



# MassHunter Software Overview, Tips, & Tricks

Anne Blackwell, AE

Mark Sartain, AE

Sumit Shah, AE

David Weil, AE

Nathan Miller, PS

ASTS – Vancouver, BC May 8<sup>th</sup>

La Jolla, CA May 20<sup>th</sup>

# MassHunter Workstation

One software for all your Agilent mass specs

Minimize the learning and optimize the use of software in your lab across different mass spec instrument platforms

- Control and data processing for Agilent GC/MS, LC/MS, and ICP-MS instruments



LC/MS



GC/MS



ICP-MS

- From GC and LC Single Quad to Accurate Mass QTOF's

# MassHunter Software for your Key Applications

- **Qualitative Analysis** for confident identifications and to set up methods

Food



- **Quantitative Analysis** for fast and accurate results

Pharma



- **Acquisition** for innovative techniques such as tMRM to confirm compounds

Veterinary Drugs



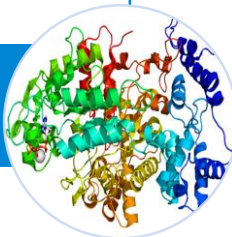
- **Personal Compound Database and Libraries (PCDLs)** for rapid identification

Forensic Toxicology



- **Spectrum Mill** for accurate identification of proteins

Proteomics



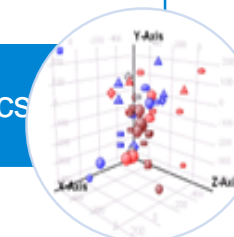
- **BioConfirm** for characterization of intact proteins, peptides, and monoclonal antibodies

Biopharma



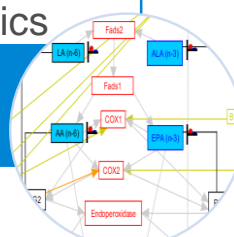
- **Mass Profiler Professional (MPP)** for differential profiling

Metabolomics



- **Pathway Architect** for bringing together genomics, proteomics, and metabolomics

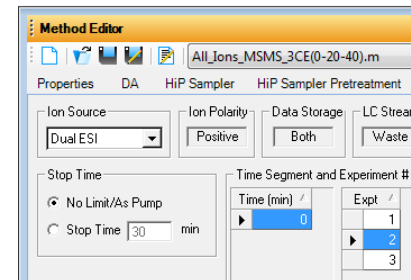
Integrated Biology



# Agilent MassHunter Core Programs

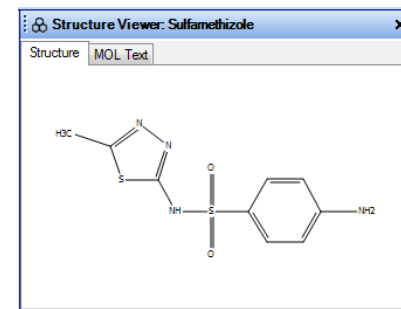
## Acquisition

- Support for all Agilent LCs, GCs, and mass spectrometers
- Superior compound detection (LC/MS) tMRM, All Ions MS/MS, and Ion Mobility



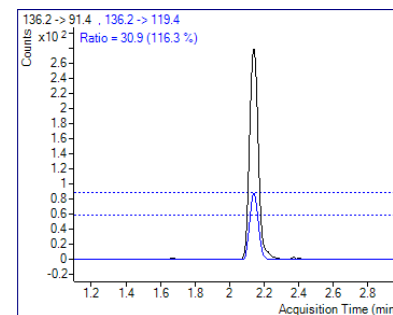
## Qualitative Analysis

- Application Focused Solutions Kits: Software, Libraries, Methods
- Patented Data mining & identification software algorithms formula/structure

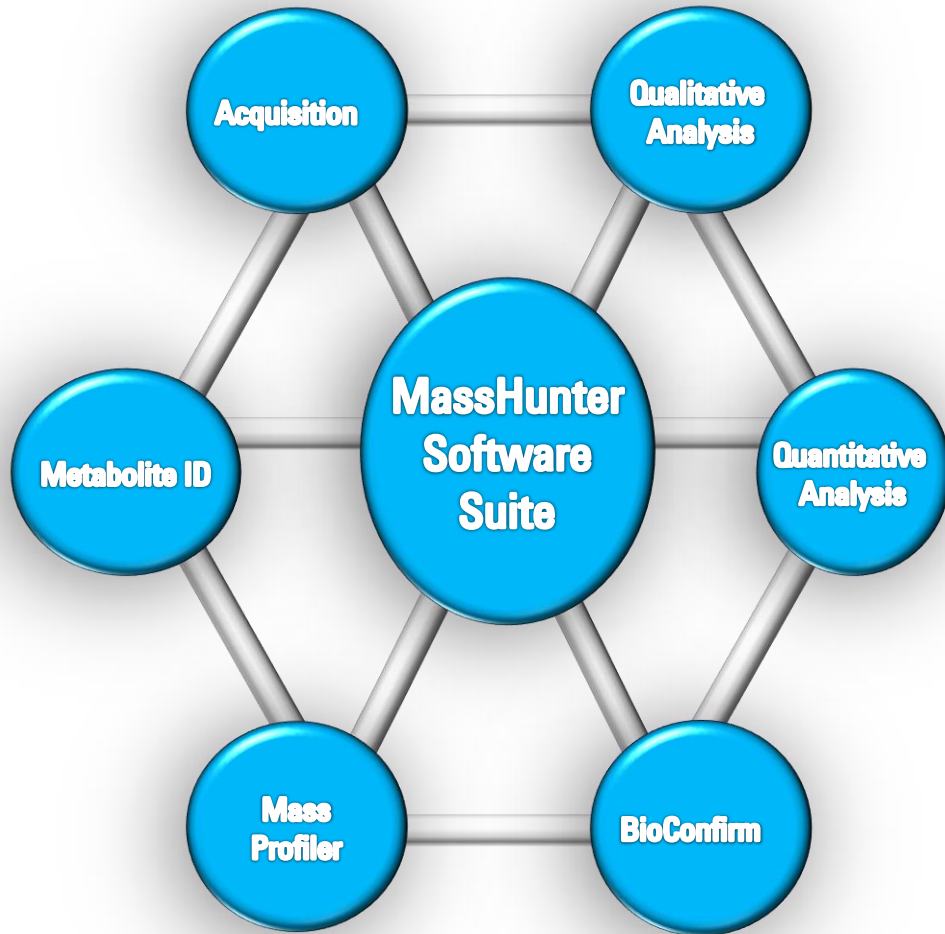


## Quantitative Analysis

- High-throughput quantitation of target compounds
- Easily visualize results using the Batch Table or Compounds-at-a-Glance from ALL Agilent LCs, GCs, and Mass Specs



# MassHunter Suite of Software:



- Qualitative Analysis (Qual)
- BioConfirm
- Spectrum Mill B.04.01
- Molecular Structure Correlator (MSC)
- PCDL Manager
- Profinder
- Pathways to PCDL
- Mass Profiler (MP)
- Mass Profiler Professional (MPP)
- SimLipid (Premier Biosoft)

**Fully integrated workflows to enable you to identify, plan, and execute your next experiment**

# MassHunter Software Window 7

## Current Versions (May 2014)

- MassHunter Acquisition for QQQ B.07.00 **NEW**
- MassHunter Qualitative Analysis B.06.00 SP1\*
- MassHunter Quantitative Analysis B.07.00 **NEW**
- MassHunter BioConfirm B.06.00
- MassHunter PCDL Manager B.04.00 SP1
- MassHunter METLIN Metabolite PCDL B.05.00
- MassHunter Mass Profiler Professional 12.65 **NEW**
- MassHunter Profinder B.06 **NEW**
- Accurate Mass Libraries Pesticide/Vet Drugs/Forensics
- Pathway to Database Creator Software
- ChemStation SQ (LC/MS and GC/MS) to MassHunter file translator

**All run on Windows 7 Pro 64 bit with Excel 2013**

# Keep Your MassHunter Current!

Online service patches and updates found at [www.agilent.com](http://www.agilent.com)

The screenshot shows the Agilent Technologies website interface. At the top, there is a navigation bar with the Agilent logo, 'Global Sites', and 'Contact Us'. Below this is a secondary navigation bar with links for 'Products & Services', 'Solutions', 'Technical Support', 'Library', 'Training & Events', and 'Buy'. A search bar is located on the right side of this bar. The main content area is titled 'Home > Buy'. On the left, there is a 'FILTERS APPLIED' section with two filters: 'Patches' and 'In the Last 12 Months'. Below this is a 'NARROW YOUR CHOICES' section. The main search results area shows '1-1 of 1 results for MassHunter Qualitative Data Analysis Software'. The result is for 'MassHunter Qualitative Analysis B.06.00 Service Pack 1 (SP1)', which is categorized as 'Patches'. The description states: 'Software patches available for download to fix defects in MassHunter Qualitative Analysis B.06.00 Service Pack 1 (SP1)'.

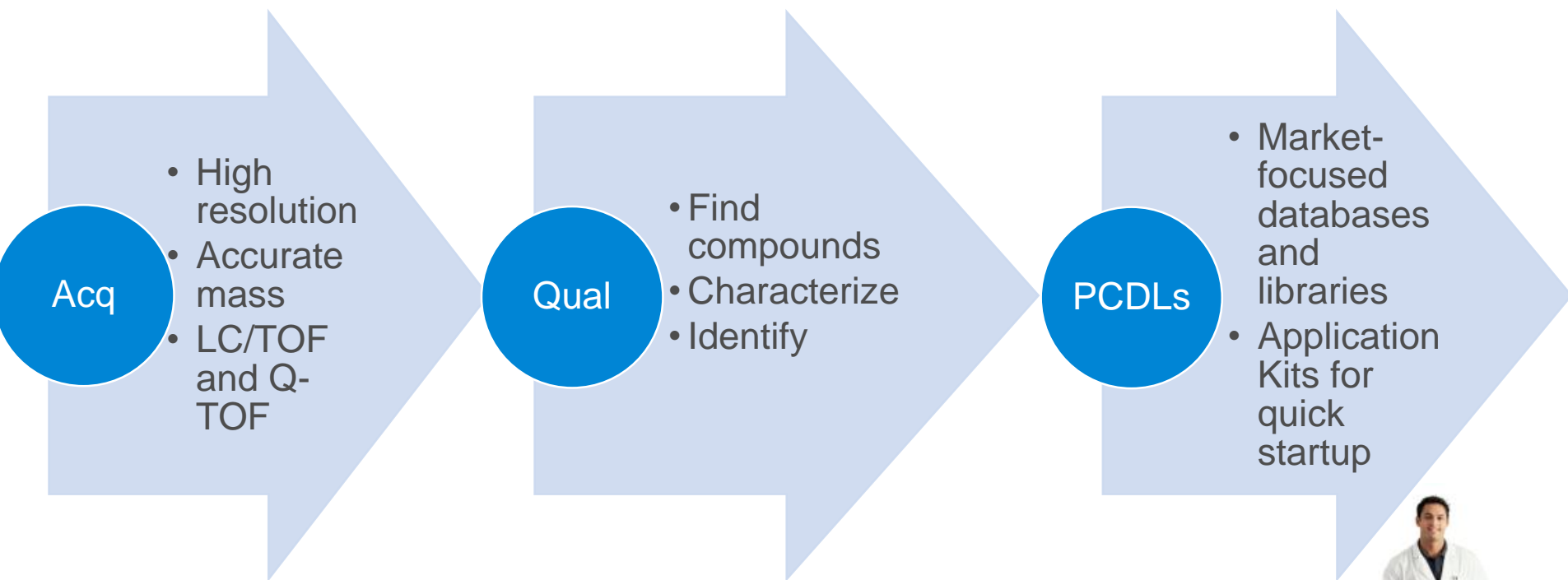
<http://www.chem.agilent.com/en-US/Technical-Support/Software-Informatics/MassHunter-Qualitative-Data-Analysis-Software/Pages/default.aspx>

General Software Technical Support with Patches and Updates

<http://www.chem.agilent.com/en-US/Technical-Support/Software-Informatics/Pages/default.aspx>

# The MassHunter Qualitative Workflow

Identify with confidence



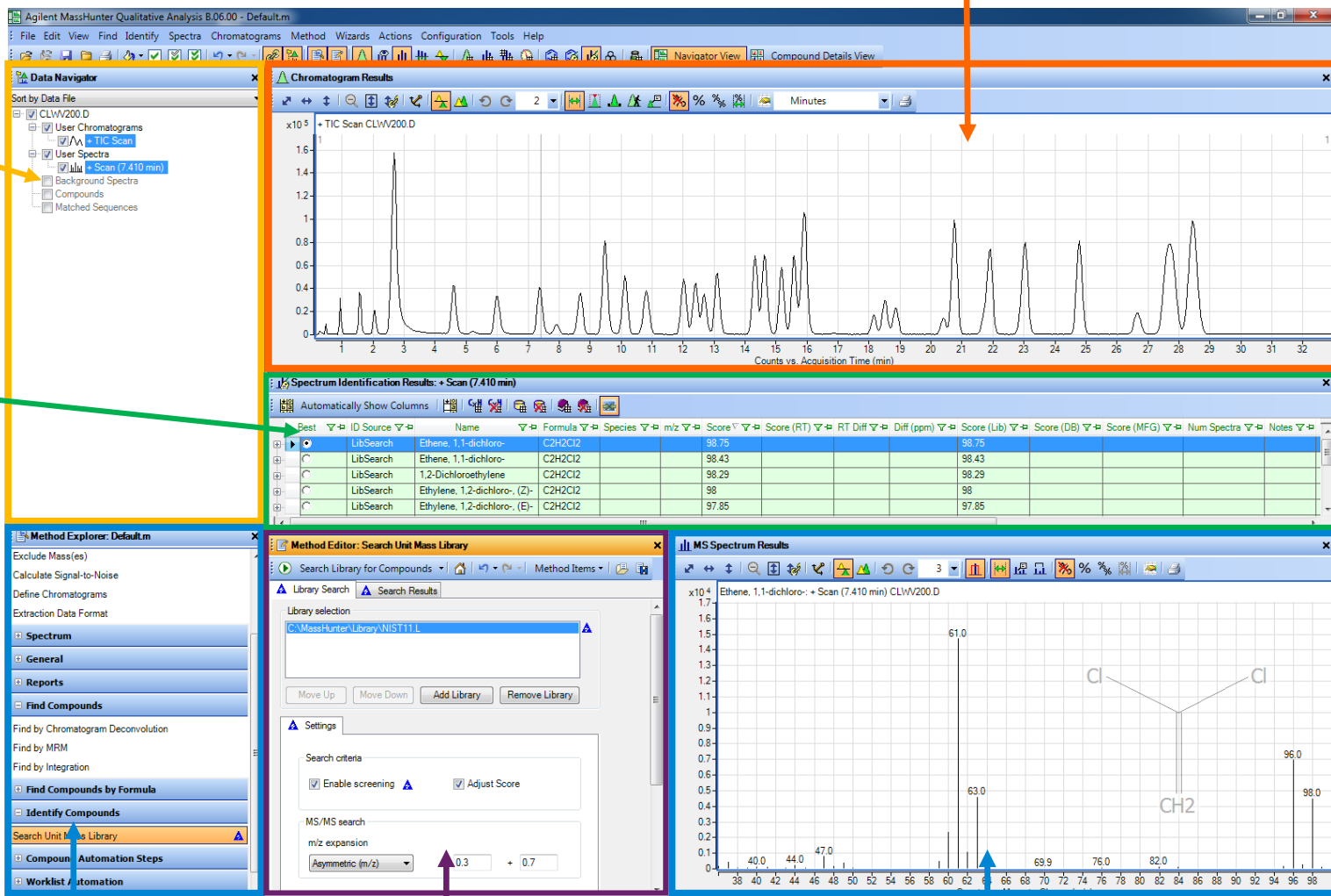
Agilent provides a complete suite of tools, consumables and consulting to set up for the rapid identification of unknowns





# Qualitative Analysis

## Chromatogram Display



Data Navigator

Results Table

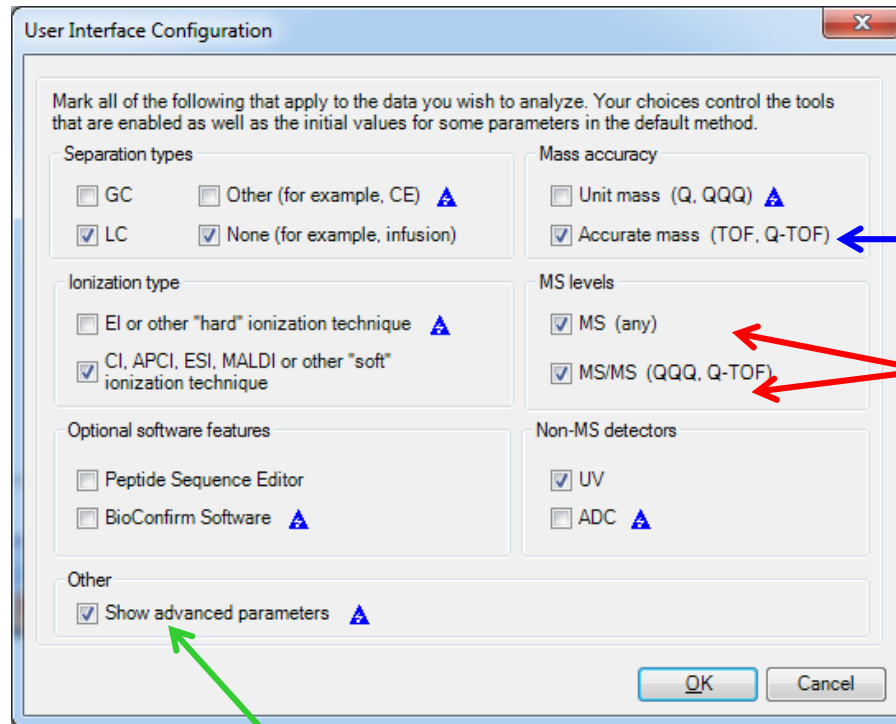
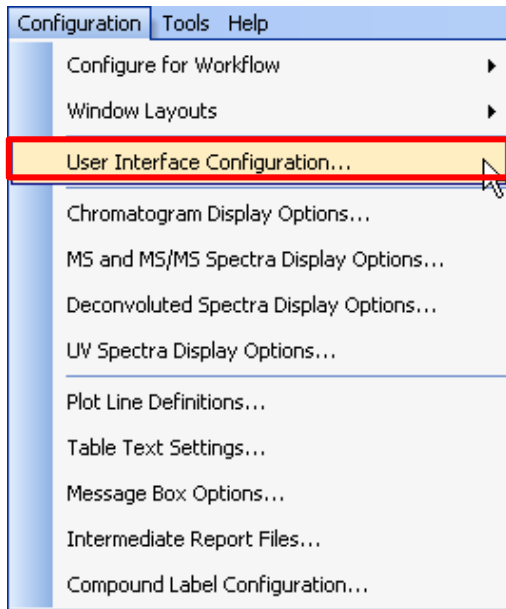
Method Explorer

Method Editor

Spectrum Display

# Qual is used for All Data Type: MSD, QQQ, TOF

## So Setup User Interface for Data File Type



Accurate Mass

Both Levels

Show Advanced Parameters

Setting data file type automatically changes the method options, display and search capabilities

# Selecting Data Types Changes Display

**Find Compounds**

Find by Chromatogram Deconvolution

Find by Integration

## GC/MSD

Separation types

GC     Other (for example, CE)

LC     None (for example, infusion)

Ionization type

EI or other "hard" ionization technique

CI, APCI, ESI, MALDI or other "soft" ionization technique

Mass accuracy

Unit mass (Q, QQQ)

Accurate mass (TOF, Q-TOF)

MS levels

MS (any)

MS/MS (QQQ, Q-TOF)

## LC/QQQ

**Find Compounds**

Find by MRM

Find by Integration

Mass accuracy

Unit mass (Q, QQQ)

Accurate mass (TOF, Q-TOF)

MS levels

MS (any)

MS/MS (QQQ, Q-TOF)

## LC/QTOF

**Find Compounds**

Find by Auto MS/MS

Find by Targeted MS/MS

Find by Molecular Feature

Find by Integration

Mass accuracy

Unit mass (Q, QQQ)

Accurate mass (TOF, Q-TOF)

MS levels

MS (any)

MS/MS (QQQ, Q-TOF)

## LC/TOF

**Find Compounds**

Find by Molecular Feature

Find by Integration

Mass accuracy

Unit mass (Q, QQQ)

Accurate mass (TOF, Q-TOF)

MS levels

MS (any)

MS/MS (QQQ, Q-TOF)

**TIP:** To use low res libraries you must have the GC checked

# And Changes Compound Identification

## Accurate Mass Q(TOF)

### ☐ Identify Compounds

Search Database

Search Accurate Mass Library

Generate Formulas

Combine Identification Results

## Unit Mass MSD/QQQ

### ☐ Identify Compounds

Search Accurate Mass Library

Combine Identification Results

---

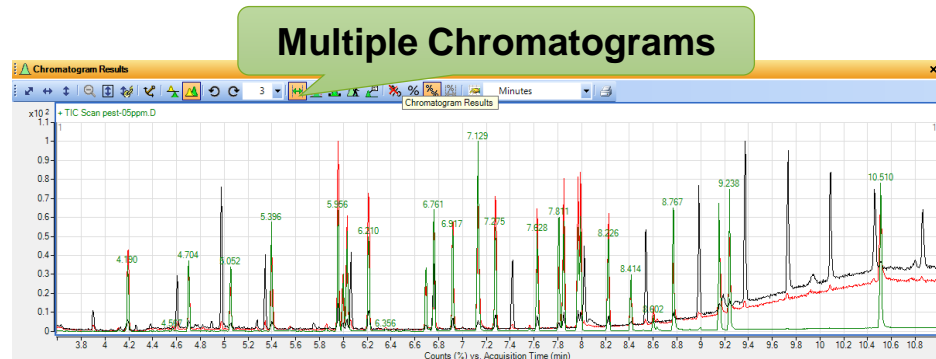
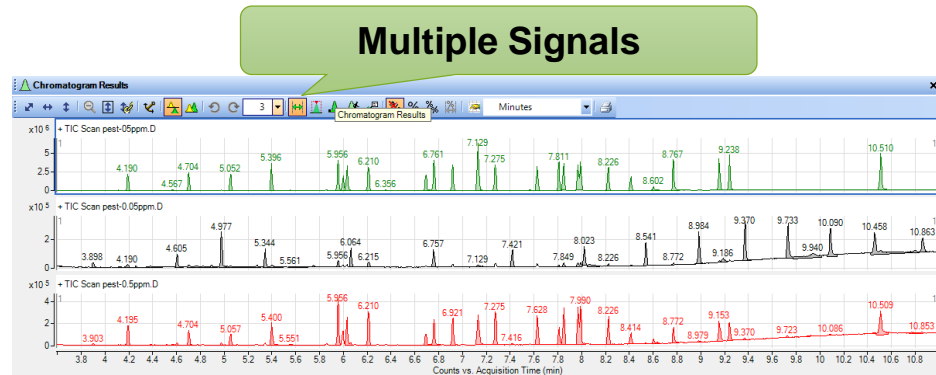
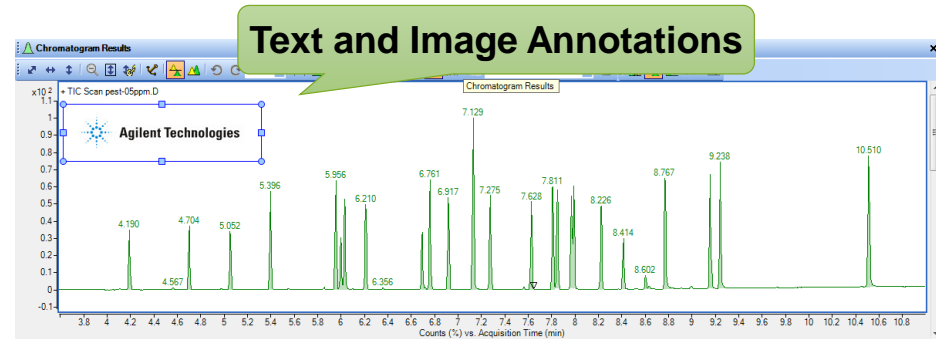
**Tip:** The low resolution \*.L file should be copied to the X:\\MassHunter\\Library\\ subdirectory and one can use the NIST library if you have a license

# Chromatogram Display

## Comprehensive Display Options

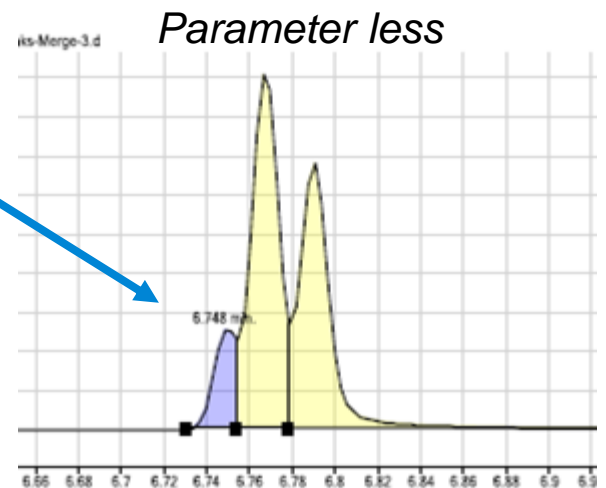
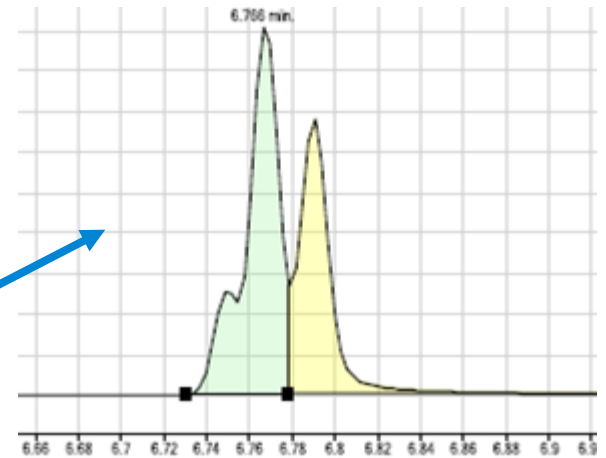
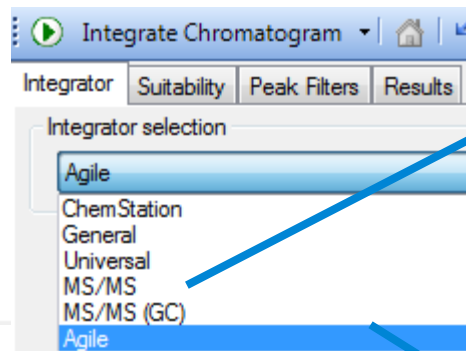
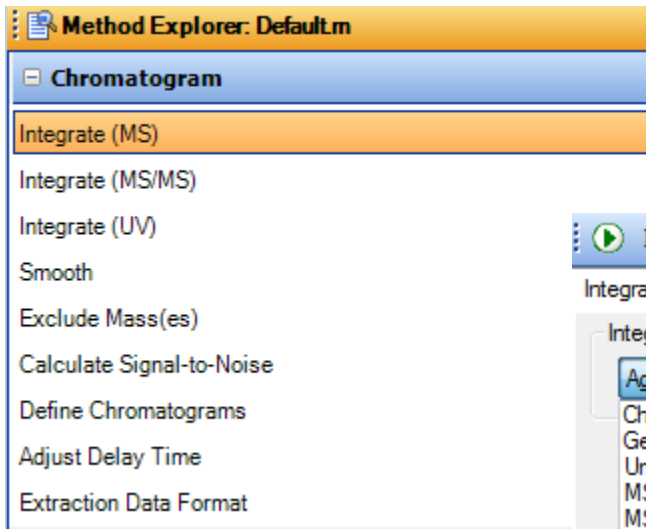
- Display **multiple** Chromatograms, from one or many data files.
- Extract **multiple signal types**, i.e. TIC, EIC, UV, FID, Instrument curves, etc.
- Annotate peaks or chromatograms with text or images

Definition of chromatograms can be stored in the method and used with automation.



# Improved Parameter-less Integrators

## MS/MS and Agile what's the difference?



The Agile integrator requires 75% fewer data points for Integration typically 15 points minimum

**Agile2 Now in QUANT B.07**

# For Accurate Mass Systems

**Use Advanced Tab to Narrow Extraction Limits (10 ppm)**

- Extract Peak Spectrum
- Extract MS Peak Spectrum from UV Peaks
- Extract Chromatograms...**
- Extract Defined Chromatograms
- Use Highlighted Chromatograms

Type:   Integrate when extracted

MS Chromatogram **Advanced** Excluded Masses

MS level:  Polarity:

Scans:

m/z of interest:

m/z value(s):

MS Chromatogram **Advanced** Excluded Masses

Fragmentor:  Ionization:

Collision energy:

Single m/z expansion for this chromatogram

±

- 10
- 20
- 50
- 100
- 200
- 500

## Set to Exclude Reference and Background Ions

MS Chromatogram **Advanced** Excluded Masses

Do not exclude masses

Exclude masses (or m/z ranges) from all new chromatograms

m/z value(s):

Single m/z expansion for this chromatogram

±

# Spectra Display

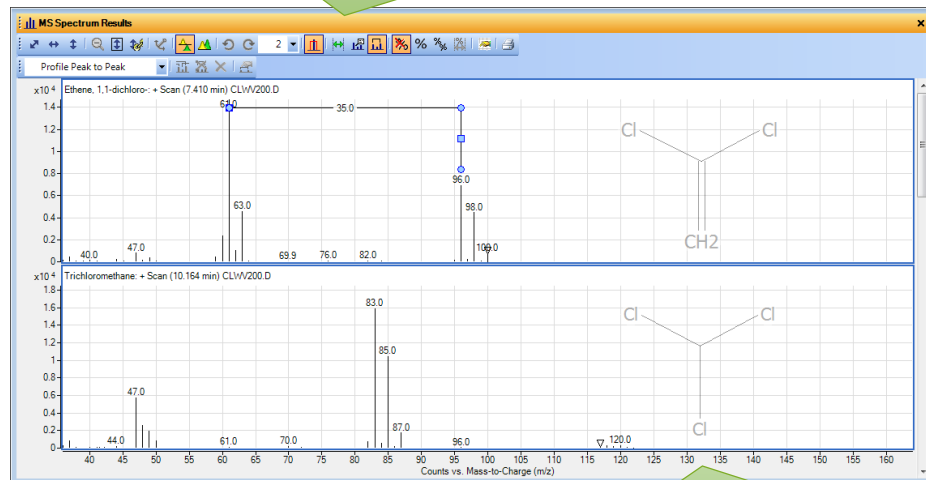
## Extract Spectra via:

- Manual spectra selection
- Integrated peaks
- **Multiple Find-by-Methods**
  - By Deconvolution
  - By Integration
  - By Molecular Feature
  - Find by Formula (Ion)

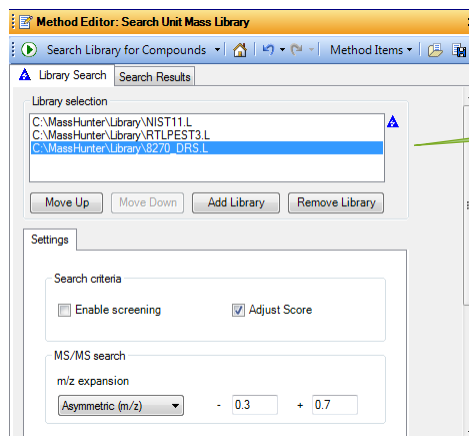
## Identify from Library Searching GCMS

- Multiple Libraries (\*.L)
- Link to NIST MS Search

### Mass Difference Annotations



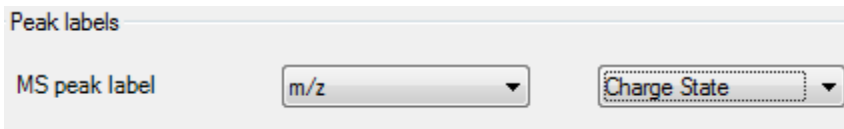
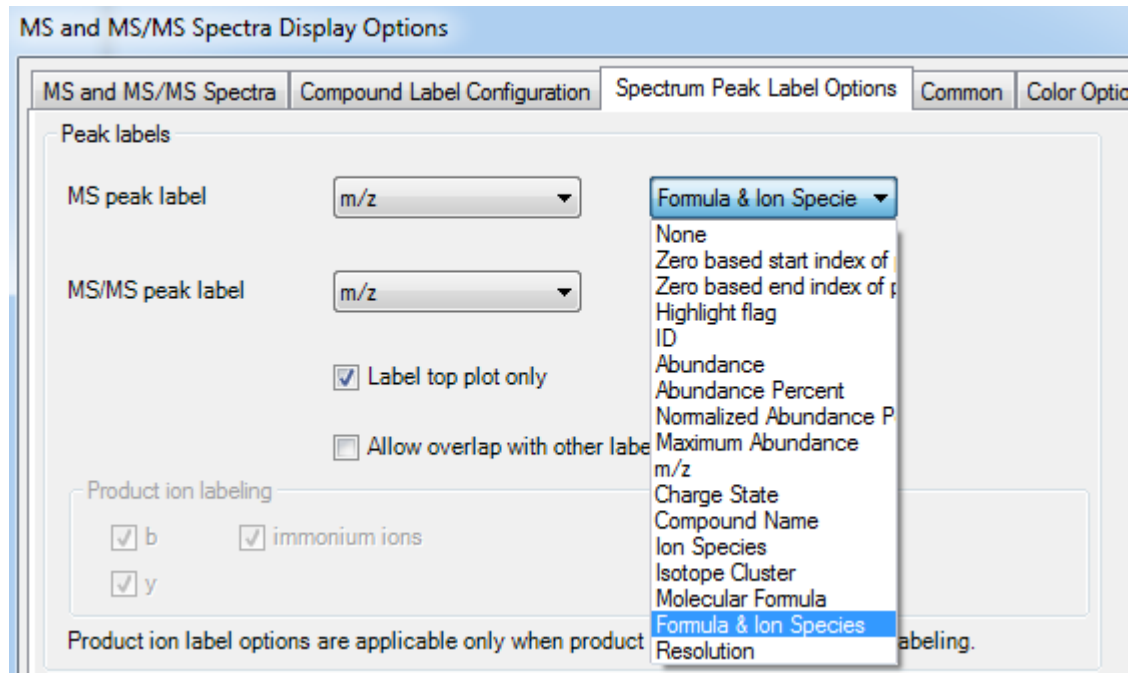
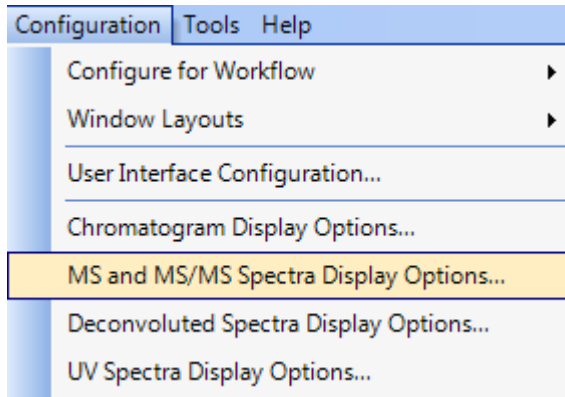
### Structure Annotations



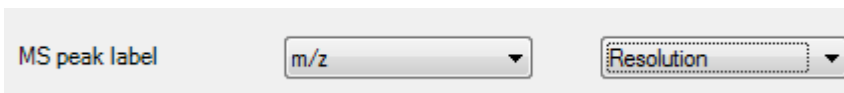
### Search Multiple Libraries



# How to Set Labels on MS and MS/MS Spectra



Multiply Charged Species



In Profile Mode Resolution of MS Peak

# Using Extract Peak Parameters – Saturation Correction

Method Editor: Extract (MS)

Peak Location | Peak Filters | Charge State

Manual Extraction | Peak Spectrum Extraction (MS)

Spectra to include

- At apex of peak
- Average scans > 5 % of peak height

TOF spectra

- Exclude if above 10.0 % of saturation
- In the m/z ranges used in the chromatogram
- Anywhere
- In these m/z ranges 100.0000-2000.0000
- Never return an empty spectrum

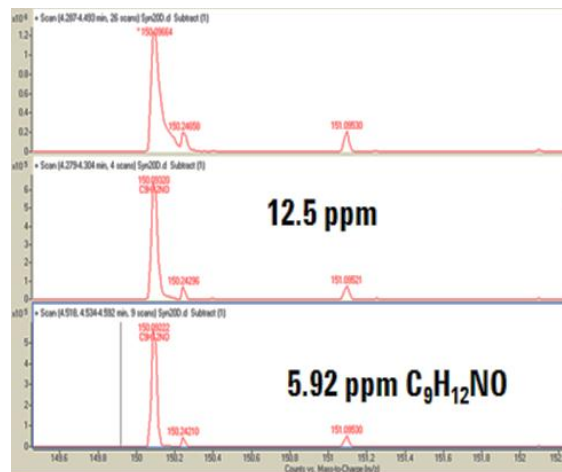
Peak spectrum background

MS: Average of spectra at peak start and end

Time range: 0.000

Also evaluate with no background

Change 10% to 5%  
Change 40% to 10%

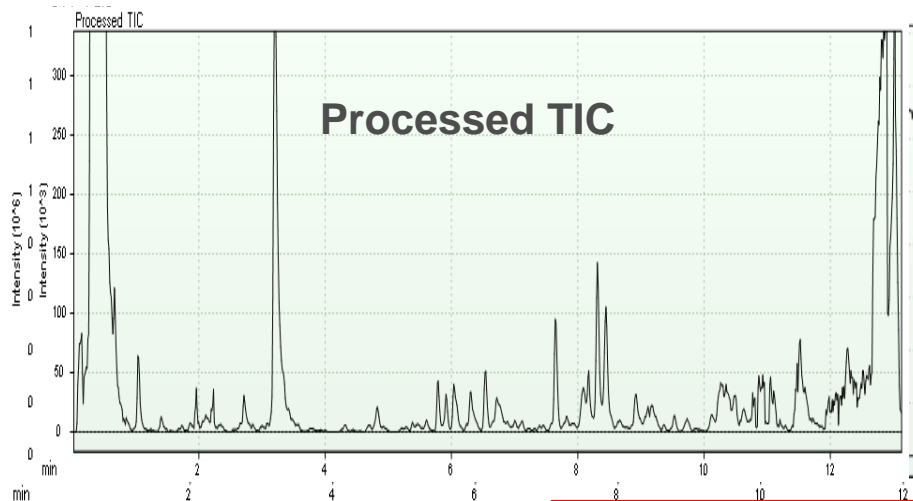


For Narrow Peaks  
Remember to Check Never  
Return an Empty Spectrum

# Unsupervised Naïve data mining

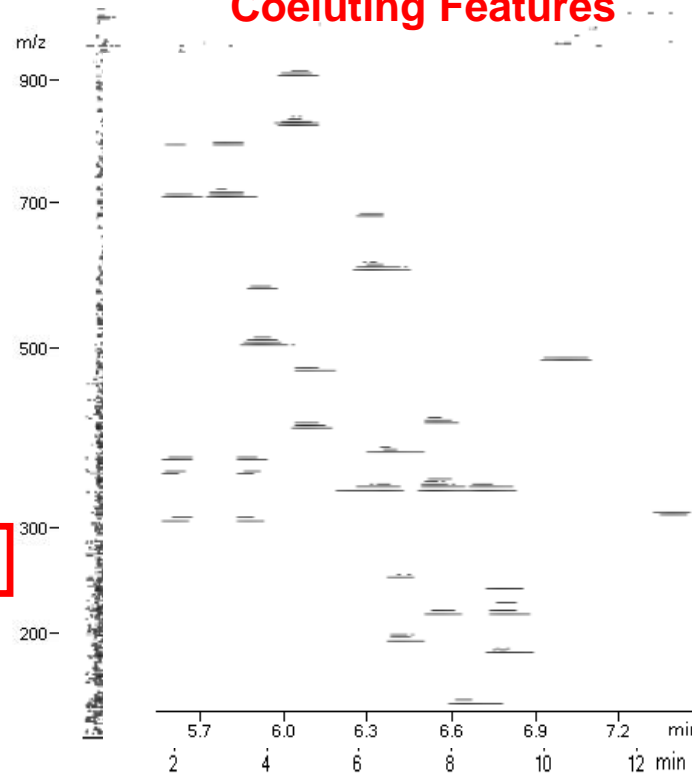
## Molecular Feature Extraction (MFE)

### Finds Features in TOF/QTOF Data



species	RT	m/z	mass	abund.
M	8.162	342.1467	130643	
M+H	8.165	343.1547	342.1474	11889
M+H+1	8.162	344.1581		2290
M+H+2	8.157	345.1748		369
M+H4N	8.164	360.1807	342.1469	8420
M+H4N+	8.156	361.1893		1227
M+Na	8.162	365.1359	342.1466	75678
M+Na+1	8.163	366.1394		15324
M+Na+2	8.162	367.1429		1901
2M+Na	8.164	707.2810	342.1459	4629
2M+Na+1	8.162	708.2860		1808
2M+Na+2	8.173	709.2895		336

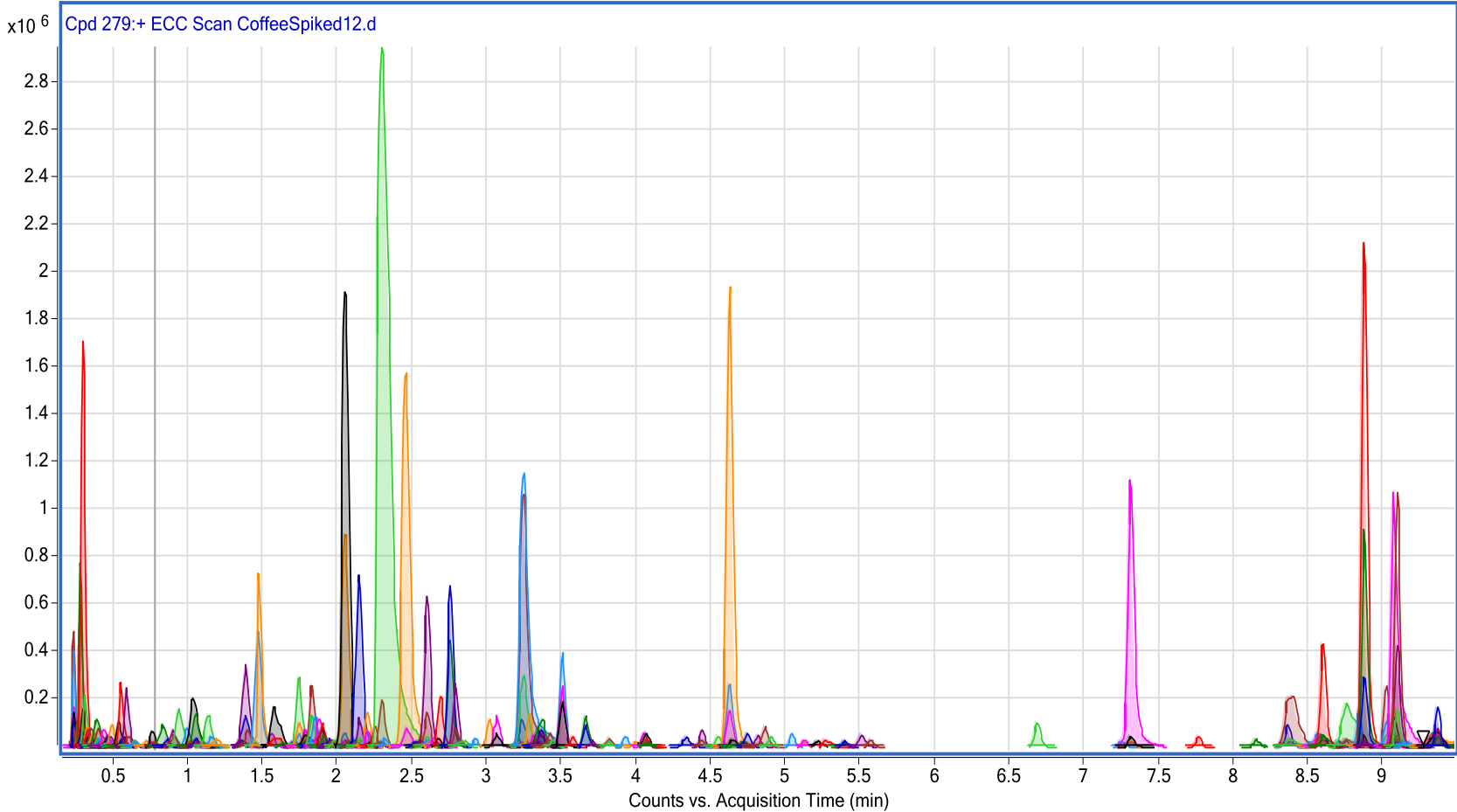
### 3D Plot Before Coeluting Features



Data Reduced sum intensities of isotopes, adducts, clusters and multiply charges ions together.



# Graphical Results Displayed



**Over 280 Compounds Found in Coffee Spiked with Pesticide**

# Choose Isotope Model to Match Application

Peak Location	Peak Filters	Charge State
Isotope grouping		
Peak spacing tolerance:	<input type="text" value="0.0025"/> m/z, plus	<input type="text" value="7.0"/> ppm
Isotope model:	<div style="border: 1px solid gray; padding: 2px;"><p>Common organic molecules ▼</p><p>Common organic molecules</p><p>Peptides</p><p>Unbiased</p><p>Glycans</p></div>	
Charge state		
<input checked="" type="checkbox"/> Limit assigned charge sta	<input type="text" value="2"/>	
<input type="checkbox"/> Treat ions with unassigned charge as singly-charged		

## TIP:

For Compounds containing metals or elemental such as B, Li, Si select **Unbiased**

## Check Limit Assigned Charge States Maximum Values

**For Small Molecule Applications: Set to 2**

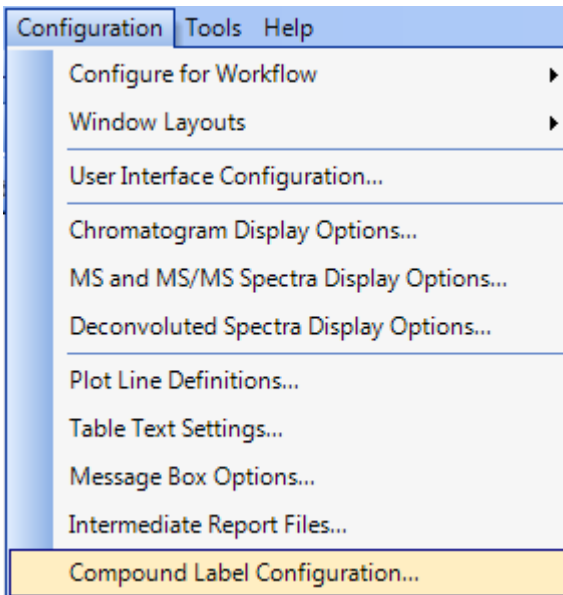
**For High Molecular Weight Apps: Uncheck or Max 10**

# Compounds Labels Display

Sort by Data File

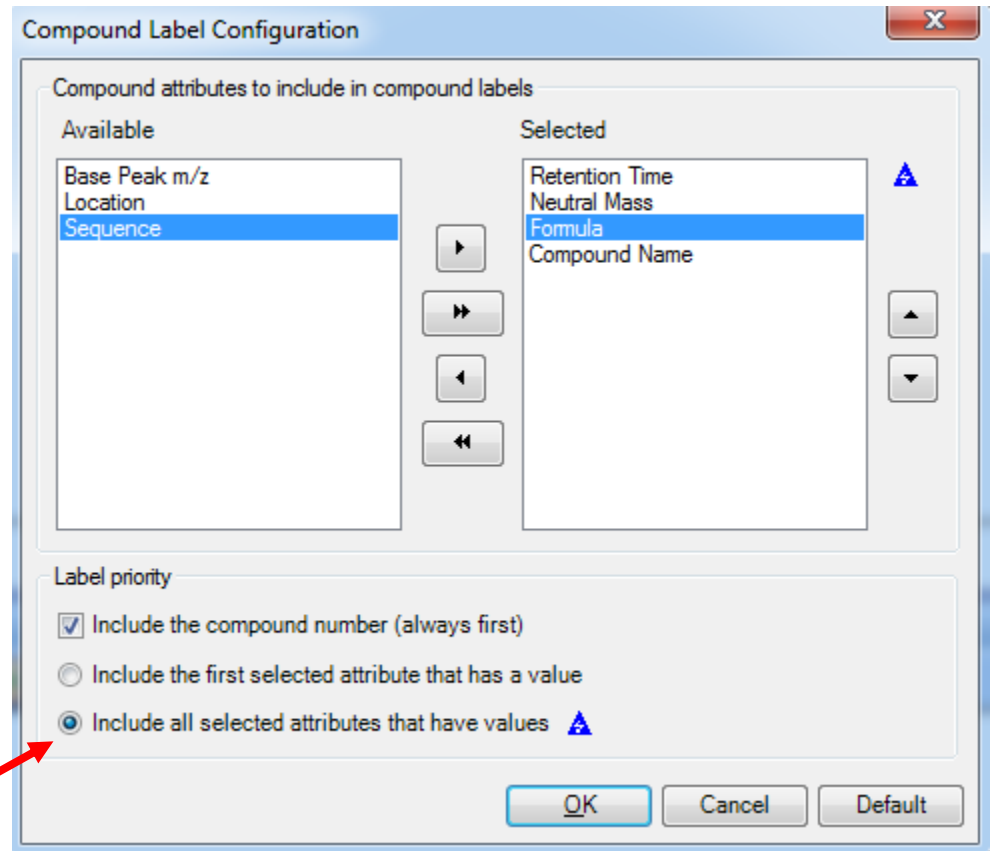
<input checked="" type="checkbox"/>	Compounds
<input checked="" type="checkbox"/>	Cpd 13: 1.020 169.0848; C7 H11 N3 O2; C7 H11 N3 O2; N(pai)-Methyl-L-histidine
<input checked="" type="checkbox"/>	Cpd 14: 1.039 103.0996; C5 H13 N O
<input checked="" type="checkbox"/>	Cpd 16: 1.068 161.1047; C7 H15 N O3
<input checked="" type="checkbox"/>	Cpd 17: 1.114 113.0586; C4 H7 N3 O; C4 H7 N3 O; Creatinine
<input checked="" type="checkbox"/>	Cpd 20: 1.146 115.0992; C6 H13 N O
<input checked="" type="checkbox"/>	Cpd 23: 1.193 85.0892; C5 H11 N
<input checked="" type="checkbox"/>	Cpd 24: 1.195 140.0581; C6 H8 N2 O2; C6 H8 N2 O2; Ethyl-imidazole carboxylate
<input checked="" type="checkbox"/>	Cpd 25: 1.215 170.0687; C7 H10 N2 O3; C7 H10 N2 O3; 2,3,4-Trihydroxybenzylhydrazide
<input checked="" type="checkbox"/>	Cpd 26: 1.232 228.1104; C10 H16 N2 O4
<input checked="" type="checkbox"/>	Cpd 27: 1.278 143.0945; C7 H13 N O2; C7 H13 N O2; Triparanol
<input checked="" type="checkbox"/>	Cpd 28: 1.318 137.0476; C7 H7 N O2; C7 H7 N O2; 2-Pyridylacetic acid
<input checked="" type="checkbox"/>	Cpd 29: 1.328 175.0955; C6 H13 N3 O3; C6 H13 N3 O3; Citrulline
<input checked="" type="checkbox"/>	Cpd 30: 1.346 202.1316; C9 H18 N2 O3; C9 H18 N2 O3; Ala Ile
<input checked="" type="checkbox"/>	Cpd 32: 1.420 85.0895; C5 H11 N
<input checked="" type="checkbox"/>	Cpd 33: 1.450 203.1164; C9 H17 N O4; C9 H17 N O4; L-Glutamic acid n-butyl ester
<input checked="" type="checkbox"/>	Cpd 34: 1.464 159.1257; C8 H17 N O2; C8 H17 N O2; DL-2-Aminooctanoic acid
<input checked="" type="checkbox"/>	Cpd 35: 1.471 211.0948; C9 H13 N3 O3; C9 H13 N3 O3; Zalcitabine
<input checked="" type="checkbox"/>	Cpd 37: 1.499 145.0857; C5 H11 N3 O2; C5 H11 N3 O2; 4-(diaminomethylideneamino)butanoic acid
<input checked="" type="checkbox"/>	Cpd 38: 1.539 216.1468; C10 H20 N2 O3; C10 H20 N2 O3; Val Val
<input checked="" type="checkbox"/>	Cpd 39: 1.613 268.1168; C11 H16 N4 O4; C11 H16 N4 O4; Isobutylglycine
<input checked="" type="checkbox"/>	Cpd 40: 1.623 244.0697; C9 H12 N2 O6; C9 H12 N2 O6; Uridine
<input checked="" type="checkbox"/>	Cpd 42: 1.646 192.0265; C6 H8 O7; C6 H8 O7; 2,3-Dioxogulonic acid
<input checked="" type="checkbox"/>	Cpd 43: 1.647 137.9956; C6 H2 O4
<input checked="" type="checkbox"/>	Cpd 44: 1.648 174.0159; C6 H6 O6; C6 H6 O6; Dehydroascorbic acid
<input checked="" type="checkbox"/>	Cpd 45: 1.655 180.0643; C7 H8 N4 O2; C7 H8 N4 O2; Theobromine
<input checked="" type="checkbox"/>	Cpd 46: 1.660 228.1470; C11 H20 N2 O3; C11 H20 N2 O3; Leu Pro
<input checked="" type="checkbox"/>	Cpd 47: 1.667 216.1223; C8 H16 N4 O3
<input checked="" type="checkbox"/>	Cpd 48: 1.685 169.0844; C7 H11 N3 O2; C7 H11 N3 O2; N(pai)-Methyl-L-histidine
<input checked="" type="checkbox"/>	Cpd 49: 1.685 141.0791; C7 H11 N O2; C7 H11 N O2; Ethosuximide
<input checked="" type="checkbox"/>	Cpd 51: 1.775 129.0425; C5 H7 N O3; C5 H7 N O3; Pyroglutamic acid
<input checked="" type="checkbox"/>	Cpd 52: 1.776 158.1415; C8 H18 N2 O

# Specify Compound Label Configuration



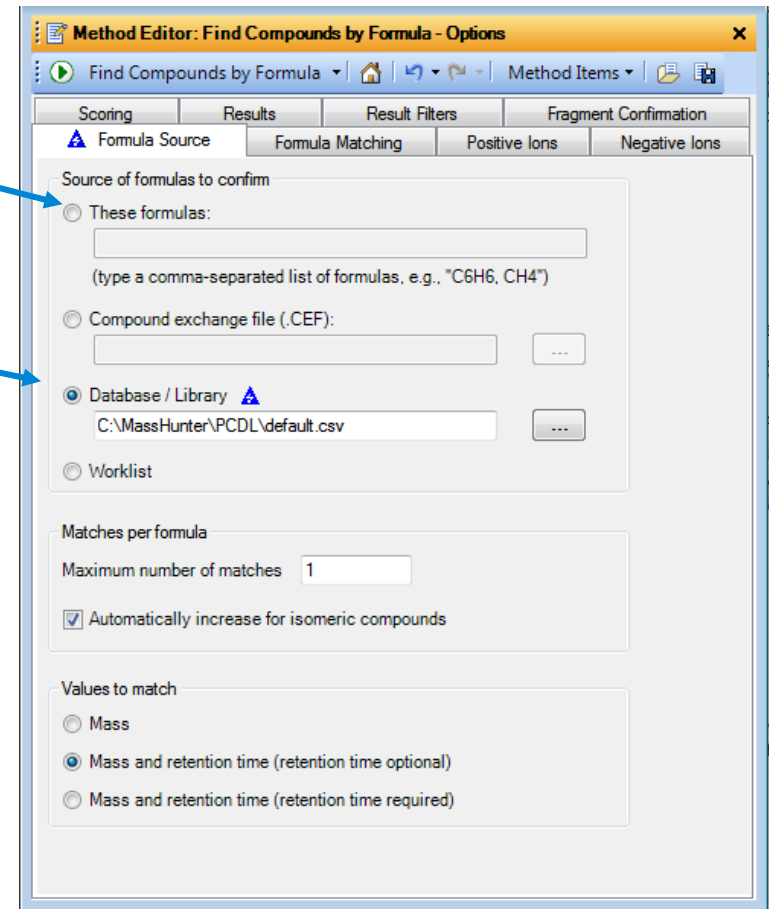
Highlight Parameter in list and use > and < to move to and from **Selected**.

Check **Include all selected attributes that have values** to display all attributes in table.



# Targeted Data Mining: Find by Formula (FBF)

- **Sources from:**
  - Chemical formulae
  - CEF file
  - PCD/PCDL
- Takes input formula, calculates mono-isotopic mass and isotope pattern filtering
- Extracts and integrates EICs from the data, extracts peak spectra
- Calculates score based on accurate mass, isotope abundance pattern, and isotope spacing
- **Retention Time Matching Optional**

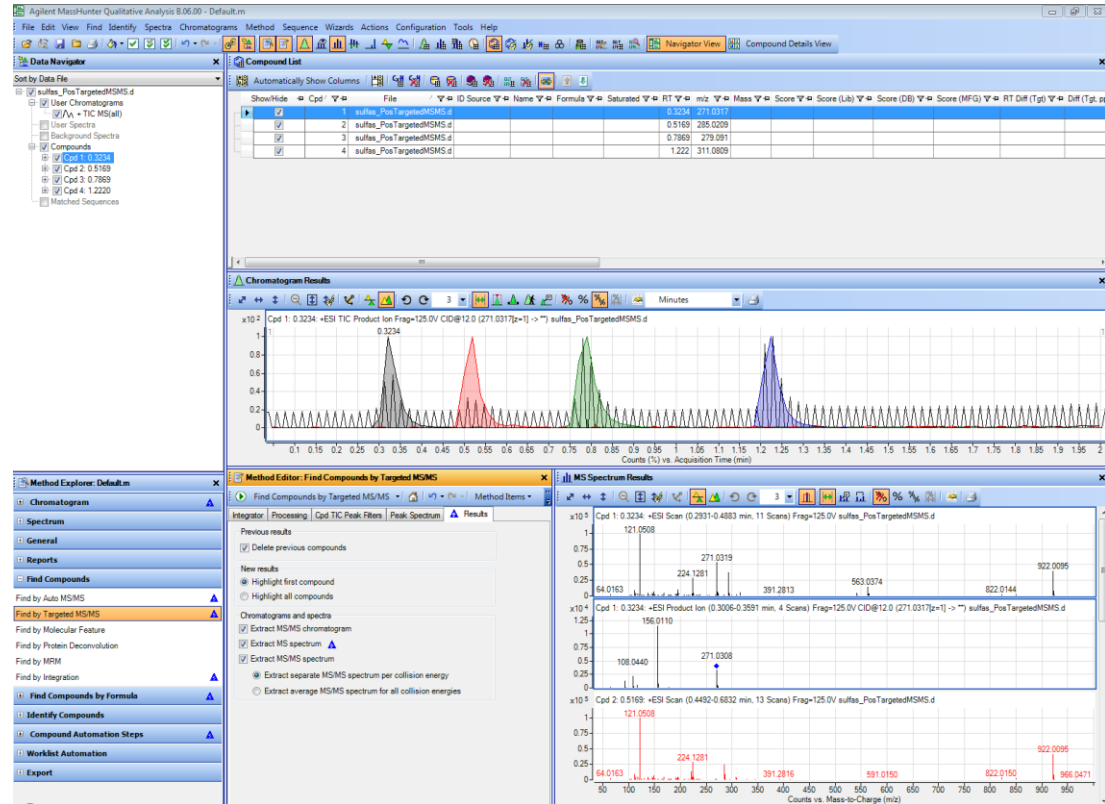




# Analysis of MS/MS Data: Multiple Options

Depends on how the data was acquired:

- **MRM for QQQ Data**
- **MFE Extracting MS/MS Data**
- **Auto MS/MS for QTOF**
- **Targeted MS/MS for QTOF**
  - Extracts chromatogram for each targeted mass listed in the acquisition method
- Each compound can have an associated EIC, MS spectrum and MS/MS spectra either an **average** of collision energy or **separated** by collision energy



# MFE Extracting MS/MS Data

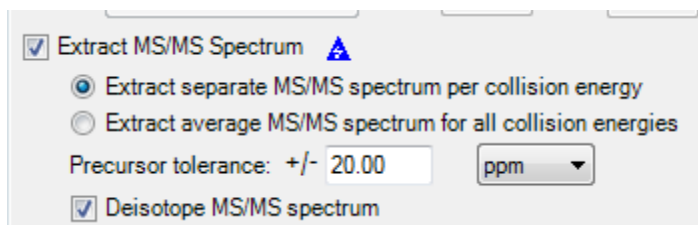
## Benefit:

- Identifies Adducts and Groups Them Together
- MS/MS Spectra separated by CE or Combined
- Deisotope MS/MS Spectrum
- Identifies Compounds in which MS/MS Missed
- Easy to Setup MS/MS Inclusion List

## Disadvantage:

- No MS/MS Fragment ion Filtering
- Compound List Larger with MS and MS/MS

### Results Tab



Extract MS/MS Spectrum ▲

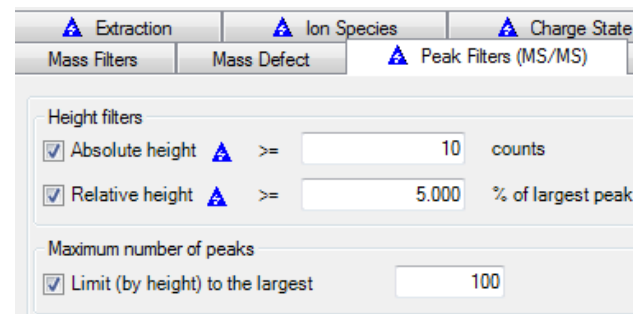
Extract separate MS/MS spectrum per collision energy

Extract average MS/MS spectrum for all collision energies

Precursor tolerance: +/- 20.00 ppm

Deisotope MS/MS spectrum

**Remember to set  
MS/MS Peak Filters**



▲ Extraction    ▲ Ion Species    ▲ Charge State

Mass Filters    Mass Defect    ▲ Peak Filters (MS/MS)

Height filters

Absolute height ▲ ≥ 10 counts

Relative height ▲ ≥ 5.000 % of largest peak

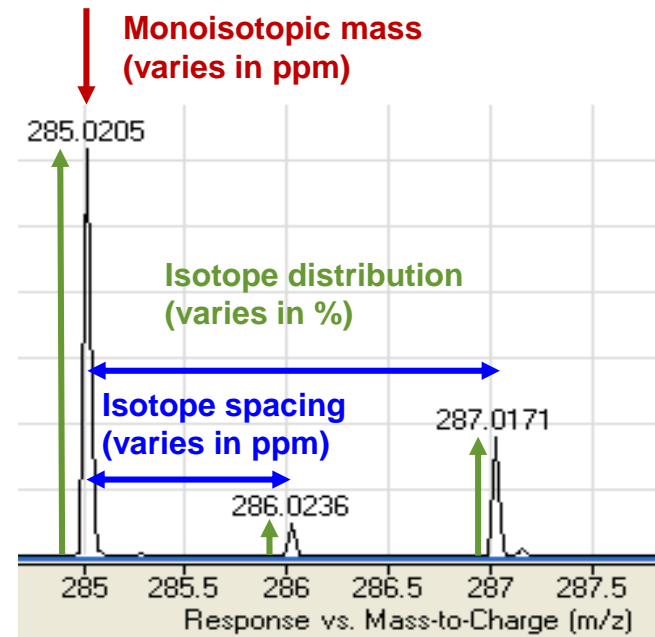
Maximum number of peaks

Limit (by height) to the largest 100

# Database Searching

- After feature extraction, search for identifications
- Search Database: searches .csv file or PCD
- Search Accurate Mass Library: searches PCDL
- Scoring based on
  - Accurate mass match
  - Isotope abundance
  - Isotope spacing
  - Retention time (if selected)
  - Dot product scoring of MS/MS spectral match
- Forward and/or reverse scoring

## Scoring based on



# Molecular Formula Generation

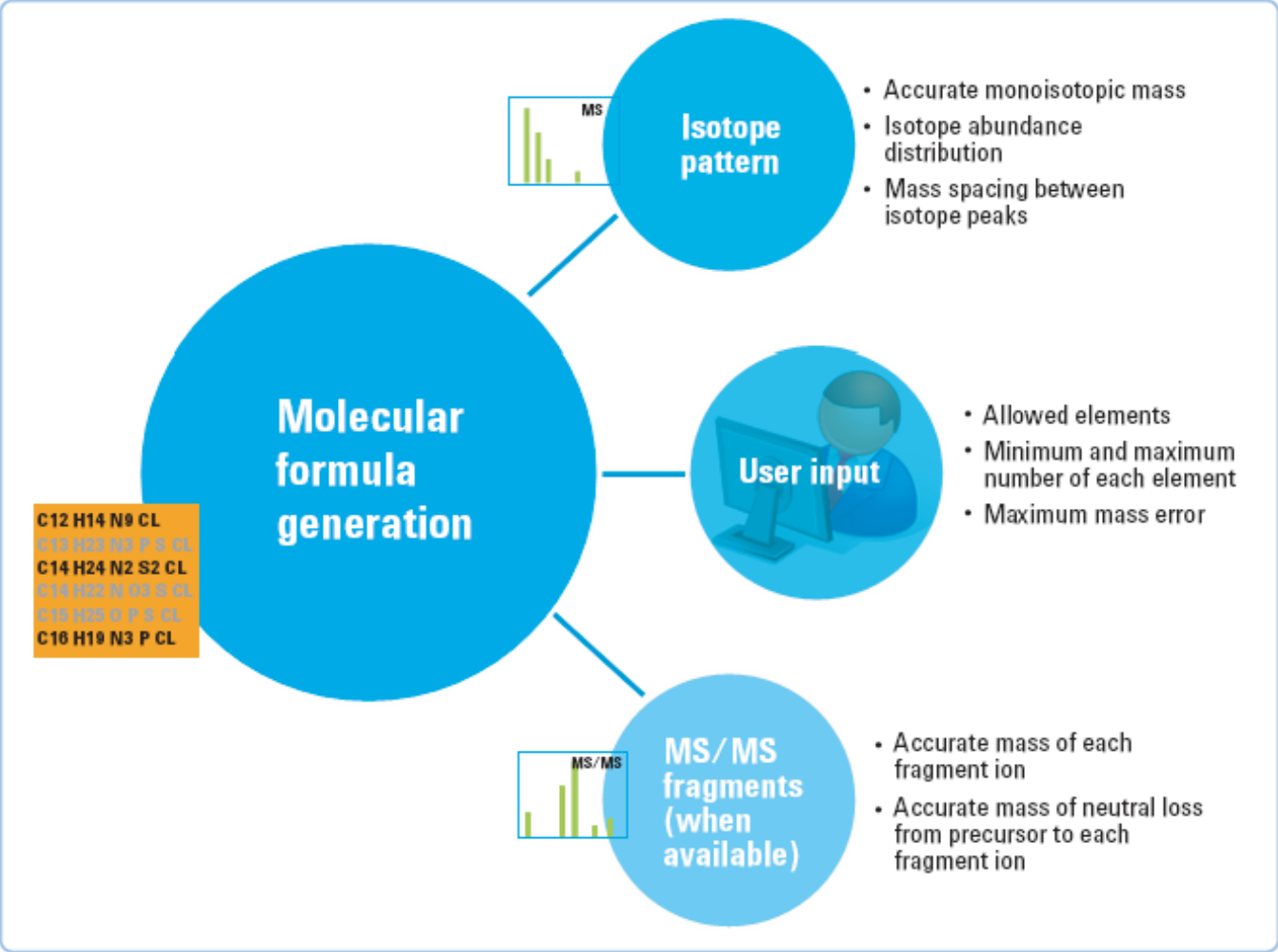
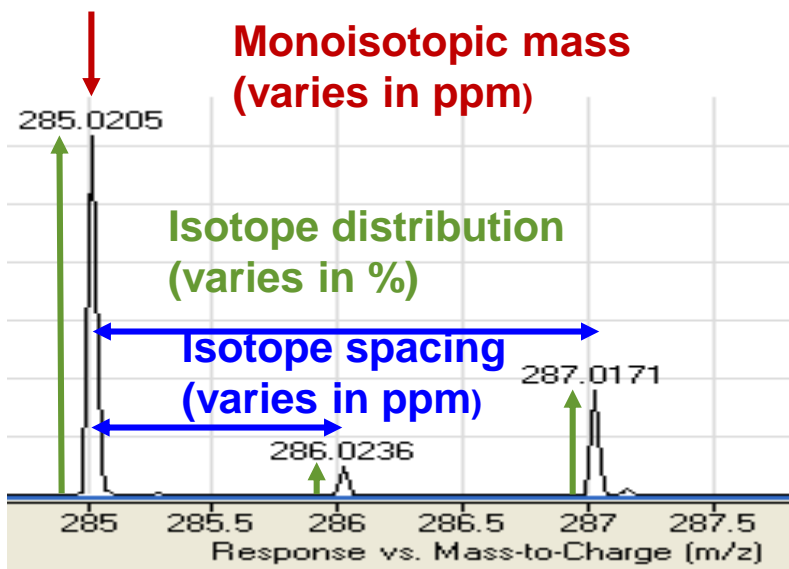


Figure 1. Agilent's molecular formula generation software uses multiple dimensions of information to generate and score lists of possible molecular formulas. It has been optimized for analysis of accurate-mass data from Agilent 6200 Series TOF and 6500 Series Q-TOF LC/MS systems.

# Agilent's Molecular Formula Generation Software

Scoring based on



**Mass Match +**

**Abund. Match +**

**Spacing Match =**

Overall Score

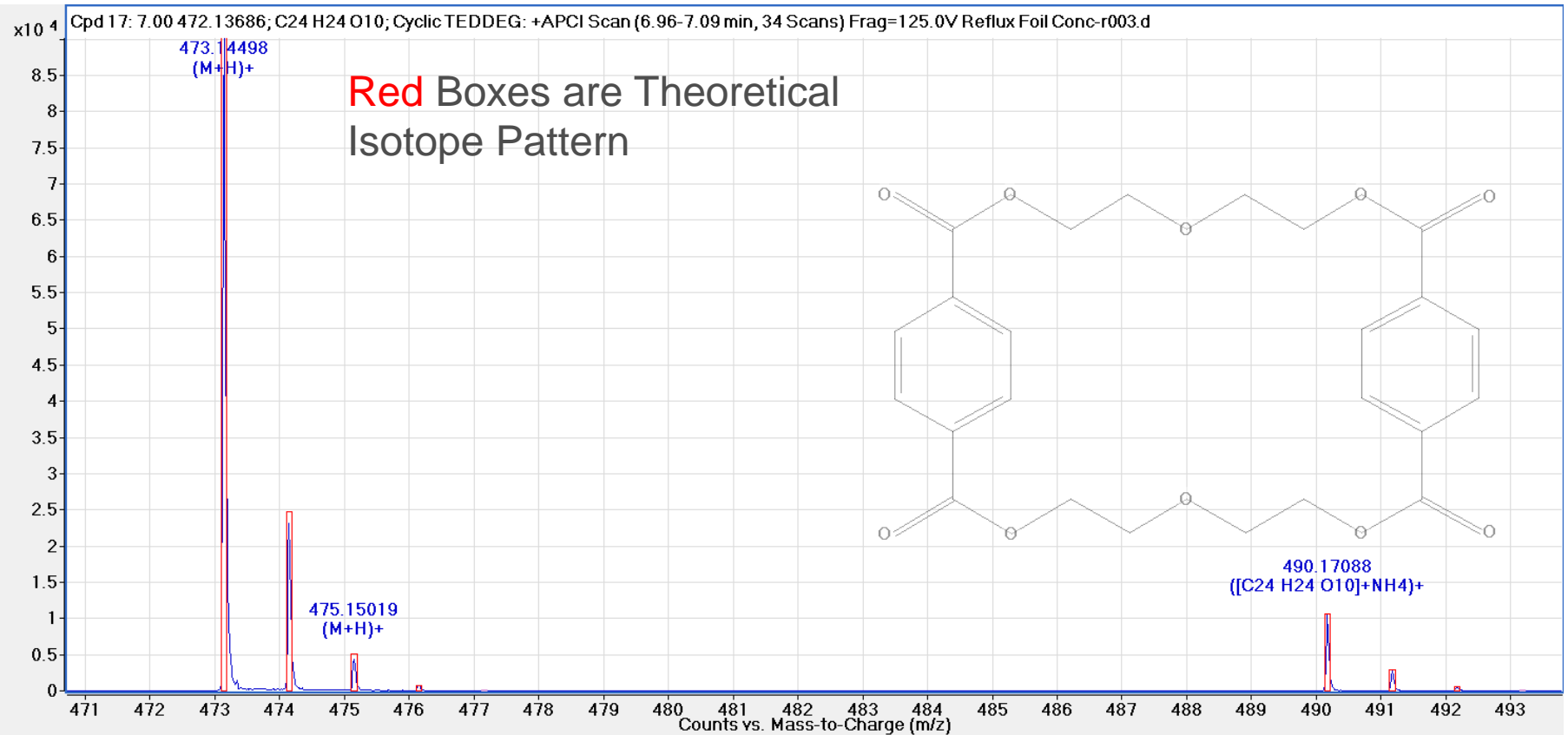
MS Formula Results: Cpd 2: C<sub>10</sub>H<sub>9</sub>CIN<sub>4</sub>O<sub>2</sub>S

m/z	Ion	Formula	Abundance
285.021	(M+H) <sup>+</sup>	C <sub>10</sub> H <sub>10</sub> LN <sub>4</sub> O <sub>2</sub> S	24506.1

Best	Formula (M)	Calc m/z	Score	Cross Score	Mass	Calc Mass	Diff (ppm)	Abs Diff (p)	Spacing Matc	Abund Matc	Mass Match	m/z	DBE
<input checked="" type="checkbox"/>	C <sub>10</sub> H <sub>9</sub> CIN <sub>4</sub> O <sub>2</sub> S	285.0208	99.55		284.0137	284.0135	-0.71	0.71	99.19	99.26	99.69	285.021	8
<input type="checkbox"/>	C <sub>7</sub> H <sub>12</sub> N <sub>2</sub> O <sub>6</sub> S <sub>2</sub>	285.021	77.28		284.0137	284.0137	0.01	0.01	99.54	1.93	100	285.021	3
<input type="checkbox"/>	C <sub>7</sub> H <sub>13</sub> CIN <sub>4</sub> O <sub>2</sub> S <sub>2</sub>	285.0241	75.57		284.0137	284.0168	11.12	11.12	99.87	83.87	46.22	285.021	3

# Isotope Pattern Matching



# Molecular Formula Generation

## Isotope Pattern Matching and MS/MS for Formula confirmation

Identify Compounds

Agilent MassHunter Qualitative Analysis - Default.m

MS Formula Results: Compound 41

m/z	Species	Formula	Abundance
285.01973	(M+H) <sup>+</sup>	C <sub>10</sub> H <sub>10</sub> N <sub>4</sub> O <sub>2</sub> SCl	58153

Best	Formula	Score	Mass	Calc Mass	Difference (ppm)	Abs Diff (ppm)	MS Score	MS/MS Score	Coverage	DBE
<input checked="" type="checkbox"/>	C <sub>10</sub> H <sub>9</sub> N <sub>4</sub> O <sub>2</sub> SCl	100	284.01246	284.01347	3.59	3.59	100	100	100	8

Isotope	Abund%	Calc Abund%	m/z	Calc m/z	Difference (ppm)
1	100	100	285.01973	285.02075	3.57
2	12.81	13.26	286.02167	286.0232	5.37
3	33.92	37.7	287.01714	287.0179	2.65
4	4.23	4.92	288.01833	288.02023	6.58
5	1.63	1.89	289.01491	289.0157	2.72
6	0.17	0.22	290.01673	290.01726	1.83

**MS Score based on:**

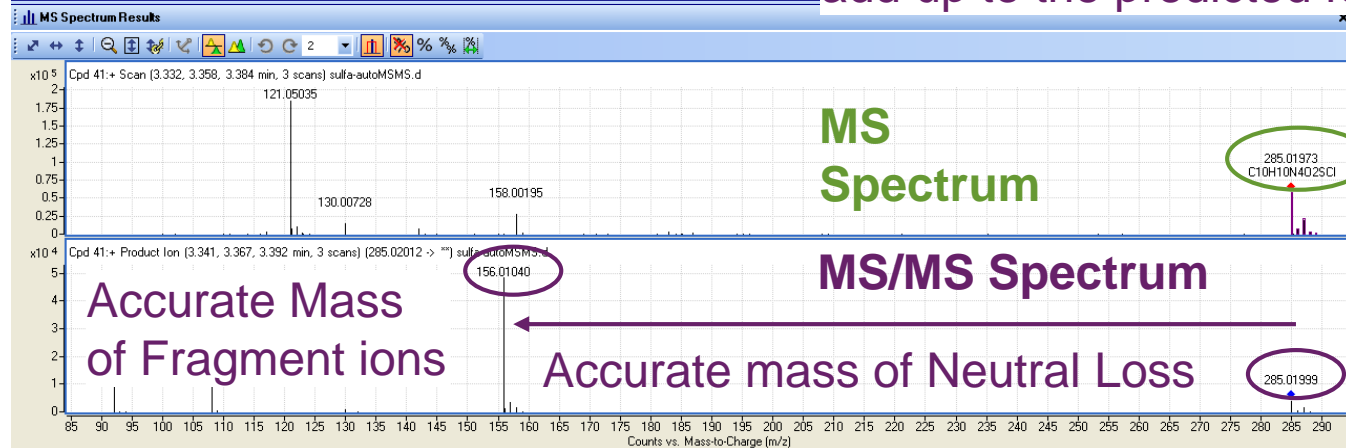
- Mass main Isotope
- Isotope Pattern
- Mass M+1 and M+2

MS/MS Formula Details: Compound 41 C<sub>10</sub>H<sub>9</sub>N<sub>4</sub>O<sub>2</sub>SCl

m/z	Abund	Formula	Mass	Frag Mass	Difference (ppm)	Loss Mass	Loss Formula
92.04927	9722	C <sub>6</sub> H <sub>5</sub> N	91.04199	91.0422	2.27	192.97127	C <sub>4</sub> H <sub>4</sub> N <sub>3</sub> O <sub>2</sub> SCl
92.04927	9722	C <sub>3</sub> H <sub>5</sub> N <sub>3</sub>	91.04199	91.04557	39.3	192.9679	C <sub>7</sub> N <sub>3</sub> O <sub>2</sub> Cl
92.04927	9722	CH <sub>5</sub> N <sub>3</sub> O <sub>2</sub>	91.04199	91.03818	-41.91	192.9753	C <sub>9</sub> H <sub>4</sub> N <sub>3</sub> Cl
108.04397	10541	C <sub>6</sub> H <sub>5</sub> NO	107.03669	107.03711	3.92	176.97636	C <sub>4</sub> H <sub>4</sub> N <sub>3</sub> O <sub>2</sub> SCl
108.04397	10541	C <sub>3</sub> H <sub>5</sub> N <sub>3</sub> O <sub>2</sub>	107.03669	107.04048	35.41	176.97299	C <sub>7</sub> N <sub>3</sub> O <sub>2</sub> Cl
156.0104	52240	C <sub>6</sub> H <sub>5</sub> N <sub>2</sub> O <sub>2</sub>	155.00312	155.0041	6.29	129.00937	C <sub>4</sub> H <sub>4</sub> N <sub>3</sub> Cl
156.0104	52240	C <sub>9</sub> H <sub>5</sub> N <sub>2</sub> O	155.00312	155.00073	-15.45	129.01275	CH <sub>8</sub> N <sub>3</sub> SCl

**MS/MS Score based on:**

- Ability to calculate molecular formulas for each fragment & the corresponding neutral loss which add up to the predicted formula for the precursor



**Accurate mass information used:**

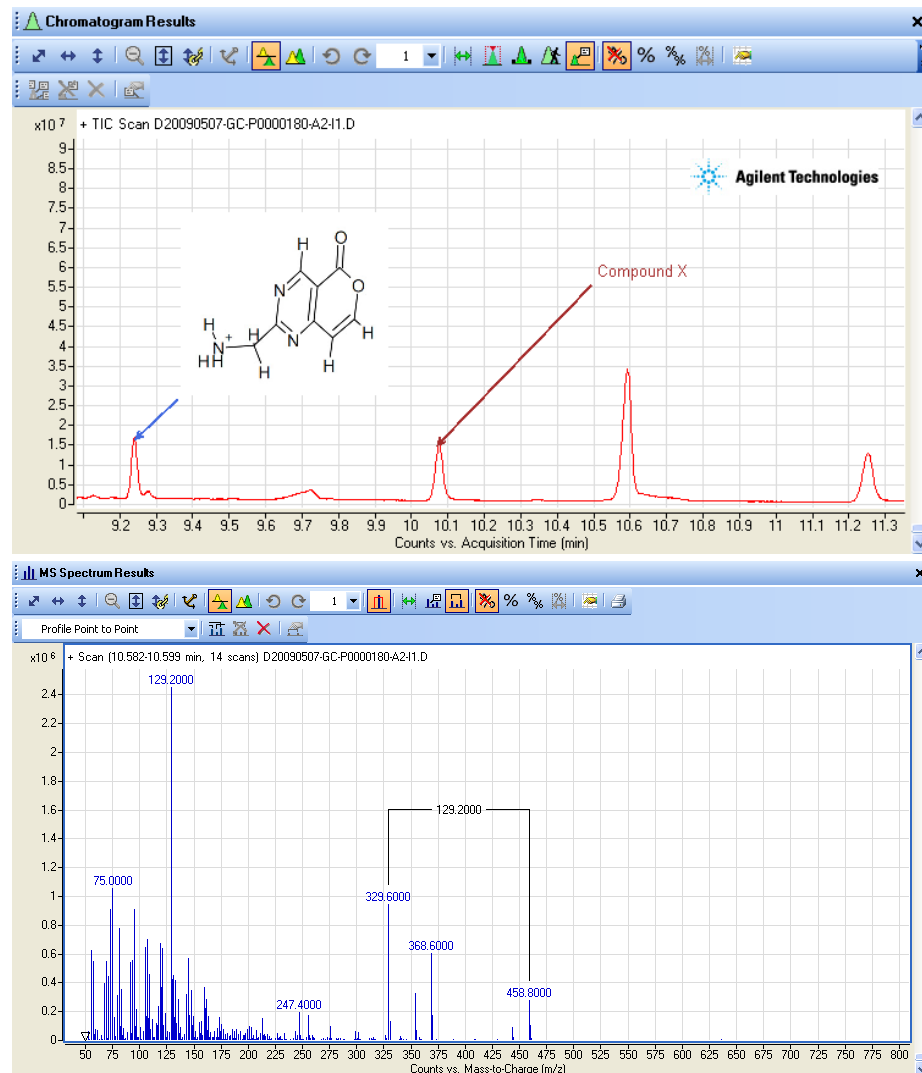
- Precursor ion
- Isotopes M+1, M+2
- Fragment ion
- Neutral loss

# Annotate and Document

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

Use *Mass Caliper* to document fragmentation and losses in spectrum

Export or use copy & paste to add graphics or results into presentations and documents



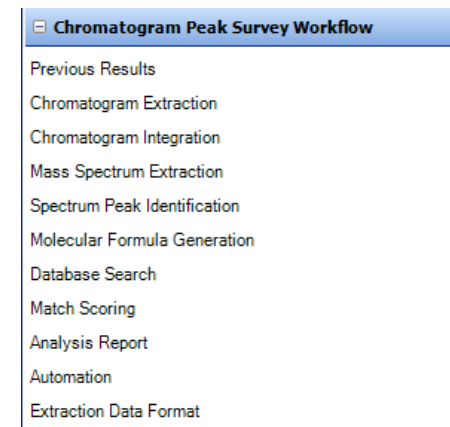
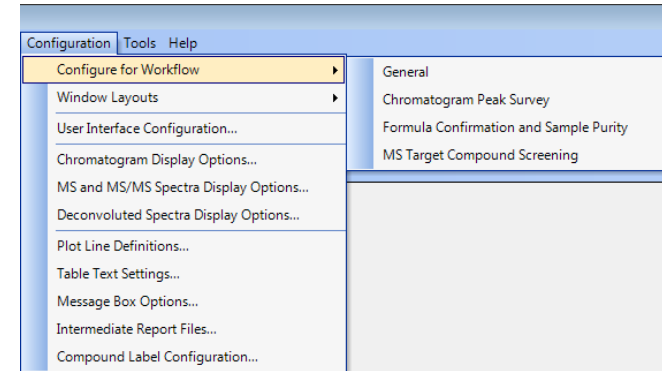


# Workflows in Qual

- **Workflows guide users through Qual functions needed for specific tasks**

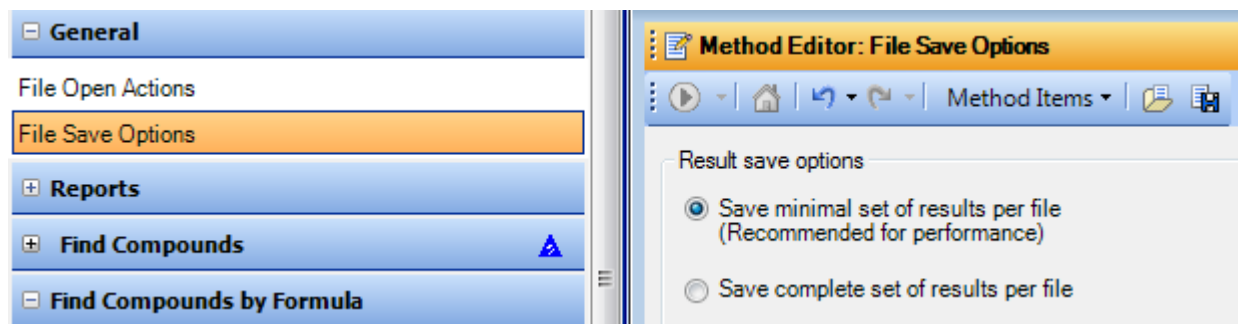
- Load via Configuration Menu on Toolbar
- Default method with default parameters and report templates
- Specified layout of user interface limited to needed windows
- Section at the top of the Method Explorer grouping together the relevant functions

- **Helpful as a starting point for new users and as a preliminary analysis before “deep dive” type data analysis**



# Saving Results

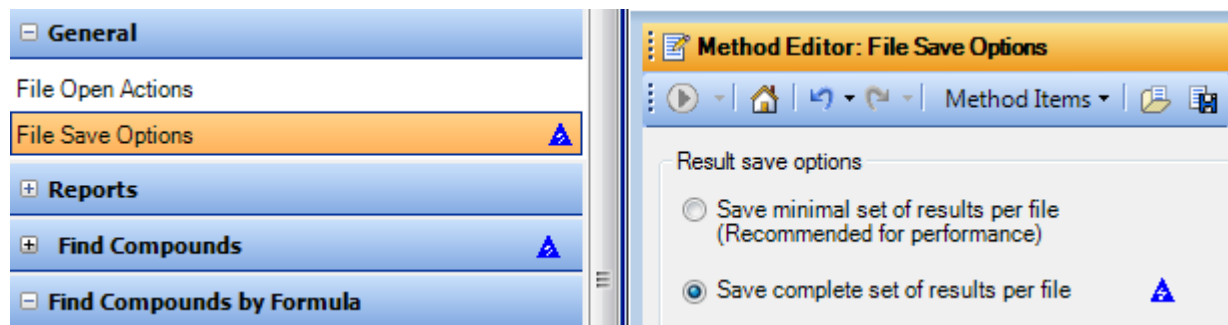
The Method default saves Minimal Amount of Graphics



**Default Setting**

**Graphics not saved  
only compound list**

Change to “Save Complete Results”



**All Graphics Saved**

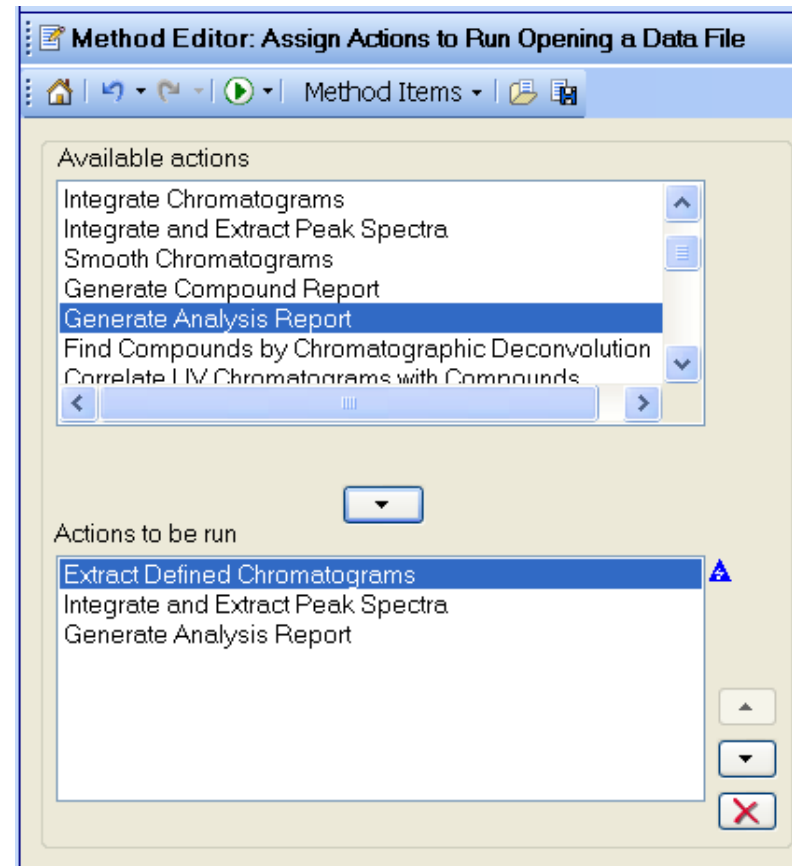
# Automation - File Open Actions & Post Acquisition Worklist Processing

## Automate common file open actions in manual review

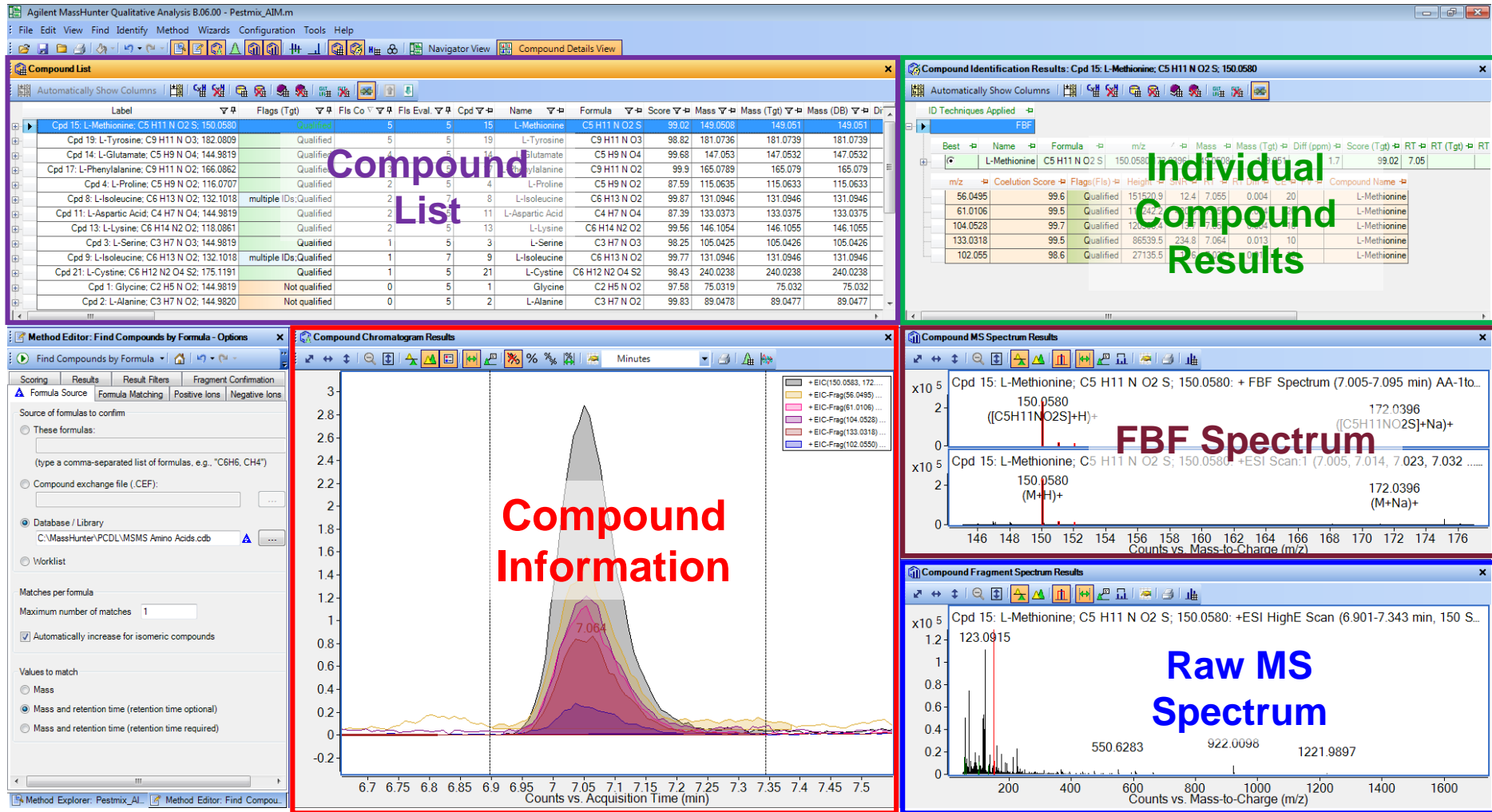
- Standardize review processes
- Automate common actions, i.e. extract EIC.

## Define Qualitative methodology for sequence computation.

- No user interaction required.

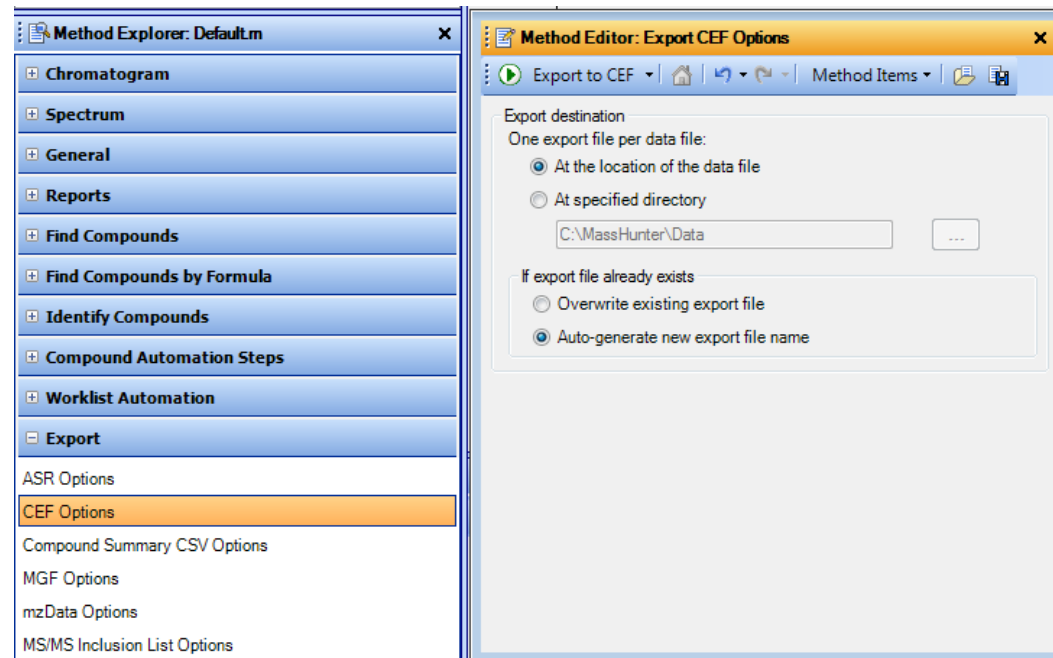


# Compound Details View

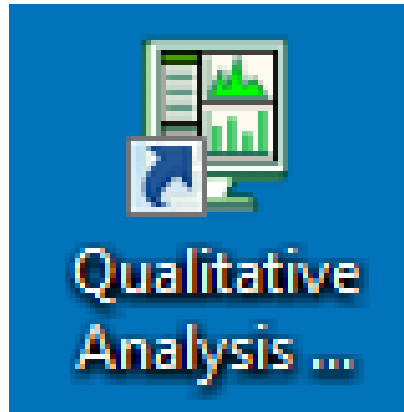


# What is a .cef file?

- **C**ompound **E**xchange **F**ormat file
- Agilent-specific file format that moves compound information back and forth between Qual, MPP, and other Agilent software
- XML-based – the amount of information contained depends on what the user has extracted
  - Accurate mass, retention time
  - Formulas
  - Spectra
- Can be edited manually

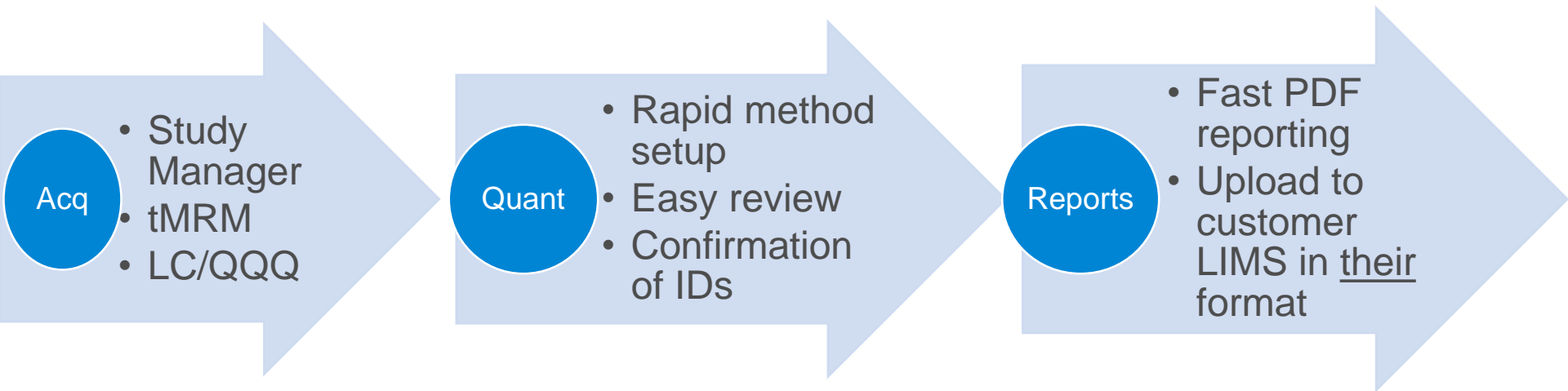


# Questions about MassHunter Qual?



# The MassHunter Quantitative Workflow

## Quantify with confidence

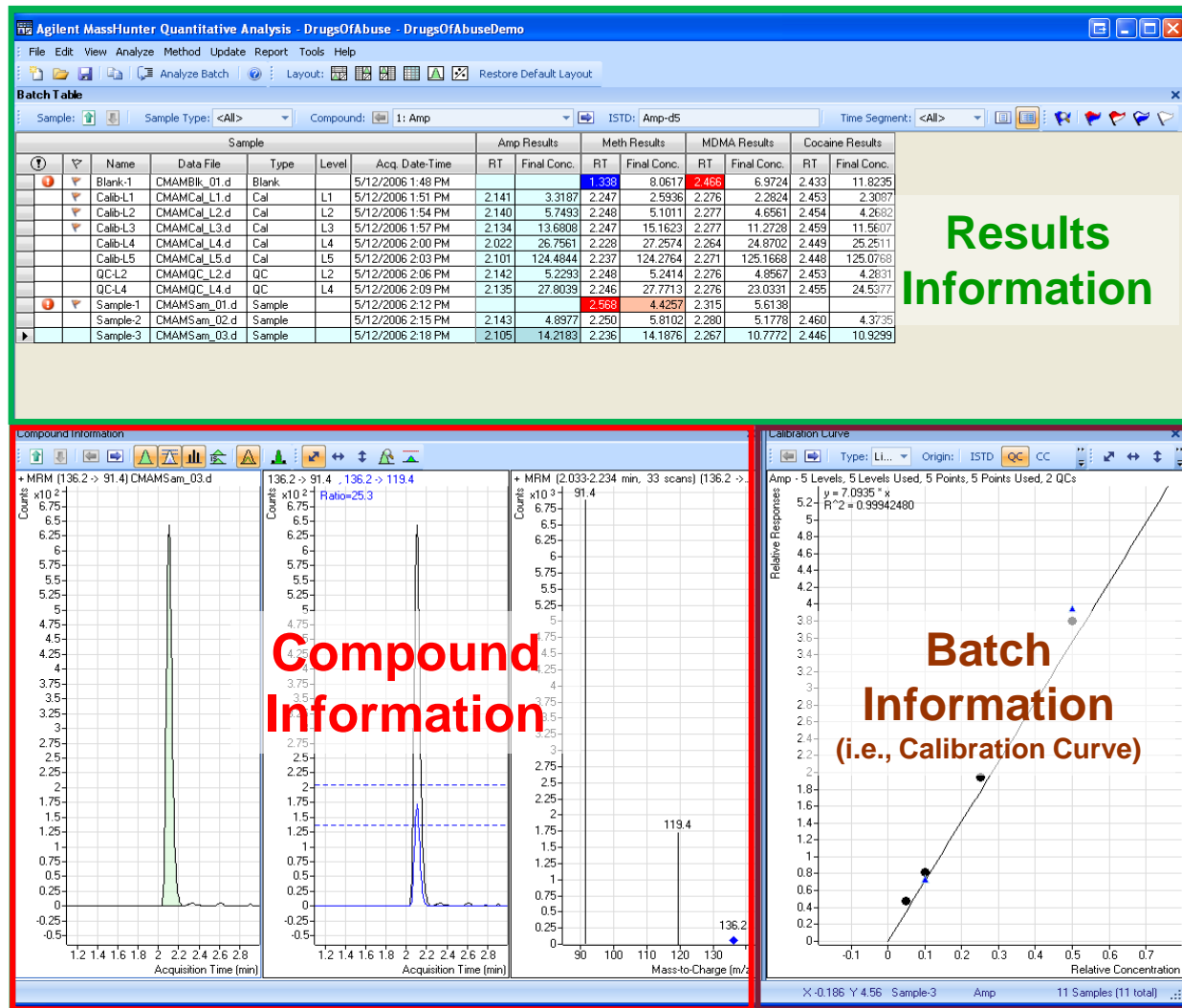


**Agilent provides fast setup and running of quantitative methods from acquiring samples to the final report**

# Quantitative Analysis

## The Quant Batch screen:

- 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.





# Batch Screen – Sample & Results Information

In **Results Information**, the Quantitation Message 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

More than 40 quality checks can be specified to highlight outliers in **results**.

- Set high and low limits.

Custom Calculations can be added for User defined quality checks

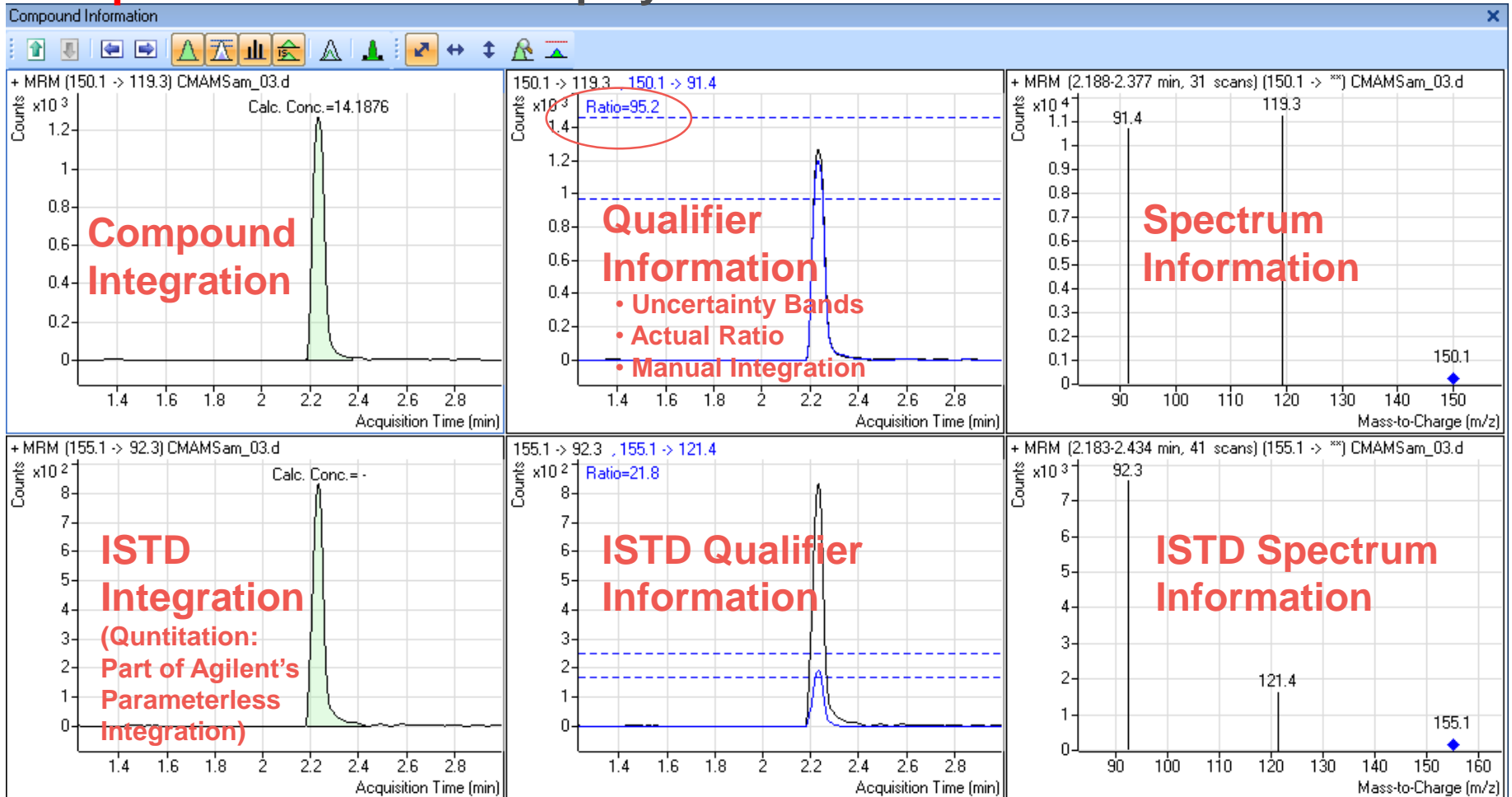
Amp Results		
RT	Final Conc.	Accuracy
2.141	3.3187	132.7
2.140	5.7493	115.0
2.134	13.6808	109.4
2.022	26.7561	107.0
2.101	124.4844	99.6
2.142	5.2293	104.6
2.135	27.8039	111.2
2.143	4.8977	
2.105	14.2183	

**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

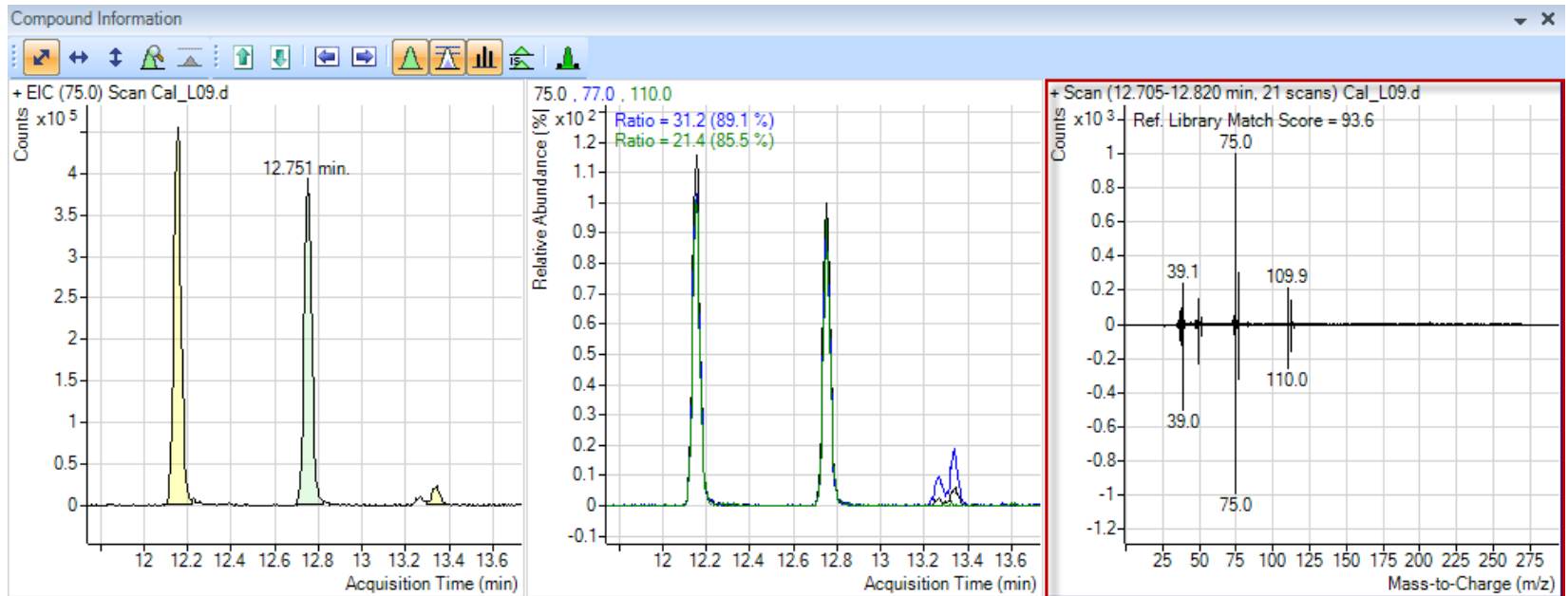
# Batch Screen - Compound Information

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



# Batch Screen - Library Reference Spectra

- Confirmation of Compound Identification
- Visual comparison of Sample and Library Spectra
- Seen in Batch-at-a-Glance and on Reports
- Extracts Spectra from Library by matching on CAS number based in Quant method and creates a small reference library (reflibrary.xml)

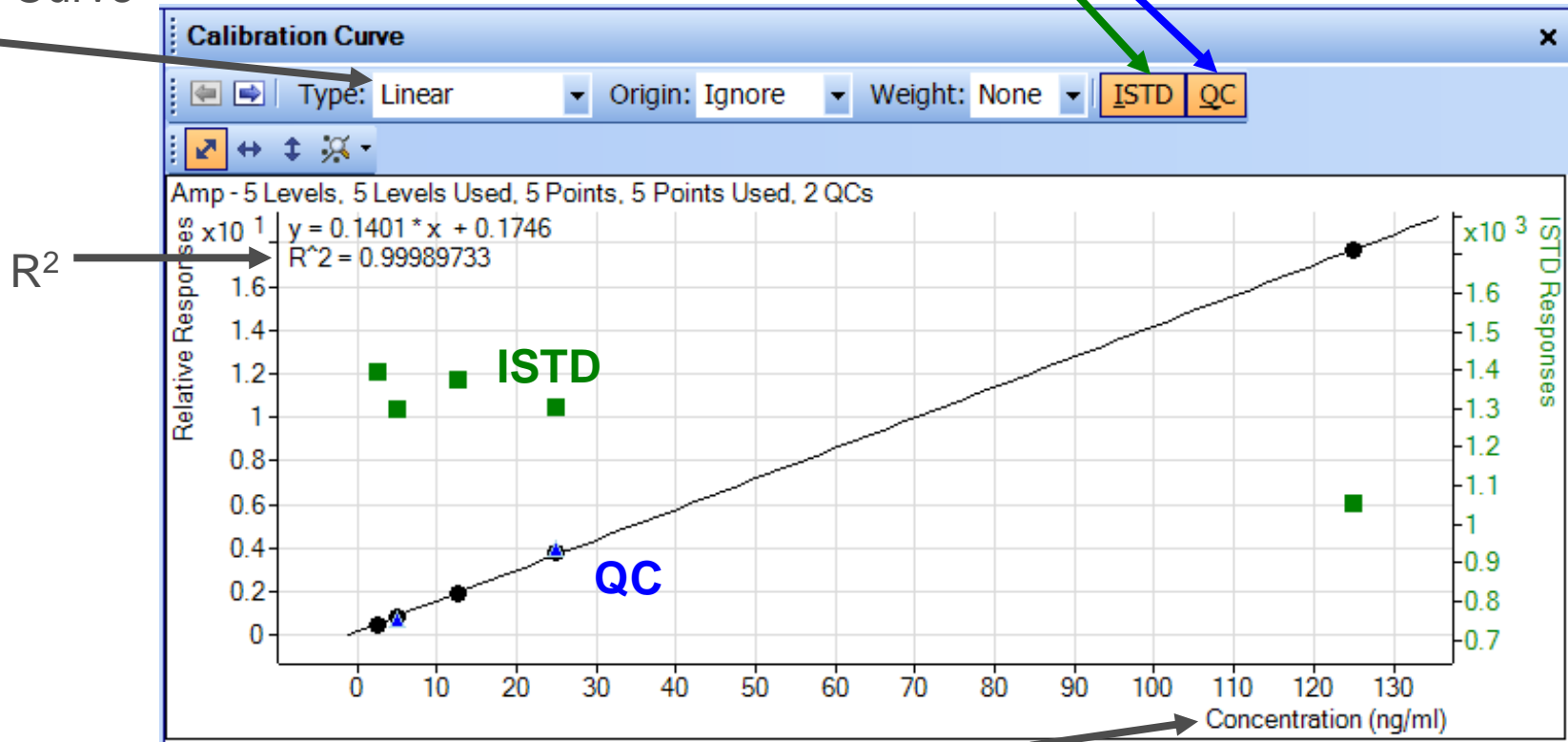


# Batch Screen – Calibration Curve

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

To view ISTD responses or display QC samples click either the ISTD or QC button.

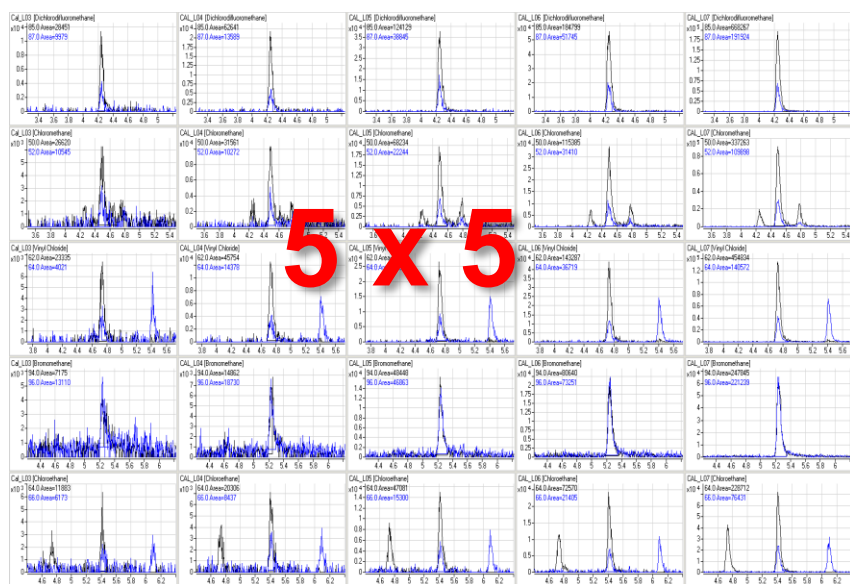
Change Curve Fit



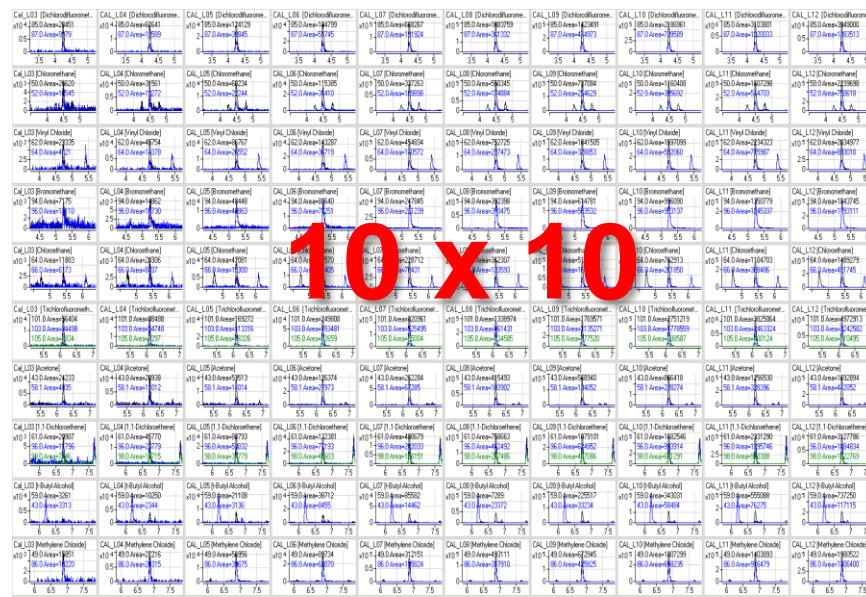
Concentration can be set as relative (to ISTD) or actual.

# Compounds-at-a-Glance

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



5 x 5

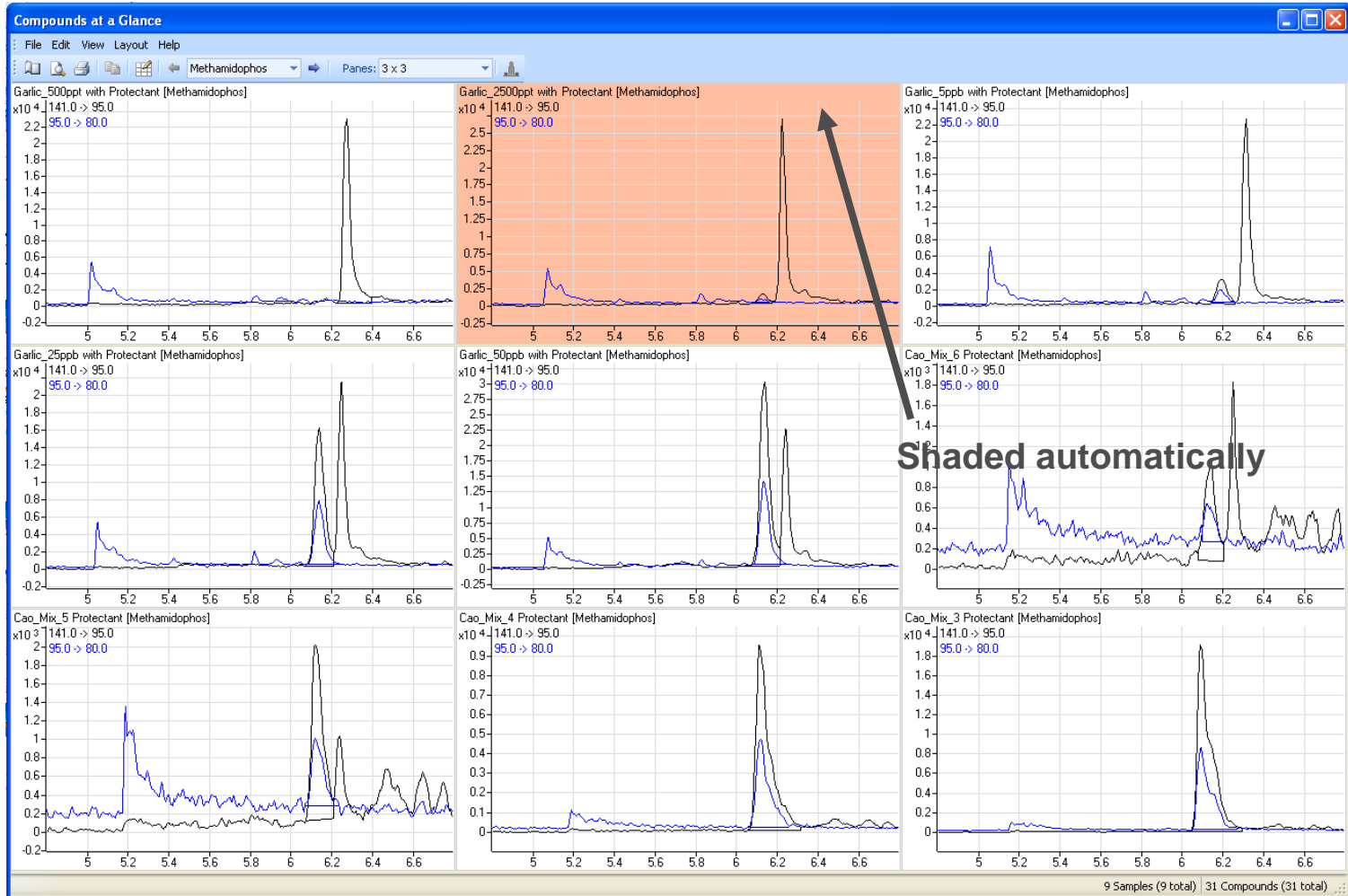


10 x 10

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

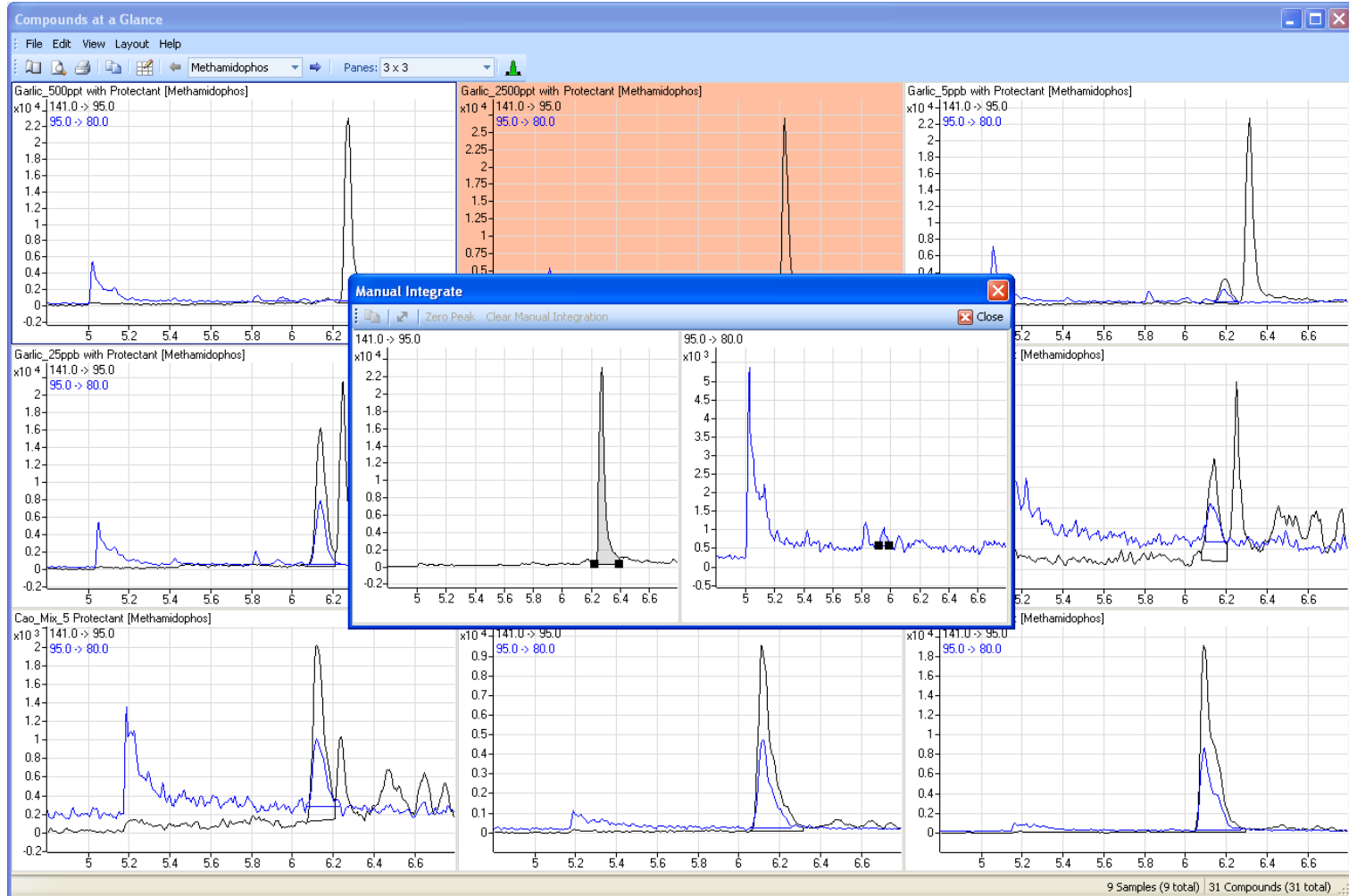
# Compounds-at-a-Glance

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



# Compounds-at-a-Glance

You can perform manual integration of compounds-at-a-glance.





# Simplify Quantitation Method Creation

Easily create a target method from acquired data (SIM or Scan).

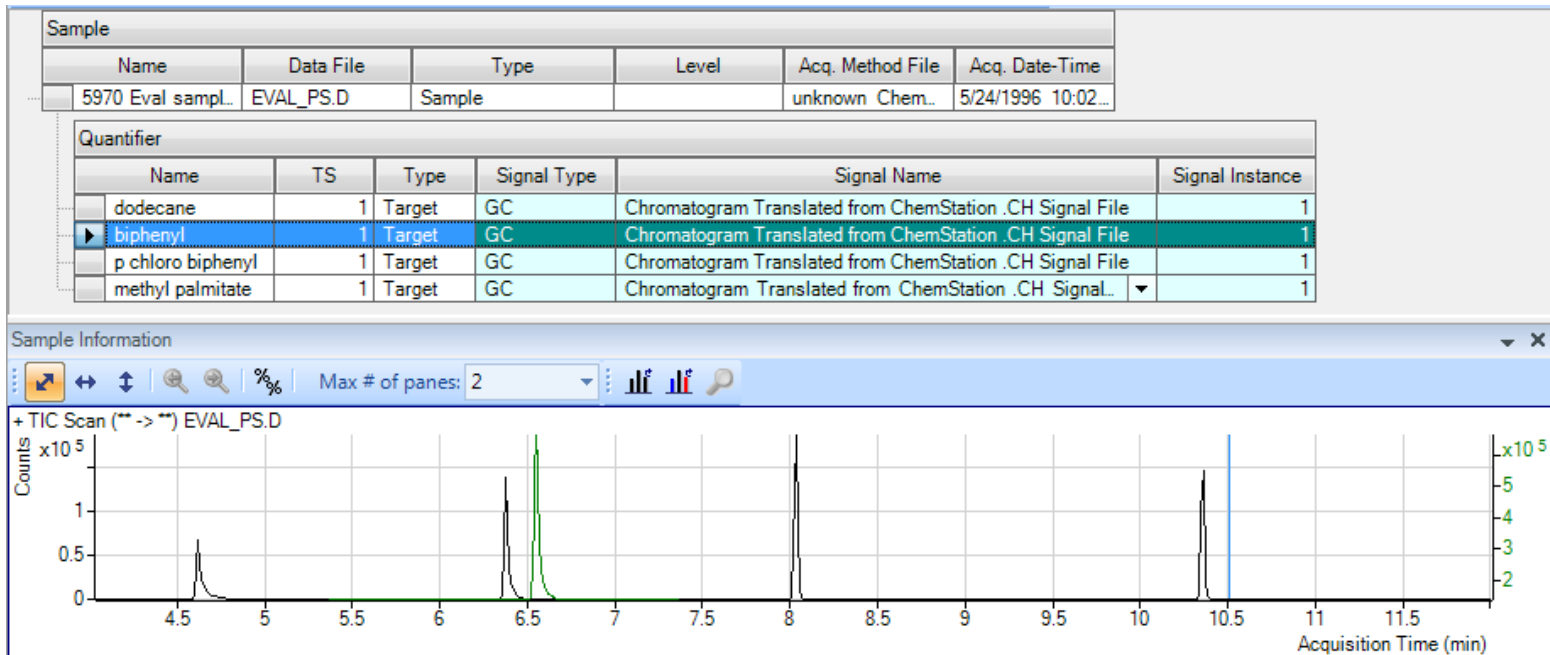
- Compound Information from a data file - populates Compound Name, Retention Time, Quant and Qual ions, and ion ratios automatically.

The screenshot displays the Agilent MassHunter Quantitative Analysis software interface. The main window shows the 'Method Table' with columns for Name, Data File, Type, Level, Acq. Method File, and Acq. Date-Time. A dialog box is open, listing options for creating a new method: 'New Method from Acquired MRM Data...', 'New Method from Acquired Scan Data...', 'New Method from Acquired Scan Data with Library', 'New Method using Manual Setup', and 'New Method from File...'. The 'New Method from Acquired MRM Data...' option is highlighted with a red box. The 'Method Table' window shows a table with columns for Name, TS, Transition, Collision, Scan, Type, and RT. The table contains three rows of data, with the first row highlighted. The first row is 'Amp' with TS 136.2, Transition 91.4, Collision 5.0, Scan MRM, Type Target, and RT 2.020. The second row is 'Amp-d5' with TS 141.1, Transition 93.4, Collision 5.0, Scan MRM, Type ISTD, and RT 1.990. The third row is 'Cocaine' with TS 304.1, Transition 182.0, Collision 5.0, Scan MRM, Type Target, and RT 2.449. The 'Transition' and 'Rel. Resp.' columns are circled in red in the original image.

Name	TS	Transition	Collision	Scan	Type	RT
Amp	136.2	91.4	5.0	MRM	Target	2.020
Amp-d5	141.1	93.4	5.0	MRM	ISTD	1.990
Cocaine	304.1	182.0	5.0	MRM	Target	2.449

# Quantitate Using 2-D Signals (GC and LC)

In addition to Scan and SIM data, MassHunter can also quantitate with 2-D signals, such as FID and UV. Set-up and Quantitation of GC and LC signals is the same as for GC/MS or LC/MS data.



# Compound Specific Integration Choice: Including parameterless integration

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	APCIautotune.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			
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			
Cocaine	1	304.1 > 182.0	MRM	Target	2.449	Universal	

Compound Information

+ MRM (136.2 > 91.4) CMAMCaL5.d  
RT=2.102 min.  
Name=Amp  
Area=19301

136.2 > 91.4 , 136.2 > 119.4  
Ratio=27.0

+ MRM (141.1 > 93.4) CMAMCaL5.d  
RT=2.076 min.  
Name=Amp-d5  
Area=1048

141.1 > 93.4 , 141.1 > 124.4  
Ratio=26.5

Integration

Integrator: Agile

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

Apply to All OK Reset Default Cancel Apply

Agile2 NEW

# Questions about Quant?



Look for “Quant Schema” on your Quant install disc  
for very detailed help and descriptions!

# Personal Compound Databases and Libraries

Confident identification using your mass spec

Identify  
Compounds

PCDs (accurate mass database) and PCDLs (MS/MS libraries) allow you to search your data to identify compounds using accurate mass against reference spectra

PCD/PCDL	Market	Compounds	Compounds with MS/MS Spectra
Pesticides	Food Safety	1669	733
Forensics/Tox	Forensics/Tox	9008	3019
Veterinary Drugs	Food / Forensics	1049	630
METLIN	Metabolomics	64,092	8040

# PCDL Manager

- Allows user to view, edit, and rearrange PCDs and PCDLs
- Can create custom PCDs and PCDLs, including addition of MS/MS spectra from acquired data
- **Custom Databases:** Polymer Additives, Coffee, Lipids, HMDB, Natural Products

MassHunter PCDL Manager for Metabolomics - C:\MassHunter\PCDL\MSMS Amino Acids.cdb

File Edit View PCDL Links Help

Find Compounds

Single Search Batch Search Batch Summary Edit Compounds Spectral Search Browse Spectra Edit Spectra

Mass: [ ] [M+H]<sup>+</sup> Neutral [M-H]<sup>-</sup>  
Mass tolerance: 10.0 ppm mDa  
Retention time: [ ] Require  
RT tolerance: 0.1 min  
Ion search mode:  
 Include neutrals  
 Include anions  
 Include cations

Formula: [ ] Name: valine Notes: [ ]  
IUPAC: [ ]  
CAS: [ ] KEGG: [ ]  
ChemSpider: [ ] HMP: [ ]  
METLIN: [ ] LMP: [ ]

Molecule: Structure MOL Text  
C[C@@H](O)C(=O)O

Notes: Positive MS/MS  
Endogenous Metabolite  
Geigy vol. 3 p. 92

Single Search Results: 1 hit for

Compound Name	Formula	Mass	Anion	Cation	RT (min)	CAS	ChemSpider	METLIN	HMP	KEGG	LMP	IUPAC Name	Num Spectra
L-Valine	CSH11NO2	117.07898	<input type="checkbox"/>	<input type="checkbox"/>	72:18.4		35	HMDB008...	C00183				4

MassHunter PCDL Manager for Metabolomics - C:\MassHunter\PCDL\MSMS Amino Acids.cdb

File Edit View PCDL Links Help

Find Spectra

Single Search Batch Search Batch Summary Edit Compounds Spectral Search Browse Spectra Edit Spectra

Mass: [ ] Precursor ion: [ ] Ion polarity: (Any)  
Tolerance: 200 ppm mDa Ionization mode: (Any)  
Collision energy: [ ]  
Tolerance: 2.0 eV

Spectra for compound: L-Valine

Compound Name	Precursor Ion	Collision Energy	Ion Polarity	Ionization Mode	Instrument Type
L-Valine	118.08626	10	Positive	ESI	QTOF
L-Valine	118.08626	20	Positive	ESI	QTOF
L-Valine	118.08626	40	Positive	ESI	QTOF
L-Valine	116.07170	10	Negative	ESI	QTOF

Single Search Results: 1 hit for

Compound Name	Formula	Mass	Anion	Cation	RT (min)	CAS	ChemSpider	METLIN	HMP	KEGG	LMP	IUPAC Name	Num Spectra
L-Valine	CSH11NO2	117.07898	<input type="checkbox"/>	<input type="checkbox"/>	72:18.4		35	HMDB008...	C00183				4

Graphic: Mass List

Library spectrum

# PCD versus PCDL

- Personal Compound Database (PCD)
  - Required: name, accurate mass
  - Optional: structure, retention time, formula, structure, CAS or other ID numbers
- Personal Compound Database Library (PCDL)
  - All of the above, *plus* MS/MS spectra
- Scoring based on
  - Accurate mass match
  - Isotope abundance
  - Isotope spacing
  - Retention time (if selected)
  - Dot product scoring of MS/MS spectra match
    - Forward and/or reverse scoring

# Pathways to PCDL for Metabolomics

Pathway Database Creator

Settings Tools Help

Pathway Data

Source: BioCyc/MetaCyc

Organism/Database: Add/Remove

All Organisms

Search Text: Clear

Selection Mode

Pathway Names

Fellow Pathway Members

Reaction Partners

Prefer Compound Names from

BioCyc/MetaCyc

METLIN

Create PCDL View unsolved

0 Unique Compound Selected Clear All

ID	Name	# of Member Cmpds
PWY-2582	brassinosteroid biosynthesis II	20
PWY-699	brassinosteroid biosynthesis I	24
PWY-5461	betanidin degradation	4
PWY-6999	theophylline degradation	12
PWY-6538	caffeine degradation III (bacteria, via demethylation)	17
PWY-6552	caffeine degradation I (main, plants)	5
PWY-6553	caffeine degradation II	5
PWY-6633	caffeine degradation V (bacteria, to trimethylurate)	5
PWYD-1297	purine deoxyribonucleosides degradation	18
PWY-6430	thymine degradation	10
PWYD-1298	pyrimidine deoxyribonucleosides degradation	17
PWY-6556	pyrimidine ribonucleosides degradation II	6
PWYD-1295	pyrimidine ribonucleosides degradation I	7
GLUCONSUPER-PWY	D-gluconate degradation	0
PWY-2361	3-oxoadipate degradation	6

Organism	Selection Mode	Entry ID	Name	# of Cmpd	Del.
----------	----------------	----------	------	-----------	------

## Convert pathway metabolite information into Agilent personal compound databases

- Pathway database source - WikiPathways, BioCyc and KEGG
- Select one to many pathways
- Removes redundant metabolites
- Adds compound information – **Formula**, Compound ID(s), Name, Structure

## Can link to METLIN PCDL to add compound information

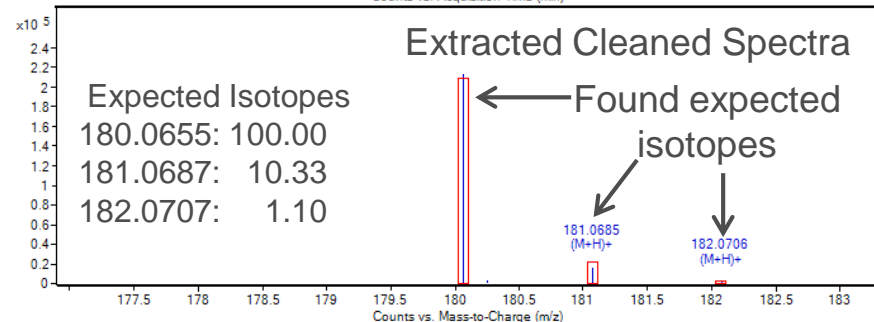
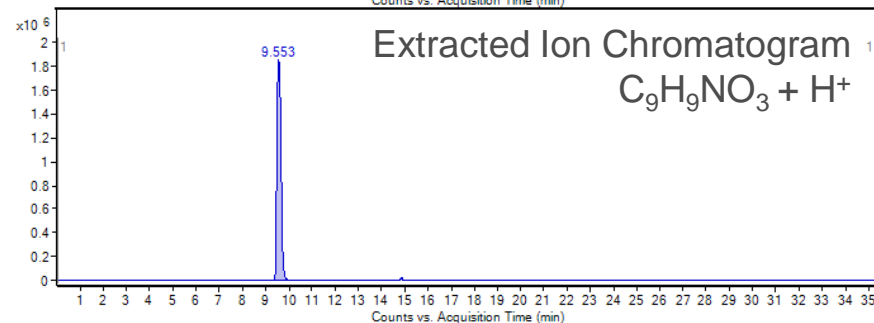
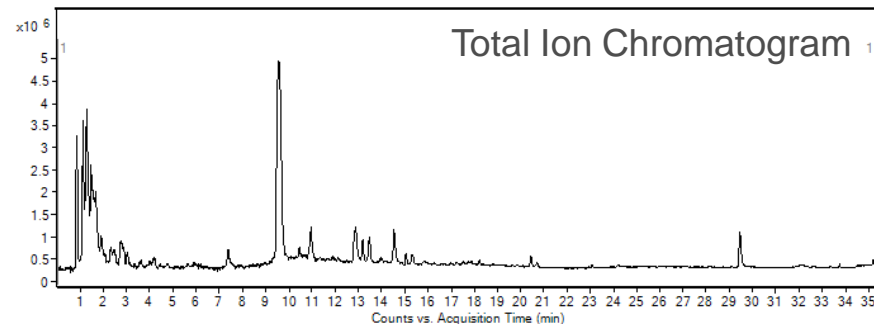
- Retention time or MS/MS spectra



# Power of Pathway Directed Data Mining

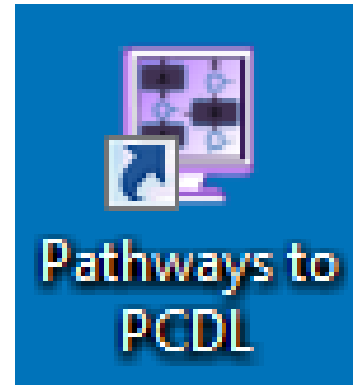
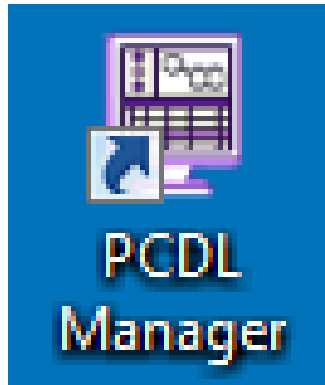
## Mine Data Using Find by Formula and Database

- Extract chromatogram and spectra using empirical formula and user-set rules
  - Use a metabolite database created by Pathways to PCDL
- Create Find by Formula method
- Chromatograms extracted and integrated
- Spectra scored from empirical formula
- User specifies match criteria threshold
  - Spectra score
  - Retention time (optional) increases specificity
- User can review and edit results
- Produce a CEF file for import into MPP



**Targeted Data Mining of Qualitative Data for Greater Specificity**

# Questions about PCDL Manager or Pathways to PCDL?



# Molecular Structure Correlator (MSC)

Identify  
Compounds

- Utilizes centroid MS/MS data to help elucidate structures for unknown compounds that are *not* found in PCDs or PCDLs by:

- Calculating formulas for a precursor, fragment ions, and neutral losses
- Can Search Online Databases: Chemspider for possible structures
- Matches experimental fragments those from proposed structure by a systematic bond breaking, and displaying the best matches

Precursor MFG results

Loaded mol file

Compound formula: C23H31NO2

ID	Formula	Ions	Peak	d(M/z)	Product	
1	C23H31NO2	767	604	2.7	2.7	94
2	C19H27NO5	0	0	0.7	0.7	80
3	C20H29NO25	41	41	6.9	6.9	80
4	C19H27NO7	36	33	10.3	10.3	92
5	C19H29NO45	0	0	4.5	4.5	63
6	C19H27NO55	0	0	6.4	6.4	48
7	C19H27NO10	0	0	10.1	10.1	61

Fragment formulas for C23H31NO2

m/z	Intensity	Formula	d(M/z)
101.0607	92989.85	C8H9	1.6
167.0857	86414.21	C13H11	-6.8
209.1330	72955.48	C15H17	-2.3
100.1119	72103.65	C8H14N	2.2
91.0544	55205.42	C7H7	-1.5
131.0852	41825.77	C13H11	2.9
281.1526	16947.35	C19H21O2	0.4
149.0587	12370.42	C9H10O2	9.1
210.1363	11961.80	C16H18	19.1
168.0879	10736.67	C13H12	32.5
106.0726	8174.76	C8H10	48.3
73.0285	5765.78	C7H10O	-1.6
132.0880	4301.33	C13H12	40.7
101.1146	4243.73	C8H15N	53.1
72.0816	3229.49	C6H10N	-11.3
92.0574	3225.02	C7H8	50.6
101.1622	2475.53	C13H12O	1.8
282.1565	2347.47	C19H22O2	17.4
188.1071	2216.98	C15H18O	1.8
167.1288	2142.96	C15H17NO	9.8
209.1584	2074.37	C15H23NO	-14.2
101.2262	2055.64	C13H22O	1.8
101.1440	1885.64	C13H22O	1.8
100.2252	1756.18	C13H22O	1.8
209.2670	1553.03	C15H23O	1.8
100.0291	1482.47	C7H8O	4.3
91.0880	1326.02	C7H8O	4.3
101.1170	1322.02	C7H8O	4.3
90.4492	1211.88	C7H8O	4.3

Compound formula: C23H31NO2

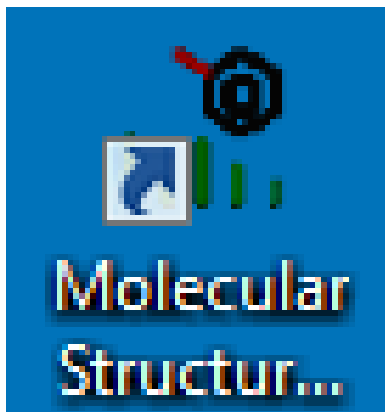
Fragments of structure #1 - elucidated: 56.7% ions, 97.8% Weight

Mass	Intensity	Weight(%)	No. of cand.	Best score	
1	281.1526	16947.35	41.7	1	95.5
2	100.1119	72103.65	0.4	1	94.3
3	73.0285	5765.78	0.0	1	97.7
4	209.1330	72955.48	31.6	2	93.8
5	167.0857	86414.21	9.6	1	96.7
6	72.0816	3229.49	0.0	2	95.9
7	149.0587	12370.42	0.7	3	69.0
8	91.0544	55205.42	0.2	1	66.3
9	105.0687	82889.85	0.4	2	66.3
10	210.1363	11961.80	5.1	2	60.3
11	131.0852	41825.77	1.1	6	58.3
12	282.1565	2347.47	6.0	1	52.2
13	168.0879	10736.67	1.2	1	36.4

Proposed structure of fragment ions and scores

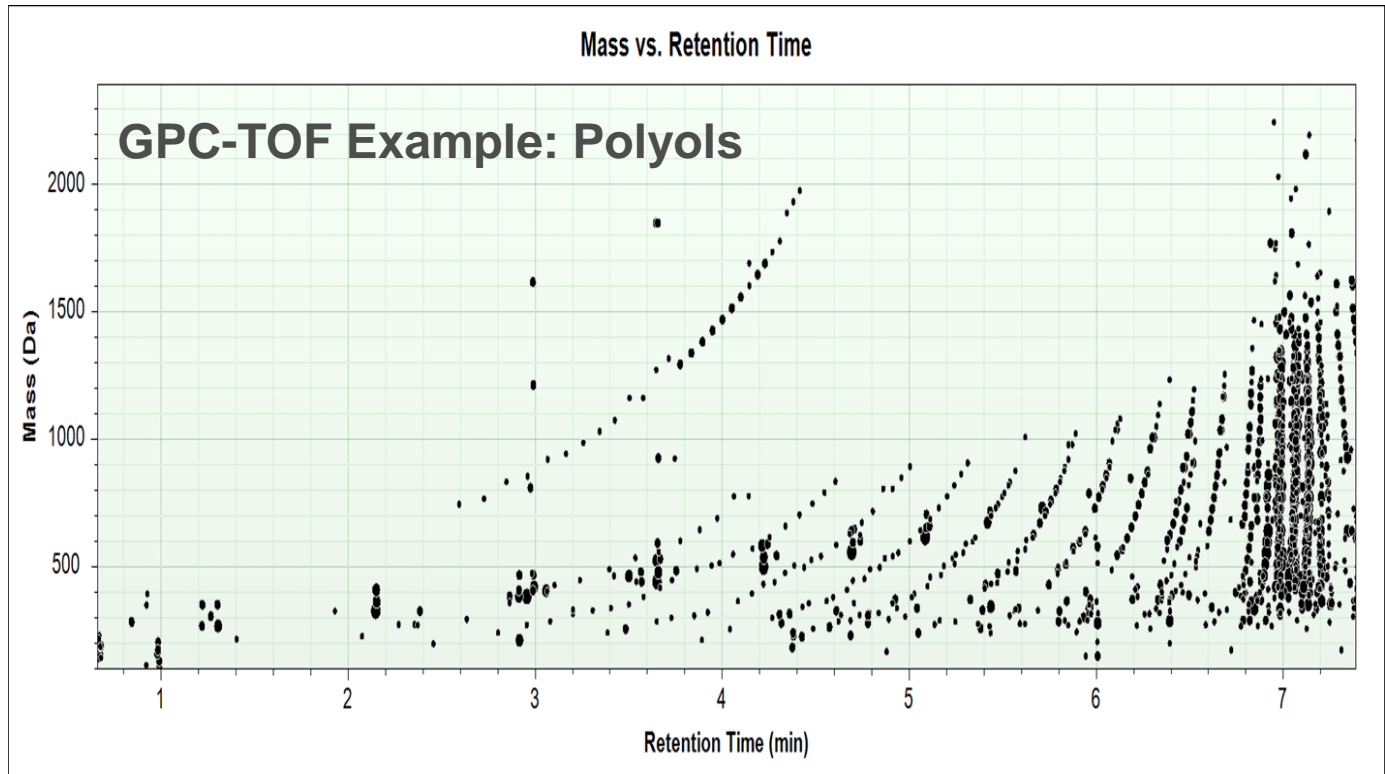
Product ion MFG results

# Questions about MSC?



# Mass Profiler (MP) Differential Analysis Program

- Feature alignment
- Single-variate statistics for binary experiments
- IDBrowser for compound identification

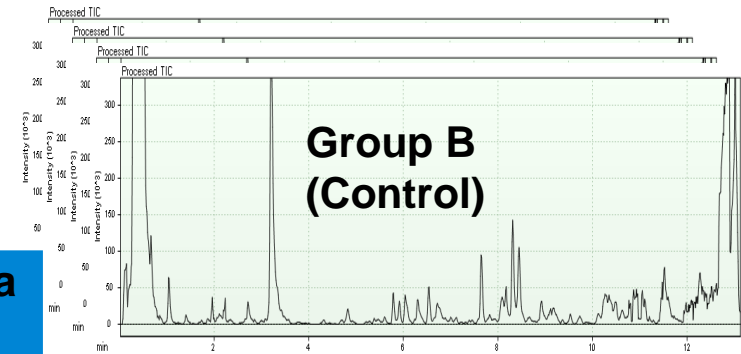
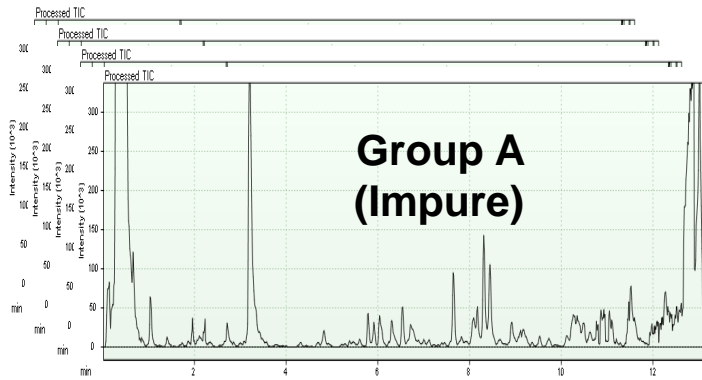


Clearly see  
repeating  
units of 44  
and 58 m/z

# Mass Profiler

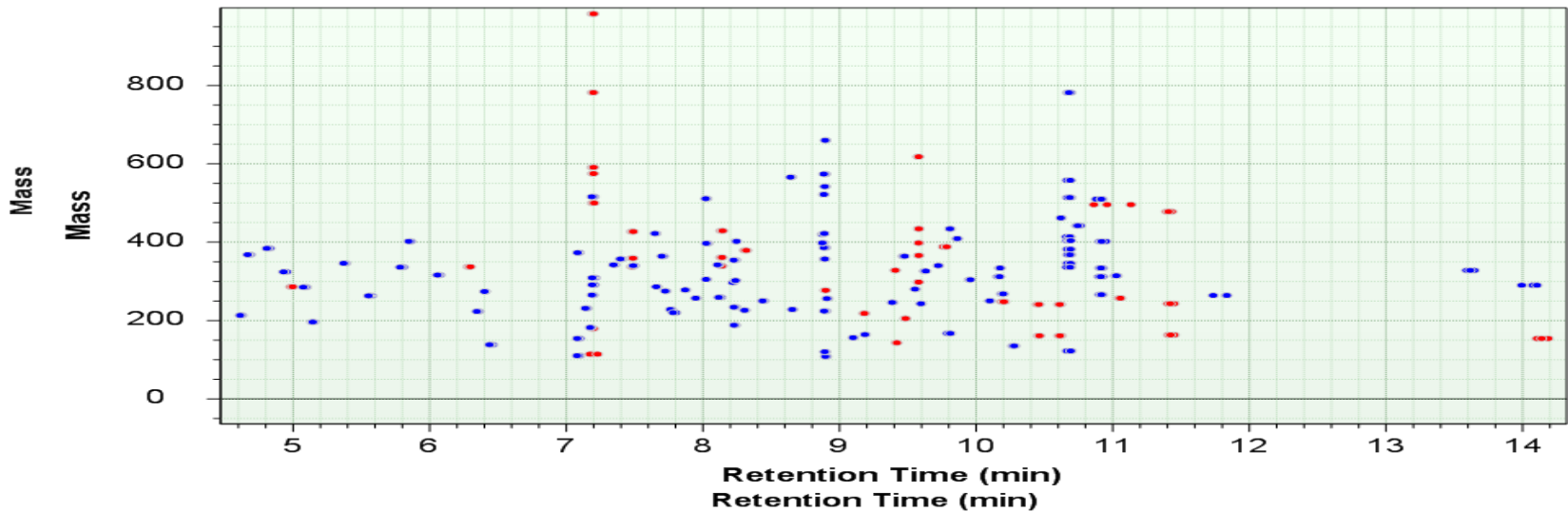
- Impurity Profiling/Differential Analysis Software
- Graphical Displays
  - Mass vs Retention Time
  - Log2 Ratio (Group1/Group2) vs Retention Time
  - Log2 Abundance Group 2 vs Log2 Abundance Group 1
  - Unique to Group 1 vs RT and Unique to Group 2 vs RT (New)
- Feature Identification
  - Molecular Formula Generation and AMRT database
  - Single Feature or Batch Processing (summary report)
  - Web Internet Database Searching

# Mass Profiling Software



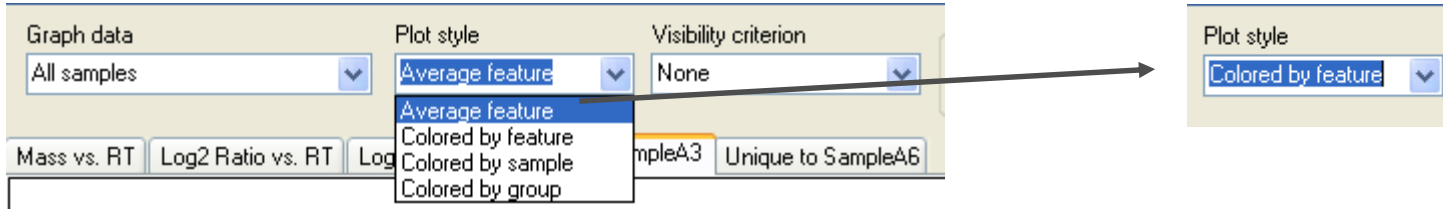
Aligns Data  
RT, Mass,  
Abundance

What's Changed? Mass/RT No Fold Change  
Mass vs. Retention Time

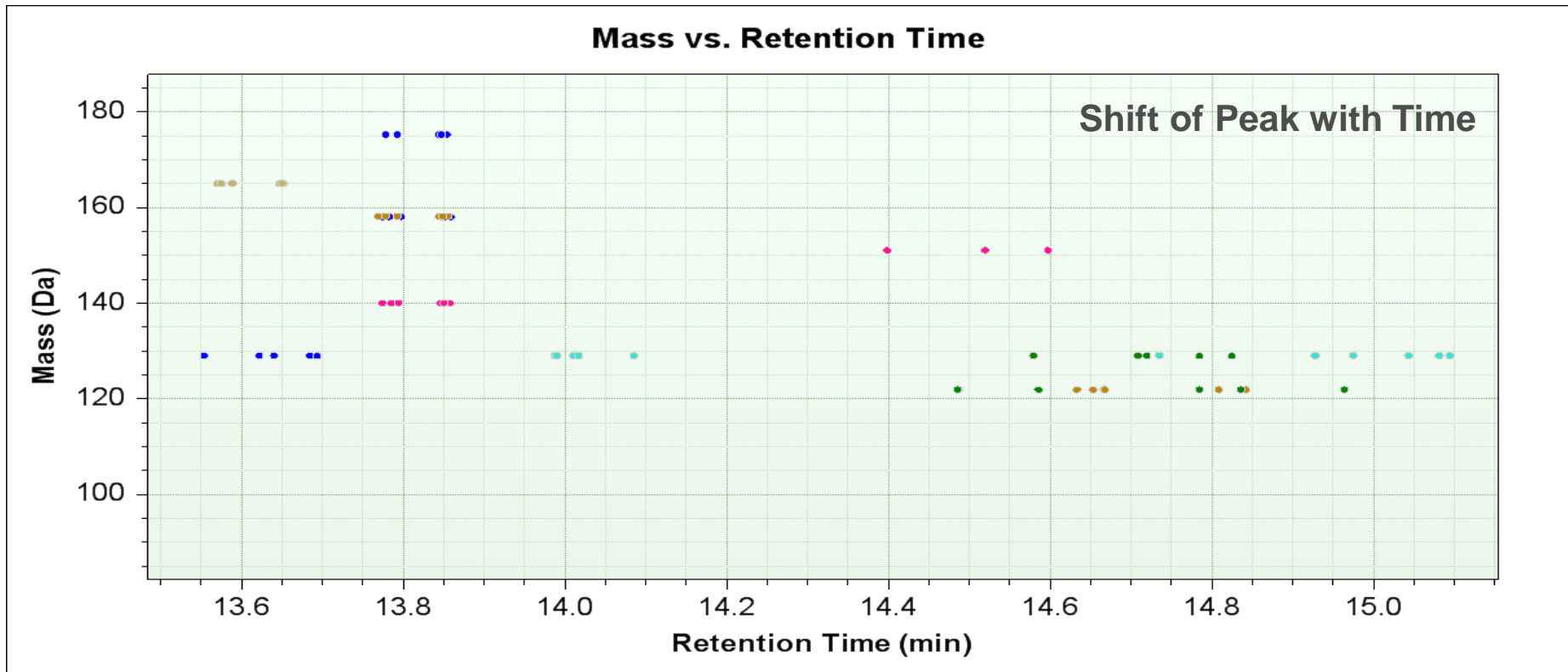


What's Unique? Impurity Control

# Mass Profiler – Reproducibility of Results

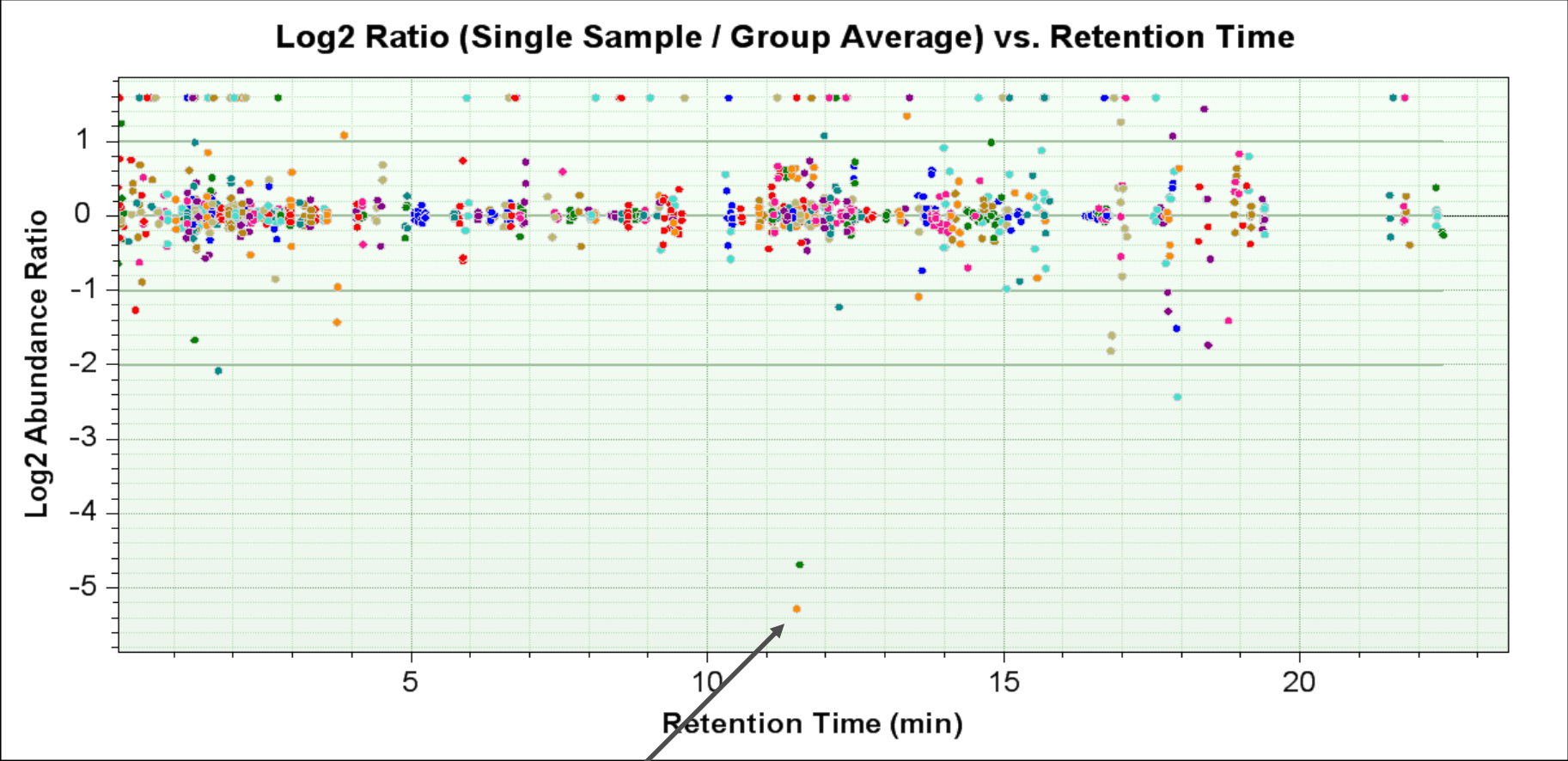


## Reproducible Retention Time Stability



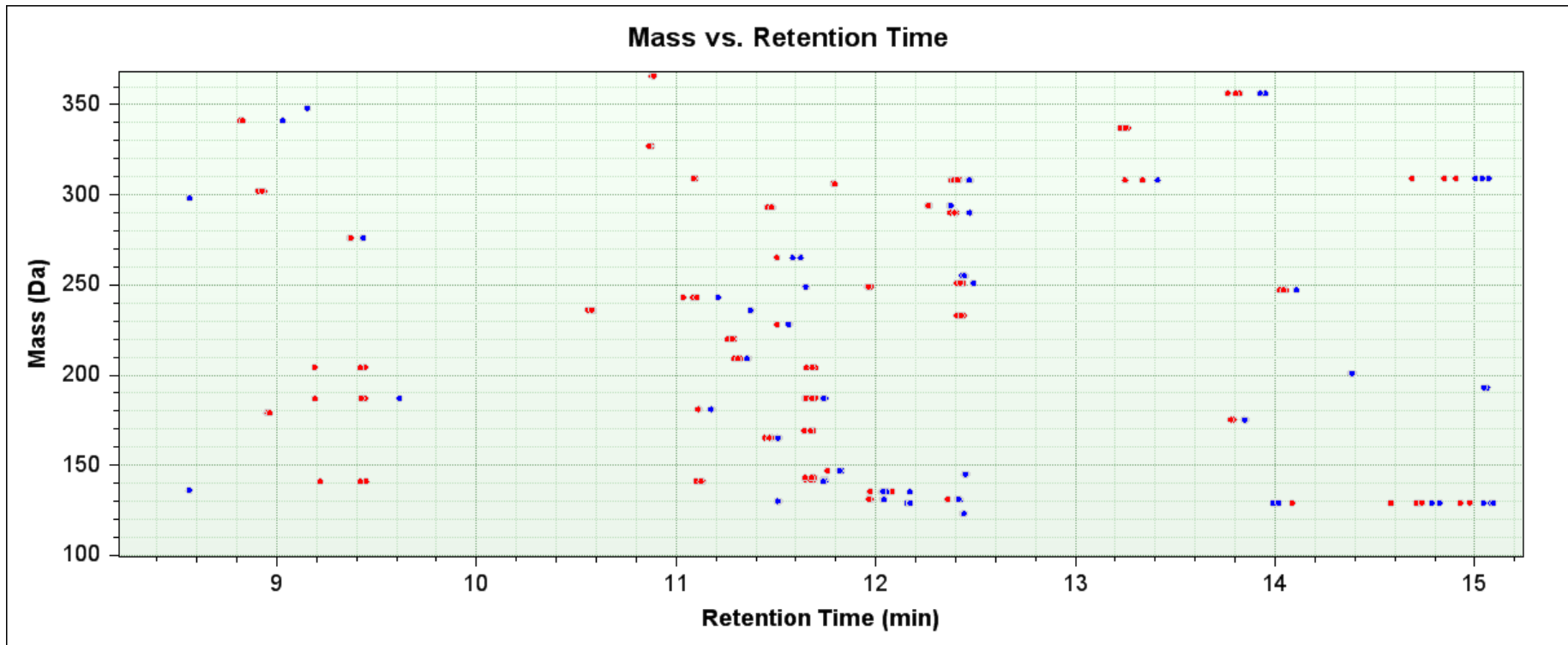
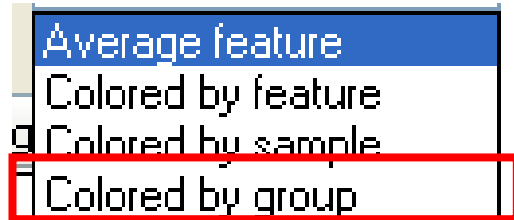


# Mass Profiler – Reproducibility of Results



**Outlier Sample or Feature**

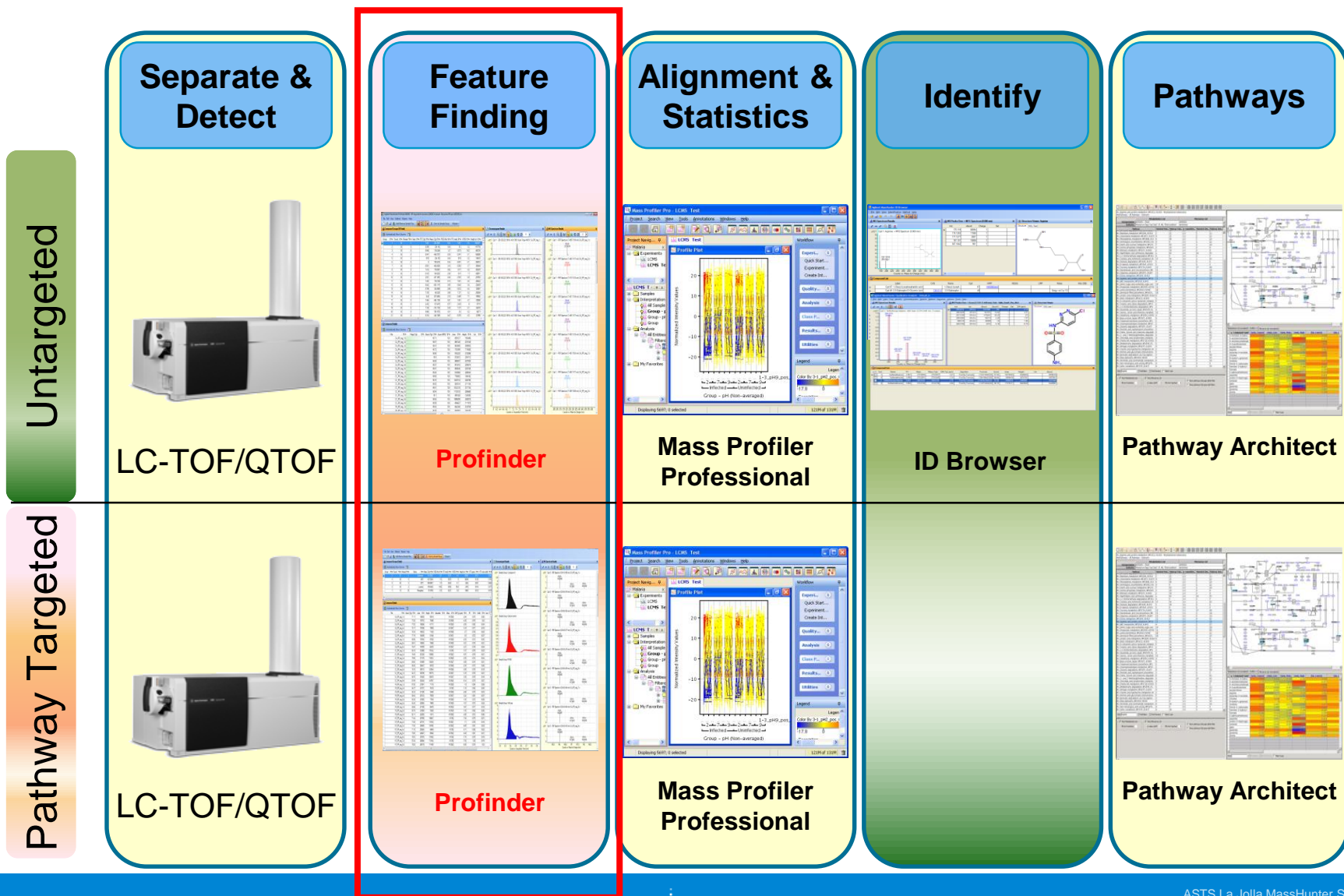
# Unique Group 1 and Unique Group 2



# Questions about Mass Profiler?

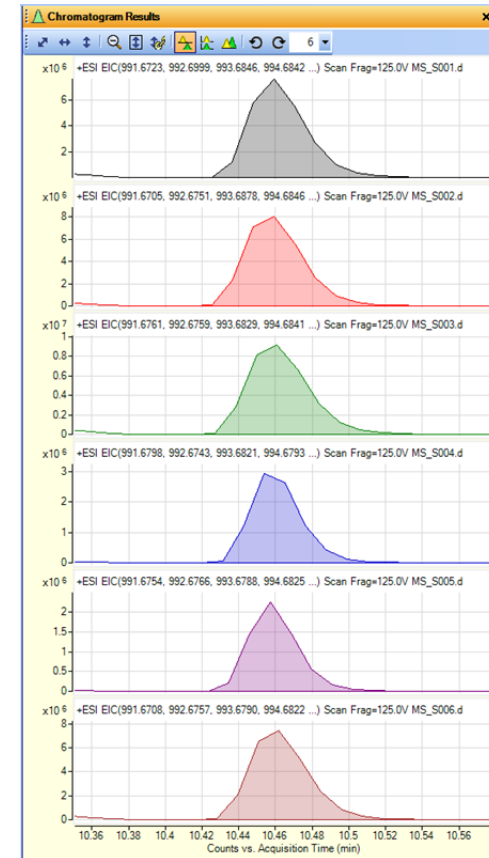
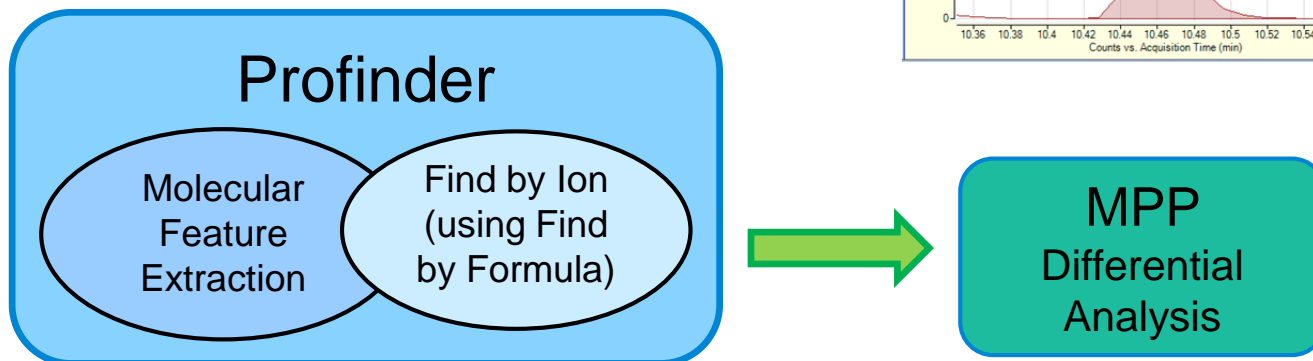


# Untargeted Data Acquisition & Analysis



# Mass Hunter Profinder - **NEW**

- Batch based or “project” based logic
- Extracts and aligns features prior to statistical analysis in MPP
- Can replace previous recursive workflow in Qual
- More efficient, fewer manual steps
- Visualize, review, and edit results across the batch for higher quality results



# Profiler Workflows

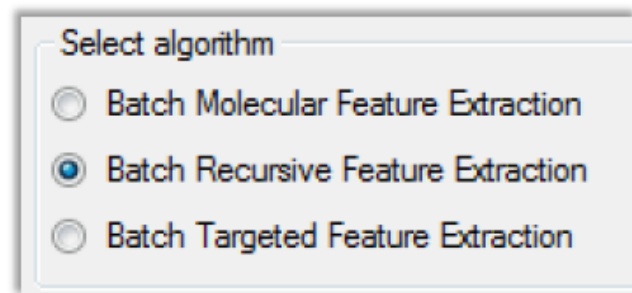
1. Batch **Molecular** Feature Extraction
  - Reduces False Positives, No Editing



2. Batch **Recursive** Feature Extraction
  - Reduces False Negatives, Allows Editing



3. Batch **Targeted** Feature Extraction
  - Uses database targets, Allows Editing

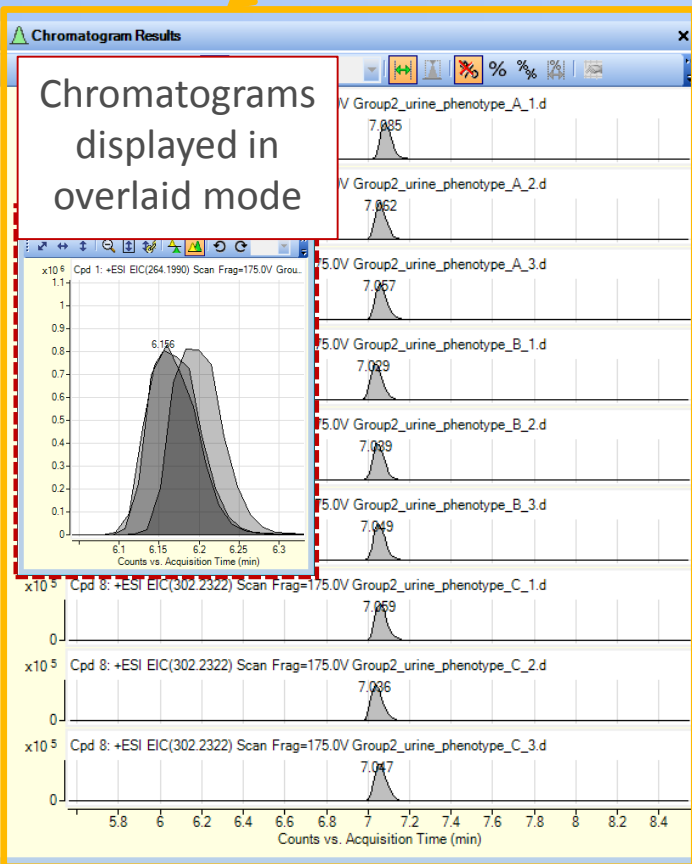


# Profinder Results Navigation

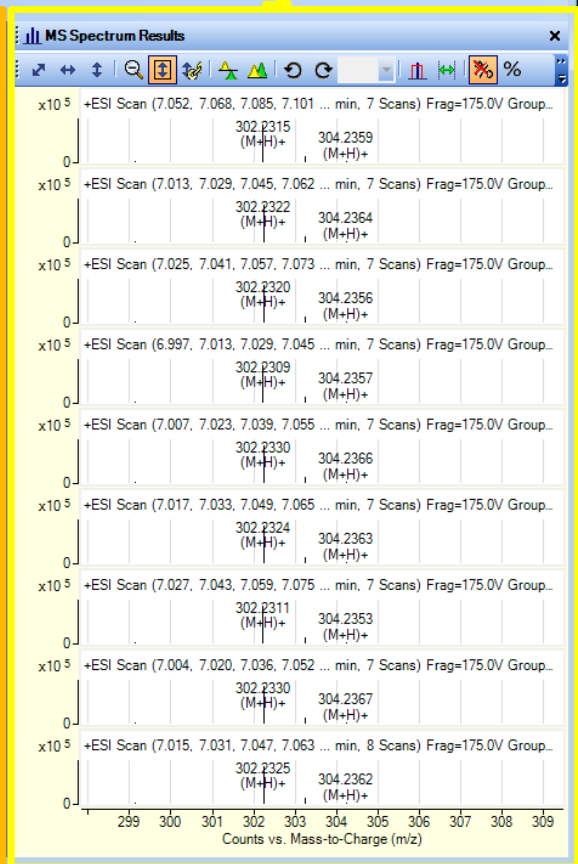
Compound Groups Table

Group	Found	Missed	Mass (Tgt)	Mass (med)	RT (Tgt)
1	9	0	263.1915	263.1911	6.166
2	9	0	439.2207	439.2213	5.732
3	9	0	314.1409	314.1409	5.783
4	9	0	113.0592	113.0591	0.67
5	9	0	137.0479	137.0478	0.785
6	9	0	93.0585	93.0578	0.833
7	6	3	288.2088	288.2095	8.291
8	9	0	301.2249	301.2249	7.057
9	9	0	116.0779	116.0778	0.667
10	9	0	269.0826	269.0829	5.796
11	8	1	179.0577	179.058	5.271
12	2	7	104.0294	104.0299	5.435
13	9	0	151.002	151.002	1.249

Chromatogram Results



Spectrum Results



File	Score	Mass	Diff (Tgt, ppm)
Group2_urine_phenotype_A_1.d	97.07	301.2242	-2.36
Group2_urine_phenotype_A_2.d	99.73	301.2249	-0.1
Group2_urine_phenotype_A_3.d	99.88	301.2247	-0.67
Group2_urine_phenotype_B_1.d	94.27	301.2236	-4.37
Group2_urine_phenotype_B_2.d	97.86	301.2256	2.44
Group2_urine_phenotype_B_3.d	99.64	301.2251	0.7
Group2_urine_phenotype_C_1.d	97.27	301.2238	-3.64
Group2_urine_phenotype_C_2.d	97.58	301.2257	2.45
Group2_urine_phenotype_C_3.d	99.46	301.2251	0.78

Compound Details Table

# Questions about Profinder?





# DA Reprocessor

Use this, it saves memory and works in the background!

Run Qual method on a batch of samples

DA Reprocessor - Offline Utilities B.06.00 (B269)

START STOP

	<input checked="" type="checkbox"/>	Sample Name	Sample Position	Data File	Method
1	<input checked="" type="checkbox"/>	Benzo urine 1	P1-E1	C:\MassHunter\Data\BenzosInUrine\Benzo urine 0011.d	C:\MassHunter\Methods\B.06.00\MFE+cef.m
2	<input checked="" type="checkbox"/>	Benzo urine 2	P1-E2	C:\MassHunter\Data\BenzosInUrine\Benzo urine 0012.d	C:\MassHunter\Methods\B.06.00\MFE+cef.m
3	<input checked="" type="checkbox"/>	Benzo urine 3	P1-E3	C:\MassHunter\Data\BenzosInUrine\Benzo urine 0013.d	C:\MassHunter\Methods\B.06.00\MFE+cef.m
4	<input checked="" type="checkbox"/>	Benzo urine 4	P1-E4	C:\MassHunter\Data\BenzosInUrine\Benzo urine 0014.d	C:\MassHunter\Methods\B.06.00\MFE+cef.m
5	<input checked="" type="checkbox"/>	Benzo urine 5	P1-E5	C:\MassHunter\Data\BenzosInUrine\Benzo urine 0015.d	C:\MassHunter\Methods\B.06.00\MFE+cef.m
6	<input checked="" type="checkbox"/>	Benzo urine 6	P1-E6	C:\MassHunter\Data\BenzosInUrine\Benzo urine 0016.d	C:\MassHunter\Methods\B.06.00\MFE+cef.m

Right click upper left corner to add one or multiple samples

Populates automatically

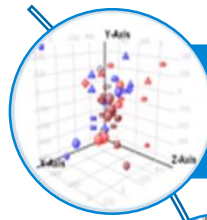
Open your Qual method

# Questions about DA Reprocessor?

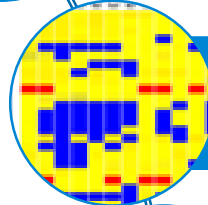


# Mass Profiler Professional

Find differences in mass spec data sets and reach statistically valid conclusions



Get from data to answers using statistical tests such as PCA



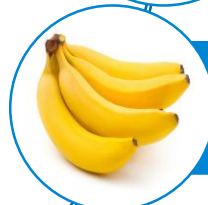
Dive deeper into results using visualizations e.g. heat maps



Accurate identifications using ID Browser



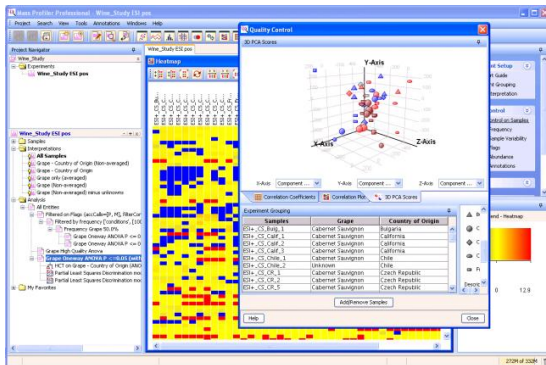
Use data from LC/MS, GC/MS, ICP-MS, and NMR



Run QC assays using the Sample Class Predictor

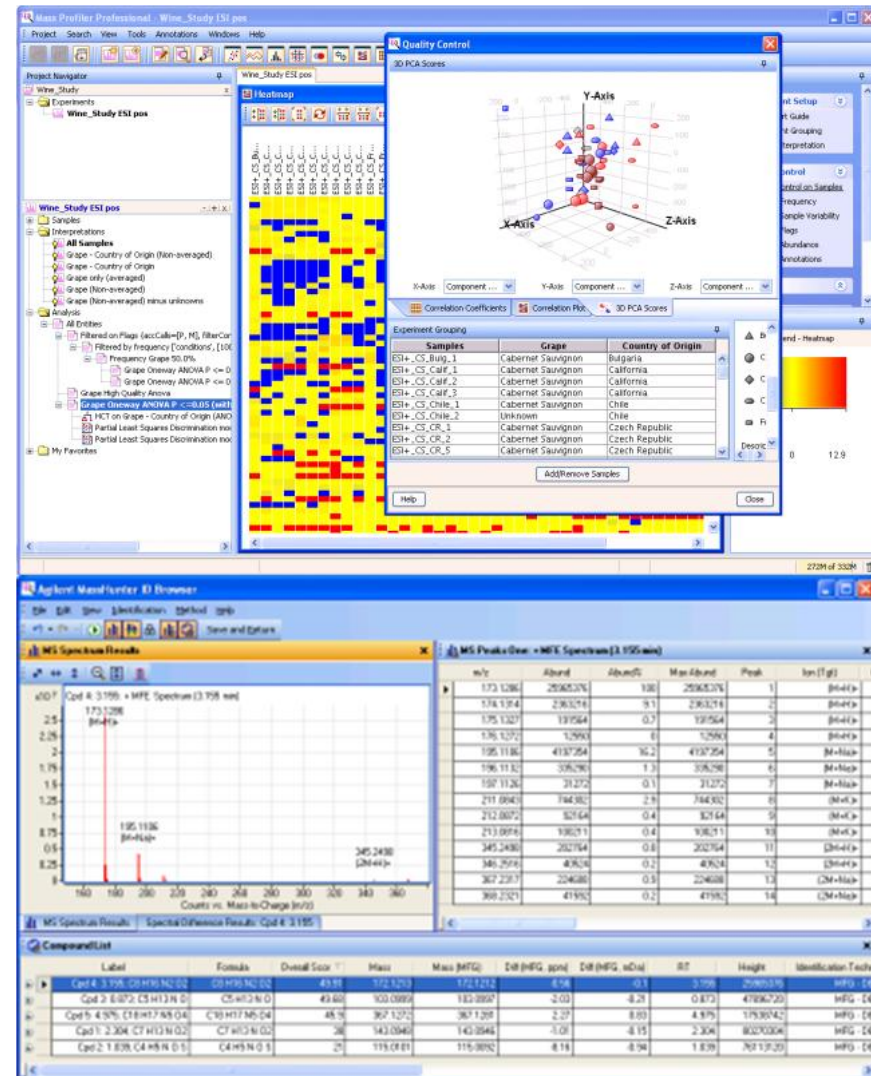


Bring genomics, proteomics, and metabolomics together



# Mass Profiler Professional (MPP)

- Compound alignment
- Filtering
- Single- and multi-variate statistics
  - t-test, ANOVA, clustering, fold change, PCA
- IDBrowser for compound identification
- Sample Class Prediction
- Pathway Architect
- Multiple data types and sources
  - Metabolomics, lipidomics, proteomics, other small molecule profiling
  - LC-MS, GC-MS, ICP-MS, generic import
  - Targeted, untargeted



# ID Browser

Searches against csv or PCD files to identify compounds

The screenshot displays the Agilent MassHunter ID Browser B.05.00 interface. The main window is divided into several panes:

- MS Spectrum Results:** Shows a mass spectrum plot for "Cpd 4: 19-Oxotestosterone; C19 H28 O2; 8.293; + FBF Spectr...". The x-axis is "Counts vs. Mass-to-Charge (m/z)" and the y-axis is "x10<sup>4</sup>". The base peak is at m/z 289.2158 (M+H)<sup>+</sup>. Other significant peaks are at m/z 290.2190 (M+H)<sup>+</sup> and 291.2209 (M+H)<sup>+</sup>. A chemical structure of 19-Oxotestosterone is shown next to the spectrum.
- MS Peaks One: + FBF Spectrum (8.293 min):** A table listing the following peaks:

m/z	Abund	Abund % (Norm)
289.2158	52412.47	
290.219	10196.8	
291.2209	1140.85	
292.2209	179	
311.1977	13018.88	
312.2011	2644.13	
313.1999	297.23	
314.195	29	
577.4243	3829.87	
578.4274	1561.83	
579.4311	332.57	
580.4234	25.5	
- Structure Viewer: 19-Oxotestosterone:** Displays the chemical structure of 19-Oxotestosterone, a steroid with a ketone group at C-3, a double bond at C-4, and a hydroxyl group at C-19.
- Compound List:** A table listing search results for various compounds. The top results are:

Label	Name	Score (DB)	Hits (DB)	Formula	Score (MFG)	Score
Cpd 2: 2,6-Methano-2H-quinolizine...	2,6-Methano-2H-quinolizine(MDL...	75.85	2	C19 H22 N2 O3		75.85
Cpd 3: 12-oxo-ETE; C20 H30 O3;...	12-oxo-ETE	89.29	10	C20 H30 O3		89.29
Cpd 4: 19-Oxotestosterone; C19 H...	19-Oxotestosterone	98.56	7	C19 H28 O2		98.56
Cpd 7: epsilon-Caprolactam; C6 H...	epsilon-Caprolactam	86.68	1	C6 H11 N O		86.68
Cpd 9: epsilon-Caprolactam; C6 H...	epsilon-Caprolactam	86.88	1	C6 H11 N O		86.88
Cpd 8: C17 H30 N4 O5; 8.288				C17 H30 N4 O5	98.51	98.51
Cpd 6: C13 H18 N6 O4; 8.308				C13 H18 N6 O4	98.19	98.19
Cpd 1: C39 H54 N2 S2; 8.294				C39 H54 N2 S2	97.72	97.72
Cpd 5: C20 H32 N2 O3; 8.288				C20 H32 N2 O3	95.02	95.02

# ID Browser

Searches against csv or PCD files to identify compounds

Measured and theoretical isotope ratios

Ion species and isotope abundance values

Compound structure

The screenshot displays the Agilent ID Browser interface. The top section shows three panels: 'MS Spectrum Results' (left), 'MS Peaks One: + FBF Spectrum (8.293 min)' (middle), and 'Structure Viewer: 19-Oxotestosterone' (right). The 'MS Spectrum Results' panel shows a mass spectrum with peaks at m/z 289.2158, 290.2190, and 291.2209. The 'MS Peaks One' panel shows a table of peaks with their m/z, abundance, and normalized abundance. The 'Structure Viewer' panel shows the chemical structure of 19-Oxotestosterone. Below these panels is a search results table with columns for Label, Name, Score (DB), Hits (DB), Formula, Score (MFG), and Score. The table lists several compounds, with 19-Oxotestosterone (Cpd 4) highlighted in blue. Red arrows point from the labels above to the corresponding panels. Blue, green, and purple boxes highlight specific columns in the table, with labels below them: 'Database match score' (blue), 'Number of hits' (green), 'Database match or MFG formula' (white), 'MFG score' (red), and 'Overall Score' (purple).

Label	Name	Score (DB)	Hits (DB)	Formula	Score (MFG)	Score
Cpd 2: 2,6-Methano-2H-quinolizine...	2,6-Methano-2H-quinolizine(MDL...	75.85	2	C19 H22 N2 O3		75.85
Cpd 3: 12-oxo-ETE; C20 H30 O3;...	12-oxo-ETE	89.29	10	C20 H30 O3		89.29
Cpd 4: 19-Oxotestosterone; C19 H...	19-Oxotestosterone	98.56	7	C19 H28 O2		98.56
Cpd 7: epsilon-Caprolactam; C6 H...	epsilon-Caprolactam	86.68	1	C6 H11 N O		86.68
Cpd 9: epsilon-Caprolactam; C6 H...	epsilon-Caprolactam	86.88	1	C6 H11 N O		86.88
Cpd 8: C17 H30 N4 O5; 8.288				C17 H30 N4 O5	98.51	98.51
Cpd 6: C13 H18 N6 O4; 8.308				C13 H18 N6 O4	88.10	88.10
Cpd 1: C39 H54 N2 S2; 8				C39 H54 N2 S2		
Cpd 5: C20 H32 N2 O3; 8				C20 H32 N2 O3		

Measured and theoretical isotope ratios

Database match score

Number of hits

Database match or MFG formula

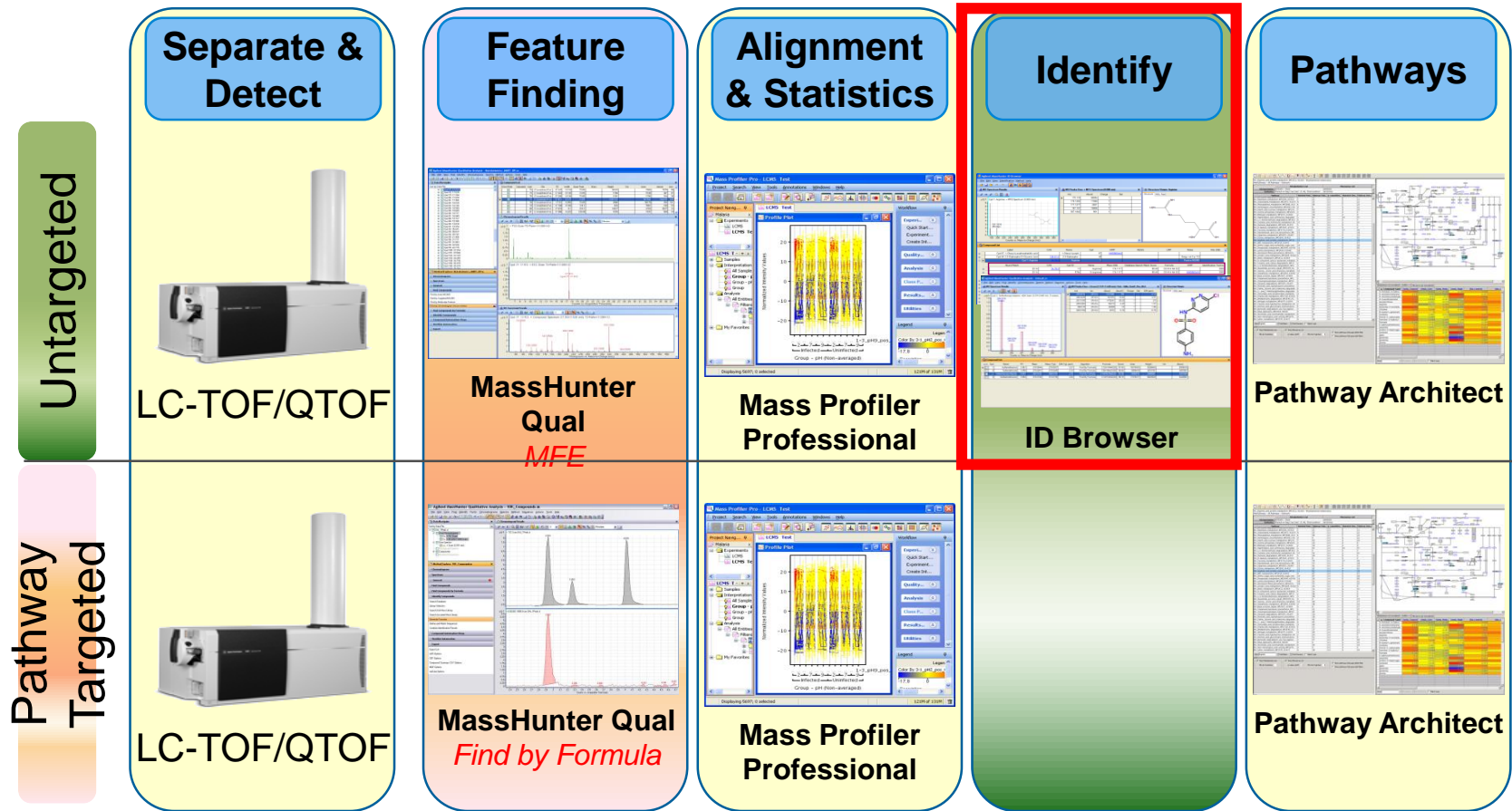
MFG score

Overall Score



# SimLipid from PREMIER Biosoft International

One way to think of SimLipid is like “ID Browser for Lipids”



# SimLipid vs. METLIN PCD

METLIN PCD has 31,011 lipid compounds. It is suited in lipidomics for customers who:

- Are agreeable to an **MS-only workflow** (i.e. database search)
- Want to use Agilent's ID Browser for identifications (part of MPP) instead of SimLipid
- Want to have the other ~33,000 metabolite compounds in METLIN
- Lower cost solution – perpetual license

SimLipid has 36,224 lipids in its database. It is suited for customers who:

- Want to identify lipids using **MS/MS pattern matching** (in addition to database search)
- Have instruments other than Agilent's
- Are familiar with or already own SimLipid for lipid identifications
- Requires an annual subscription



# The MPP Lipidomics Workflow



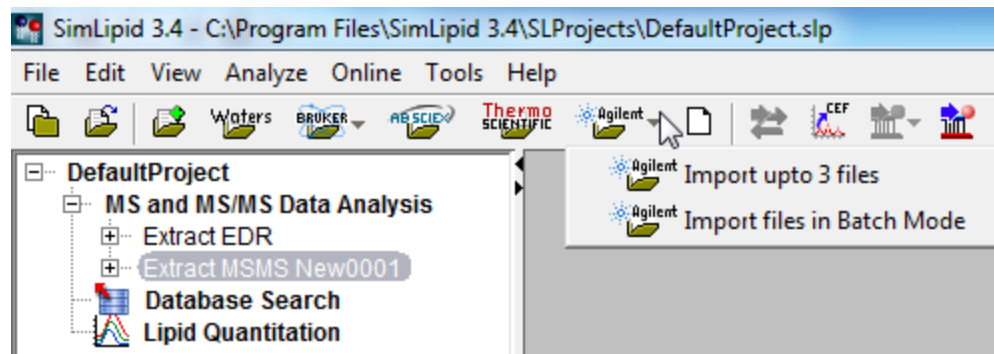
- SimLipid 3.3 and higher supports import and export of Agilent's Compound Exchange Format (.CEF) file. Compounds found in Qual and exported as .CEF can be
  - annotated in SimLipid as lipid compounds using
    - MS database searching
    - MS/MS pattern matching for features that have MS/MS
  - export annotated results in .CEF file format
  - import annotated .CEF file into MPP,
    - use Pathway Architect to give biological contextualization.

# Overview of SimLipid Process

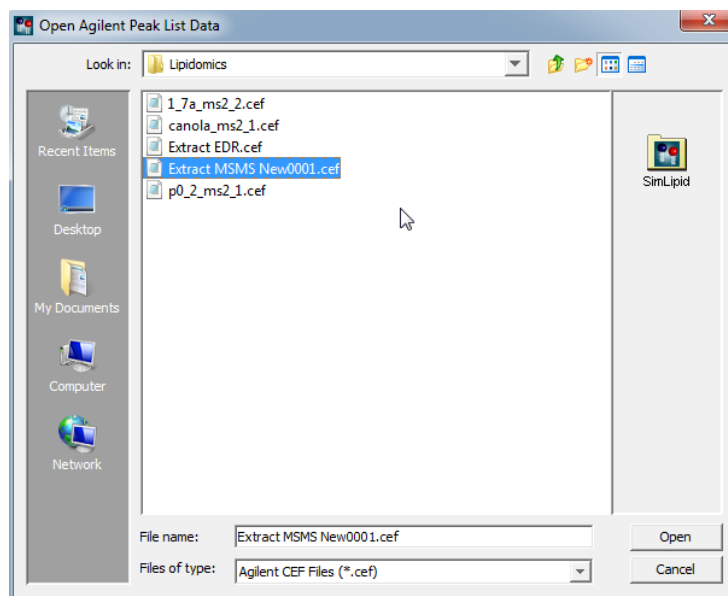
- Import CEF files into SimLipid
- Run High Throughput Search on CEF files
- Load HTP Results from SimLipid server
- Generate HTP Report (optional)
- Export annotated CEF files for analysis in MPP

# Import Agilent CEF Files

Choose the Agilent icon on the SimLipid menu bar and select either Import up to 3 files or Batch Mode.

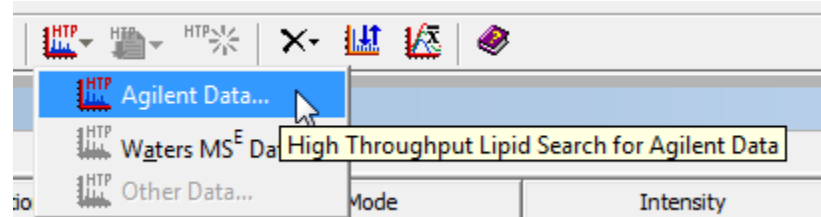


Select your CEF files.

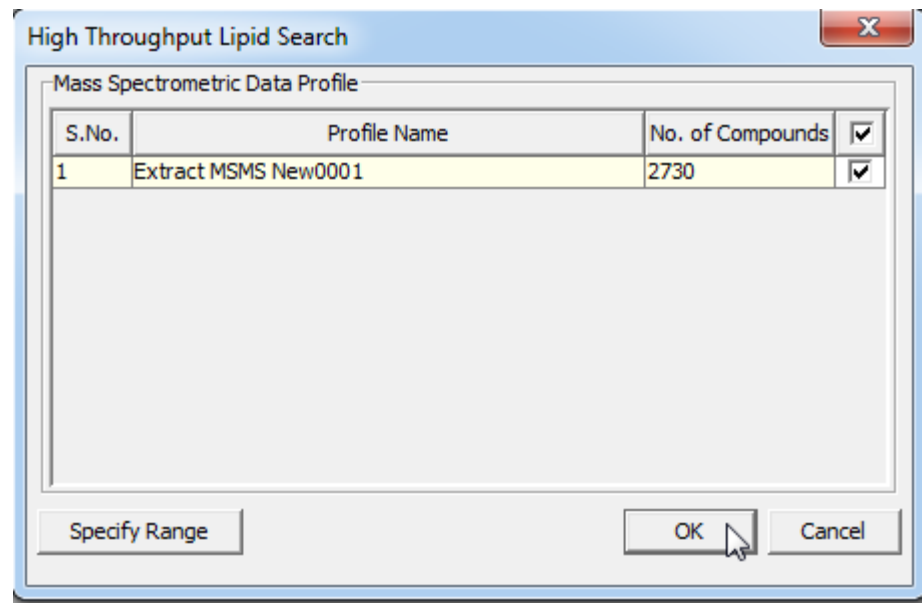


# Run High Throughput Search on the CEF Files

Select High Throughput Lipid Search (“HTP”) in the menu bar

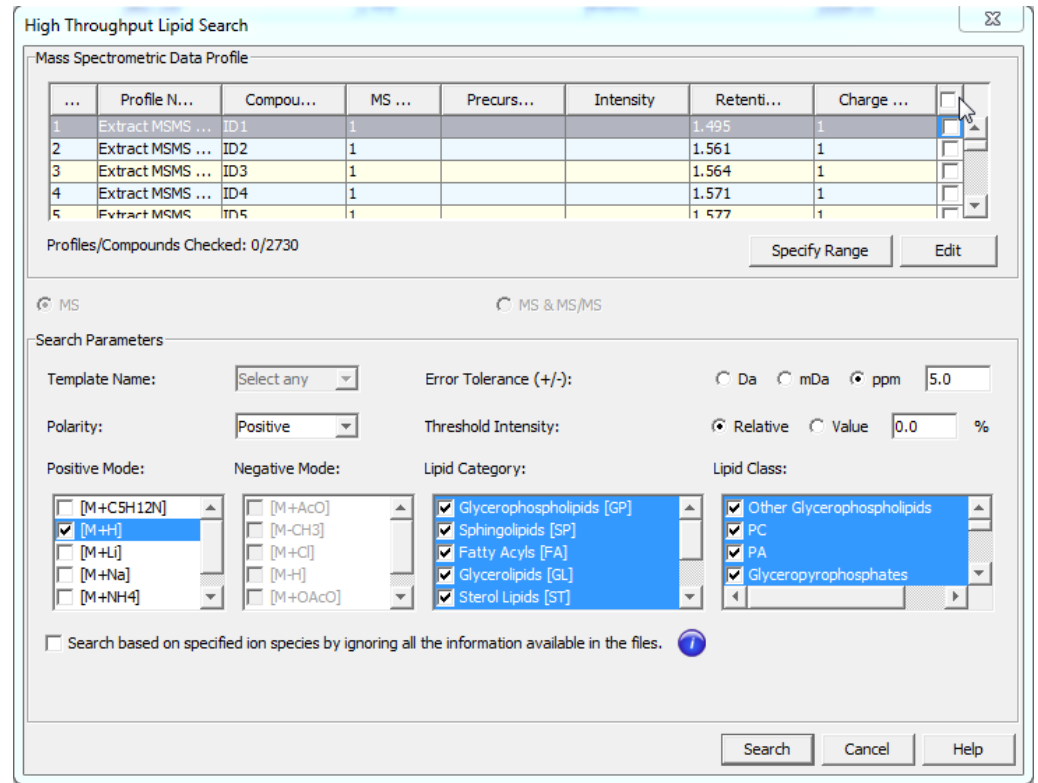


Select CEF files to run High Throughput search on and click OK.



# Run High Throughput Search on the CEF Files

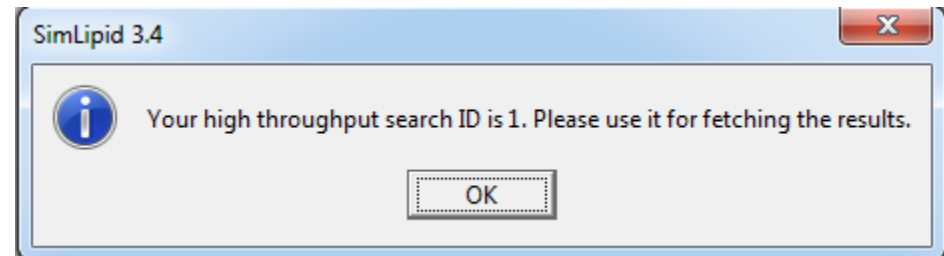
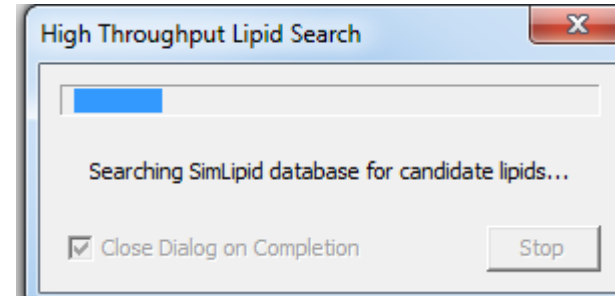
Select the compounds to run HTP search on and the specific search parameters, then press the Search button.



2000 compounds (aka “profiles” in SimLipid) can be searched at one time

# Run High Throughput Search on the CEF Files

The High Throughput search runs and then you are given a search ID (even on individually installed instance, i.e. non-server)

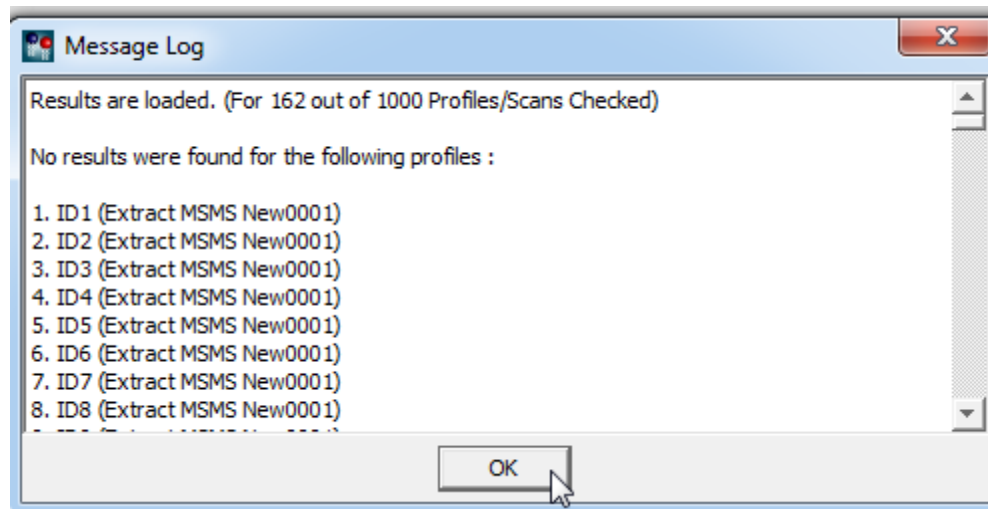


# Load HTP Results

Go to the HTP icon on the menu bar and select to load your HTP search request.

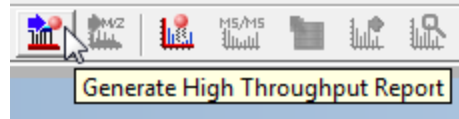
A message log will return how many of the compounds were identified (e.g. 162 out of 1000)

Searches are cumulative—the next time you search it will automatically select the second 1000 compounds.

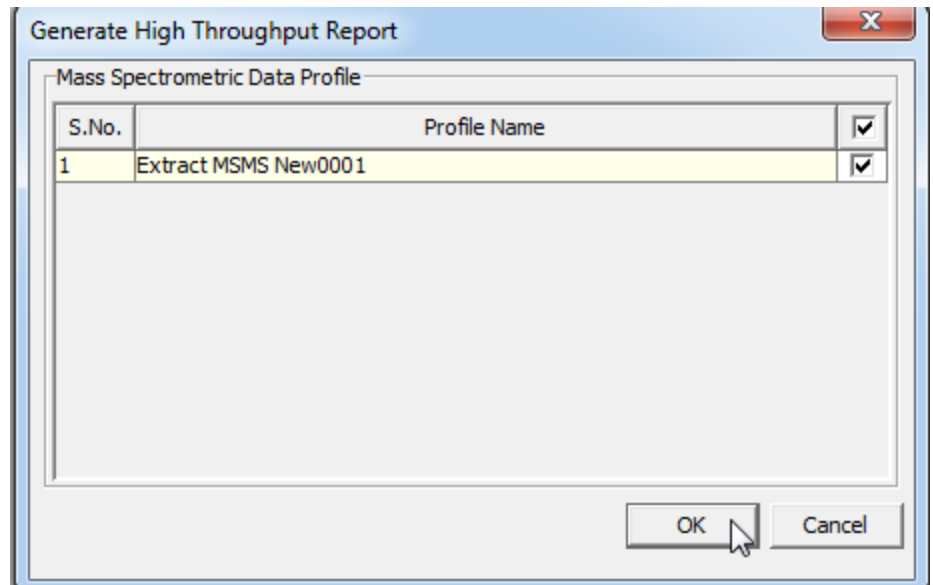


# Generate High Throughput Report (optional)

Select the Generate High Throughput Report icon in the menu bar



Select CEF files to generate High Throughput report on and click OK.





# Generate High Throughput Report (optional)

Select the compounds (aka profiles) to include in the report and the parameters to be displayed.

Generate High Throughput Report

Mass Spectrometric Data Profile

S.No.	Profile Name	Scan Name	MS Level	Precurso...	Intensity	Retentio...	Charge...	<input checked="" type="checkbox"/>
1	Extract MSMS N...	ID13	1			1.594	1	<input checked="" type="checkbox"/>
2	Extract MSMS N...	ID36	1			1.632	1	<input checked="" type="checkbox"/>
3	Extract MSMS N...	ID37	1			1.632	1	<input checked="" type="checkbox"/>
4	Extract MSMS N...	ID48	1			1.639	1	<input checked="" type="checkbox"/>
5	Extract MSMS N...	ID64	1			1.671	1	<input checked="" type="checkbox"/>

Profiles/Scans Checked: 162/162 Specify Range

MS | MS/MS |

MS Search

Select All  Select  matched lipids

Lipid Options

Retention Time  m/z  Intensity  
 No. of Hits  Chemical Composition  Abbreviation/Common Name  
 Delta Mass  Lipid Structure

Select All Clear All

Output Options

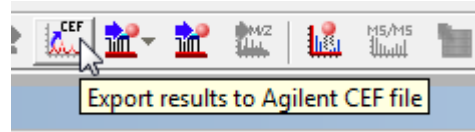
File Type:

Export to Folder:  Browse...

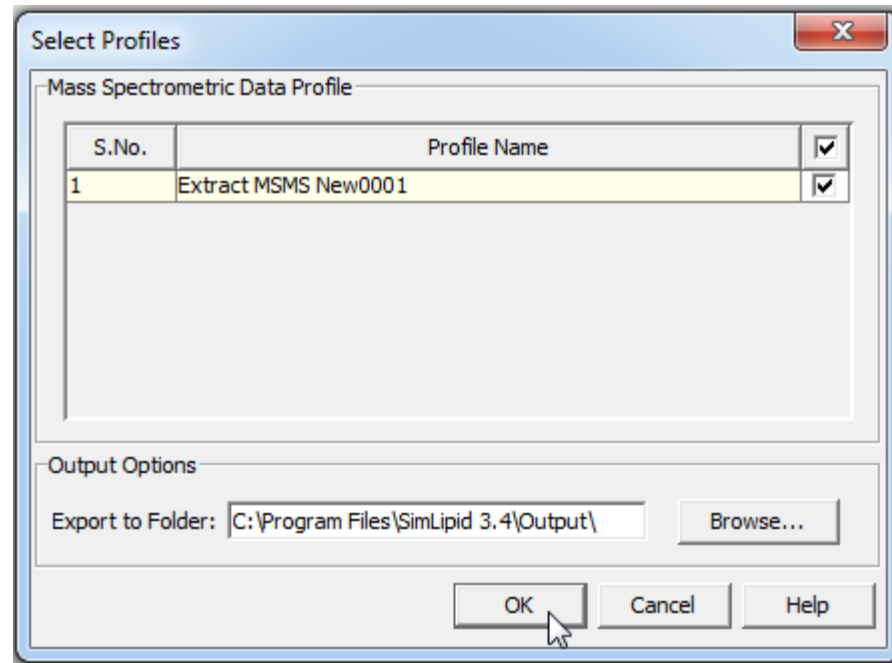
OK Cancel

# Export Annotated CEF files for Analysis in MPP

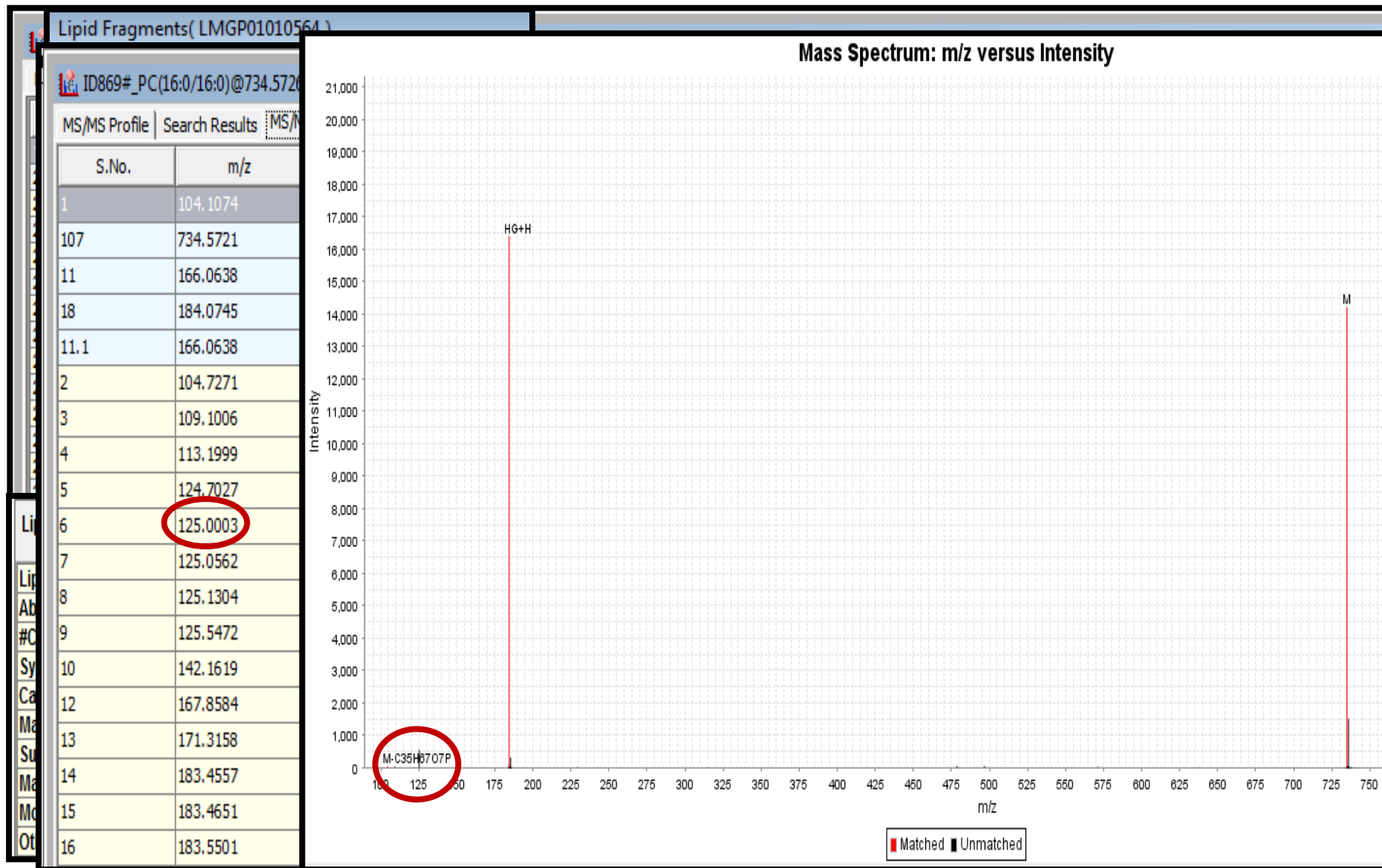
Select the CEF icon in the menubar.



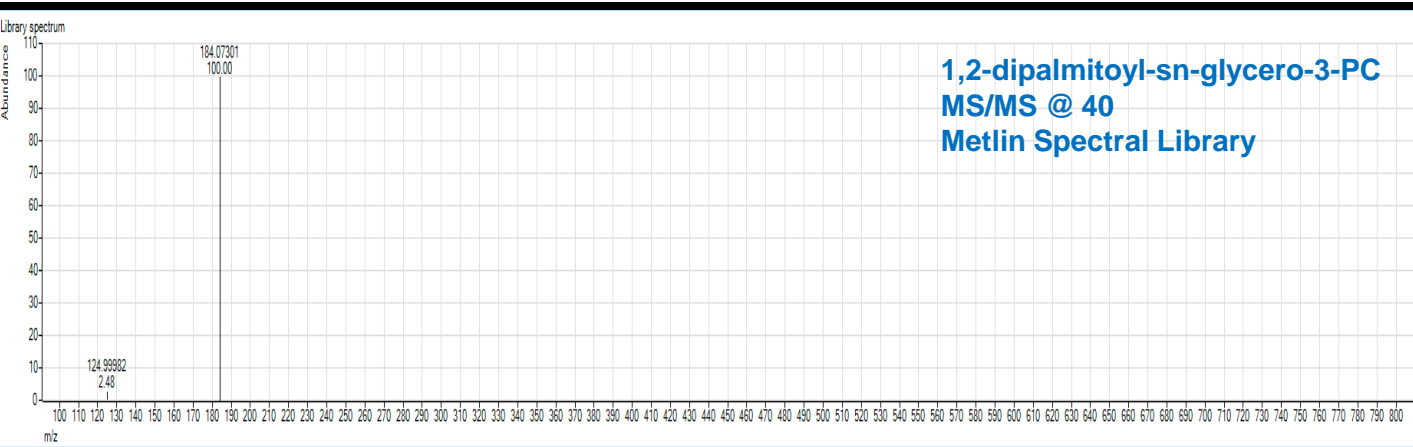
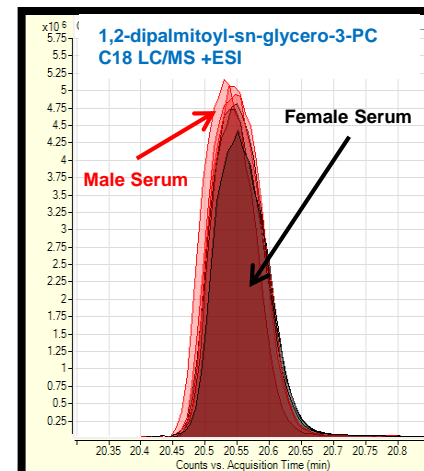
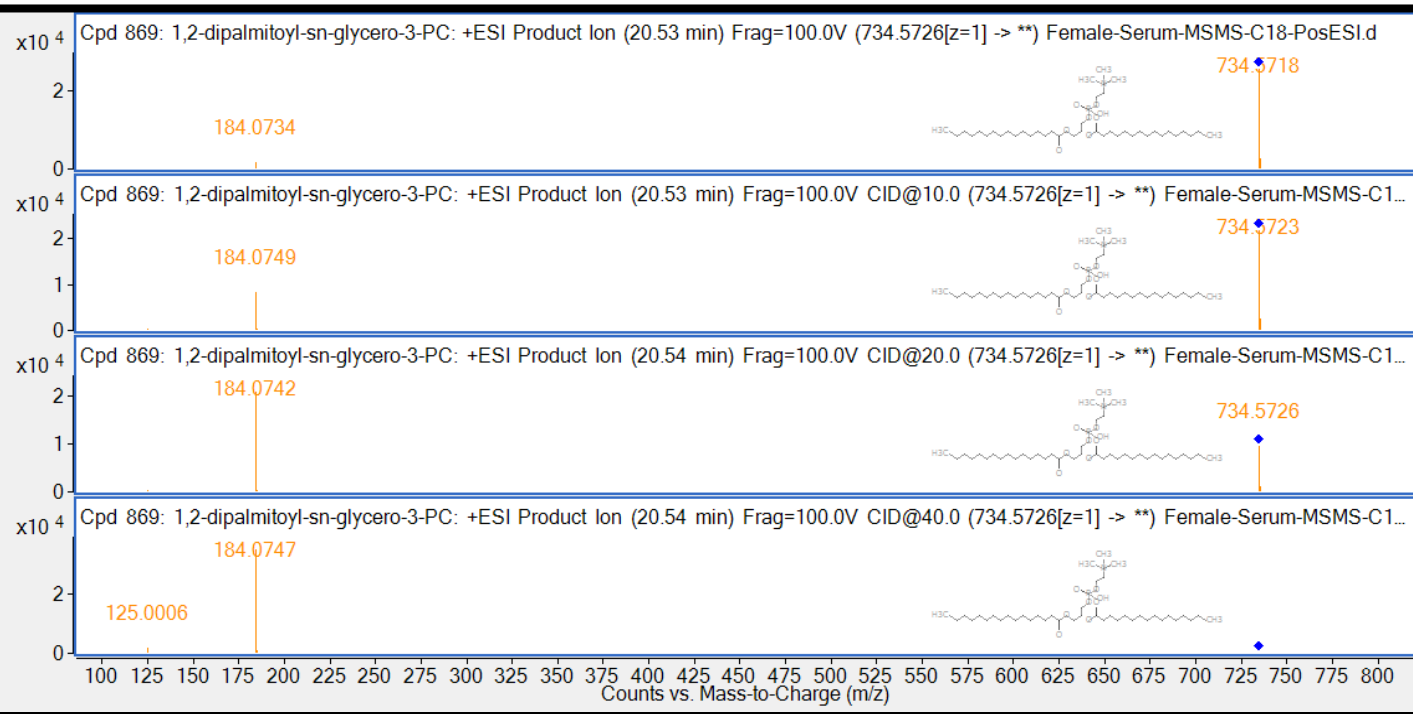
Select CEF files to export and click OK.



# LC/MS/MS Identification of 1,2-dipalmitoyl-sn-glycero-3-PC



# LC/MS/MS Identification of 1,2-dipalmitoyl-sn-glycero-3-PC



# Ordering SimLipid

SimLipid is available from PREMIER Biosoft International through their website:

<http://www.premierbiosoft.com/lipid/index.html>

They can be contacted through [sales@premierbiosoft.com](mailto:sales@premierbiosoft.com)

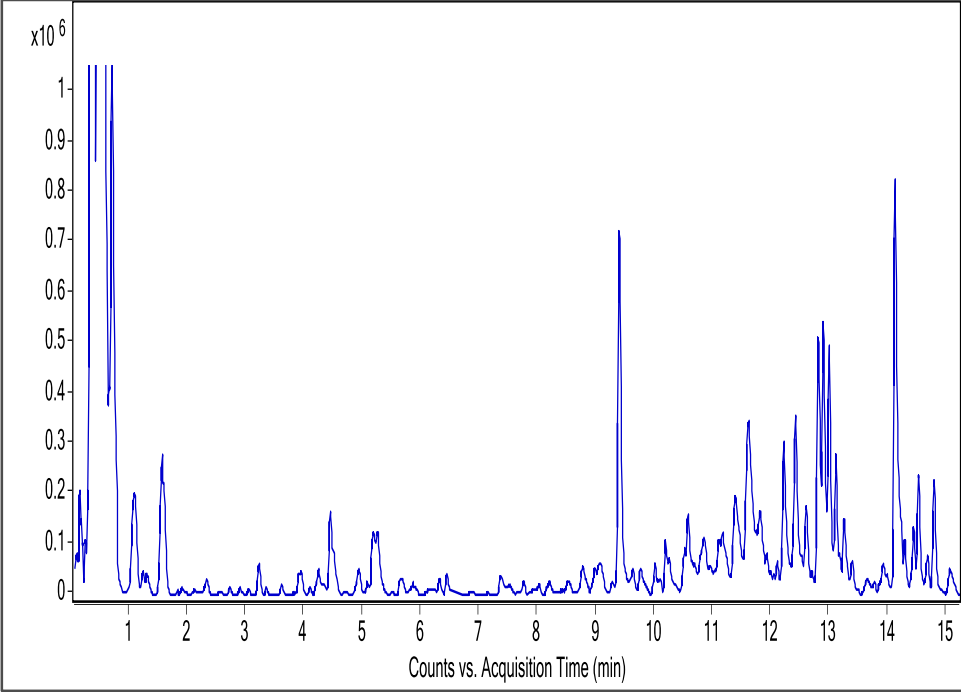
Phone: +1-650-856-2703

On their website, they offer temporary licenses for customers to try out the product before buying.

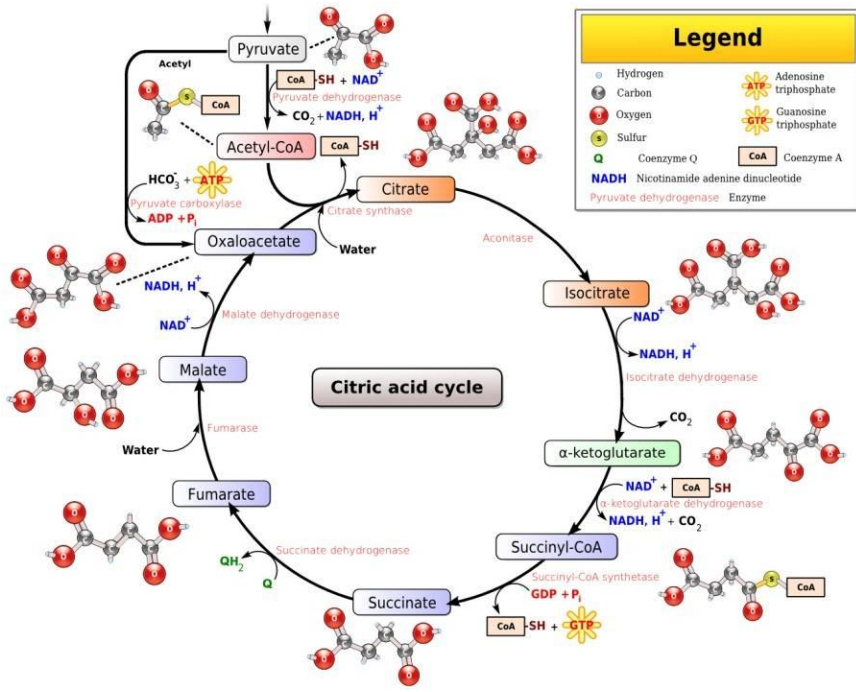
# Pathway Architect

## Pathway analysis using multi-omic data

Start here



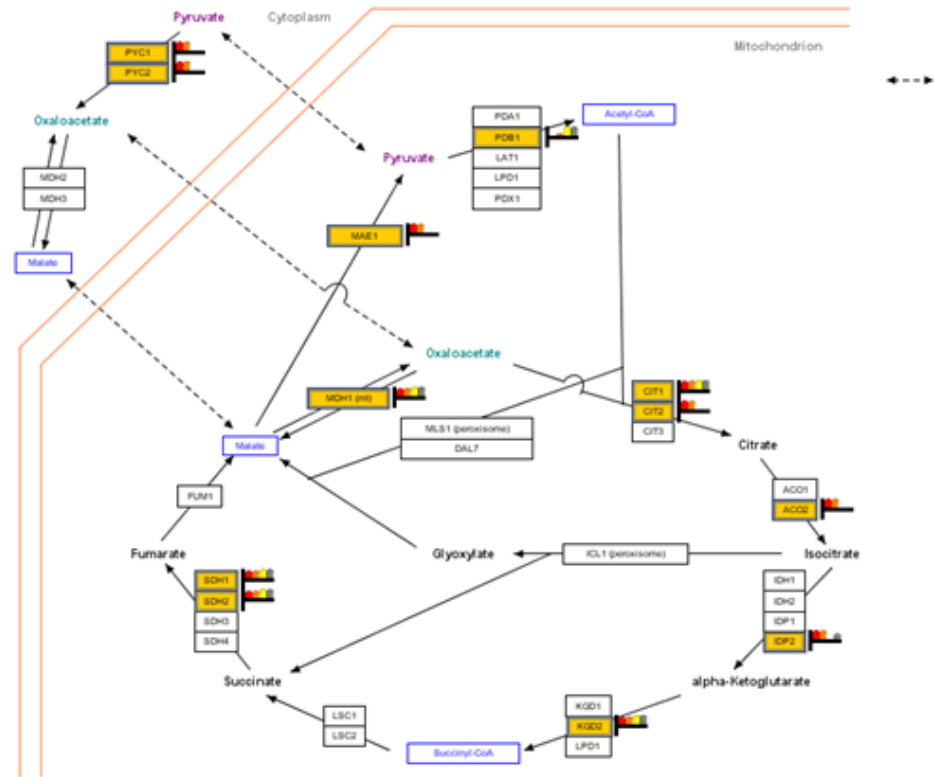
Finish here



# Pathway Architect

Customers can take the value of their data to another level. Pathway Architect helps them make sense of the data by:

- Visualizing it on
  - Wikipathways
  - BioCyc/MetaCyc
- Overlaying genomics, proteomics and metabolomics data
- Designing their next experiment for MS/MS analysis or custom microarrays



**TCA Cycle**

# Starting Pathway Architect

**Multi-Omic Analysis (Step 1 of 4)**

**Input Experiments**  
The active experiment in the open project is set as Experiment 1 by default. Select the second experiment for Multi-Omic Analysis, choose a Pathway Organism, and the sources from which you want to match pathways for the selected organism. Any pathway organism can be selected from the drop-down, regardless of the organisms associated with the chosen experiments; for example, if you know that your research area is more extensively described in another organism.

Experiment Chooser

Experiment 1  
Experiment 1: MicroArray (Choose...)  
Organism 1: Mycobacterium tuberculosis

Experiment 2  
Experiment 2: Metabolomics\_Neg (Choose...)  
Organism 2: Mycobacterium Tuberculosis

Choose Pathway Organism: Mycobacterium tuberculosis

Curated pathways only  
 Literature Derived Networks only  
 Both

Curated pathways | Literature Derived Networks

- WikiPathways - Analysis (8 pathways)
- WikiPathways - Reactome (0 pathways)
- WikiPathways - GenMAPP (0 pathways)
- WikiPathways - Other (104 pathways)
- BioCyc (224 pathways)
- BioPAX (Imported) (0 pathways)
- GPML (Imported) (0 pathways)
- Hand created (0 pathways)
- Legacy (0 pathways)

Buttons: Help, << Back, Next >>, Finish, Cancel

Transcriptomics results

Metabolomics results

Pathway Organism

Pathway database



# Pathway Architect Navigation

Mass Profiler Professional - Differentiation by Infection and Treatment

Project Navigator

- Two-Variable Data Set
  - Experiments
    - Differentiation by Infection and Treat
      - One Variable Data Set
- One Variable Data Set
  - Samples
  - Interpretations
    - Analysis
      - All Entities
        - Filtered on Flags {accCalls=[P, M], filterC
        - Filtered by frequency ['conditions'], [1]
        - 2way ANOVA
          - 2Way ANOVA p (Corr) (Infe
          - 2Way ANOVA p (Corr) (Infe
          - 2Way ANOVA p (Corr) (Treat)
          - Union 2Way ANOVA cut-off p
          - SEA-Filtered by frequency [Condi
          - SEA-Filtered by frequency [Condi

Global Lists

- My Lists

Legend

- Heatstrip
- Heatmap
- Color Settings

Differentiation by Infection and Treatment

- [Infected, 0]
- [Infected, 250]
- [Not Infected, 0]
- [Not Infected, 250]

Description

Pathway List View

Differentiation by Infection and Treatment

Interpretation Infection - Treatment

Entity List Filtered by frequency ['condit...

Pathway	Matche...	Pathwa...
Hs_TCR_signaling_WP1927_45...	1	10
Hs_Signaling_by_Robo_receptor...	1	5
Hs_Sphingolipid_Metabolism_W...	2	29
Hs_Fatty_acid_triacylglycerol_a...	2	81
Hs_Signaling_by_EGFR_WP1910...	1	8
Hs_Metabolism_of_amino_acids...	5	135
Hs_Factors_involved_in_megaka...	1	9
Hs_L1CAM_interactions_WP184...	1	5
Hs_Neurotransmitter_uptake_a...	1	6
Hs_Membrane_Trafficking_WP1...	1	5
Hs_Integration_of_energy_meta...	2	21
Hs_Metabolism_of_water-solubl...	6	71
Hs_Peroxisomal_lipid_metabolis...	1	37
Hs_Aspargine_N-linked_glycos...	1	55
Hs_GPCR_downstream_signalin...	2	19
Hs_Metabolism_of_carbohydrat...	3	63
Hs_Eukaryotic_Translation_Ter...	1	1
Hs_Platelet_homeostasis_WP18...	1	17
Hs_Fanconi_Anemia_pathway_W...	1	1
Hs_Mitotic_G2-G2-M_phases...	1	4
Hs_Protein_folding_WP1892_42...	1	4
Hs_Semaphorin_interactions_WP...	1	5
Hs_Metabolism_of_RNA_WP185...	1	8
Hs_Respiratory_electron_transp...	1	13
Hs_Metabolism_of_nucleotides...	3	81
Hs_Signaling_by_Insulin_recepto...	2	11
Hs_Telomere_Maintenance_WP...	1	10
Hs_Phase_1_-_Functionalization...	1	102
Hs_Metabolism_of_porphyrins...	1	31
Hs_Eukaryotic_Translation_Elon...	1	2

Find:  Find Next Find Previous

Show Differentiation by InfeC

Min # of matches:

Differentiation by Infection and Treatment (normalized) - Conflicts : 1

Entity Name	Compound Name	[Infected, 0]	[Infected, 250]
MoCo			
sulfurated MoCo			
oxidized glutathione	Glutathione, oxidized	-4.606	-0
Orthophosphate/Ortho...	Phosphoric acid	-4.876	0
Pantothenate	Pantothenic Acid	0	16
Nicotinamide	Niacinamide	-1.132	1
Pyridoxine	Pyridoxine (Vitamin B6)	-8.362	-3
▶ AMP	Adenosine5'-monopho...	-0.317	1

Find:  Find Next Find Previous Match Case

Profile plot (Log2 Normalized) SEA-Filtered by frequency ['conditions', [100, 0, 1]] - Pathway View SEA-Filtered by frequency ['conditions', [100, 0, 1]] - Pathway View

Workflow

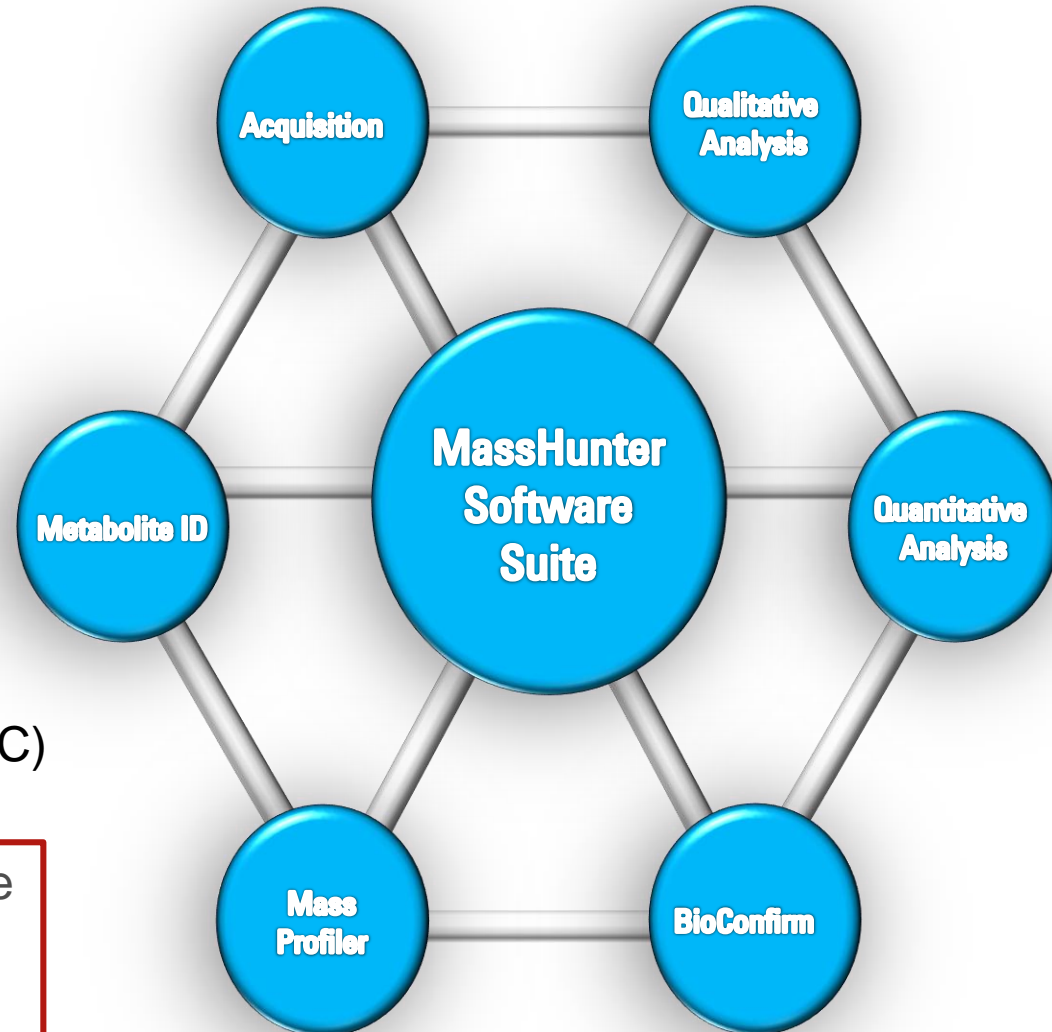
- Experiment Setup
  - Quick Start Guide
  - Experiment Grouping
  - Create Interpretation
- Quality Control
- Analysis
- Class Prediction
- Results Interpretations
  - Find Similar Entity Lists
  - Export for Recursion
  - IDBrowser Identification
  - Export for Identification
  - Export Inclusion List
  - Import Annotations
- Pathway Analysis
  - Single Experiment Analysis
  - Multi-Omic Analysis
  - Launch IPA
  - Export to MetaCore
  - Connect to Cytoscape
- NLP Networks
- Utilities

221M of 396M

# Mass Hunter Qualitative Analysis and Its “Accessories”

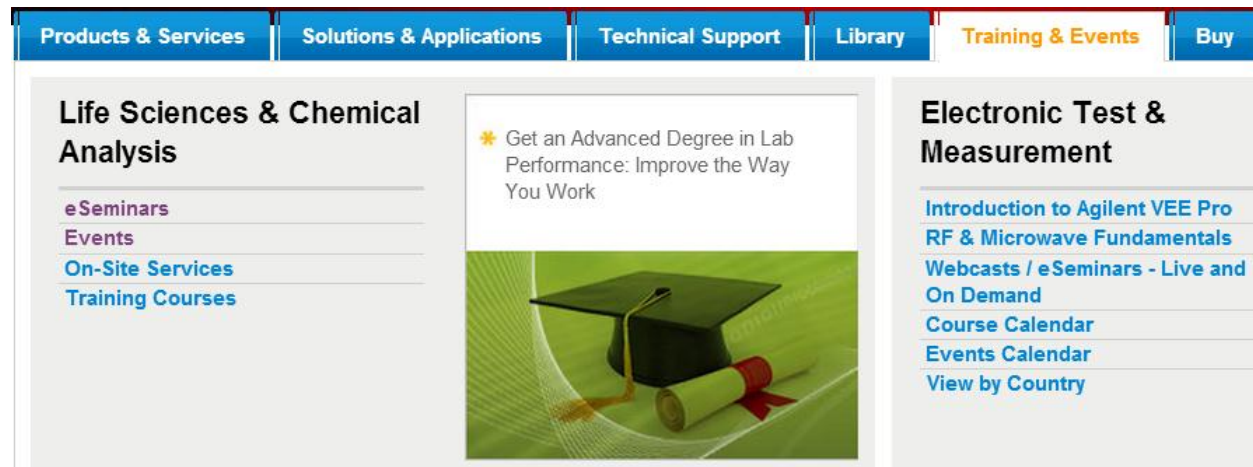
- Qualitative Analysis (Qual)
- PCDL Manager
- Pathways to PCDL
- Profinder
- Mass Profiler (MP)
- Mass Profiler Professional (MPP)
- ID Browser
- SimLipid (Premier Biosoft)
- Molecular Structure Correlator (MSC)

Fully integrated workflows to enable you to identify, plan, and execute your next experiment



# How can you learn more about MassHunter software?

- Read the PDF manuals and guides that shipped with your instrument or software
- Watch the videos that shipped with your instrument or software
- Read the Workflow Overviews and Workflow Guides specific to your application area
- Use the Help feature in the software!
  - Especially good for unfamiliar terms or software features
- Attend a training class – contact your Account Manager if interested
  - QTOF operation
  - QQQ operation
  - MPP
- View eSeminars – search Agilent website



The screenshot shows a portion of the Agilent website. At the top, there is a navigation bar with several tabs: "Products & Services", "Solutions & Applications", "Technical Support", "Library", "Training & Events" (highlighted in orange), and "Buy". Below the navigation bar, the page is divided into three main sections. The left section is titled "Life Sciences & Chemical Analysis" and contains a list of links: "eSeminars", "Events", "On-Site Services", and "Training Courses". The middle section features a promotional banner with a star icon and the text "Get an Advanced Degree in Lab Performance: Improve the Way You Work", accompanied by an image of a graduation cap and a rolled-up diploma. The right section is titled "Electronic Test & Measurement" and contains a list of links: "Introduction to Agilent VEE Pro RF & Microwave Fundamentals", "Webcasts / eSeminars - Live and On Demand", "Course Calendar", "Events Calendar", and "View by Country".

# Familiarization Guides

## Remember LC/MS and GC/MS Versions!



**Agilent MassHunter  
Workstation Software**  
Qualitative Analysis

**Familiarization Guide**

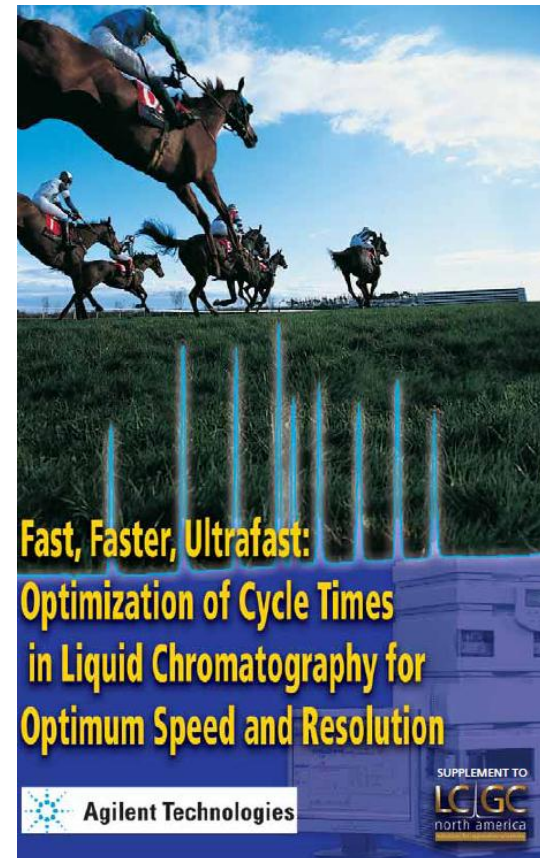


**Agilent MassHunter  
Workstation Software**  
Qualitative Analysis

**Familiarization Guide for  
GC/MS**



# Training: Learn about Liquid Chromatography Online Primers and Basic Concept Guides





[http://www.chem.agilent.com/search/?N=68+4294964917&Nr=OR%28part\\_language%3Aen%2Cg\\_rec\\_type%3ASharePoint%29&Ntt=primers](http://www.chem.agilent.com/search/?N=68+4294964917&Nr=OR%28part_language%3Aen%2Cg_rec_type%3ASharePoint%29&Ntt=primers)




# Updated Manuals/Training Materials Available on Website directly from the Help Page

**Getting Started**

 **What's new**

 **Available Manuals**

 [Visit our Web Site](#)

Searching  
Literature  
Mass Spectrometry  
Manuals  
Last 6 Months  
PDF's of new manuals

Home > Buy

**FILTERS APPLIED**

- Library
- Mass Spectrometry
- User Manuals
- In the Last 6 Months
- MassHunter Workstation Software
- English

**NARROW YOUR CHOICES**

**Solutions**

- Proteomics & Protein Sciences (3)

**Product**

- 6560 Ion Mobility Q-TOF LC/MS (3)
- MassHunter Data Acquisition Software (1)
- MassHunter Quantitative Data Analysis Software (2)
- MassHunter Workstation (2)
- MassHunter Workstation with MSD ChemStation DA (1)

All (5) | Explore (0) | Shop (0) | Support (5)

1-5 of 5 results for **Manuals** 1

**PDF**  
User Manual

**MassHunter Quantitative Analysis for GC/MSD Familiarization Guide (PDF)**

This Familiarization Guide presents step-by-step exercises to help you learn to use the Quantitative Analysis program.  
Publication Part Number: G3335-90200 | Created: 31 Jan 2014 | File Size: 13 MB

**PDF**  
User Manual

**6200 Series TOF and 6500 Series Q-TOF LC/MS System Quick Start Guide B.06.00 (PDF)**

6200 Series TOF and 6500 Series Q-TOF LC/MS System Quick Start Guide B.06.00  
Publication Part Number: G3335-90163 | Created: 23 Jan 2014 | File Size: 4 MB

**PDF**  
User Manual

**MassHunter Workstation Software Data Acquisition for 6200 Series TOF and 6500 Series Q-TOF Familiarization Guide B.06.00 (PDF)**

6200 Series TOF and 6500 Series Q-TOF Familiarization Guide B.06.00  
Publication Part Number: G3335-90161 | Created: 23 Jan 2014 | File Size: 4 MB

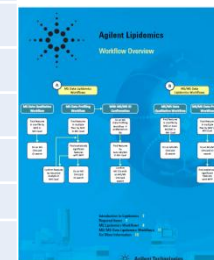
**PDF**  
User Manual

**6200 Series TOF and 6500 Series Q-TOF LC/MS System Concepts Guide B.06.00 (PDF)**

6200 Series TOF and 6500 Series Q-TOF LC/MS System Concepts Guide B.06.00  
Publication Part Number: G3335-90162 | Created: 23 Jan 2014 | File Size: 6 MB

# Application Specific LC/MS Workflow Guides:

Publ #	Title	Pages
5990-7061EN	QQQ LC/MS Bioanalysis Workflow Overview	9
5990-7060EN	QQQ LC/MS Bioanalysis Workflow Guide	40
5990-7063EN	Drug Discovery Screening Workflow Overview	12
5990-7062EN	Drug Discovery Screening Workflow Guide	50
5990-7065EN	TOF, QTOF LC/MS BioPharma Workflow Overview	12
5990-7064EN	TOF, QTOF LC/MS BioPharma Workflow Guide	50
5990-7068EN	TOF, QTOF LC/MS Metabolomics Discovery Workflow Overview	16
5990-7067EN	TOF, QTOF LC/MS Metabolomics Discovery Workflow Guide	168
5990-7069EN	TOF, QTOF LC/MS Screening of Pesticides Workflow Overview	12
5990-7072EN	TOF, QTOF LC/MS Screening of Pesticides Workflow Guide	84
5990-7074EN	QQQ LC/MS Quantitation of Pesticides Workflow Overview	8
5990-7073EN	QQQ LC/MS Quantitation of Pesticides Workflow Guide	54
5990-9886EN	QQQ LC/MS Peptide Quantitation with Skyline Workflow Overview	12
5990-9887EN	QQQ LC/MS Peptide Quantitation with Skyline Workflow Guide	54
5991-1644EN	Agilent Lipidomics Workflow Overview	14
5991-1643EN	Agilent Lipidomics Workflow Guide	66
5991-1910EN	Integrated Biology with Mass Profiler Professional Workflow Overview	18
5991-1909EN	Integrated Biology with Mass Profiler Professional Workflow Guide	124
5991-1995EN	Agilent All Ions MS/MS - Workflow Overview	8
5991-1994EN	Agilent All Ions MS/MS Workflow Guide	36



<http://www.chem.agilent.com/en-us/search/library/Pages/default.aspx>

# Any Other Questions?



Qualitative  
Analysis ...



PCDL  
Manager



Pathways to  
PCDL



Profinder  
B.06.00



Mass Profiler  
Professional



Molecular  
Structur...



DA  
Reprocessor



SimLipid 4

