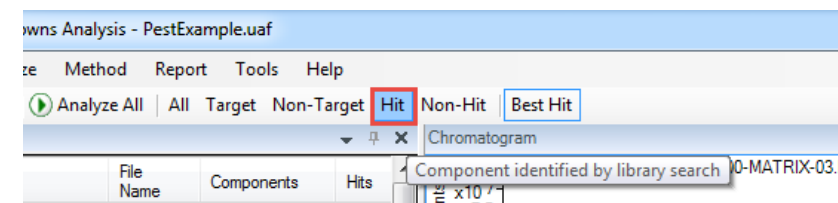
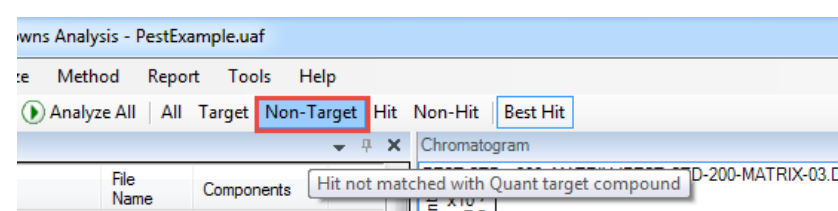
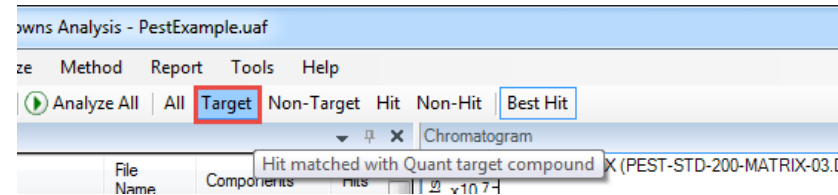
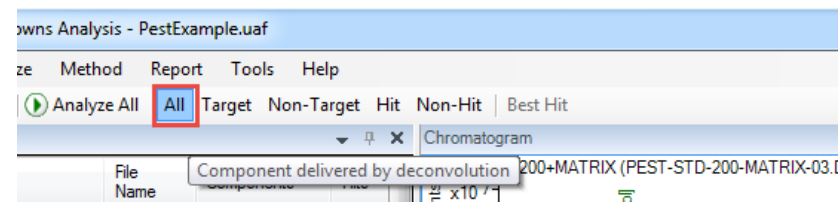
Move Up Move Down

OK Reset Default Cancel

Component Review

Filtering of the Components Table

- All – All components are displayed.
- Target – Components that match a library entry and match Quant Batch compounds.
- Non-Target – Components that match a library entry, but don't match Quant batch compounds.
- Hits – Components that have a library match.
- Non-Hit – Components that don't match any library entry within the defined parameters.



Component Review

Best Hit

When **Best Hit** is **disabled** all library hits are displayed.

Agilent MassHunter Unknowns Analysis - Webinar VOA 2.uaf

File Edit View Analyze Method Report Tools Help

Analyze All | All Target Non-Target **Hit** Non-Hit Best Hit

Components

Sample Name	Component RT	Compound Name	Match Factor	Best Hit	CAS#
CAL_L08	7.1777	Carbon disulfide	89.7	<input checked="" type="checkbox"/>	75-15-0
CAL_L08	7.1777	Arsine	60.7	<input type="checkbox"/>	7784-42-1
CAL_L08	7.1777	4,4'-Diisothiocyanatostilbene...	61.1	<input type="checkbox"/>	53005-05-3
CAL_L08	7.1777	Carbon disulfide	89.7	<input type="checkbox"/>	75-15-0
CAL_L08	7.1777	Glycine, N-(dithiocarboxy)-N-...	63.4	<input type="checkbox"/>	40520-03-4
CAL_L08	7.6578	Ethylene, 1,2-dichloro-, (Z)-	96.4	<input checked="" type="checkbox"/>	156-59-2
CAL_L08	7.6578	Ethylene, 1,2-dichloro-, (Z)-	95.4	<input type="checkbox"/>	156-59-2
CAL_L08	7.6578	Ethylene, 1,2-dichloro-, (E)-	95.7	<input type="checkbox"/>	156-60-5
CAL_L08	7.6578	Ethylene, 1,2-dichloro-, (E)-	96.1	<input type="checkbox"/>	156-60-5
CAL_L08	7.6578	1,2-Dichloroethylene	95.5	<input type="checkbox"/>	540-59-0

When **Best Hit** is **enabled** only the highest Match Factor hit is displayed.

Agilent MassHunter Unknowns Analysis - Webinar VOA 2.uaf

File Edit View Analyze Method Report Tools Help

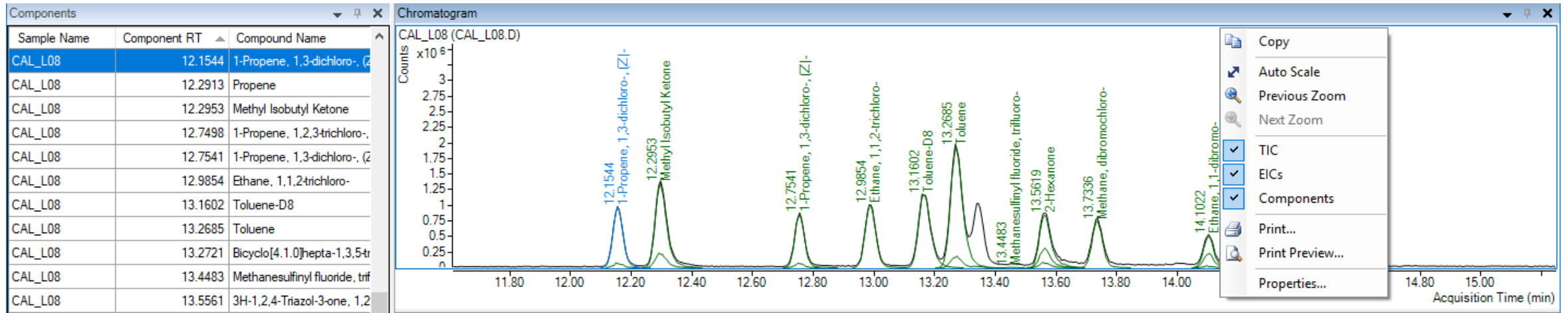
Analyze All | All Target Non-Target **Hit** Non-Hit **Best Hit**

Components

Sample Name	Component RT	Compound Name	Match Factor	Best Hit	CAS#
CAL_L08	7.1777	Carbon disulfide	89.7	<input checked="" type="checkbox"/>	75-15-0
CAL_L08	7.6578	Ethylene, 1,2-dichloro-, (Z)-	96.4	<input checked="" type="checkbox"/>	156-59-2
CAL_L08	7.8052	Propane, 2-methoxy-2-methyl-	92.7	<input checked="" type="checkbox"/>	1634-04-4
CAL_L08	7.9579	Ethane, 1,1-dichloro-	94.8	<input checked="" type="checkbox"/>	75-34-3
CAL_L08	8.0616	Acetic acid ethenyl ester	80.5	<input checked="" type="checkbox"/>	108-05-4
CAL_L08	8.4326	2-Butanone	83.8	<input checked="" type="checkbox"/>	78-93-3
CAL_L08	8.6509	Ethene, 1,1-dichloro-	95.2	<input checked="" type="checkbox"/>	75-35-4
CAL_L08	8.8910	Trichloromethane	94.8	<input checked="" type="checkbox"/>	67-66-3
CAL_L08	9.0056	Propane, 2,2-dichloro-	78.7	<input checked="" type="checkbox"/>	594-20-7
CAL_L08	9.3275	Tetrahydrofuran	76.9	<input checked="" type="checkbox"/>	109-99-9

Tip: Must have more than 1 Max. hit count.

Component Review Chromatogram

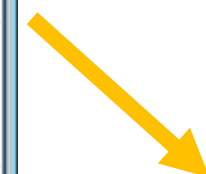
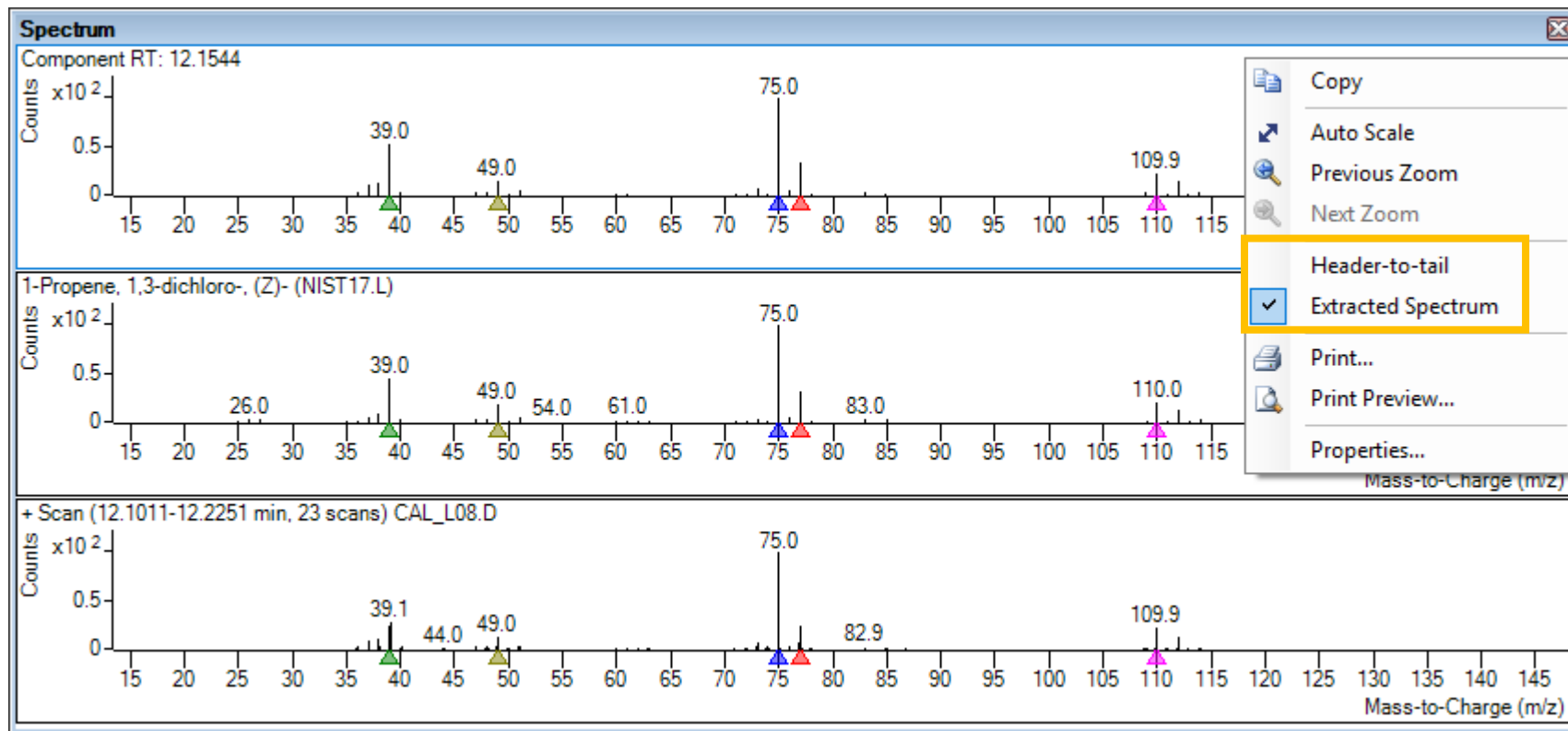


- Various displays of the Chromatogram window are available.
- TIC displayed in **Black**.
- All non-selected ions (EIC) displayed in **Green**.
- Chromatogram displays selected component(s) in **Blue**.
- Clicking in the Chromatogram display selects the nearest peak and selects it in Components table.

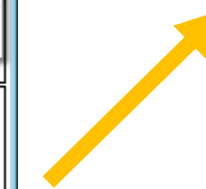
Spectrum Views

Extracted Spectrum

Allows comparison of the deconvoluted spectrum (top) to the library spectrum (middle) and the averaged spectrum (bottom).

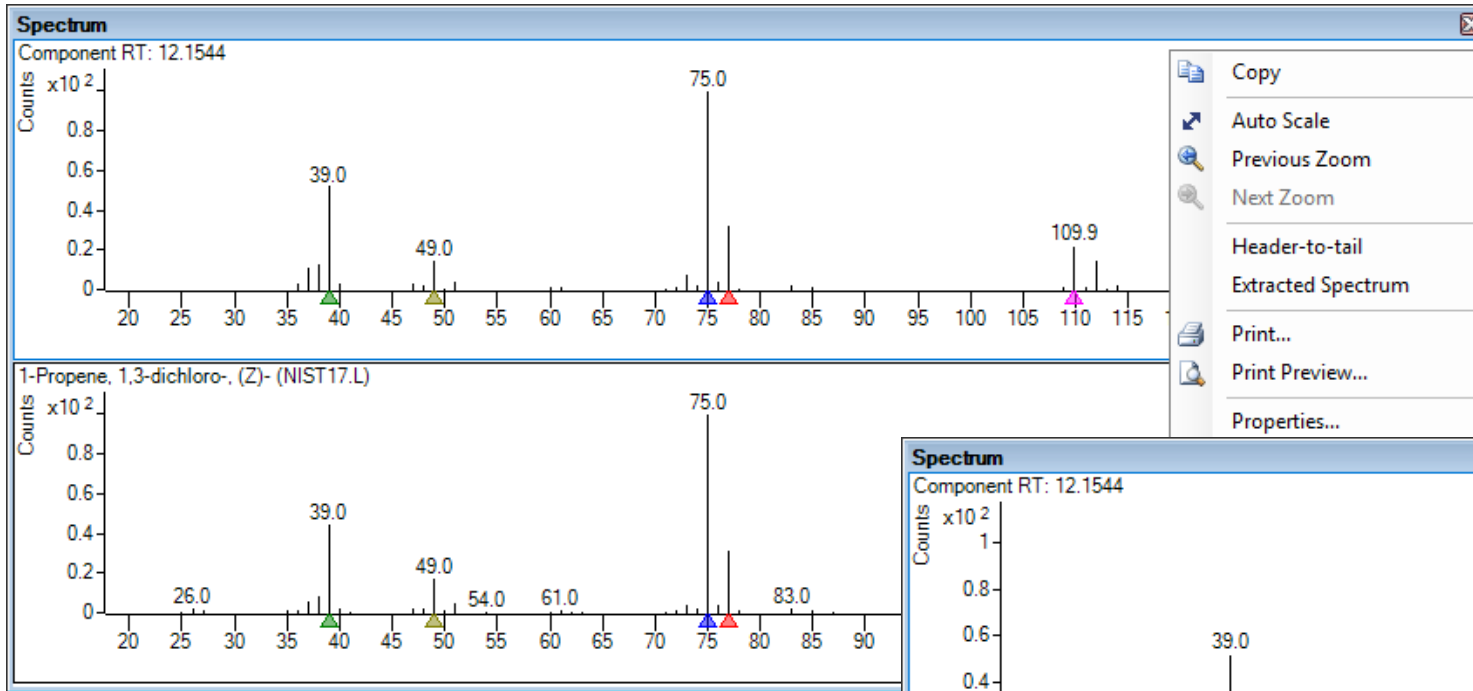


Purity



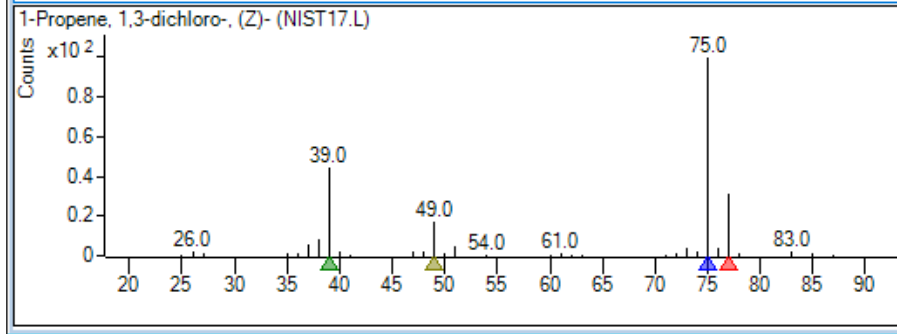
Spectrum Views

Head-To-Tail

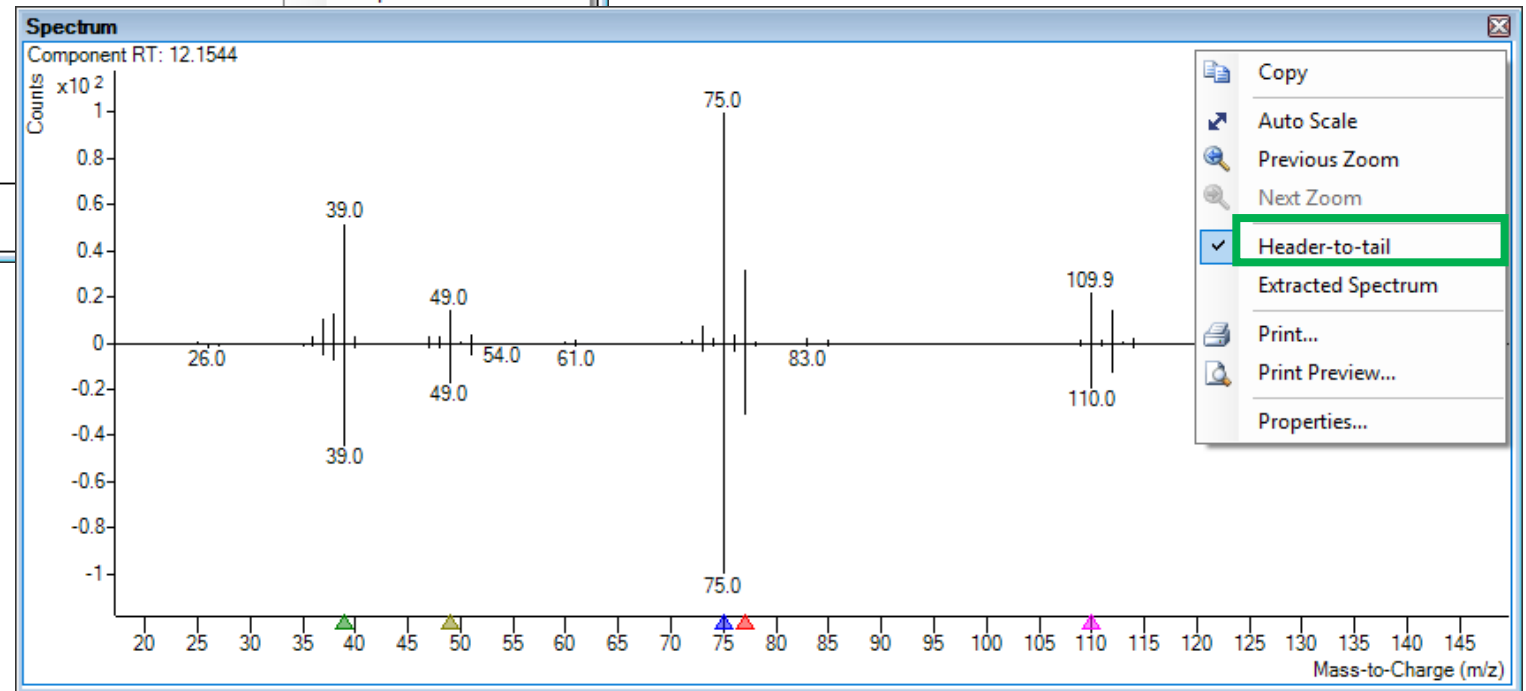


Right click to view Head-to-Tail.

Head to Tail View



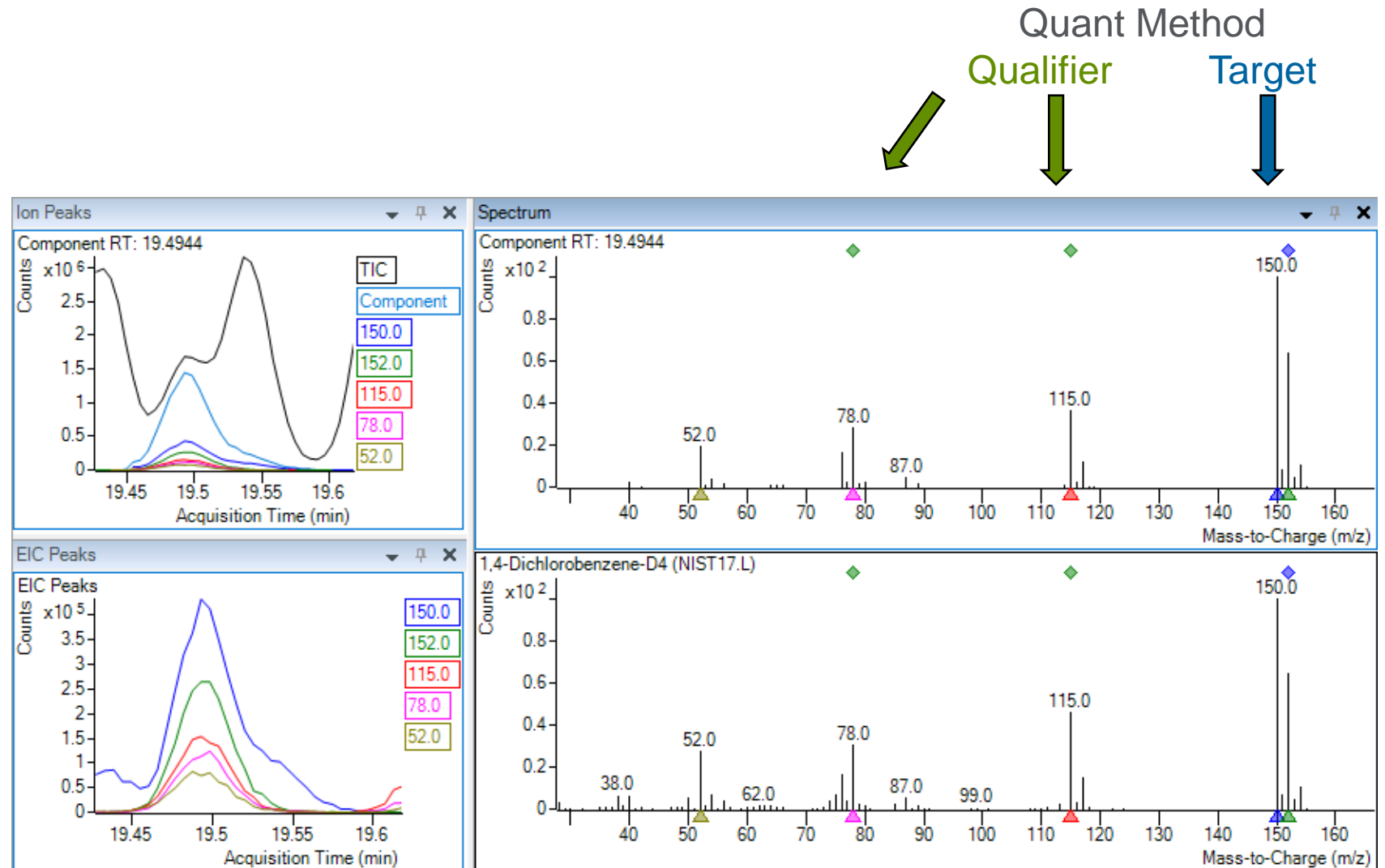
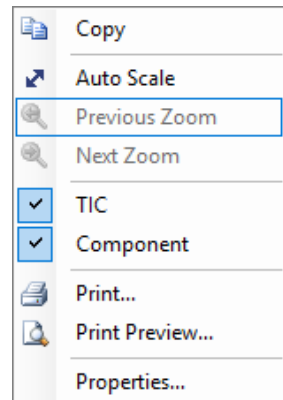
Head to Head View



Component Review

Ion Peaks and EIC Peaks

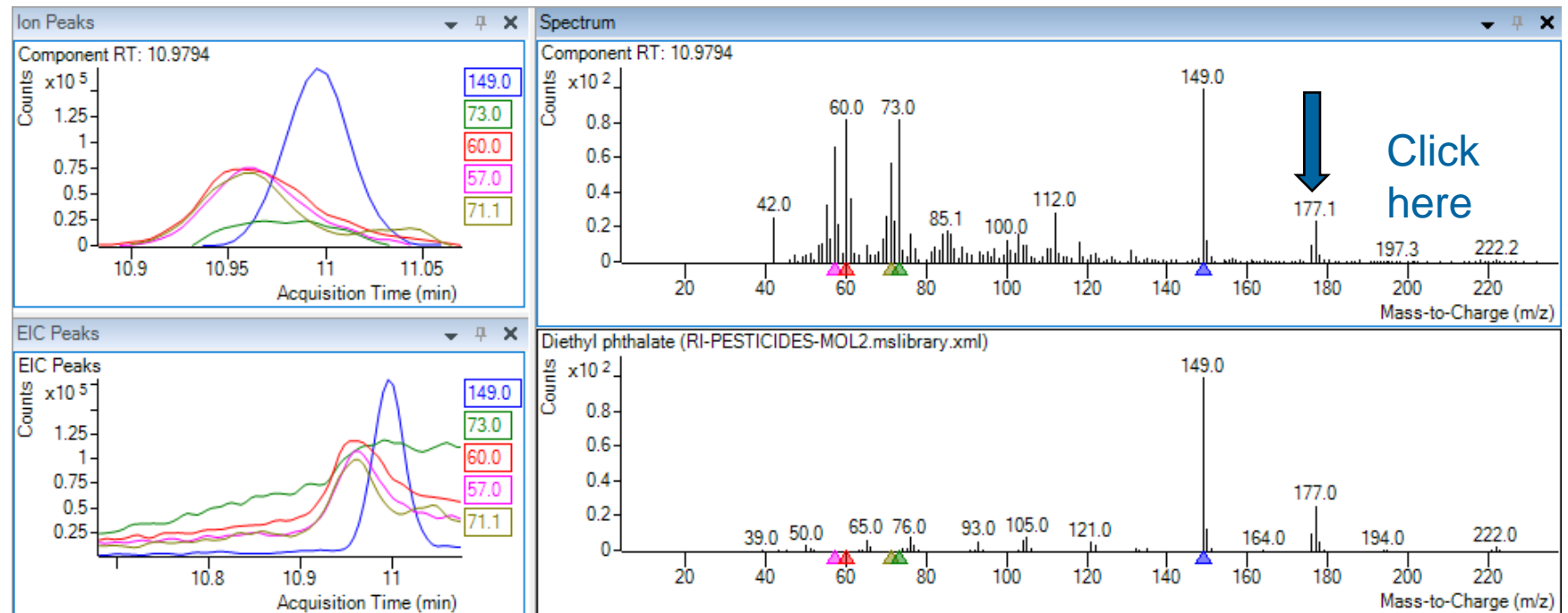
- Activated from **View > EIC Peaks**.
- Useful for visualizing co-eluting peaks.
- Click on ion in Spectrum to make it add/remove in Ion Peaks or EIC Peaks.
- Use menu to add TIC & Component.



Component Review

Ion Peaks and EIC Peaks

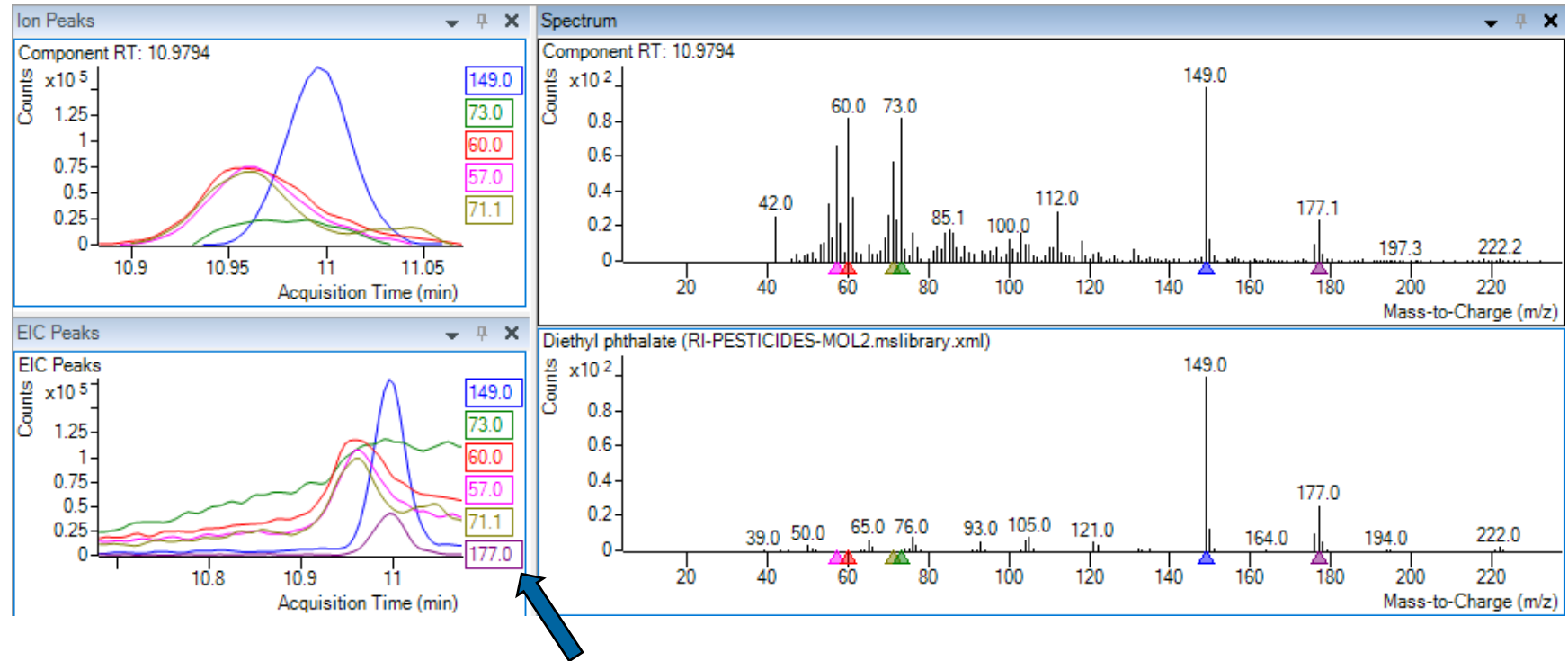
- Adding another Extracted Ion Chromatogram (EIC)
- Click on the peak in either the component or library window.
- Best done without head-to-tail.
- Is the 177.0 mass part of the first component or the second component?



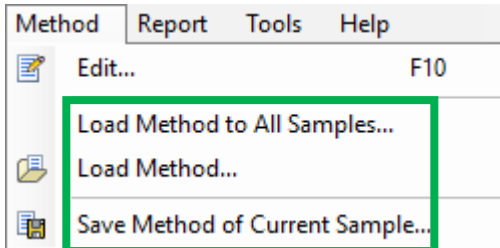
Component Review

Ion Peaks and EIC Peaks

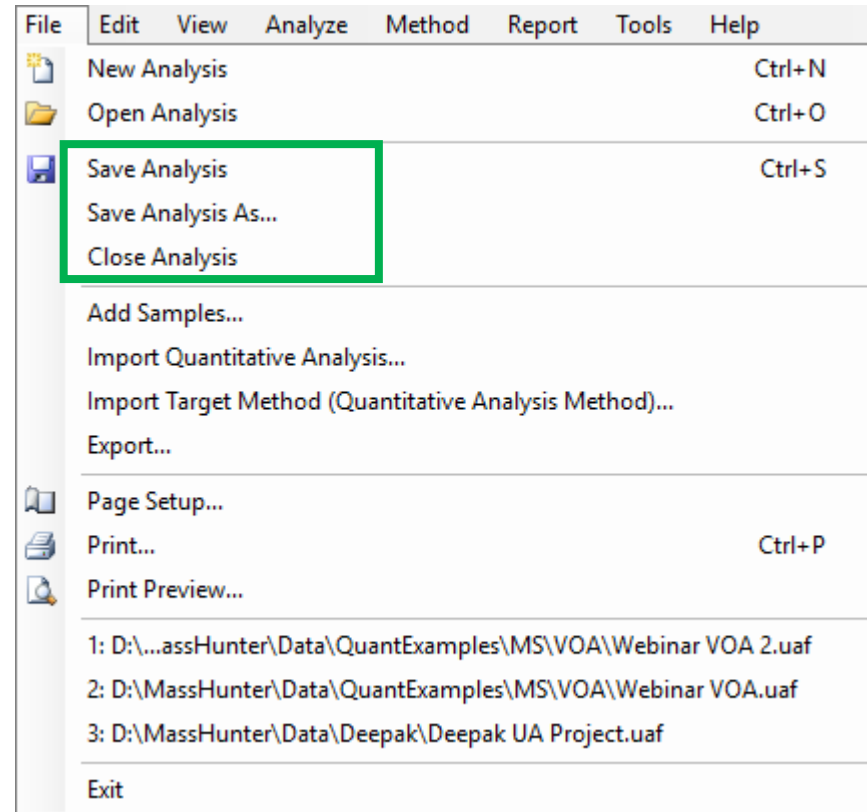
- EIC for mass is displayed in the window.
- Is the 177.0 mass part of the first component or the second component?



Unknowns Analysis Method



- Method can be saved and loaded from .M folder (unified method) or as uamethod.xml file.
- Previously stored methods can be used multiple times.



- Method id also saved as part of the Analysis.
- Method is stored in the .uaf file.

Export Components to Library Editor

Sample Name	Component RT	Compound Name	Match Factor	Best Hit	Window Size Factor
CAL_L08	3.8275	(2-Aziridinylethyl)amine	50.5	<input checked="" type="checkbox"/>	25.0
CAL_L08	4.7823	1-Propene, 2-methyl-	89.4	<input checked="" type="checkbox"/>	25.0
CAL_L08	9.5948	Cyclopentene, 1-chl...	62.0	<input checked="" type="checkbox"/>	25.0
CAL_L08	12.2960	Methyl Isobutyl Keto...	94.6	<input checked="" type="checkbox"/>	25.0
CAL_L08	18.5872	Ethane, pentachloro-	61.1	<input checked="" type="checkbox"/>	25.0
CAL_L08	19.1328	Benzene, 1,2,4-trime...	97.7	<input checked="" type="checkbox"/>	25.0

- Select desired components (3).
- Right click and select **Export**.
- Choose **Selected Components/Hits**.
- Choose format as **Library**.
- Three components and spectra in library.

Export Component Table

Export from:

All components/hits

Selected components/hits

Export to:

Library

Automatically name compounds for non-hit components

Prefix:

Unknown

Add index

Add retention time

OK Cancel

Library Editor - Webinar 1.mslibrary.xml*

File Edit Tools Help

Compound Table

Compound ID	Compound Name	CAS#	Formula	Molecular Weight	Retention Index	Retention Time
1	1-Propene, 2-methyl-	115-11-7	C4H8	56.063	386.0000	4.7823
2	Methyl Isobutyl Keto...	108-10-1	C6H12O	100.089	690.0000	12.2960
3	Benzene, 1,2,4-tri...	95-63-6	C9H12	120.094	1020.0000	19.1328

Spectrum View

Max. # of panes: 8

SingleQuadrupole +1-Propene, 2-methyl- (115-11-7)

x10⁴

0.75

0.5

0.25

0

20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 240 250 260 270

41.1

56.1

62.0

78.7 88.4 102.7 120.0 134.0 146.6 159.6 179.8 191.0 207.8 233.1 260.1

Displayed Compounds: 3 | Total Compounds: 3 | Spectra: 3

Export Components to .CSV

Sample Name	Component RT	Compound Name	Match Factor	Best Hit	Window Size Factor
CAL_L08	4.2466	Dichlorodifluorometh...	97.7	<input checked="" type="checkbox"/>	200.0
CAL_L08	4.4921	Chloromethane	98.6	<input checked="" type="checkbox"/>	200.0
CAL_L08	4.6131	2-(Dibromomethane)...	55.4	<input checked="" type="checkbox"/>	25.0
CAL_L08	4.7325	Ethene, chloro-	95.3	<input checked="" type="checkbox"/>	100.0
CAL_L08	4.7821	2-Butene	99.3	<input checked="" type="checkbox"/>	200.0
CAL_L08	4.7871	2-Butyne	59.2	<input checked="" type="checkbox"/>	25.0



- Add/Remove Columns...
- Copy
- Set Best Hits
- Show Alternate Hits...
- Delete Components/Hits Del
- Restore All Components/Hits
- Set Hits as ISTDs
- Format Column...
- Export...**
- Print...
- Print Preview...



Export Component Table

Export from:

All components/hits

Selected components/hits

Export to:

CSV File

Automatically name compounds for non-hit components

Prefix:

Unknown

Add index

Add retention time

OK Cancel



- Select three different components.
- Right click and select **Export**.
- Choose **Selected Components/Hits**.
- Choose format as **CSV File**.
- Three components in CSV File.

	A	B	C	D	E	F	G
1	Sample Name	Component RT	Compound Name	Match Factor	Best Hit	Window Size Factor	
2	CAL_L08	4.492109814	Chloromethane	98.603205	TRUE	200	
3	CAL_L08	4.732524655	Ethene, chloro-	95.327862	TRUE	100	
4	CAL_L08	4.787117711	2-Butyne	59.193042	TRUE	25	

Export Components to Quantitative Analysis Method

Sample Name	Component RT	Compound Name	Match Factor	Best Hit	Window Size Factor
CAL_L08	4.2466	Dichlorodifluorometh...	97.7	<input checked="" type="checkbox"/>	200.0
CAL_L08	4.4921	Chloromethane	98.6	<input checked="" type="checkbox"/>	200.0
CAL_L08	4.6131	2-(Dibromomethane)...	55.4	<input checked="" type="checkbox"/>	25.0
CAL_L08	4.7325	Ethene, chloro-	95.3	<input checked="" type="checkbox"/>	100.0
CAL_L08	4.7821	2-Butene	99.3	<input checked="" type="checkbox"/>	200.0
CAL_L08	4.7871	2-Butyne	59.2	<input checked="" type="checkbox"/>	25.0

One compound added to QDB
With two Qualifiers

- Add/Remove Columns...
- Copy
- Set Best Hits
- Show Alternate Hits...
- Delete Components/Hits Del
- Restore All Components/Hits
- Set Hits as ISTDs
- Format Column...
- Export...**
- Print...
- Print Preview...

Export Component Table

Export from:

All components/hits

Selected components/hits

Export to:

Quantitative Analysis Method

Automatically name compounds for non-hit components

Prefix:

Unknown

Add index

Add retention time

OK Cancel

Export Quantitative Method

Destination method path:

D:\MassHunter\Data\QuantExamples\MS\VOA\Webinar QDB.m

Browse...

Target ion:

Most abundant

Number of qualifiers to add:

2

OK Cancel

Sample	Name	Data File	Type	Level
	CAL_L08	CAL_L08.D	Cal	8

Quantifier	Name	TS	Scan	Type	MZ	Uncertainty
	2-(Dibromometh...	1	Scan	Target	45.0	Relative

Qualifier	MZ	Rel. Resp.	Uncertainty	Area Sum
	219.9	46.3	20.0	<input type="checkbox"/>
	217.8	13.5	20.0	<input type="checkbox"/>

Layouts

- Preset Layouts
- Create custom layouts

View Analyze Method Report Tools Help

All Target **Non-Target** Hit Non-Hit

- Samples
- Chromatogram
- Components
- Ion Peaks
- EIC Peaks
- Spectrum
- Molecular Structure
- Analysis Messages
- Preset Layout**
 - Standard
 - All - Extended
 - All - Condensed**
 - Sample - Component
 - Chromatogram - Spectrum
 - Component - Spectrum
 - Component - Spectrum - Ion
 - Spectrum - Ion
- Load Layout...
- Save Layout...

Agilent MassHunter Unknowns Analysis - Webinar VOA 2.uaf

File Edit View Analyze Method Report Tools Help

Analyze All All Target **Non-Target** Hit Non-Hit Best Hit

Samples

Sample Name	File Name	Components	Hits
CAL_L03	CAL_L03.D		
CAL_L04	CAL_L04.D		
CAL_L05	CAL_L05.D		
CAL_L06	CAL_L06.D		
CAL_L07	CAL_L07.D		
CAL_L08	CAL_L08.D	72	332
CAL_L09	CAL_L09.D		
CAL_L10	CAL_L10.D		
CAL_L11	CAL_L11.D		
CAL_L12	CAL_L12.D		
CC_L07	CC_L07.D		
QC_L06	QC_L06.D		
Blank01	BLANK01.D		
Blank02	BLANK02.D		
SAMPLE01	SAMPLE01.D		
SAMPLE02	SAMPLE02.D		
SAMPLE03	SAMPLE03.D		

Chromatogram

Components

Component RT	Compound Name	Match Factor	Best Hit	F1
16.1809	Methane, tribromo-	92.4	<input type="checkbox"/>	C1
16.1809	Dibromonitromethane	82.4	<input type="checkbox"/>	C1
16.5410	Bicyclo[4.2.0]octa-1,3,5-triene	96.8	<input type="checkbox"/>	C8
16.5410	1,3,5,7-Cyclooctatetraene	96.7	<input type="checkbox"/>	C8
16.5410	Styrene	96.5	<input checked="" type="checkbox"/>	C8
16.5410	1,3,5,7-Cyclooctatetraene	96.2	<input type="checkbox"/>	C8
16.6645	p-Xylene	82.8	<input type="checkbox"/>	C8
16.6645	Benzene, 1,3-dimethyl-	82.5	<input type="checkbox"/>	C8
16.6645	Benzene, 1,3-dimethyl-	82.5	<input type="checkbox"/>	C8
16.6645	o-Xylene	82.1	<input type="checkbox"/>	C8
16.8793	Propane, 1,2,3-trichloro-	92.1	<input type="checkbox"/>	C3
16.8793	Propane, 1,2,3-trichloro-	92.1	<input type="checkbox"/>	C3
16.8793	Propane, 1,2,3-trichloro-	94.5	<input type="checkbox"/>	C3
16.8793	Propane, 1,2,3-trichloro-	93.6	<input type="checkbox"/>	C3
17.2879	Benzene, (1-methylethyl)-	80.9	<input type="checkbox"/>	C9
17.2879	Benzene, (1-methylethyl)-	80.7	<input type="checkbox"/>	C9
17.2879	Benzene, (1-methylethyl)-	80.2	<input type="checkbox"/>	C9
17.2879	Benzene, 1-ethyl-4-methyl-	79.3	<input type="checkbox"/>	C9
17.6572	Benzene, bromo-	96.3	<input type="checkbox"/>	C6
17.6572	Benzene, bromo-	96.1	<input type="checkbox"/>	C6
17.6572	Benzene, bromo-	96.9	<input type="checkbox"/>	C6
17.6572	Benzene, bromo-	96.9	<input type="checkbox"/>	C6

Ion Peaks

Component RT: 16.5410

Spectrum

Component RT: 16.5410

EIC Peaks

EIC Peaks

Molecular Structure

Styrene (NIST17.L)

CAL_L08.D

Unknowns Analysis



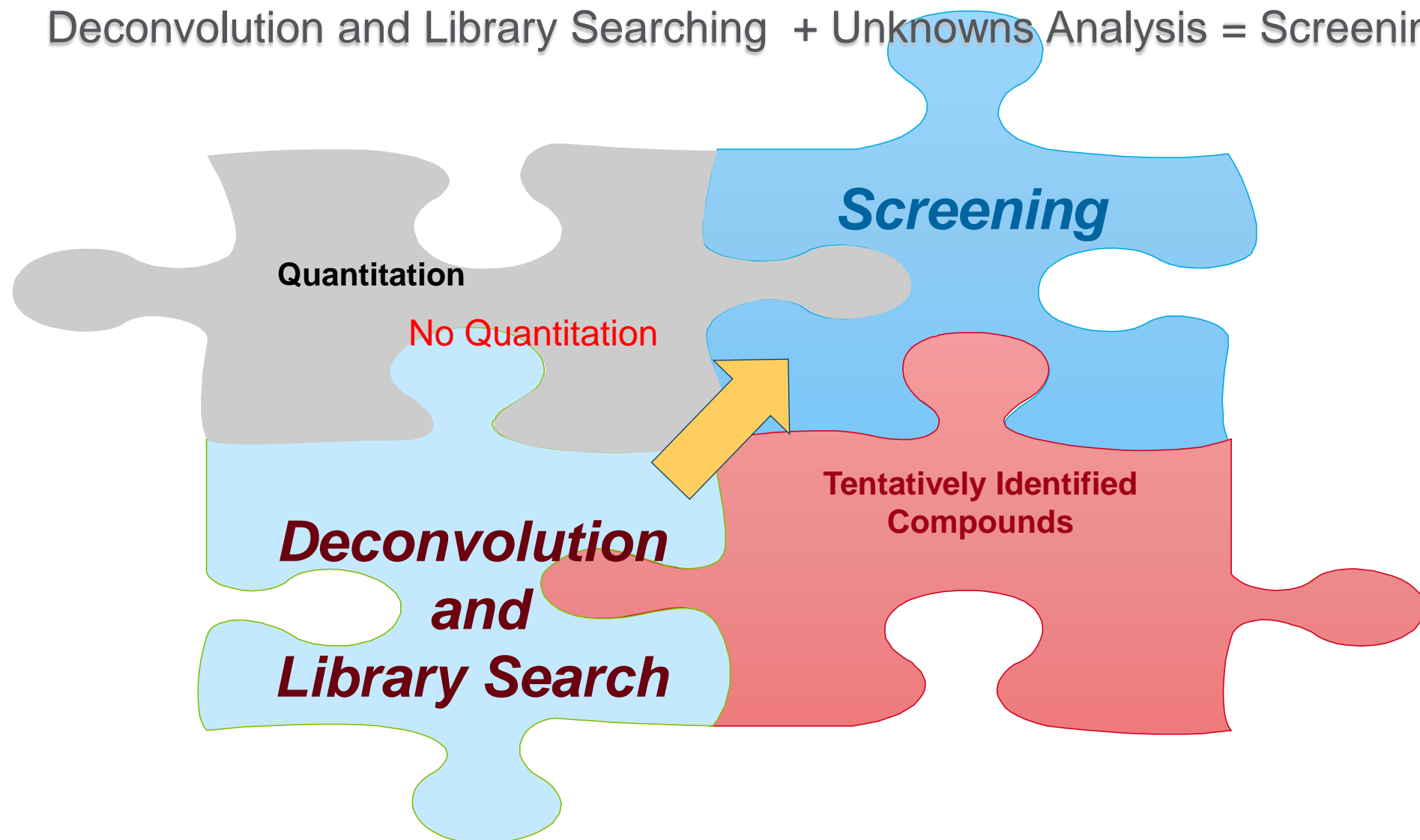
Time for a demo

Next up:
Unknowns Screening

Overview of Unknowns Analysis

Screening

Deconvolution and Library Searching + Unknowns Analysis = Screening

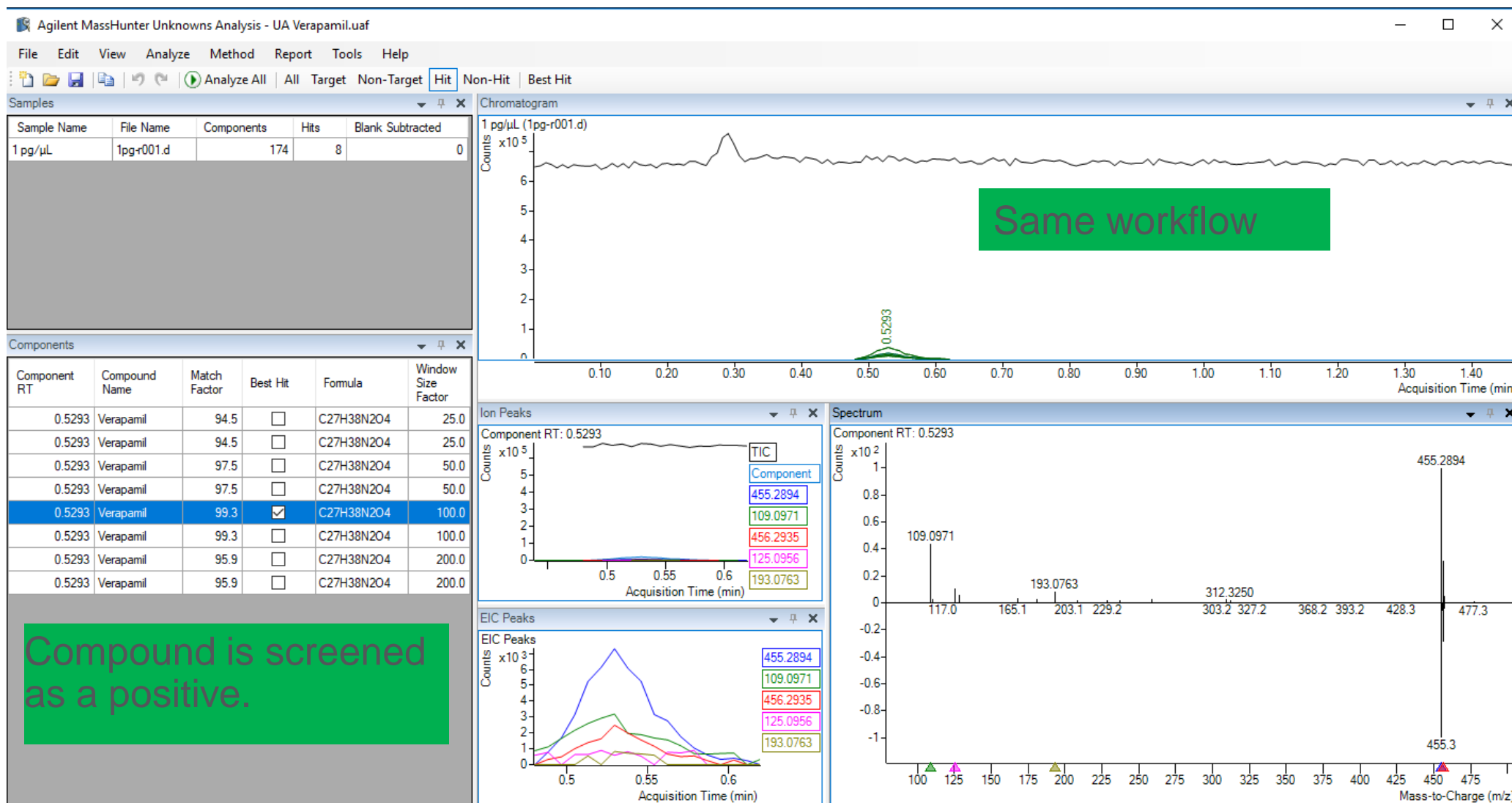


Screening Workflow

Screening methodology

- May require minimal sample preparation.
- Does not require Quantitative Analysis.
- Shorter chromatographic runs.
 - Deconvolution algorithm does most of the 'dirty' work.
 - Use multiple RT Window Size Factors to extract targets.
 - Applicable to low resolution and high resolution data.
 - Most appropriate with scan data.
- Library Searching
 - Can be commercial library.
 - Better with a smaller user generated library with 'targets'.
- Screens positive → Confirmation.
- Improves sample throughput.

Screening Workflow



Unknowns Analysis

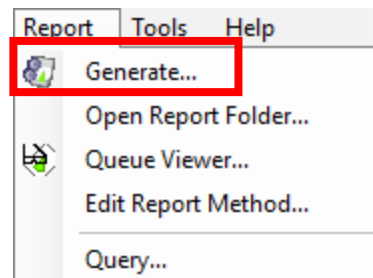


Time for a demo

Next up:
Reporting

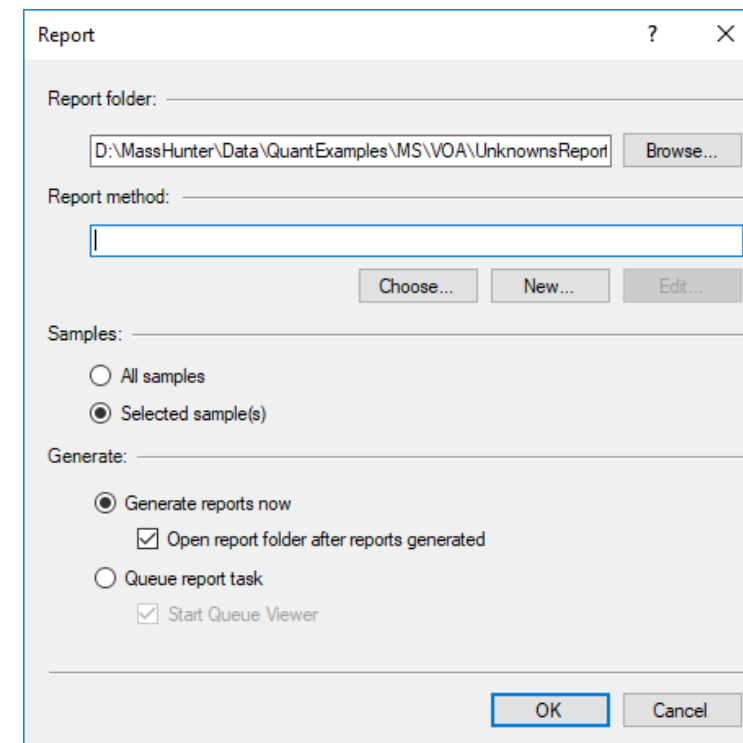
Generate Reports

Sample Name	File Name	Components	Hits
CAL_L03	CAL_L03.D		
CAL_L04	CAL_L04.D		
CAL_L05	CAL_L05.D		
CAL_L06	CAL_L06.D		
CAL_L07	CAL_L07.D		
CAL_L08	CAL_L08.D	72	69
CAL_L09	CAL_L09.D		
CAL_L10	CAL_L10.D		
CAL_L11	CAL_L11.D		
CAL_L12	CAL_L12.D		



Report > Generate

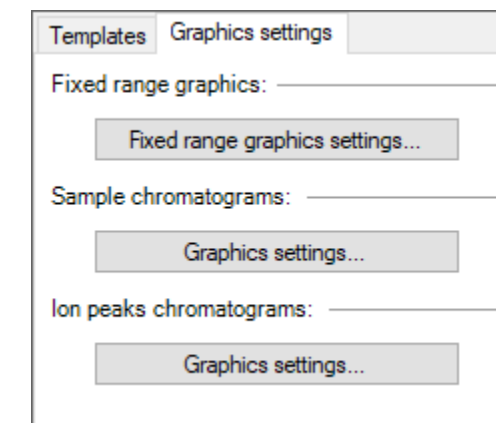
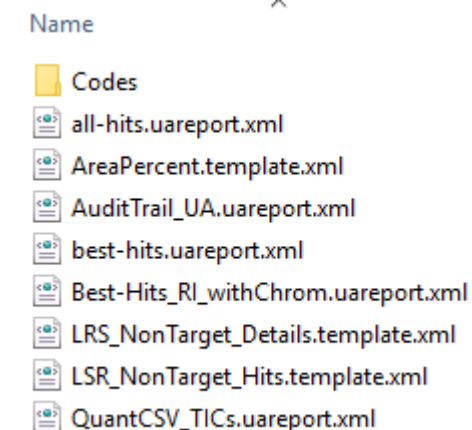
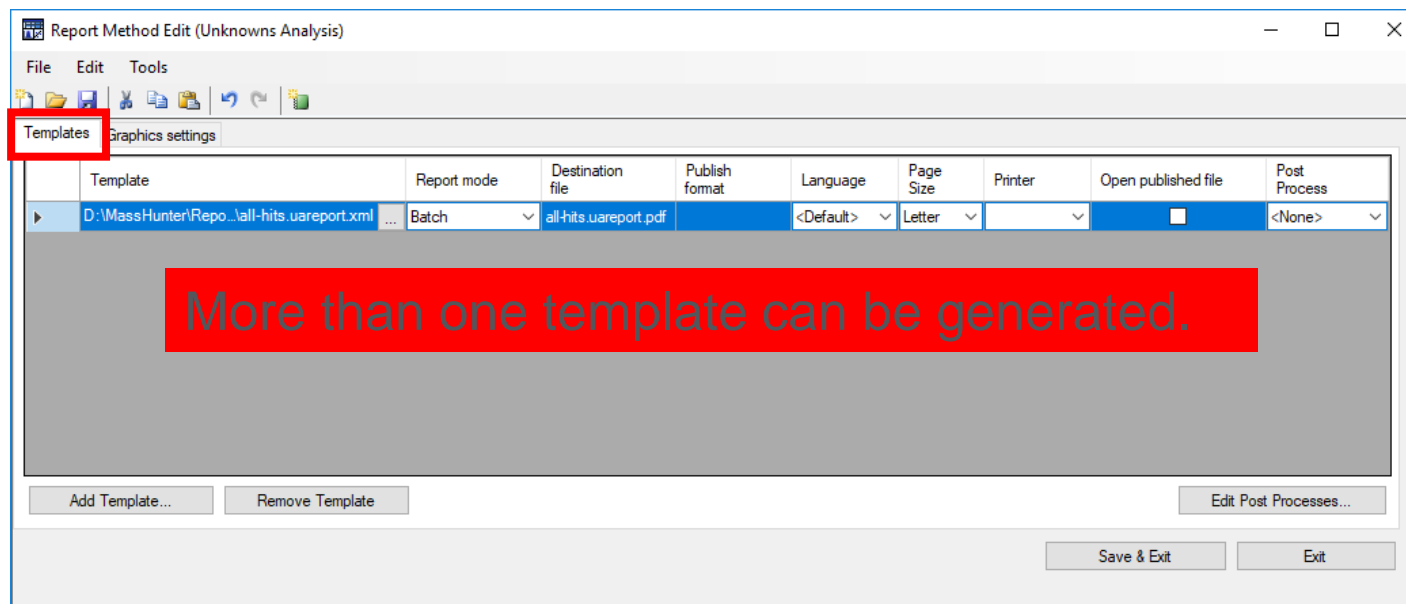
- Must “Save Analysis” first.
- If only a subset of samples is wanted select them in Samples.



Choose, create or edit a
Unknowns Analysis Report
Method.



Generate Reports



- Select the report(s).
- Numerous PDF style reports are available.
- Determine or modify the graphic settings.
- Generate the report.

Generate Reports

Graphic Settings

Report Method Edit (Unknowns Analysis)

File Edit Tools

Templates Graphics settings

Fixed range graphics: _____
Fixed range graphics settings...

Sample chromatograms: _____
Graphics settings...

Ion peaks chromatograms: _____
Graphics settings...

Graphics Range

Samples:

Min Y	Max Y	Min X	Max X
<input type="text"/>	<input type="text"/>	<input type="text"/>	<input type="text"/>

Compounds:

Compound Name	Min Y	Max Y	Min X	Max X	Min Mz	Max Mz
<input type="text"/>						

Add Delete

Import

Ion Peaks Graphics settings

General:

Background color:

Foreground color:

Gridlines color:

Font:

Font size:

Chromatogram:

TIC:

Components:

Show Ion Peaks

Show Labels

Ion Peak colors...

OK Cancel

Sample Chromatogram Graphics settings

General:

Background color:

Foreground color:

Gridlines color:

Font:

Font size:

Chromatogram:

TIC:

Components:

Display EICs

EIC colors...

Scale the TIC to the highest peak after min.

Peak Labels:

Display peak labels

Vertical labels

Allow overlap

Choose labels:

- Component RT
- Component RI
- Compound Name
- Formula
- CAS#
- Estimated Conc.

Display label names (ex. RT=2.5412)

Display units for Conc. and RT

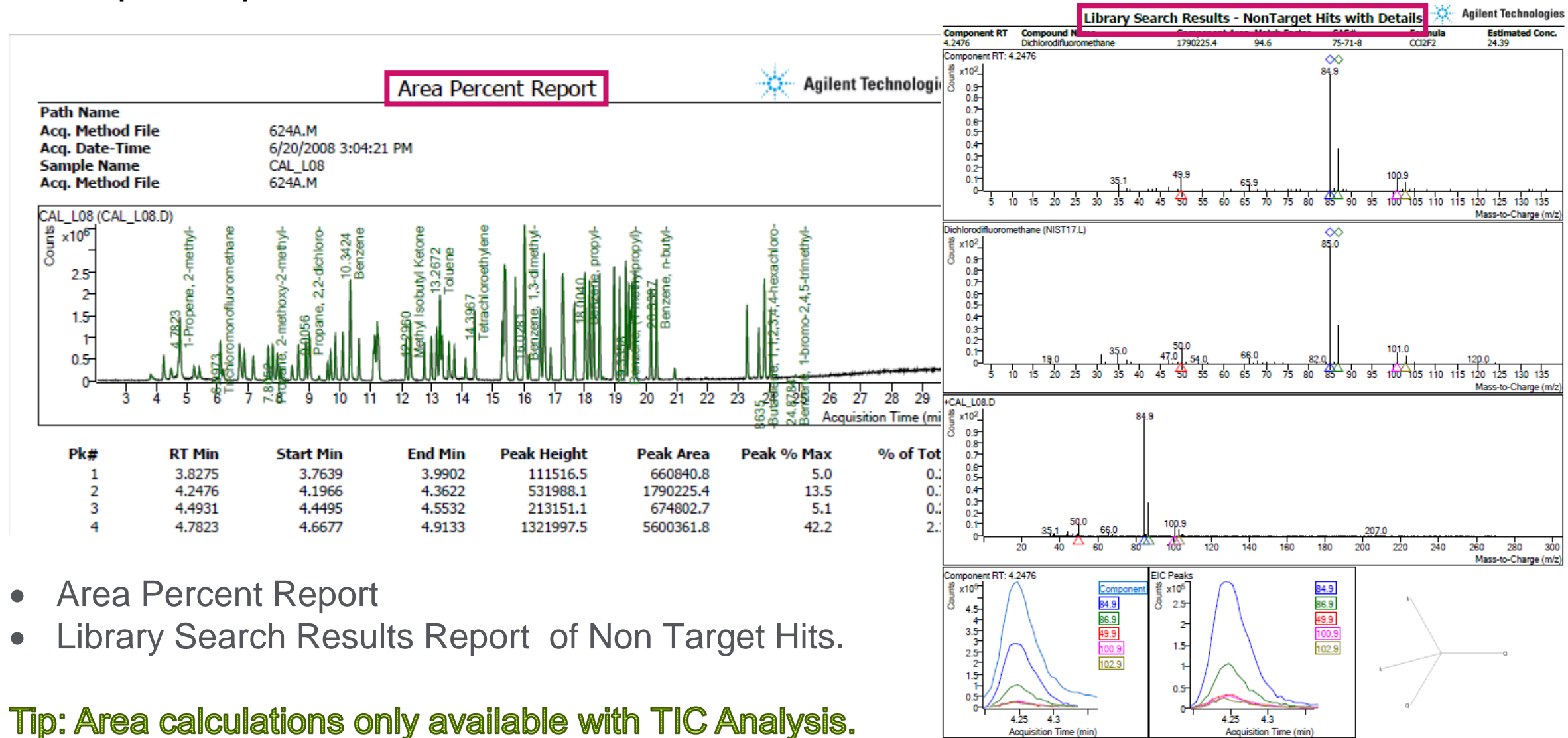
Move Up Move Down

OK Cancel

- Numerous options are available.

Generate Reports

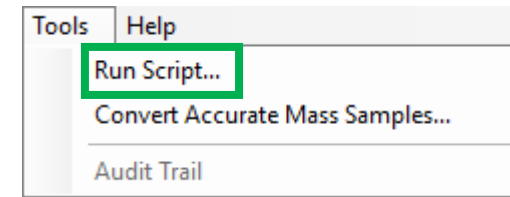
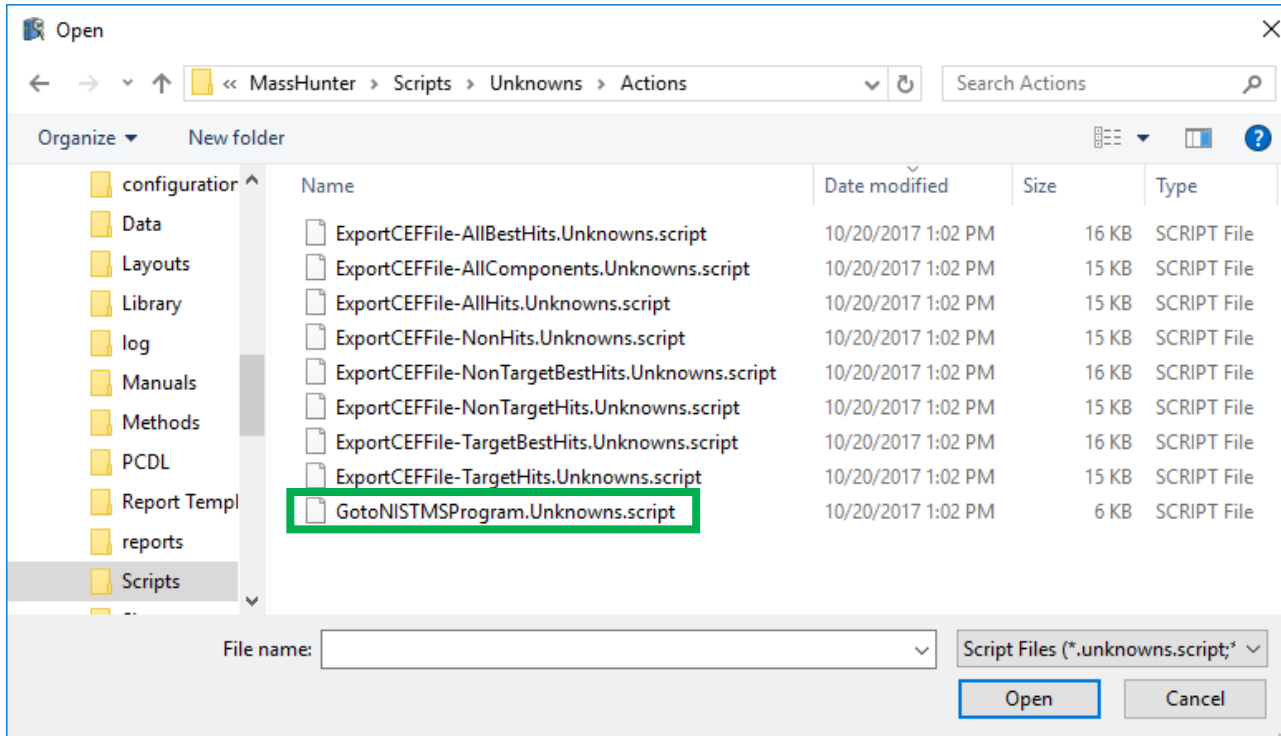
Example Reports



- Area Percent Report
- Library Search Results Report of Non Target Hits.

Tip: Area calculations only available with TIC Analysis.

Generate CEF Files



- Activated from **Tools > Run Script**.
- CEF Files (Common Exchange Format) used for exchanging data among programs, Quant, MPP, etc.
- Script to go to NIST programs. **New Feature**.
- Application – essential oils.

Customizable Report Templates

PDF Report Builder

- Both Excel and PDF Builder templates are user customizable.
- PDF Builder easier to use.

The screenshot displays the 'AreaPercent.template - Report Builder (Unknowns Analysis)' window. The interface includes a ribbon with 'File', 'Home', 'Insert', 'Page Layout', 'Formulas', 'Data', and 'Review' tabs. The 'Home' tab is active, showing options for 'Delete', 'Font', 'Alignment', 'Colors', 'Page', 'Textbox', 'Image', 'List', 'Table', and 'ScriptBox'. The main workspace shows a report template with the following content:

{L:Area Percent Report}

{C:DataFileName}	{V:DataFileName}
{C:SampleName}	{V:SampleName}
{C:AcqMethodFileName}	{V:AcqMethodFileName}
{L:Acq Date Time}	{V:AcqDateTime}

SampleChromatogram

PK#	{L:RT Min}	{C:CompoundName}	Start Min	End Min	Peak Height	L:Peak Area	L:Peak % Max	% of Total
{V:StartX}	{V:EndX}	{V:Height}	{V:Area}	AreaPercentMax	reaPercent			

{L:Page &[Page] of &[Pages]} {L:Generated at &[Time] on &[Date]}

The right-hand pane shows the 'Page1' settings, including 'General' (ID: Page1, Page Orientation: Portrait) and 'Margin' (Margins: 0.25in, 0.25in, 0.25in, 0.25in).

At the bottom, there is a 'Design-Compound' tab and a 'Ready' status bar. A tooltip at the bottom right provides instructions: 'To map repeating elements, drag the elements from the tree onto the worksheet where you want the data headings to appear.' and 'To import XML data, right click an XML mapped cell, point to XML, and then click Import.' with buttons for 'Options' and 'XML Maps...'. A 'Verify Map for Export' dropdown is also visible.

Custom Data Review Queries








- Report > Query
- Queries are useful to review data.
- Data can be viewed in subsets.
- Can Copy all the data.
- Can Copy selected data.
- Can Export Data to csv file.
- Review tentatively identified compounds or positive screening compounds.
- Requires expert programming skills (LINQ,SQL,C#)

The screenshot shows the Agilent MassHunter software interface. The 'Report' menu is open, and the 'Query...' option is highlighted. A purple arrow points from this menu item to a file explorer window. The file explorer shows a folder named 'Queries' containing several query files, including 'Batch Non-Target Hits containing Chlorine in Formula.sql.qry' and 'Sample Tentatively Identified Compound filter.linq.qry'. Another purple arrow points from the file explorer to the 'Query' window, which displays a table of query results.

SampleName	Compound	CAS	Formula	MW	Library	Score	Score
ISTD+solvent +...	Decachlorobiphe...	2051-24-3	C12Cl10	494	81.715		
PEST STD - 10+...	Oxychloridane	27304-13-8	C10H4Cl8O	420	51.085		
PEST STD - 10+...	trans-Chlordane	5103-74-2	C10H6Cl8	406	64.771		
PEST STD - 10+...	Endosulfan (alph...	959-98-8	C9H6Cl6O3S	404	62.490	23.619	
PEST STD - 10+...	Decachlorobiphe...	2051-24-3	C12Cl10	494	79.888	33.549	
PEST STD - 100...	Fenhexamid	126833-17-8	C14H17Cl2NO2	301	59.657	27.498	
PEST STD - 100...	Decachlorobiphe...	2051-24-3	C12Cl10	494	79.722	33.549	
PEST STD - 20+...	Endosulfan (alph...	959-98-8	C9H6Cl6O3S	404	72.254	23.610	
PEST STD - 20+...	Fenhexamid	126833-17-8	C14H17Cl2NO2	301	59.889	27.496	
PEST STD - 20+...	Decachlorobiphe...	2051-24-3	C12Cl10	494	75.873	33.548	
PEST STD - 200...	DDMU [1-Chloro...	1022-22-6	C14H9Cl3	282	73.369	23.268	
PEST STD - 200...	Fenhexamid	126833-17-8	C14H17Cl2NO2	301	62.037	27.499	
PEST STD - 200...	Decachlorobiphe...	2051-24-3	C12Cl10	494	78.095	33.549	
PEST STD - 50+...	Fenhexamid	126833-17-8	C14H17Cl2NO2	301	56.760	27.516	
PEST STD - 50+...	Decachlorobiphe...	2051-24-3	C12Cl10	494	76.763	33.552	















Training Resources

Familiarization Guide

Name
 G3335-90152_Quant_Familiarization-EN.pdf
 G3335-90196_QuantATM_QuickStart.pdf
 G3335-90200_Quant_Familiarization_MSD-en.pdf
 G3335-90219_Report Builder_Familiarization guide-en.pdf
 G3335-90240_Quant-My-Way_Familiarization_Guide.pdf
 G3335-90241_MassHunter_Offline_Installation-en.pdf
 G3335-90243_Unknowns_Analysis_Familiarization-en.pdf

- Uses example data located on USB in \Supplemental\MassHunter\Data\QuantExamples\MS\RI-PEST-MATRIX
- Example data can be loaded with Supplemental installer (Supplemental.msi)
- Includes RI Library and RT Calibration files.

- Familiarization Guide on USB drive in \Supplemental\MassHunter\Manuals\Quant
- Familiarization Guide covers basic operations.

Name
 ISTD-MATRIX-01.D
 PEST-STD-10-MATRIX-03.D
 PEST-STD-20-MATRIX-01.D
 PEST-STD-50-MATRIX-03.D
 PEST-STD-100-MATRIX-01.D
 PEST-STD-200-MATRIX-03.D
 QuantResults
 RTCAL
 UnknownsResults
 DEMO.uamethod.xml
 MassHunter Quant-Unknowns Analysis ASMS poster.pdf
 Pesticide spike exps 12-2010.xlsx
 RI-Libs-CF-RTL-summaries.xlsx
 RI-PESTICIDES-MOL2.mslibrary.xml

Training Resources

Help

- Help is now compiled HTML based.
- Available with a Context sensitive links.
- Searchable.

file:///C:/Program%20Files/Agilent/MassHunter/Workstation/Quant/help/en-US/UnknownsAn

Agilent | MassHunter Quantitative Analysis

Home > Unknowns Analysis

Unknowns Analysis Help

Welcome to the Agilent MassHunter Unknowns Analysis program. The program is designed to identify compounds that may be present in a sample batch beyond what has been identified in the target analysis.

Online Help

The topics listed here will help you quickly get started using the Unknowns Analysis program to analyze data for components beyond the target compounds already identified in the Quantitative Data Analysis program.

1. [Create a new analysis](#)
2. [Import data from a MassHunter quantitative analysis](#)
3. [Edit a method](#)
4. [Completely analyze](#)
5. [Generate a Report](#)

16-Sep-2017 Agilent Technologies © 2017 Agilent. All Rights Reserved

Training Resources

Available Training Resources

Convenient Training

In our classrooms, at your site or online.

From a team of industry experts that deliver a high quality learning experience.

Classroom Training

Introductory level to in-depth, hands-on for laboratory instrumentation and software.

Customized On-Site Training

Effective learning environment designed to achieve operational excellence and employ development without the need to travel.

Online

Offerings from foundation level to expert delivered at your own pace.

Agilent University

Access From Home Page

Upgraded customer experience

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

Introduce new eLearning capabilities

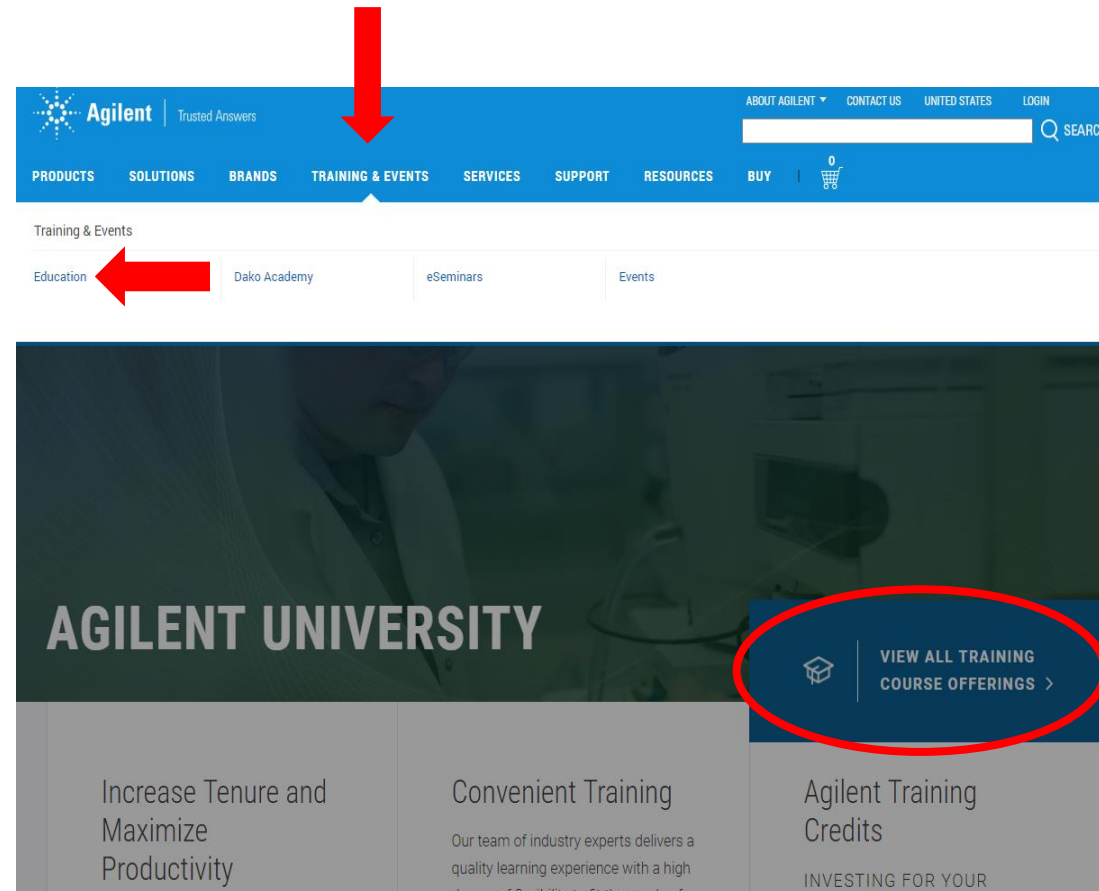
Recorded and video-based learning
Virtual online classes

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.



Agilent Community



Collaborate - Ask and answer questions.

Connect - Interact with other Agilent users.

Discover - Find relevant discussions, documents, and videos.

Share - Contribute your insights.

