

# MassHunter for Agilent GC/MS & GC/MS/MS

Next Generation  
Data Analysis Software

Presented by :  
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# Outline of Topics

**Topic 1: Introduction to MassHunter**

**Topic 2: Data Acquisition / Conversion**

**Topic 3: Qualitative Analysis**

**Topic 4: Quantitative Analysis**

**Topic 5: Reporting**

**Q & A**

**My Goal : Spark an interest in using MassHunter Data Analysis in your lab!**

# MassHunter – A Software Suite

MassHunter software is modular:

- Different modules that focus on these specific tasks:
  - ✓ Acquisition (Instrument Specific)
  - ✓ Quantitative Analysis (Quant)
  - ✓ Qualitative Analysis (Qual)
- A common reporting engine that uses different templates which are based on the specific reporting that is required.
- Suite of accessory applications which aid in specific tasks:
  - ✓ Unknown Analysis: batch versions of deconvolution and library searching
  - ✓ Library editor
  - ✓ Method development assistants
  - ✓ Data Translators



# MassHunter Data Analysis Software

MassHunter's main data analysis modules have different functions:

## Quantitative (Quant):

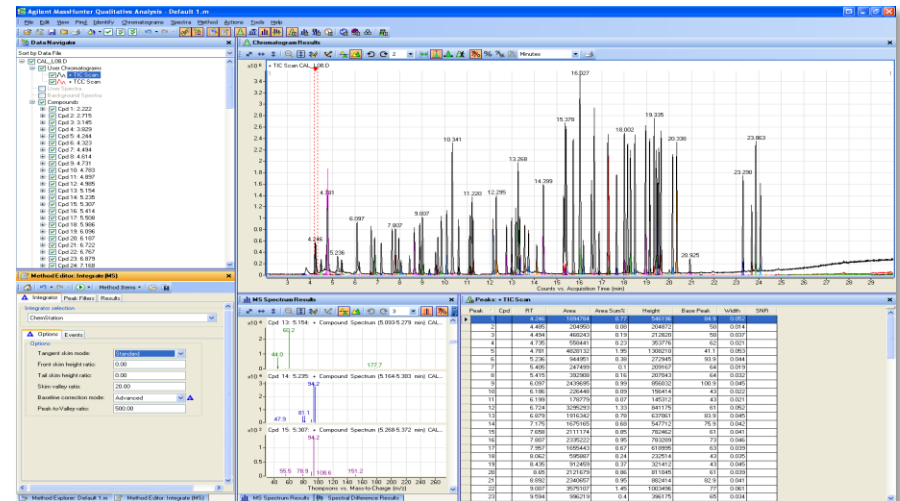
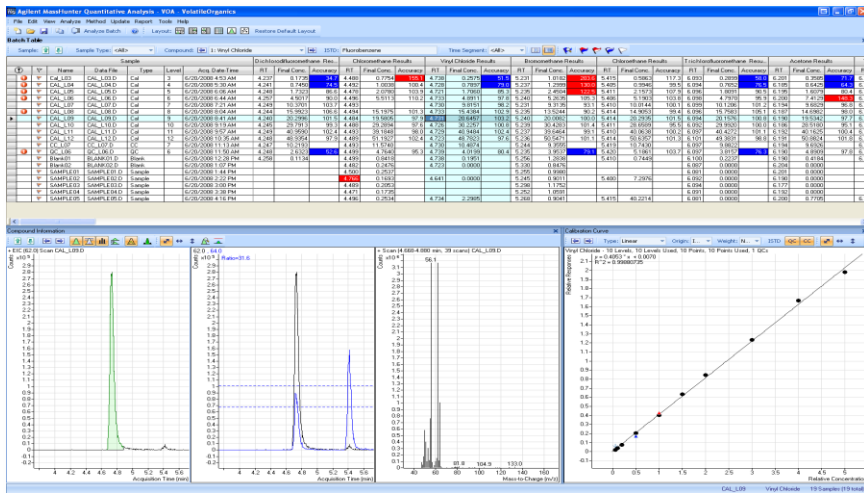
(Target Analysis - Quantitation)

- Review Batch results
- Visualize quality outliers
- Powerful quantitation engine
- Flexible result and report presentation

## Qualitative (Qual):

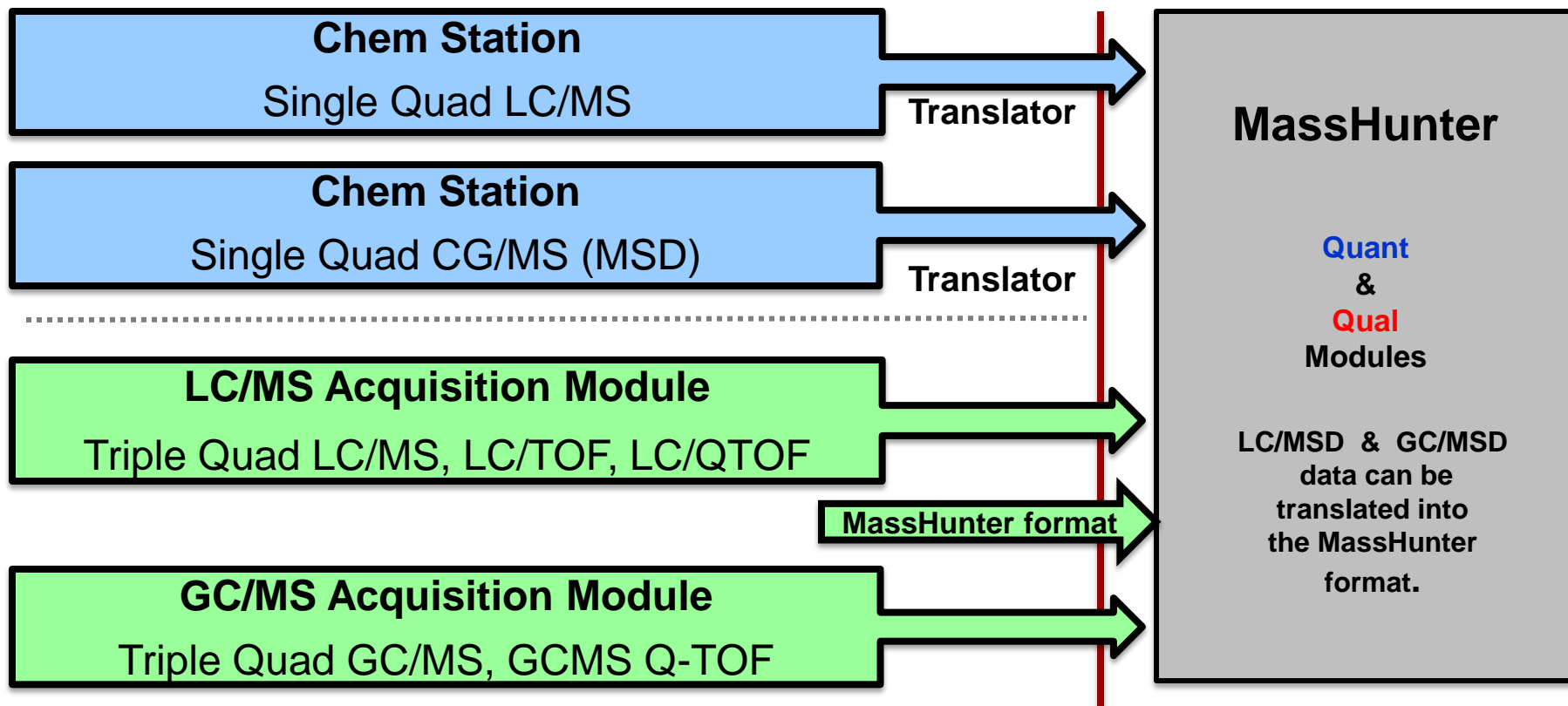
(Discovery of non-target compounds or features, & Method Development)

- Finds compounds
- Identifies compounds
- Uses chromatogram and spectra extraction tools, i.e. deconvolution
- Searches EI Libraries



# Delivering Data to MassHunter Data Analysis

**Quantitative (Quant)** and **Qualitative (Qual)** analysis modules can process data from any Agilent MassHunter software system.





**5975E SQ**  
7820 GC



**5975C SQ**  
7890 GC



**5975T LTM SQ**

# Agilent GC/MS

## Deploying MassHunter Software

# Agilent GC/MS/MS



**220 IT**  
7890 GC



**240 IT**  
7890 GC



**7000 TQ**  
7890 GC



**7200 Q-TOF**

# GCMS Translator – GC MSD



GC MSD  
Translator

GC MSD Translator converts GCMS data files to MassHunter format.

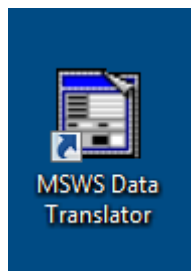
- a) single file translation
- b) Multiple file translation
- c) Automation with E.02.00 through macros



GC MSD  
ChemStation  
Quant  
Method  
Translator

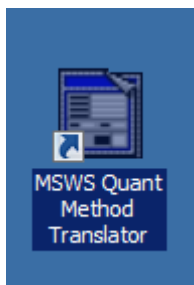
GC MSD ChemStation Quant Method Translator converts MSD Chemstation quant database to MassHunter quant format.

# GCMS Translator – Ion Trap



MSWS Data Translator converts MS Workstation data files to MassHunter format.

- a) single file translation
- b) Multiple file translation
- c) Automation with through command file



MSWS Quant Method Translator



Methods that were created by the MS Workstation can be automatically converted for use in MassHunter Quantitative Data Analysis using the GC/MS Translator software. Quantitation methods that were running successfully in the MS Workstation frequently convert and validate with no errors in MassHunter Quantitative Analysis. When validation issues are found, they are automatically identified and are correctable using the MassHunter Quantitative Analysis software.



# GCMS Translator – AIA / netCDF



GC AIA Translator converts AIA format MSD files to MassHunter format

GC/MS Translator is included with GC/MS MassHunter bundles: G7010AA, G7011AA, G6844AA, G6849AA, G6841AA *and* G6846AA

GCMS Translator is free!

Please give me contact information to receive a copy

# Outline of Topics

Topic 1: Introduction to MassHunter

Topic 2: Data Acquisition / Conversion

**Topic 3: Qualitative Analysis**

Topic 4: Quantitative Analysis

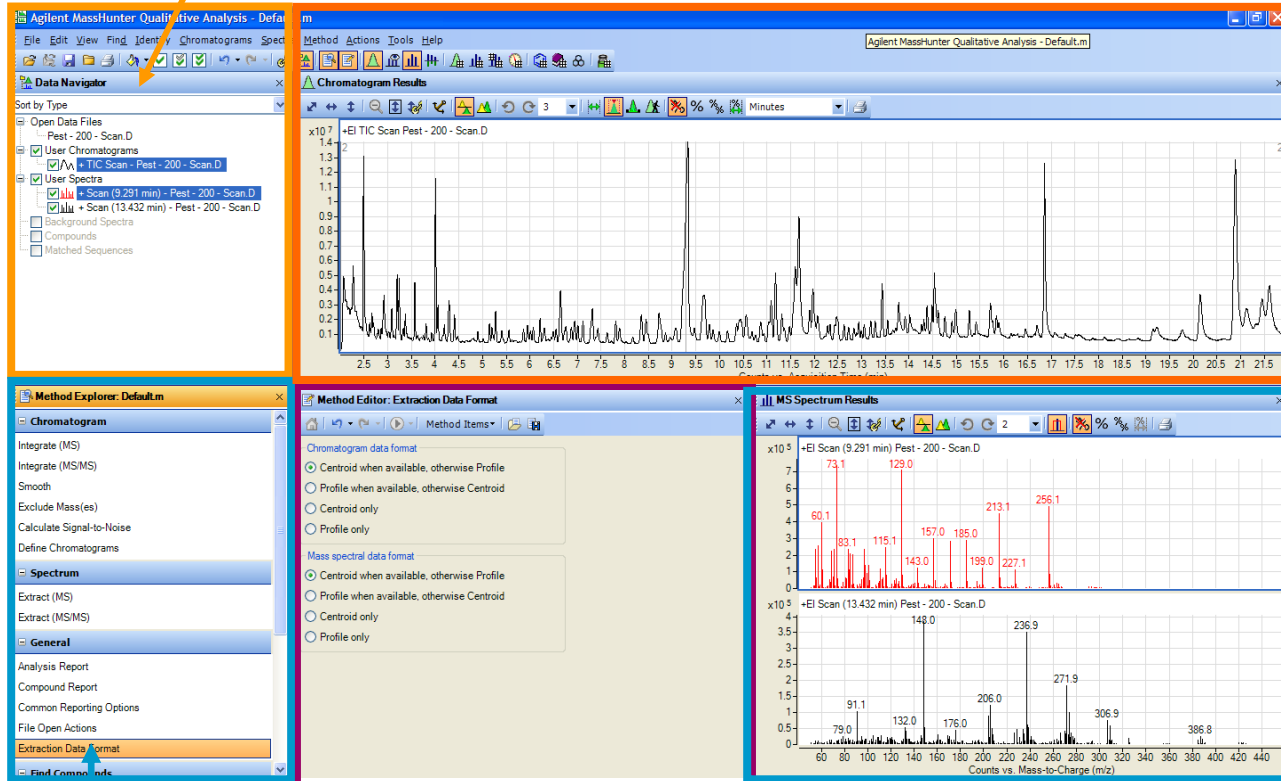
Topic 5: Reporting

Q & A

# MassHunter WorkStation Qualitative Analysis

Data Navigator

Chromatogram Results



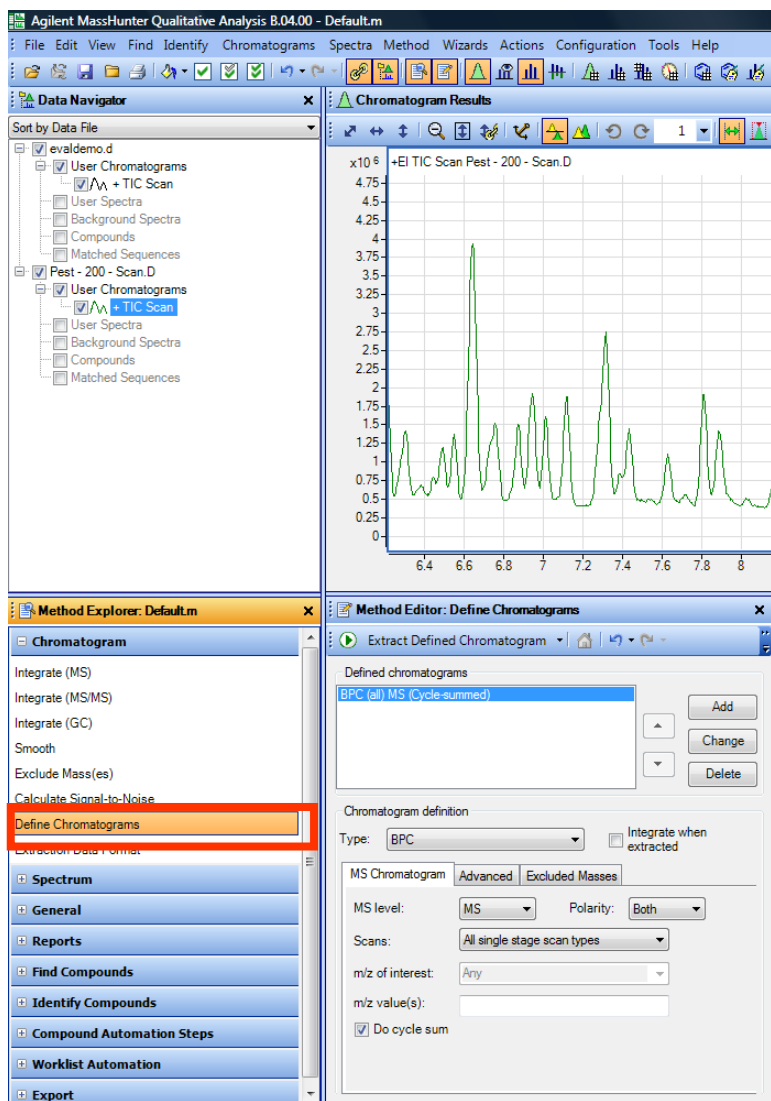
Method Explorer

Method Editor

Spectrum Results

# Extract Chromatograms

- Extract multiple signal types to create Chromatograms
- Definition of signals can be stored in the method and used with automation



## Types of Chromatograms

**TIC – Total Ion Chromatogram**

**BPC – Base Peak Chromatogram**

**EIC – Extracted Ion Chromatogram**

**SIM – Selected Ion Monitor**

**MRM – Multiple Reaction Monitor-QQQ**

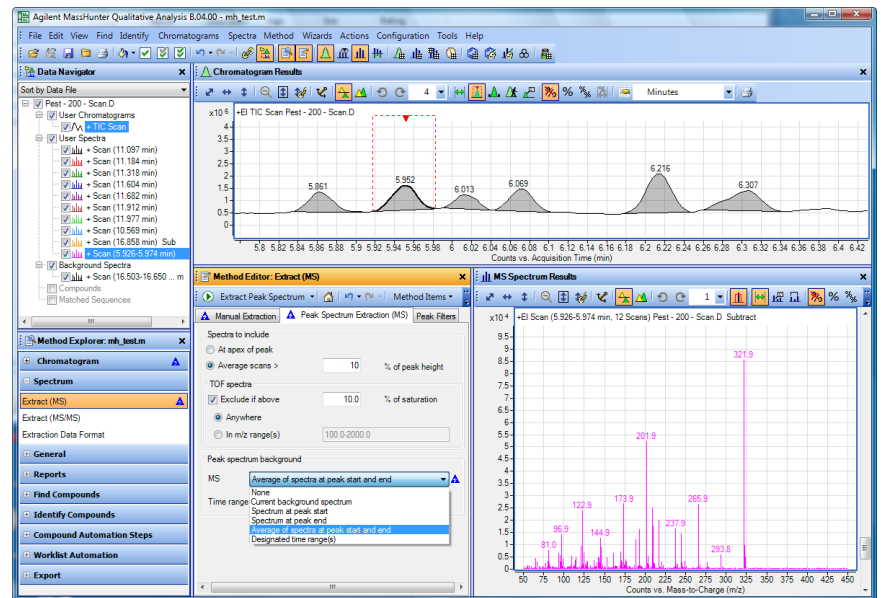
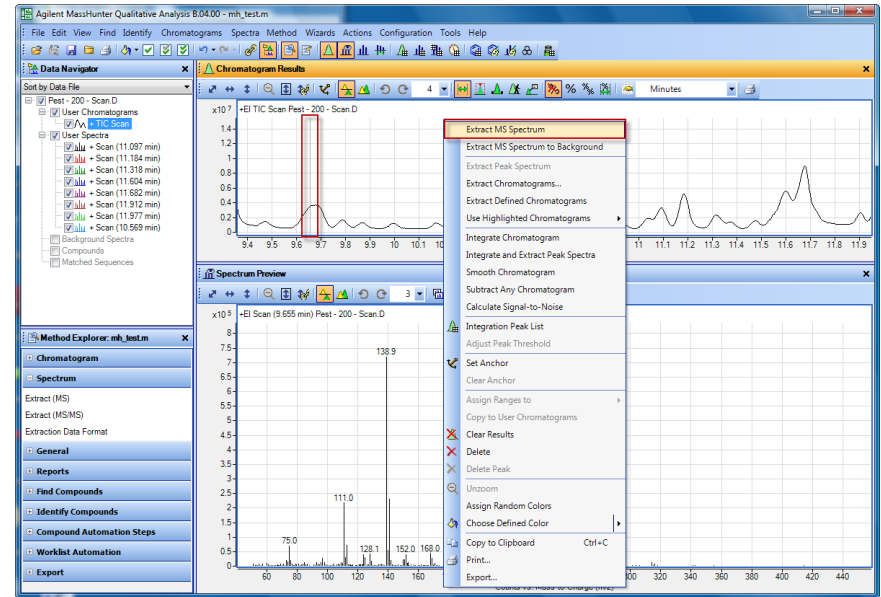
**pNLC - Precursor Neutral Loss Chromatogram**

**Other Chromatograms – DAD, VWD, ADC, GC**

**Instrument Curve - %Comp., Temps, etc.**

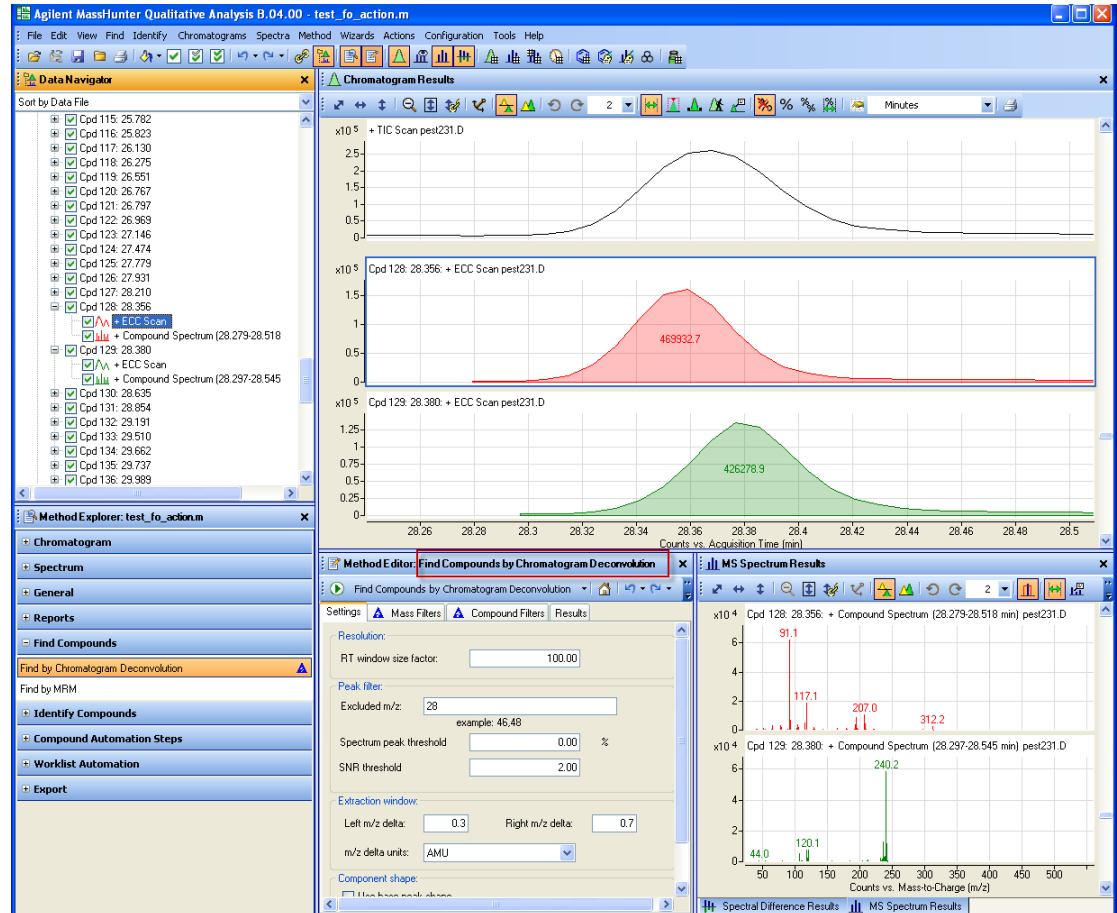
# Extract Spectra

- Manual selection or based on integrated peaks
- Background subtraction based on defined regions or peak definition



# Find Compound by Chromatogram Deconvolution

- Agilent deconvolution algorithm similar to AMDIS but not equivalent
- Creates Compounds with chromatographic and spectral components



# Identify Compounds with Library Search

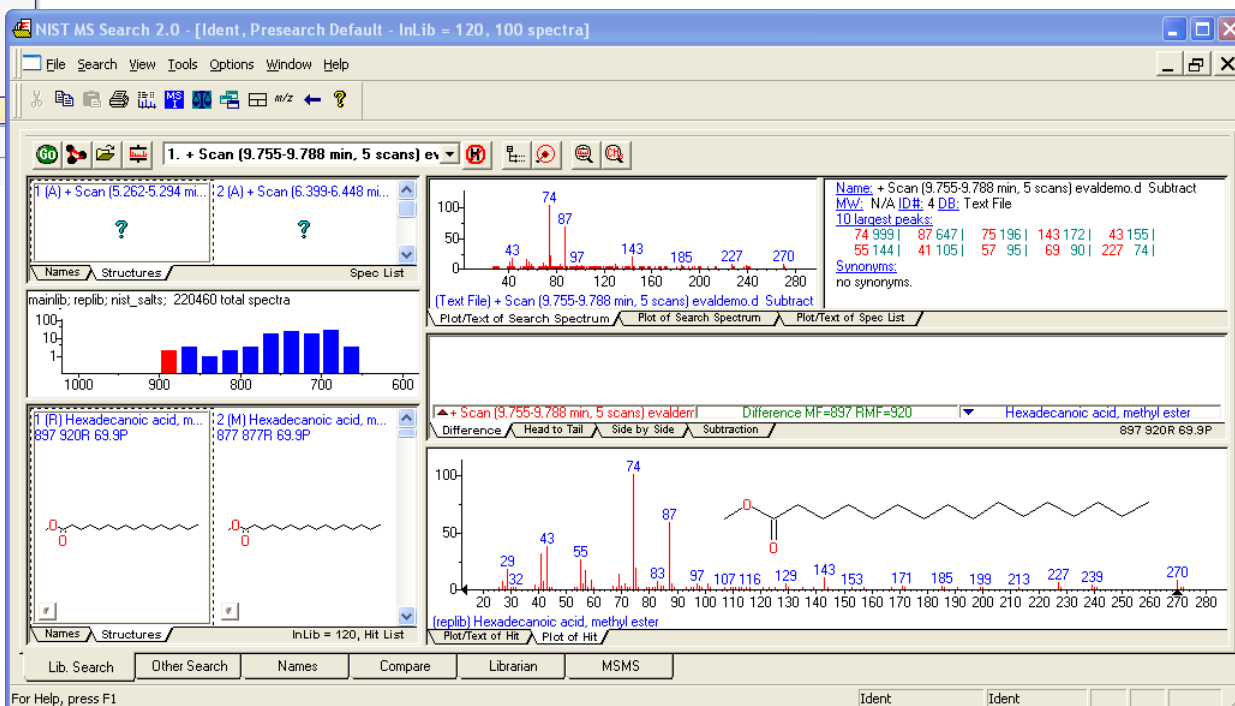
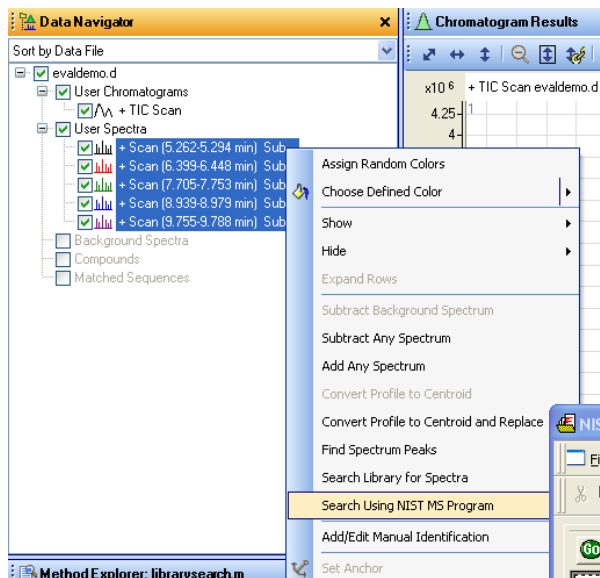
The screenshot displays the Agilent MassHunter Qualitative Analysis software interface. The main window shows 'Spectrum Identification Results' for a scan at 7.705-7.753 min. A table lists search results with columns for Best, Name, Formula, Score, Mass (DB), ID Source, Score (Lib), and CAS. The top result is 1,1'-Biphenyl, 4-chloro- with a score of 98.08. A context menu is open over the table, highlighting 'Search Library for Spectra'. A 'Structure Viewer' on the right shows the chemical structure of 1,1'-Biphenyl, 4-chloro-. Below the table, a 'Method Editor: Search Unit Mass Library' window is open, showing search criteria such as 'Spectral library path', 'Begin spectral matching at 30.00 m/z', and 'MS/MS search' options. The 'MS Spectrum Results' window shows four mass spectra plots with peaks labeled with their m/z values. A red box highlights a peak at m/z 188.2 in the third spectrum, which corresponds to the molecular ion of the identified compound.

Best	Name	Formula	Score	Mass (DB)	ID Source	Score (Lib)	CAS
1,1'-Biphenyl, 4-chloro-	C12H9Cl	98.08	188	LibSearch	98.08	2051-67-3	
1,1'-Biphenyl, 4-chloro-	C12H9Cl	109	98.08				
1,1'-Biphenyl, 4-ch	C12H9Cl	97.3	188	LibSearch	97.3	2051-62-9	
1,1'-Biphenyl, 4-ch	C12H9Cl	96.61	188	LibSearch	96.61	2051-62-9	
1,1'-Biphenyl, 2-ch	C12H9Cl	95.32	188	LibSearch	95.32	2051-60-7	
3-Chlorobiphenyl	C12H9Cl	94.54	188	LibSearch	94.54	2051-61-8	
1,1'-Biphenyl, 2-ch	C12H9Cl	94.48	188	LibSearch	94.48	2051-60-7	
1,1'-Biphenyl, 2-ch	C12H9Cl	94.36	188	LibSearch	94.36	2051-60-7	
1,1'-Biphenyl, 4-ch	C12H9Cl	92.91	188	LibSearch	92.91	2051-62-9	
1,1'-Biphenyl, 2-ch	C12H9Cl	92.23	188	LibSearch	92.23	2051-60-7	
3-Chlorobiphenyl	C12H9Cl	90.65	188	LibSearch	90.65	2051-61-8	

- Library search User Spectra or Compounds.
- Library search parameters are part of a method.
- May use Retention Time or Retention Index in search

# Using NIST library matching from Qual

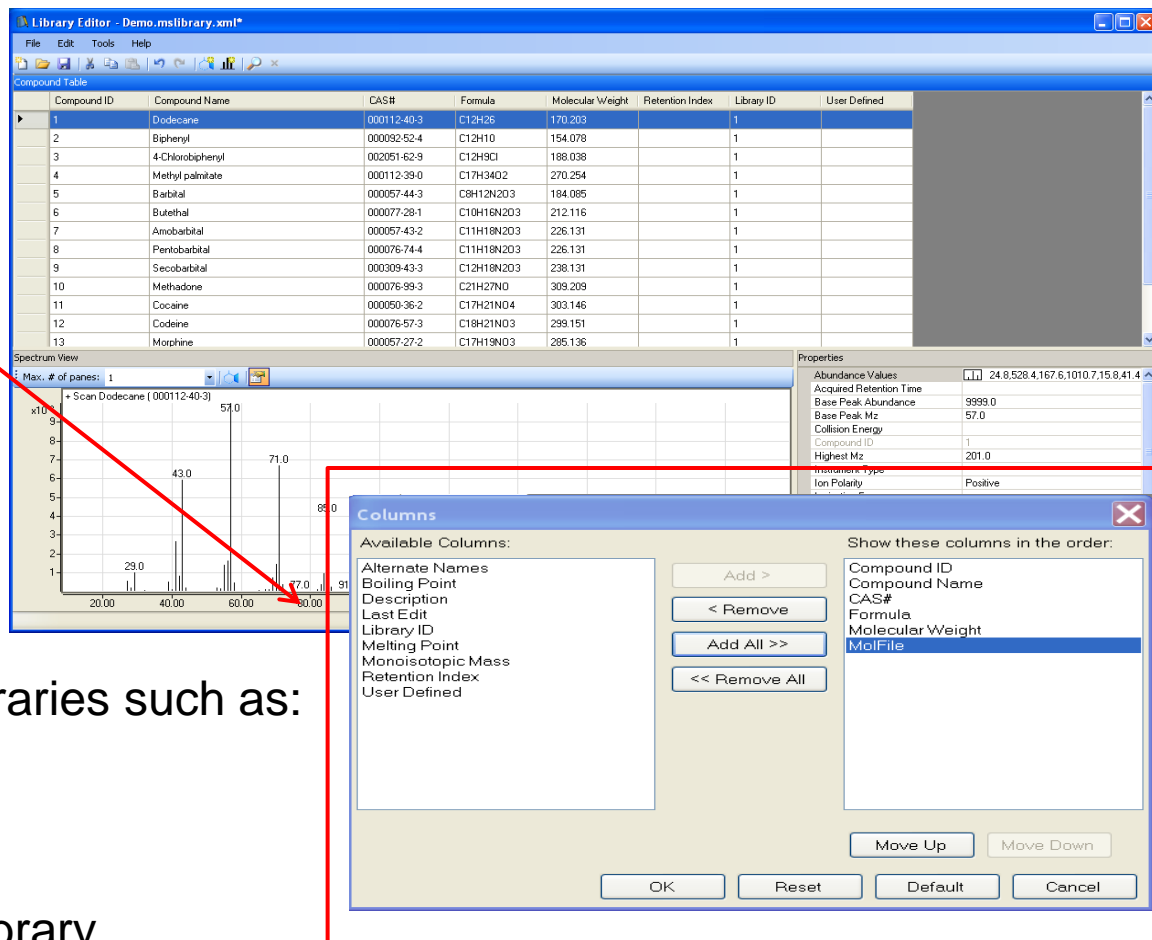
- Export spectra to NIST
- Requires NIST (not included in Qual)
- Information does not flow back to Qual / MassHunter reports





# Library Editor & Available Libraries

A dedicated application, the *Library Editor*, is used to create, edit, and modify user libraries.



The screenshot displays the Library Editor interface. At the top, a 'Compound Table' lists various compounds with columns for Compound ID, Compound Name, CAS#, Formula, Molecular Weight, Retention Index, Library ID, and User Defined. Below the table is a 'Spectrum View' showing a mass spectrum for Dodecane (000112-40-3) with peaks at 29.0, 43.0, 57.0, 71.0, and 85.0. A 'Columns' dialog box is open, showing a list of available columns and a list of columns to be displayed in the order: Compound ID, Compound Name, CAS#, Formula, Molecular Weight, and MolFile.

Compound ID	Compound Name	CAS#	Formula	Molecular Weight	Retention Index	Library ID	User Defined
1	Dodecane	000112-40-3	C <sub>12</sub> H <sub>26</sub>	170.203		1	
2	Biphenyl	000092-52-4	C <sub>12</sub> H <sub>10</sub>	154.078		1	
3	4-Chlorobiphenyl	002051-62-9	C <sub>12</sub> H <sub>9</sub> Cl	188.038		1	
4	Methyl palmitate	000112-39-0	C <sub>17</sub> H <sub>34</sub> O <sub>2</sub>	270.254		1	
5	Barbital	000057-44-3	C <sub>8</sub> H <sub>12</sub> N <sub>2</sub> O <sub>3</sub>	184.085		1	
6	Butethal	000077-28-1	C <sub>10</sub> H <sub>16</sub> N <sub>2</sub> O <sub>3</sub>	212.116		1	
7	Amobarbital	000057-43-2	C <sub>11</sub> H <sub>18</sub> N <sub>2</sub> O <sub>3</sub>	226.131		1	
8	Pentobarbital	000076-74-4	C <sub>11</sub> H <sub>18</sub> N <sub>2</sub> O <sub>3</sub>	226.131		1	
9	Secobarbital	000309-43-3	C <sub>12</sub> H <sub>18</sub> N <sub>2</sub> O <sub>3</sub>	238.131		1	
10	Methadone	000076-99-3	C <sub>21</sub> H <sub>27</sub> N <sub>0</sub>	309.209		1	
11	Cocaine	000050-36-2	C <sub>17</sub> H <sub>21</sub> N <sub>0</sub> O <sub>4</sub>	303.146		1	
12	Codine	000076-57-3	C <sub>18</sub> H <sub>21</sub> N <sub>0</sub> O <sub>3</sub>	293.151		1	
13	Morphine	000057-27-2	C <sub>17</sub> H <sub>19</sub> N <sub>0</sub> O <sub>3</sub>	285.136		1	

Properties:

- Abundance Values: 24.8,528,4,167,6,1010,7,15,8,41,4
- Acquired Retention Time: 1
- Base Peak Abundance: 9999.0
- Base Peak Mz: 57.0
- Collision Energy: 1
- Compound ID: 1
- Highest Mz: 201.0
- Retention Type: 1
- Ion Polarity: Positive

Columns:

Available Columns:

- Alternate Names
- Boiling Point
- Description
- Last Edit
- Library ID
- Melting Point
- Monoisotopic Mass
- Retention Index
- User Defined

Show these columns in the order:

- Compound ID
- Compound Name
- CAS#
- Formula
- Molecular Weight
- MolFile

Agilent provides over 15 EI Libraries such as:

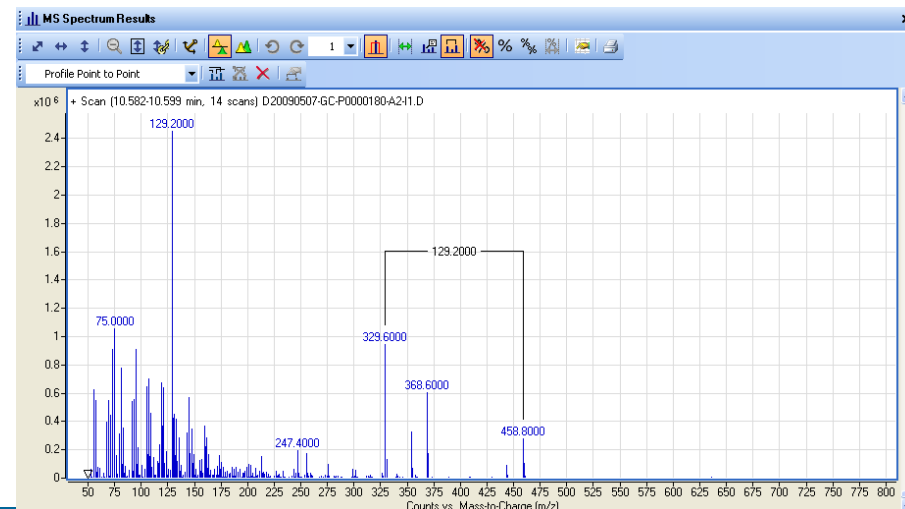
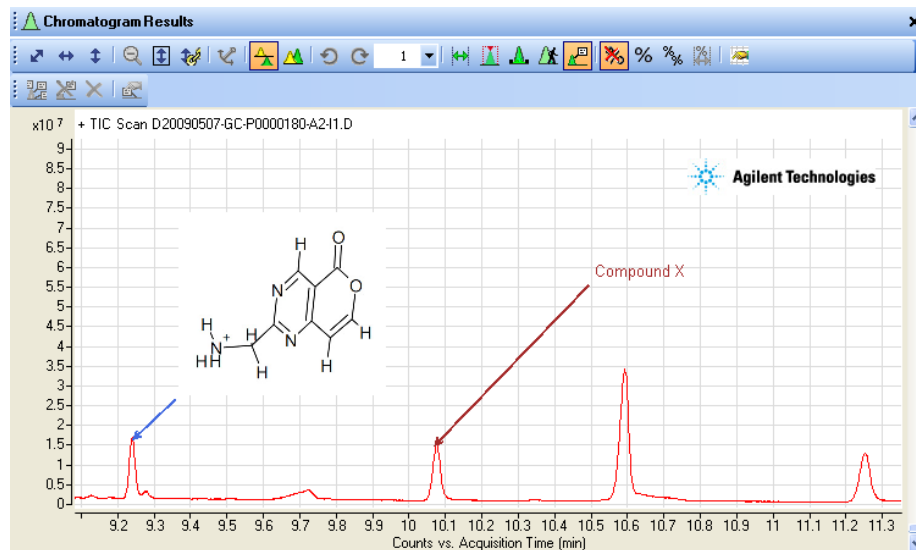
- ✓ NIST08
- ✓ Wiley8th+NIST08
- ✓ Fiehn Metabolite Library
- ✓ Japanese Pesticide list

# Annotate and Document

Annotate chromatograms and spectra using text, graphics (.jpg) and chemical structures (.mol)

Mass Caliper to document fragmentation and losses

Export or copy & paste graphics into presentations



# Automation - File Open Actions & Post Acquisition Worklist Processing

The screenshot displays two windows from the Agilent software interface. The left window, titled "Method Explorer: Defaultm", shows a tree view of method components. The "File Open Actions" component is highlighted in orange. The right window, titled "Method Editor: Assign Actions to Run Opening a Data File", shows a list of available actions and a list of actions to be run. The "Generate Analysis Report" action is selected in the available actions list, and the "Extract Defined Chromatograms" action is selected in the actions to be run list.

**Method Explorer: Defaultm**

- Chromatogram
- Spectrum
- General
  - Analysis Report
  - Compound Report
  - Common Reporting Options
  - File Open Actions**
  - Extraction Data Format
- Find Compounds
- Identify Compounds
- Compound Automation Steps
- Worklist Automation
- Export

**Method Editor: Assign Actions to Run Opening a Data File**

Available actions

- Integrate Chromatograms
- Integrate and Extract Peak Spectra
- Smooth Chromatograms
- Generate Compound Report
- Generate Analysis Report**
- Find Compounds by Chromatographic Deconvolution
- Correlate UV Chromatograms with Compounds

Actions to be run

- Extract Defined Chromatograms**
- Integrate and Extract Peak Spectra
- Generate Analysis Report

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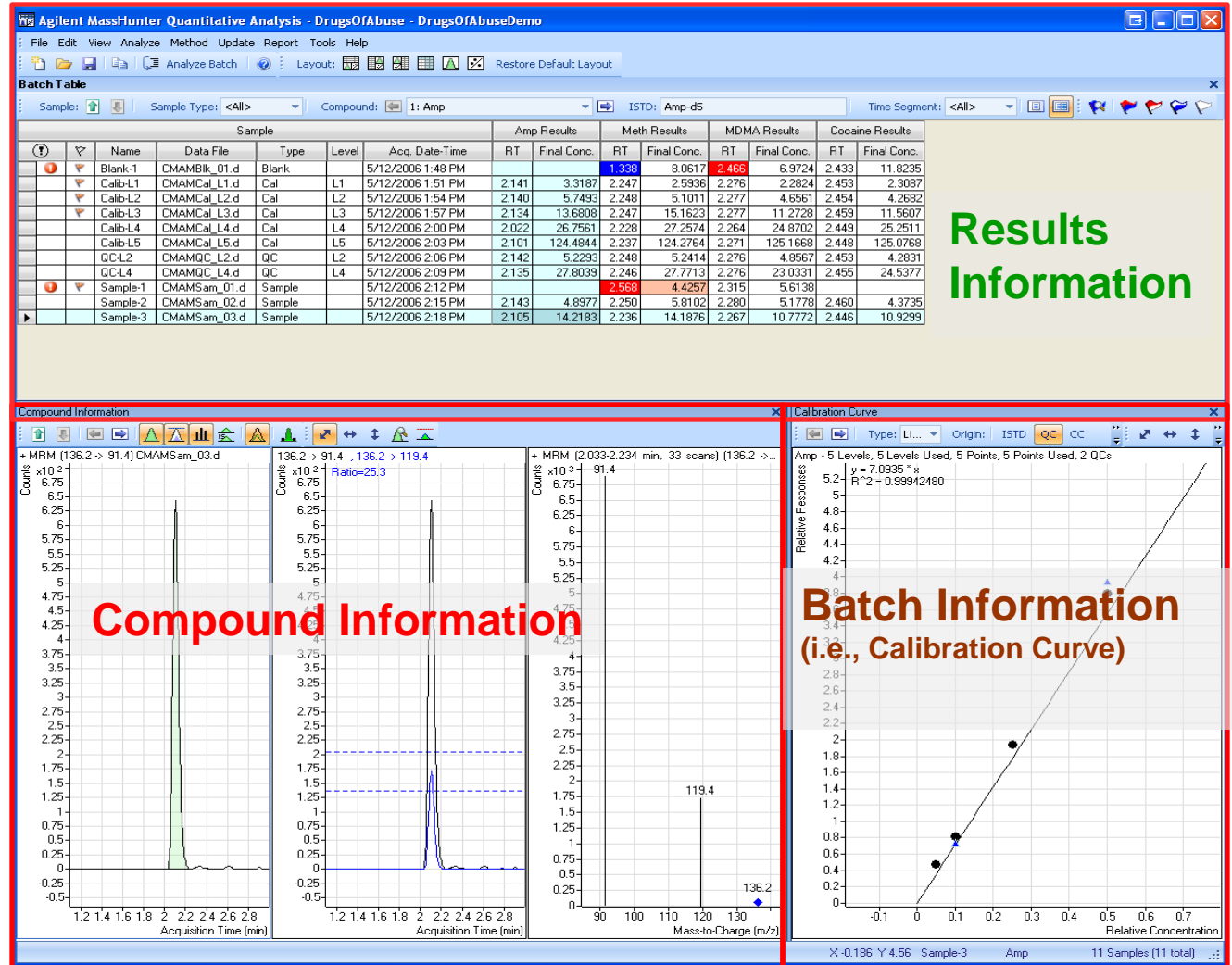
Topic 5: Reporting

Q & A

# Quantitative Analysis Screen

The **Quant Batch** screen looks like this.

- **Results Information** for the batch can be displayed. Visual guides highlight specific data that fall outside specific, predefined conditions.
- **Compound Information** displays graphical representation of the peak, qualifier information, spectral information, and the ISTD. Visual guides help identify associated data problems.
- **Batch Information** provides easy visualization and customization of relevant desired data.



Results Information

Compound Information

Batch Information (i.e., Calibration Curve)

# Batch Screen – Sample & Results Information

In **Results Information**, the **Quantitation Message** is a human-readable string that contains a list of error messages that result from a compound's quantitation.

Sample: Sample Type: <All> Compound: 1: Amp ISTD: Amp-d5 Time Segment: <All>

Compound Group: <All>

Sample						Amp Met..		Amp Results						Qualifier (136.2 -..			Amp-d5 (IS..			Qualifier (141.1 -..			
?	▽	Name	Type	Level	Acq. Date-Time	Dil.	Exp. Conc.	RT	Resp.	S/N	MI	Calc. Conc.	Final Conc.	Accuracy	Ratio	S/N	MI	RT	Resp.	Ratio	S/N	MI	
!		Blank-1	Blank		11/11/2006 11:05 AM	1.0																	
	▶	Calib-L1	Cal	L1	11/11/2006 11:10 AM	1.0	2.5000	2.141	658	49.10		2.1151	2.1151	84.6	24.3	45.47		2.129	1397	25.9	Infinity		
	▼	Calib-L2	Cal	L2	11/11/2006 11:15 AM	1.0	5.0000	2.140	1059	42.25		4.5770	4.5770	91.5	33.5	Infinity		2.128	1298	25.9	48.46		
		Calib-L3	Cal	L3	11/11/2006 11:20 AM	1.0	12.5000	2.134	2673	107.28		12.6107	12.6107	100.9	27.7	146.48		2.121	1377	26.3	46.09		
		Calib-L4	Cal	L4	11/11/2006 11:25 AM	1.0	25.0000	2.022	4952	20.26		25.8545	25.8545	103.4	29.1	49.40		1.990	1304	28.8	21.54		
		Calib-L5	Cal	L5	11/11/2006 11:30 AM	1.0	125.0000	2.101	18605	47.90		124.8426	124.8426	99.9	27.0	39.22		2.076	1053	26.4	Infinity		
		QC-L2	QC	L2	11/11/2006 11:35 AM	1.0	5.0000	2.142	1006	81.00		4.0502	4.0502	81.0	27.7	34.47		2.131	1356	31.1	42.99		
		QC-L4	QC	L4	11/11/2006 11:40 AM	1.0	25.0000	2.135	4716	91.48		26.9159	26.9159	107.7	25.1	60.79		2.121	1196	31.1	91.84		
!		Sample-1	Sample		11/11/2006 11:50 AM	1.0																	
		Sample-2	Sample		11/11/2006 11:55 AM	1.0		2.143	1004	80.65		3.7144	3.7144		30.9	70.64		2.130	1445	25.7	29.89		
		Sample-3	Sample		11/11/2006 11:59 AM	1.0		2.105	2590	74.97		13.1551	13.1551		25.3	65.40		2.089	1284	29.8	129.91		

## Quantitation Message(s)

Amp-d5: Integrator did not find any peaks  
 Amp-d5: Qualifier M/Z = 124.4: Qualifier peak not found or does not match quantitation criteria  
 Cocaine-d3: Integrator did not find any peaks  
 Cocaine-d3: Qualifier M/Z = 85.0: Qualifier peak not found or does not match quantitation criteria  
 Meth-d5: Qualifier M/Z = 121.4: Integrator did not find any peaks

## Outlier(s) Blue = low / Red = high

Amp: Qualifier ratio = 33.5 is outside the allowed range [21.2, 31.8]

These icons filter outliers in the display.

“Outliers” define and specify results of known problem samples/substances that fall outside predefined conditions.

# Results Information: Outlier Options

- 39 quality checks can be specified to highlight outliers in **results**.
- Can set high and low limits.
- User defined quality check can be added to predefined calculations.

Amp Results		
RT	Final Conc.	Accuracy
2.141	3.3187	132.7
2.140	5.7493	115.0
2.134	13.6808	109.4
2.022	26.7561	107.0
2.101	124.4844	99.6
2.142	5.2293	104.6
2.135	27.8039	111.2
2.143	4.8977	
2.105	14.2183	

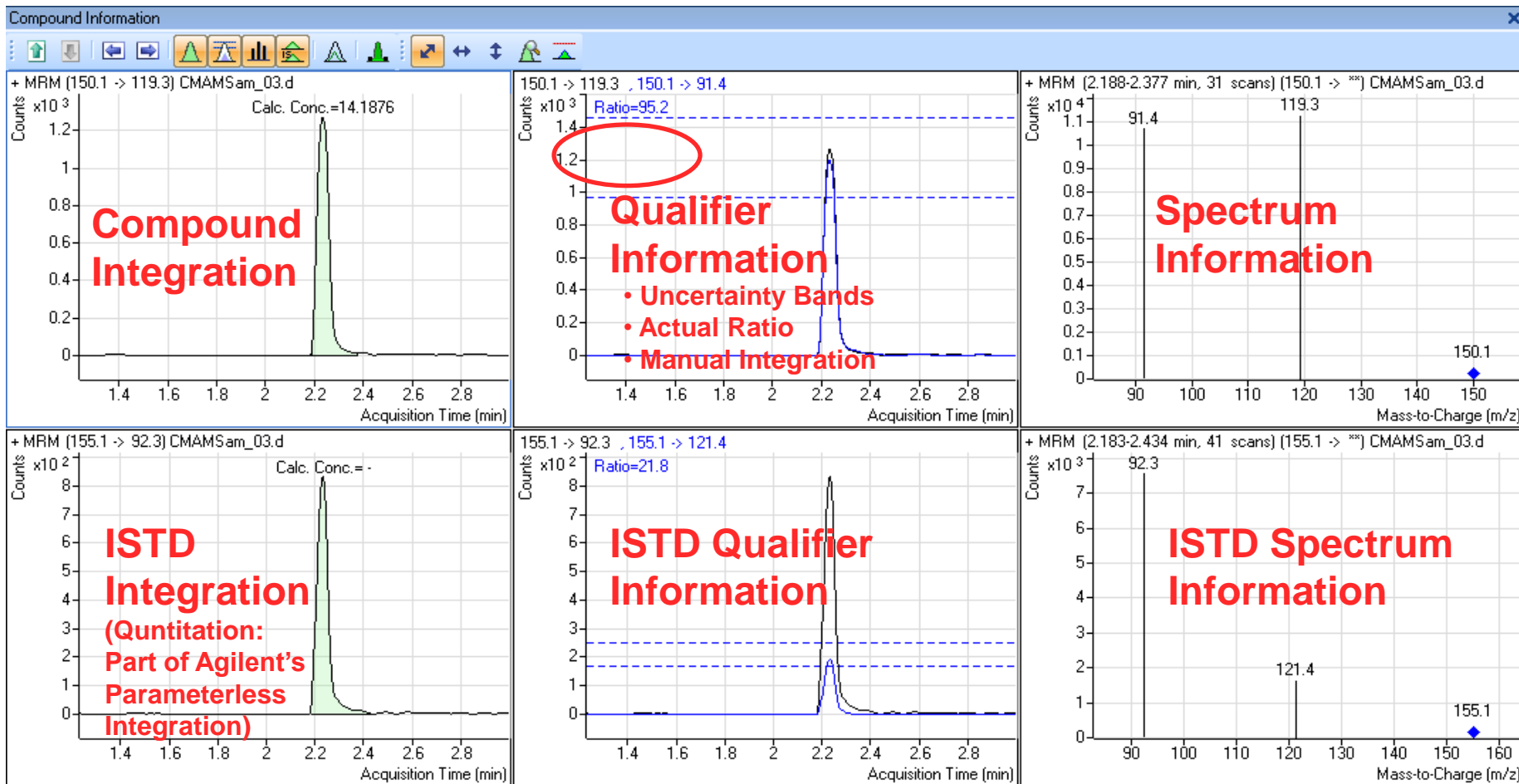
**Outlier Setup Tasks**

- Retention Time
  - Relative Retention Time
  - Peak Resolution
- Peak Symmetry
  - Peak Full Width Half Maximum
  - Peak Purity
- Signal-to-Noise Ratio
- Limit Of Detection
  - Limit Of Quantitation
  - Method Detection Limit
- Qualifier Ratio
- ISTD Response
  - ISTD Response Percent Deviation
- Sample Amount
- Sample RSD
- Blank Concentration
- Blank Response
- Accuracy
  - Average Response Factor
  - Average Response Factor RSD
- Curve Fit R2
- Relative Response Factor
- Response Factor

- QC
  - QC Relative Standard Deviation
- CC Average Response Factor
  - CC ISTD Response Ratio
  - CC Relative Response Factor
  - CC Response Ratio
  - CC Retention Time
- Matrix Spike
  - Matrix Spike Percent Difference
  - Matrix Spike Percent Recovery
  - Matrix Spike Group Recovery
- Surrogate
  - Surrogate Percent Recovery
- Response Check
- Mass Accuracy
- Custom Calculation**

# Batch Screen - Compound Information

**Compound information** displays all relevant information in one view.

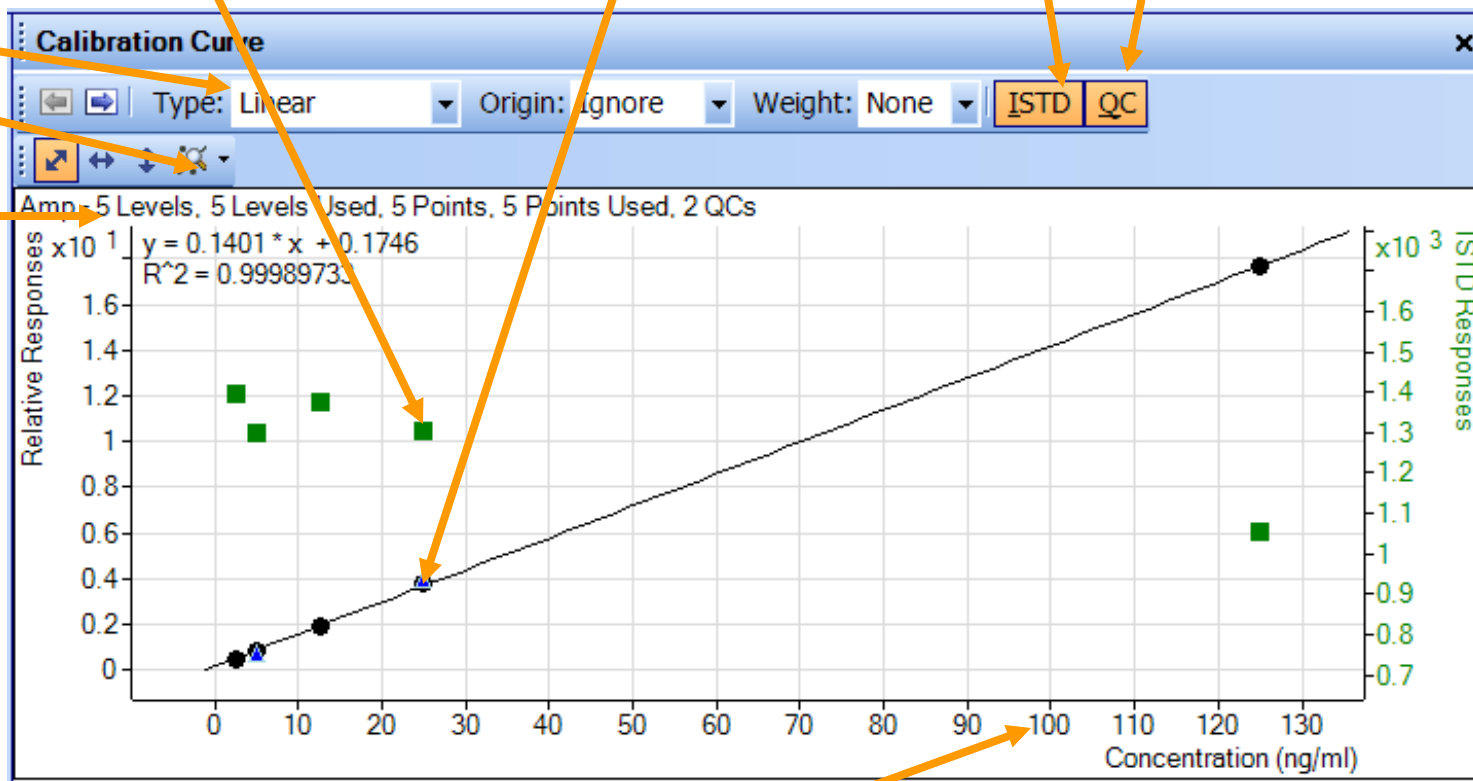




# Batch Screen – Calibration Curve

An example of **Batch Information** is this view of the Calibration Curve. The Curve fit can be changed and data can be updated instantaneously.

View ISTD responses or display QC samples - click either the ISD or QC button.



After editing the calibration curve, you must reanalyze the batch.

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

# Batch Screen - Curve Fit Assistant

**Calibration Curve** ✕

🏠 🔍 Type: Linear ▼ Origin: Ignore ▼ Weight: None ▼ ISTD QC

🔍 ↔ ⬆ 🔍

Amp - 5 Levels, 5 Levels Used, 5 Points, 5 Points Used, 2 QCs

$y = 0.1401 * x + 0.1746$   
 $R^2 = 0.99989733$   
 $y = 0.1403 * x + 0.1200$   
 $R^2 = 1.00000000$

Calculates all possible  
 calibration curve  
 combinations.

Type	Origin	Weight	# of Disabled Points	R2	Standard Error	Max % Residual	Equation
Linear	Ignore	None	3	1.00000000	0.0	0.0	$y = 0.1403 * x +$
Linear	Ignore	1/x	3	1.00000000	0.0	0.0	$y = 0.1478 * x +$
Linear	Ignore	1/x^2	3	1.00000000	0.0	0.0	$y = 0.1379 * x +$
Linear	Ignore	1/y	3	1.00000000	0.0	0.0	$y = 0.1478 * x +$
Linear	Ignore	1/y^2	3	1.00000000	0.0	0.0	$y = 0.1379 * x +$
Linear	Ignore	Log	3	1.00000000	0.0	0.0	$y = 0.1386 * x +$
Linear	Include	1/x	3	1.00000000	0.0	0.0	$y = 0.1478 * x +$
Linear	Include	1/x^2	3	1.00000000	0.0	0.0	$y = 0.1379 * x +$
Linear	Include	1/y	3	1.00000000	0.0	0.0	$y = 0.1478 * x +$
Linear	Include	1/y^2	3	1.00000000	0.0	0.0	$y = 0.1379 * x +$

📄 Copy Ctrl+C

🔍 **Curve Fit Assistant**

📄 Confidence Band

📄 Accept Assistant Curve

📄 Relative Concentration

📄 Standard Deviation Bars

🔍 Auto Scale

↔ X - Auto Scale

⬆ Y - Auto Scale

🔍 X - Log Scale

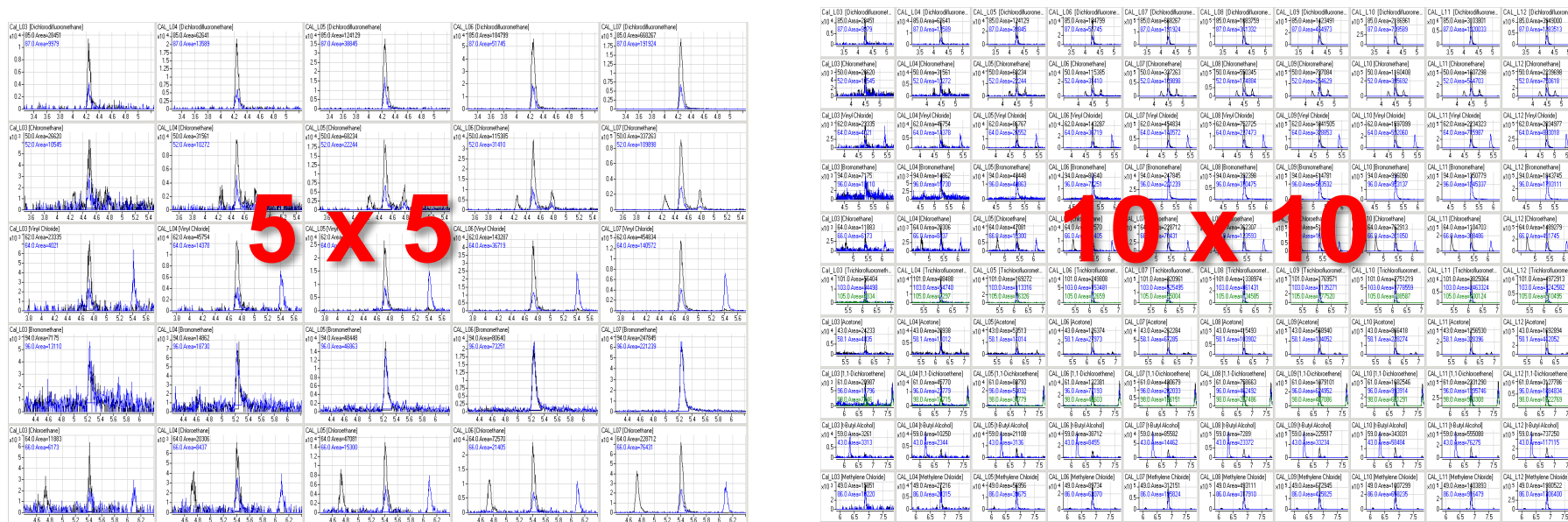
🔍 Y - Log Scale

🖨 Print... Ctrl+P

🖨 Print Preview...

# Compounds-at-a-Glance

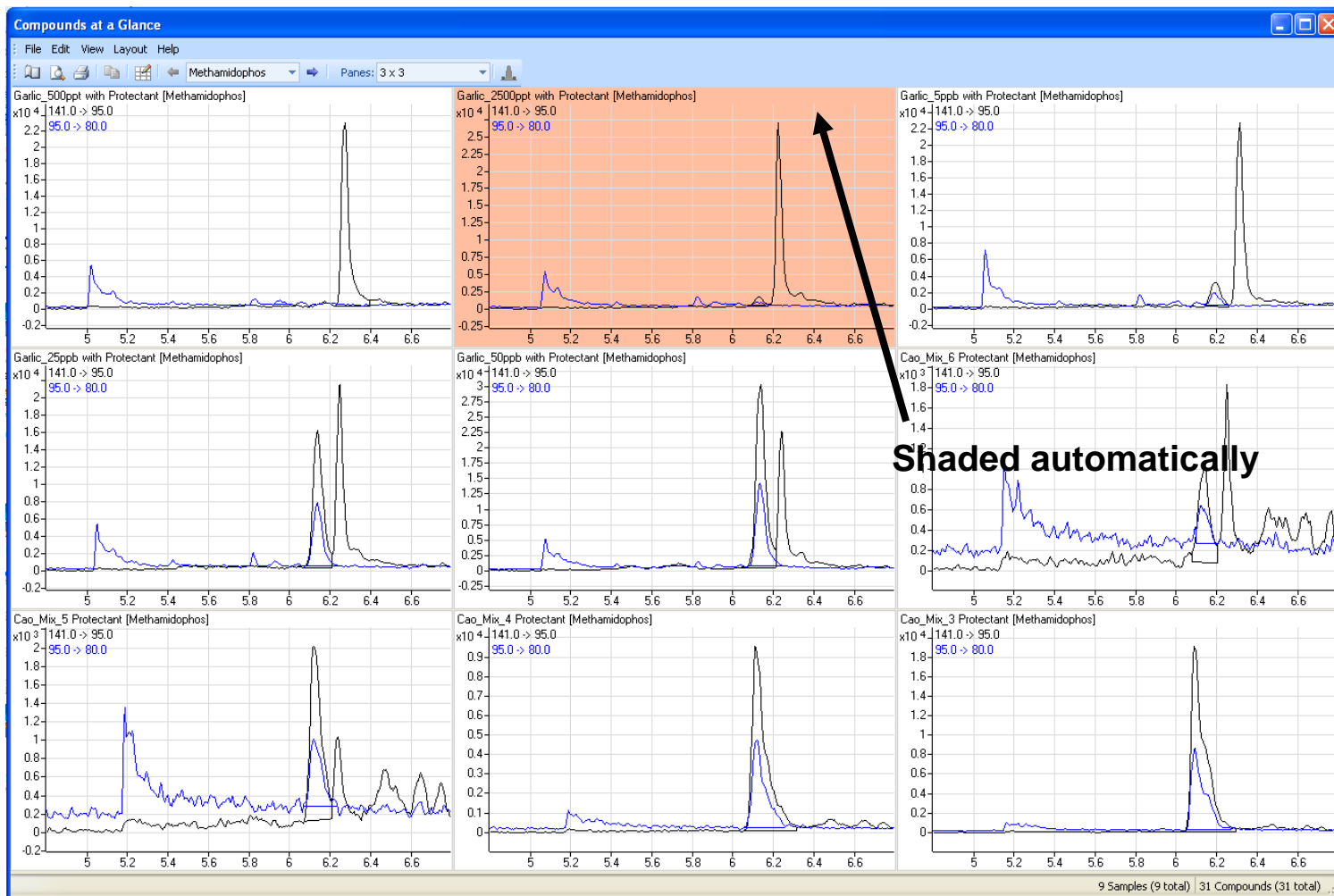
Compounds-at-a-Glance allows you to view multiple traces of compounds at a single glance.



- View up to 10 x 10 chromatograms
- Overlay Target with ISTD
- Overlay Quantifier with Qualifiers
- View chromatograms across 100 samples

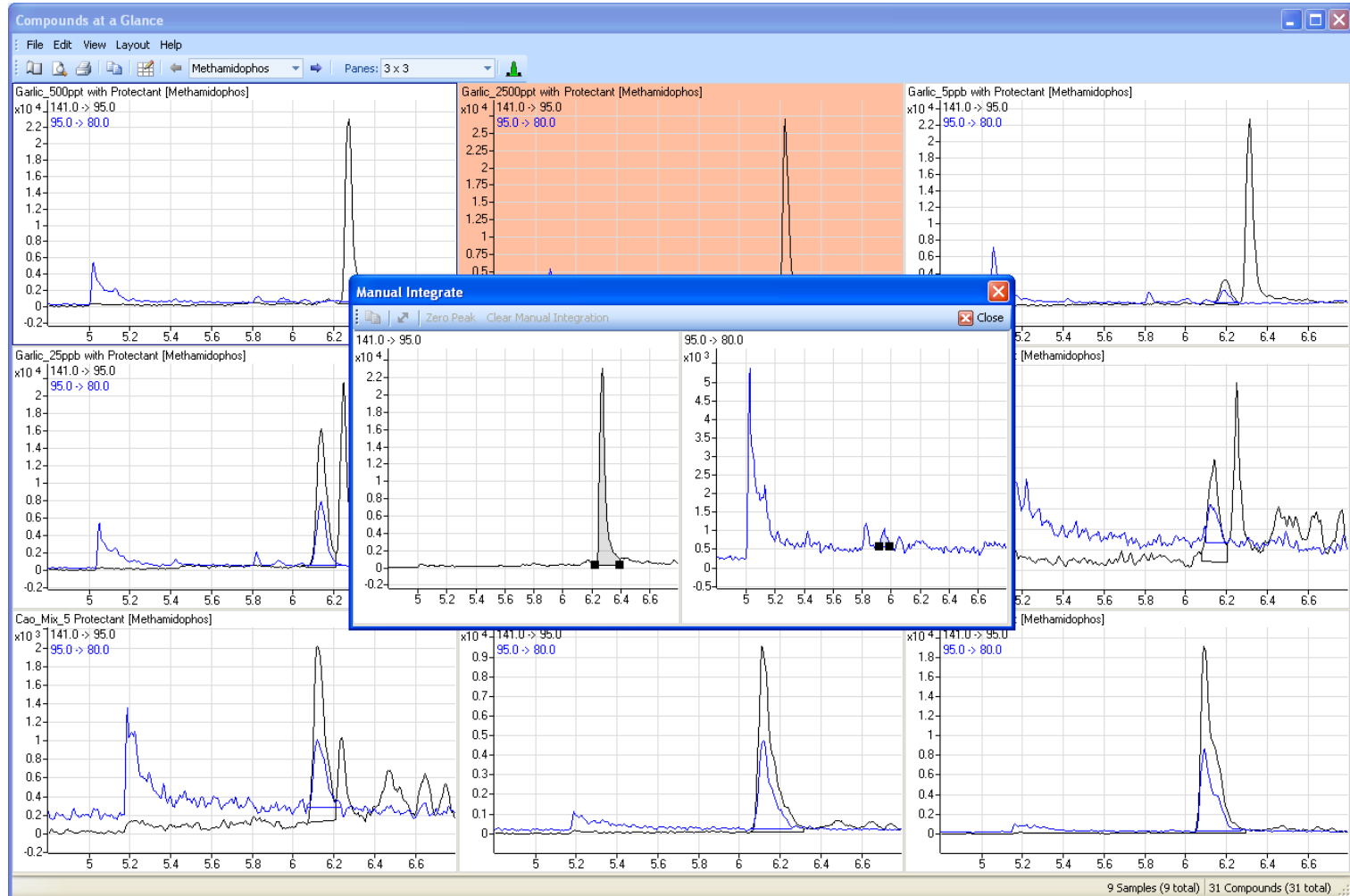
# Compounds-at-a-Glance

You can view compound outliers at-a-glance too.



# Compounds-at-a-Glance

You can view the manual integration of compounds at a glance too.



# Quantitation Method Creation

Easy way to create a target method from acquired data (MRM, SIM or Scan).  
Using information from a data file, MassHunter Quant can create a target compound list - generating Compound Name, Retention Time, Quant and Qual ions, and ratios automatically.

The screenshot displays the Agilent MassHunter Quantitative Analysis interface. The top window shows the 'Method Setup Tasks' menu with options like 'New Method from Acquired MRM Data', 'New Method from Acquired Scan Data', and 'New Method from Acquired Scan Data with Library Search'. The bottom window shows a table of quantifier data with several cells circled in red.

Name	TS	Transition	Collision	Scan	Type	RT
Amp	1	136.2 -> 91.4	5.0	MRM	Target	2.020
Qualifier						
Precursor Ion	Product Ion	Transition	Rel. Resp.	Uncertainty		
136.2	119.4	136.2 -> 119.4	28.0	20.0		
Qualifier						
Name	TS	Transition	Collision	Scan	Type	RT
Amp-d5	1	141.1 -> 93.4	5.0	MRM	ISTD	1.990
Qualifier						
Precursor Ion	Product Ion	Transition	Rel. Resp.	Uncertainty		
141.1	124.4	141.1 -> 124.4	27.9	20.0		
Qualifier						
Name	TS	Transition	Collision	Scan	Type	RT
Cocaine	1	304.1 -> 182.0	5.0	MRM	Target	2.449
Qualifier						

# Automatic Compound Detection – Scan Data

Automatic compound detection works with both MRM and Scan data.

For scan data, Library information can be used to add compound name and CAS#;

The Quant and Qual ions and ratios are taken from the data file information.

The screenshot displays the Agilent MassHunter Quantitative Analysis software interface. The main window is titled 'Agilent MassHunter Quantitative Analysis - [New Method]'. The 'Method Tasks' sidebar on the left includes sections for 'Method Setup Tasks' (MRM Compound Setup, Retention Time Setup, ISTD Setup, Concentration Setup, Qualifier Setup, Calibration Curve Setup, Globals Setup), 'Save / Exit' (Validate, Save, Save As..., Exit), 'Manual Setup Tasks', 'Outlier Setup Tasks', and 'Advanced Tasks'.

The 'Method Table' section shows the following configuration:

- Level Name Prefix:  # of Levels: 10 Create Levels Time Segment: <All>
- Sample Table:
 

Name	Data File	Type	Level	Acq. Method File	Acq. Date-Time
CMAMCal_L4.d	CMAMCal_L4.d				
- Quantifier Table:
 

Name	TS	Transition	Collision	Scan	Type	RT
Amp	1	136.2 -> 91.4	5.0	MRM	Target	2.020
- Qualifier Table:
 

Precursor Ion	Product Ion	Transition	Rel. Resp	Uncertainty
136.2	119.4	136.2 -> 119.4	28.0	20.0
- Another Quantifier Table:
 

Name	TS	Transition	Collision	Scan	Type	RT
Amp-d5	1	141.1 -> 93.4	5.0	MRM	ISTD	1.990

The 'Method Table' section at the bottom shows the following configuration:

- Level Name Prefix:  # of Levels: 10 Create Levels Time Segment: <All> Compound:
- Sample Table:
 

Name	Data File	Type	Level	Acq. Method File	Acq. Date-Time
Cal_L07.d	Cal_L07.d				
- Qualifier Table:
 

Name	TS	Scan	Type	MZ	CAS#	Library Match Score	RT	Library RT	RI	Library RI
Compound_1	1	Scan	Target	44.0			3.833			
Dichlorodifluoromethane	1	Scan	Target	84.9	75-71-8		95.6			
Methane, chloro-	1	Scan	Target	50.0	74-87-3		89.3			
Cyclobutane, ethyl-	1	Scan	Target	41.1	4806-61-5		69.3			
Compound_6	1	Scan	Target	60.0			5.168			
Methane, bromo-	1	Scan	Target	95.9	74-83-9		88.7			
Aminomethanesulfonic acid	1	Scan	Target	64.0	13881-91-9		50.2			
Trichloromonofluoromethane	1	Scan	Target	100.9	75-69-4		91.0			
Acetone	1	Scan	Target	43.0	67-64-1		81.9			

# Multiple Integrators / Compound Specific

Method Table

Level Name Prefix: # of Levels: 10 Create Levels Time Segment: <All> Compound: Amp Reset Table View

Sample	Name	Data File	Type	Level	Acq. Method File	Acq. Date-Time
	Calib-L5	CMAMCaL5.d	Cal	L5	APClautotune.m	5/12/2006 2:03...

Quantifier	Name	TS	Transition	Scan	Type	RT	Int.	Int. Params.
	Amp	1	136.2 -> 91.4	MRM	Target	2.102	Agile	
Qualifier	Precursor Ion	Product Ion	Transition	Rel. Resp.	Uncertainty	Int. Params.		
	136.2	119.4	136.2 -> 119.4	26.8	20.0			

Quantifier	Name	TS	Transition	Scan	Type	RT	Int.	Int. Params.
	Amp-d5	1	141.1 -> 93.4	MRM	ISTD	2.078	MS-MS (GC)	
Qualifier	Precursor Ion	Product Ion	Transition	Rel. Resp.	Uncertainty	Int. Params.		
	141.1	124.4	141.1 -> 124.4	26.4	20.0			

Quantifier	Name	TS	Transition	Scan	Type	RT	Int.	Int. Params.
	Cocaine	1	304.1 -> 182.0	MRM	Target	2.449	Universal	

Compound Information

Integration

Integrator: Agile

- Agile
- MS-MS
- MS-MS (GC)
- General
- Universal

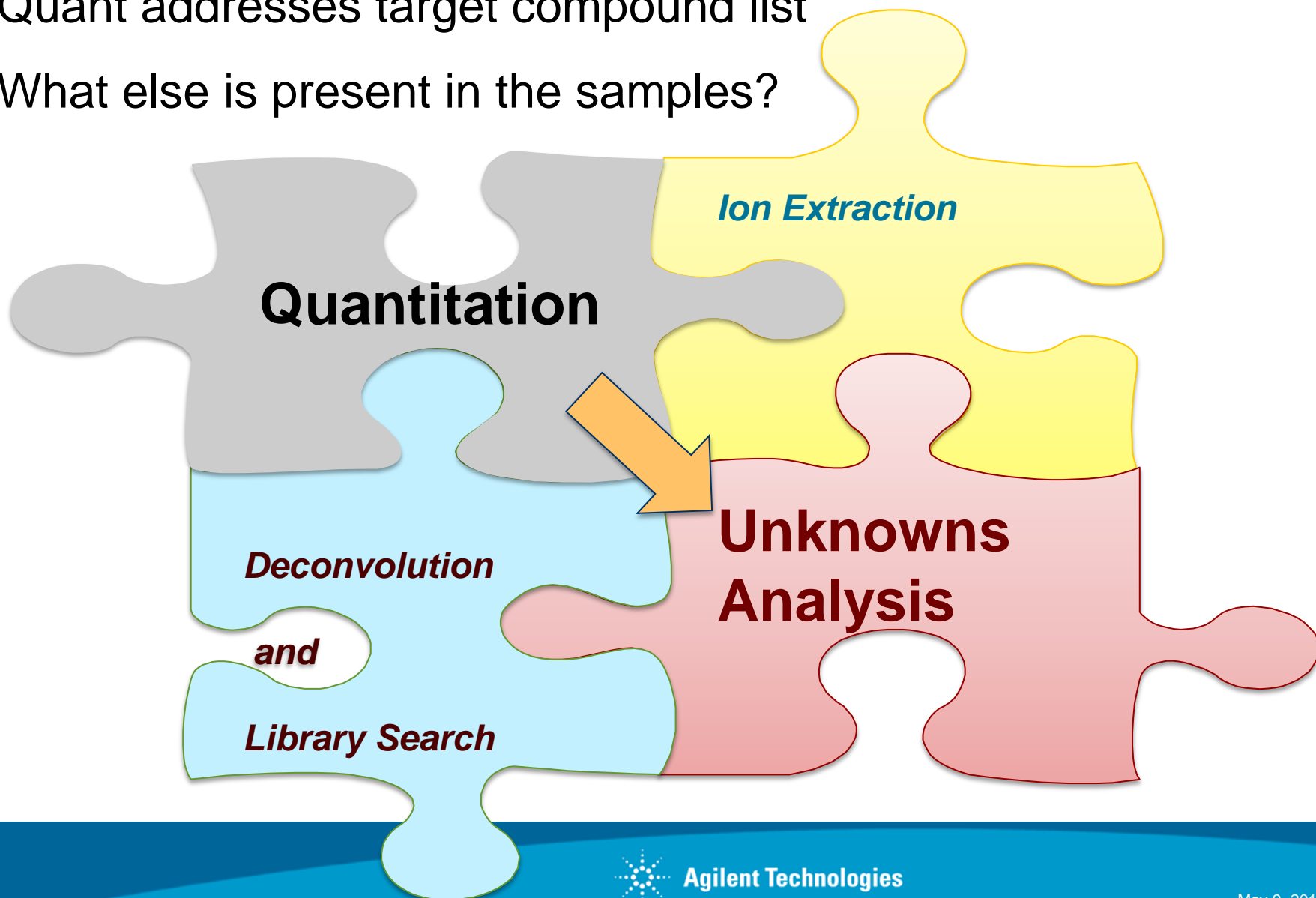
Buttons: Apply to All, OK, Reset, Default, Cancel, Apply



# Overview of Unknowns Analysis

Quant addresses target compound list

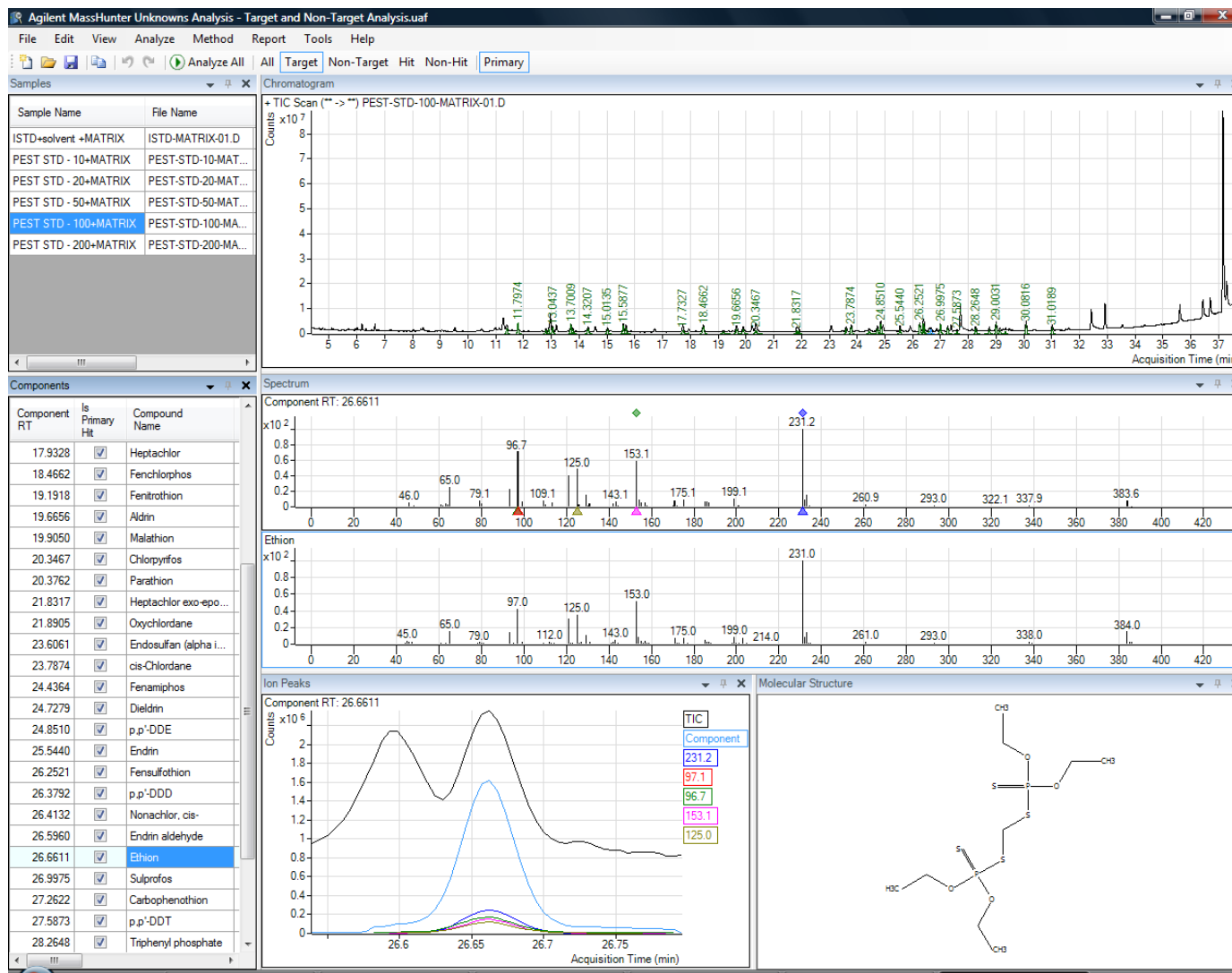
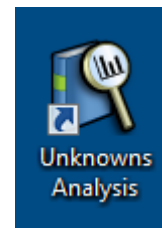
What else is present in the samples?



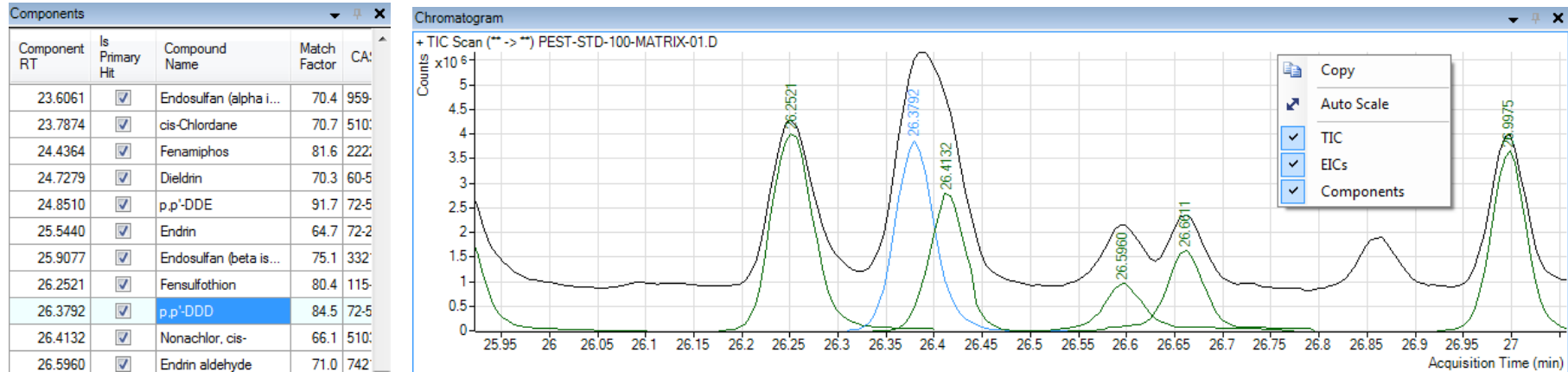
# Unknowns Analysis Workflow

- Process batch of samples in Quantitative Analysis
- Run Unknowns Analysis
- Analyze
  - Perform **deconvolution** to create **components**
  - Perform **library matching** on components, assign compound ID
  - Link **components to Quant target** compounds from
  - Assign **estimated concentrations** to non target components
- Review data
  - View component and library spectra
  - View molecular structure vs. spectrum
  - View ion peak shapes vs. component peak shape vs. TIC
  - Edit components (change compound ID, delete)
  - Run queries for custom review
- Print Report

# Unknowns Analysis



# Chromatogram



Chromatogram displays selected component(s) in **Blue**

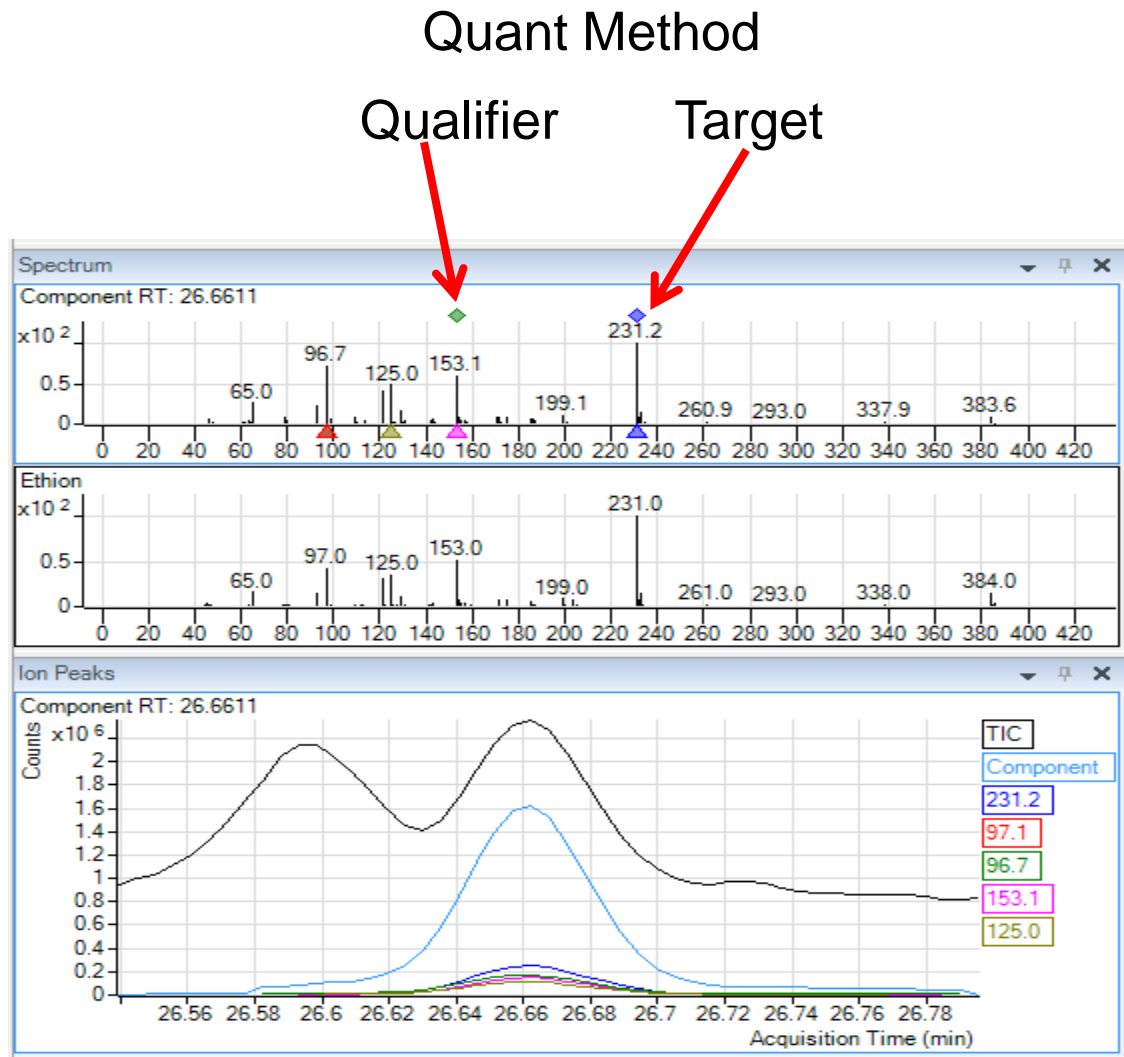
All non-selected ions (EIC) displayed in **Green**

TIC displayed in **Black**

Clicking in the Chromatogram display selects the nearest peak and selects it in Components table

# Spectrum & Ion Peaks

- Default number ions displayed in Ions Peaks is 5, limit is 10
- Click on ion in Spectrum to make it add / remove in Ion Peaks
- Click on label in Spectrum or Ion Peaks to remove



# Outline of Topics

Topic 1: Introduction to MassHunter

Topic 2: Data Acquisition / Conversion

Topic 3: Qualitative Analysis

Topic 4: Quantitative Analysis

**Topic 5: Reporting**

Q & A

# MassHunter Excel Reporting

- Excel Based (Excel 2007 & 2010 supported)
- MassHunter application exports data in XML and graphics files
- Templates define report formatting
- Over 100 shipping report templates
- Reports can be altered for desired information & appearance
- Customization using Excel features (function, formatting, code)
- Computer Based Training for report customization by users
- Some customization available through Agilent

# Shipping Quant 5.0 Templates

90 Shipping Quant Templates - 14 “New” Templates added for B.05 release

English (Letter & A4), Chinese (A4), Japanese (A4)

Significant new templates for

Compliance (1)

DrugQuant (2)

EnviroQuant (2)

Unknowns Analysis (4)

[Mockup reports for both PDF and XLSX formats](#)

	A	B	C	D	E	F
1	DIR	SUBDIR	FAST	ExcelTemplate	ExcelWorkbook	PDF
2	ESTD	Parts	FAST	QuantReport_ESTD_Summary_FAST_B_04_00.xlsx	<a href="#">HyperLink to Workbook (.xlsx)</a>	<a href="#">HyperLink to Adobe Acrobat</a>
3	ESTD	Parts		QuantReport_ESTD_Summary_B_04_00.xlsx	<a href="#">HyperLink to Workbook (.xlsx)</a>	<a href="#">HyperLink to Adobe Acrobat</a>
4	ESTD	Parts	FAST	QuantReport_ESTD_Samples_FAST_B_04_00.xlsx		
5	ESTD	Parts		QuantReport_ESTD_Samples_B_04_00.xlsx		
6	ESTD	Results	FAST	QuantReport_ESTD_ResultsSummary_FAST_B_04_00.xlsx		
7	ESTD	Results		QuantReport_ESTD_ResultsSummary_B_04_00.xlsx		
8	ESTD	Results	FAST	QuantReport_ESTD_ResultsQualifierRatios_FAST_B_04_00.xlsx		
9	ESTD	Results		QuantReport_ESTD_ResultsQualifierRatios_B_04_00.xlsx		
10	ESTD	Results	FAST	QuantReport_ESTD_ResultsComplete_FAST_B_04_00.xlsx		
11	ESTD	Results		QuantReport_ESTD_ResultsComplete_B_04_00.xlsx		
12	ESTD	Results	FAST	QuantReport_ESTD_ResultsByCompound_FAST_B_04_00.xlsx		
13	ESTD	Results		QuantReport_ESTD_ResultsByCompound_B_04_00.xlsx		
14	ESTD	NotDetected	FAST	QuantReport_ESTD_NotDetected_FAST_B_04_00.xlsx		
15	ESTD	NotDetected		QuantReport_ESTD_NotDetected_B_04_00.xlsx		
16	ESTD	NotDetected		QuantReport_ESTD_NotDetectedByCompound_B_04_00.xlsx		

Sample Sheet(s)

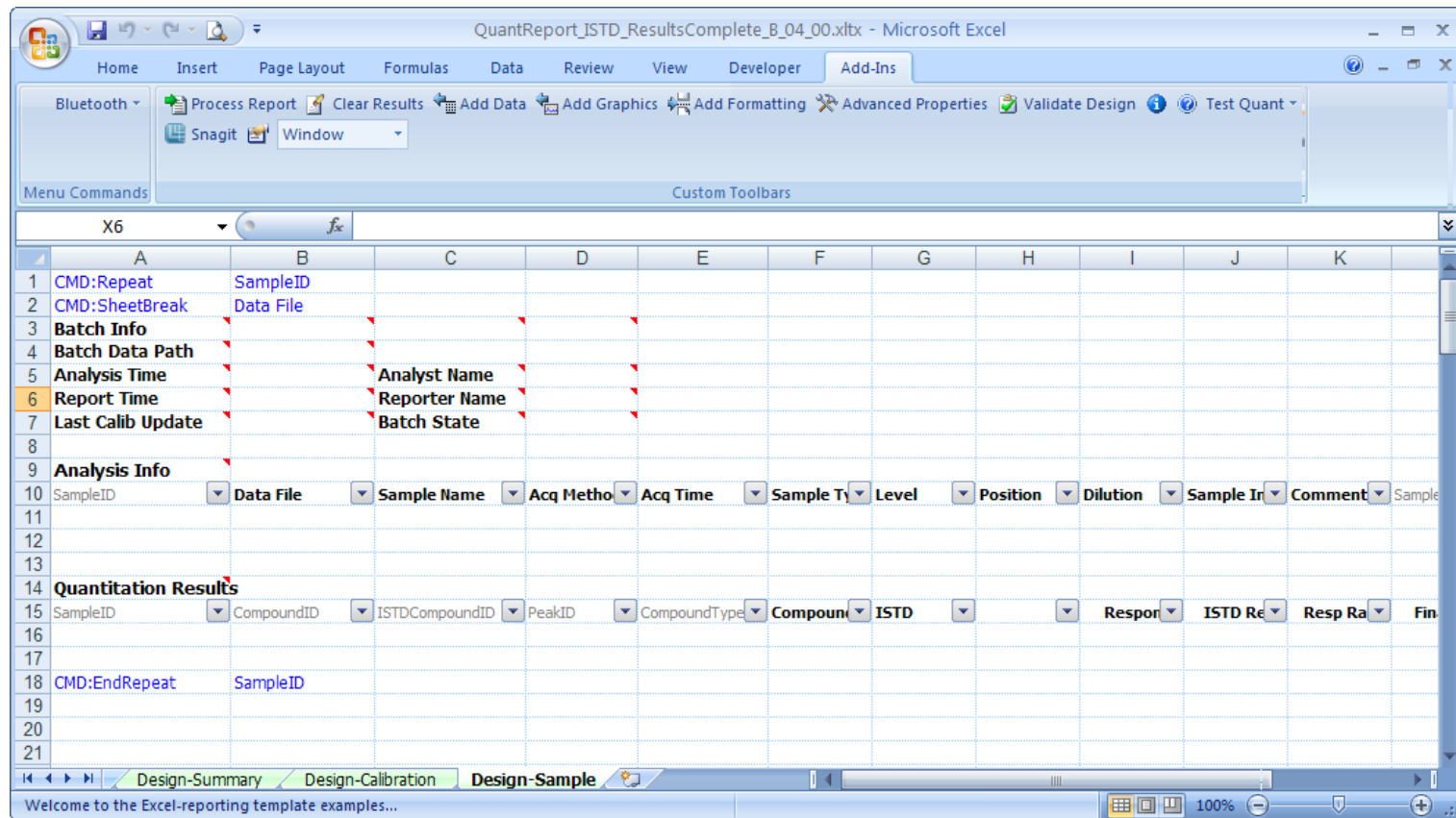
- Batch Info  
record batch identification information
- Analyze Info  
show sample specific information
- Sample Chromatogram  
Include sample chromatogram graphic
- Quantitation Results  
list results and concentration for compounds
- Compound Graphics  
display compound graphics for each compound



# Report Template Design Worksheets

Customize the template by placing data and graphics in the desired locations

Templates may have multiple Design worksheets with different layouts



# Excel XML Source Window

- Reporting uses XML mapping to import results into templates
- Drag and drop to add data to existing reports

The screenshot displays an Excel spreadsheet with a table of data and an XML Source window on the right. The table has columns A through G and rows 1 through 31. The data is organized into sections: 'Batch Info' (rows 1-5), 'CMD:Repeat' (row 7), 'CMD:SheetBreak' (row 8), a main data table (rows 9-18), and 'CMD:EndRepeat' (row 19). The XML Source window shows a tree structure of XML elements under 'QuantitationDataSet\_Map'. The element 'ns1:CompoundName' is highlighted in blue. An orange arrow points from this element to the cell at row 10, column C, which is currently empty. Below the tree, there are instructions on how to map repeating elements and import XML data.

SampleID	CompoundID	CompoundName	GraphicCalibr	RetentionTime		
SampleID	CompoundID	PeakID	CompoundID	Data File	Type	Name
SampleID	CompoundID	CompoundType	SampleName	SampleType	GraphicDeal	romatogram

**XML Source**  
XML maps in this workbook:  
QuantitationDataSet\_Map

- ns1:TargetCompound
  - ns1:BatchID
  - ns1:SampleID**
  - ns1:CompoundID**
  - ns1:AccuracyLimitMultiplierLOQ
  - ns1:AccuracyMaximumPercentDeviation
  - ns1:AreaCorrectionFactor
  - ns1:AreaCorrectionMZ
  - ns1:AverageRelativeRetentionTime
  - ns1:AverageResponseFactor
  - ns1:BlankResponseOffset
  - ns1:CASNumber
  - ns1:CCISTDResponseRatioLimitHigh
  - ns1:CCISTDResponseRatioLimitLow
  - ns1:CCRResponseRatioLimitHigh
  - ns1:CCRResponseRatioLimitLow
  - ns1:CollisionEnergy
  - ns1:CompoundGroup
  - ns1:CompoundName**
  - ns1:CompoundType

To map repeating elements, drag the elements from the tree onto the worksheet where you want the data headings to appear.

To import XML data, right click an XML mapped cell, point to XML, and then click Import.


Options XML Maps...  
Verify Map for Export...  
Tips for mapping XML

# MassHunter Reporting User Information (CBT)



## Agilent MassHunter Reporting User Information

### MassHunter Reporting User Information



#### Welcome to Agilent MassHunter Reporting User Information

Whether you want to use preconfigured reports or customize templates for special applications, this collection brings together all the training for MassHunter reporting in one location.

#### MassHunter Reporting Training

Read it, see it, hear it, do it! This self-paced curriculum incorporates multiple formats, to reinforce concepts and to allow you to adapt the training to your unique learning style. The [MassHunter Reporting Training](#) provides:

- Written topics that summarize procedures
- Demo movies to show you how to use the software
- Software reviews that allow you to interact with the programs
- No-fail quizzes with instant feedback

In addition, this DVD includes:

- Comprehensive [familiarization exercises](#) that guide you through the software step-by-step – and provide tips along the way
- Extensive online Help for MassHunter Reporting
  - [Quantitative](#)
  - [Qualitative](#)
- A [list of the demo movies](#), for quick access

#### Where do I start?

While you can customize your path through the training, we recommend the following:

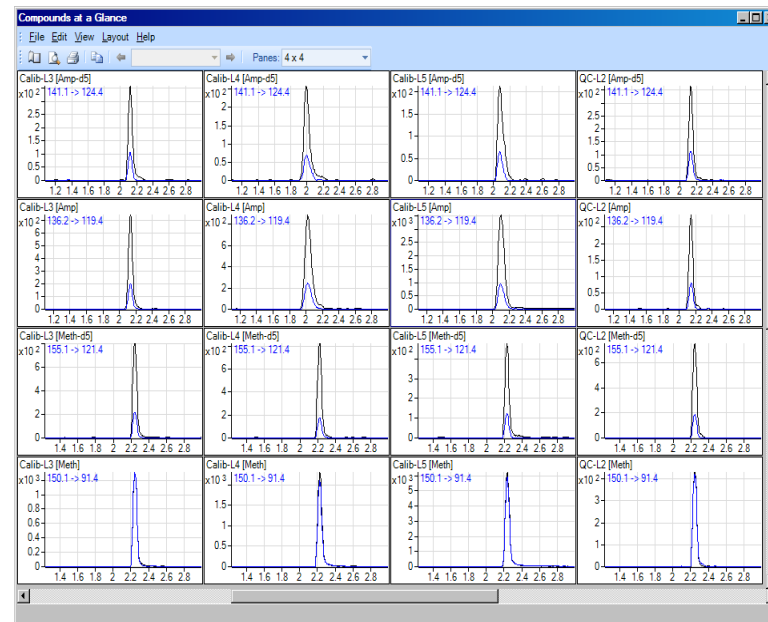
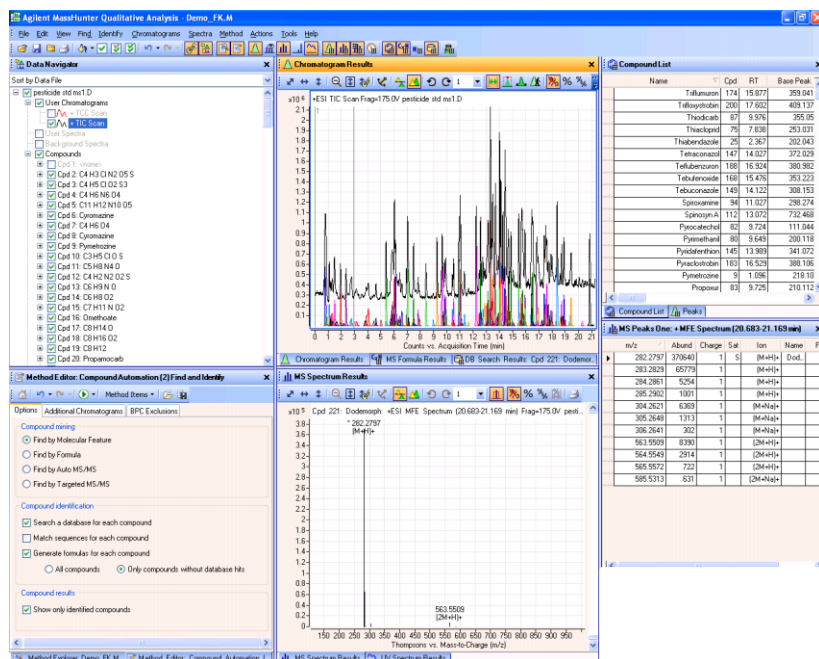
1. Start with the [MassHunter Reporting Training](#) and follow the suggested order of topics.
2. Next, work through the [Familiarization Guide](#) to solidify your knowledge. Do all the familiarization exercises at once, or intersperse them with the Reporting Training, where the topics tell you when a familiarization exercise is available.
3. When you perform a task for the first time or forget how to do it later:
  - Consult the online Help for MassHunter Reporting, which you can access from this DVD or directly from the Add-Ins tab in Microsoft® Excel.
  - View the [list of the demo movies](#) to select one for a quick refresher.

#### Quick Access

- [Reporting Training](#)
- [Familiarization Guide](#)
- [Reporting Help - Quant](#)
- [Reporting Help - Qual](#)
- [List of Demo Movies](#)

# MassHunter Workstation

## Increase your productivity significantly



# Questions?

Terry is available today for questions, software demos and problem solving.