



Agilent MassHunter Qualitative Data Analysis

Presenters: Howard Sanford

Stephen Harnos

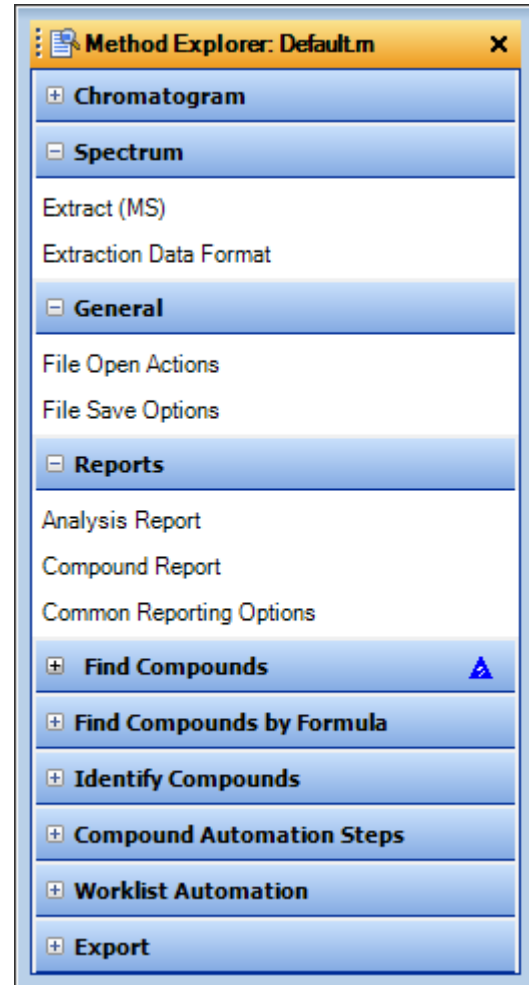
MassHunter Qualitative Analysis

Spectrum Functions

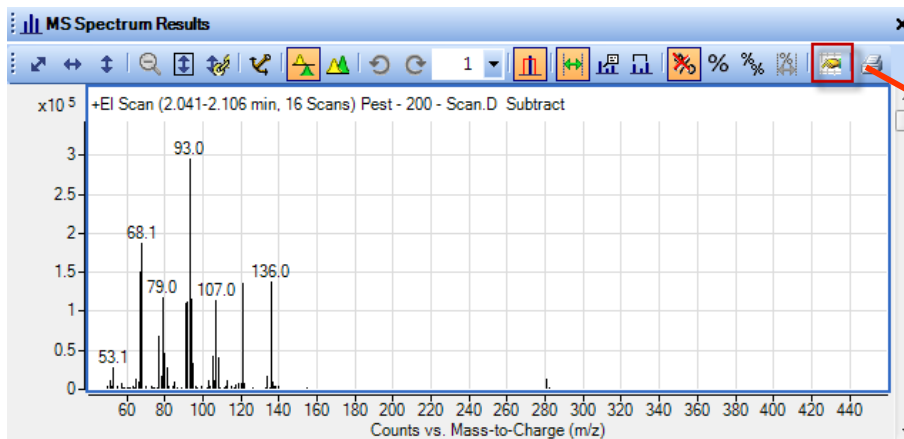
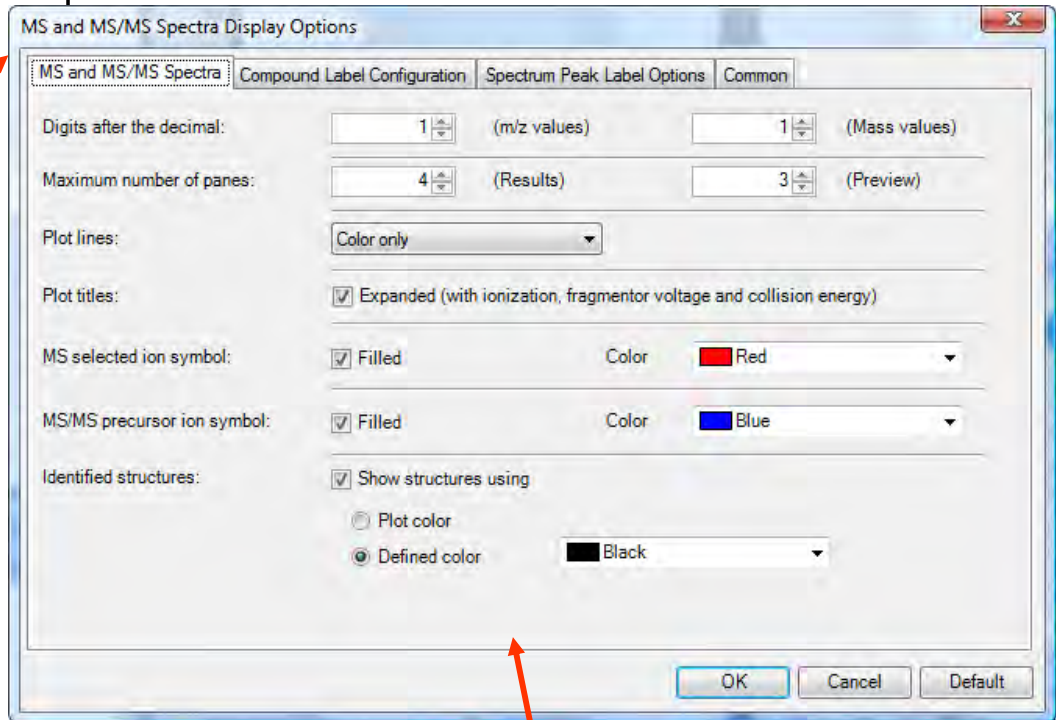
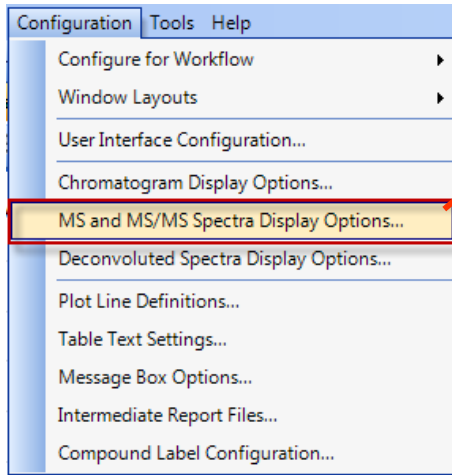
MassHunter Qualitative Analysis Software B.07.00

Topics

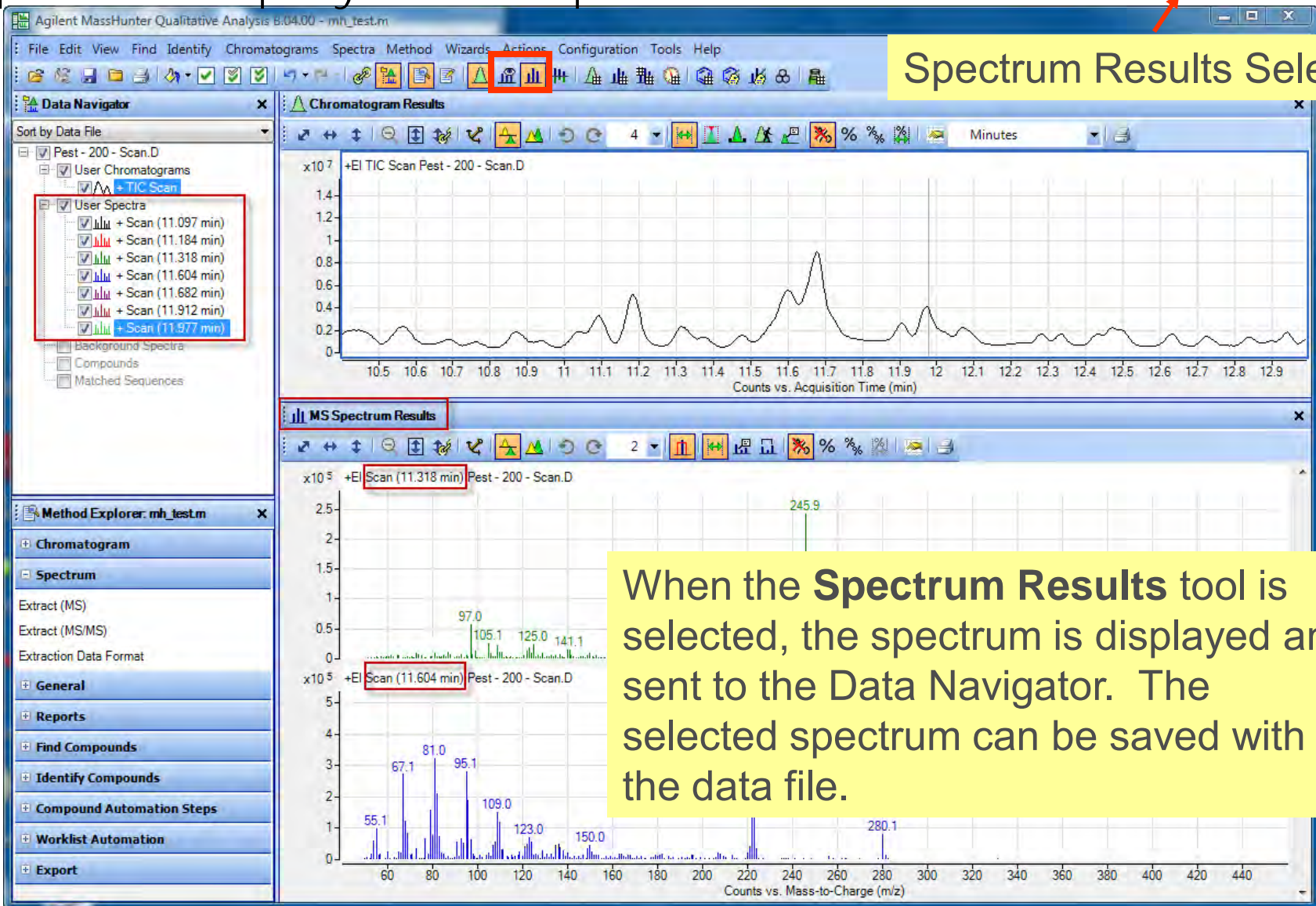
- Review Chromatogram Functions
- Spectrum Functions
 - Spectral Display
 - Extract a Spectrum and Averaging
 - Background Subtraction (MS Spectrum)
- Accurate Mass Considerations
 - Isotopic Model
- Spectrum Peak List
- Annotation
 - Text and Graphics
 - Anchoring and Floating
- Report Generation
 - Analysis and Compound Reports
- File Save Options
- Tools
- Training Resources



Mass Spectral Display Options



Spectra Display – MS Spectrum Results



Spectrum Results Selected

When the **Spectrum Results** tool is selected, the spectrum is displayed and sent to the Data Navigator. The selected spectrum can be saved with the data file.

Spectrum Display - Preview



Agilent MassHunter Qualitative Analysis B.04.00 - mh_test.m

File Edit View Find Identify Chromatograms Spectra Method Wizards Actions Configuration Tools Help

Preview

Data Navigator

Sort by Data File

Chromatogram Results

+EI TIC Scan Pest - 200 - Scan.D

When **Spectrum Preview** is selected, spectra are not saved to the Data Navigator automatically.

Spectrum Preview

+EI Scan (10.569 min) Pest - 200 - Scan.D

Easily preview spectra before saving to the Data Navigator.

Method Explorer: mh_test.m

- Chromatogram
- Spectrum
- Extract (MS)
- Extract (MS/MS)
- Extraction Data Format
- General
- Reports
- Find Compounds
- Identify Compounds
- Compound Automation Steps
- Worklist Automation
- Export

Add Preview Spectrum to Results

The screenshot displays the Agilent MassHunter Qualitative Analysis software interface. The main window is titled "Agilent MassHunter Qualitative Analysis B.04.00 - mh_test.m". The interface is divided into several panes:

- Data Navigator:** Located on the left, it shows a tree view of data files. Under "User Spectra", the entry "+ Scan (10.569 min)" is highlighted with a red box. A green arrow points from this entry to the Spectrum Preview pane.
- Chromatogram Results:** The top right pane shows a Total Ion Chromatogram (TIC) plot titled "+EI TIC Scan Pest - 200 - Scan.D". The y-axis is labeled "x10⁷" and the x-axis is "Counts vs. Acquisition Time (min)".
- Spectrum Preview:** The bottom right pane shows a mass spectrum plot titled "+EI Scan (10.569 min) Pest - 200 - Scan.D". The y-axis is labeled "x10⁵" and the x-axis is "Counts vs. Mass-to-Charge (m/z)". Two major peaks are labeled with their m/z values: 158.9 and 252.0. A yellow callout box is overlaid on this pane with the text:
 - Right-click
 - Select Copy to User Spectra
- Method Explorer:** Located on the bottom left, it shows a list of methods and actions. The "Spectrum" section is expanded, and the "Copy to User Spectra" option is highlighted with a green box.

Extract Single Scan Spectrum

Agilent MassHunter Qualitative Analysis B.04.00 - mh_test.m

File Edit View Find Identify Chromatograms Spectra Method Wizards Actions Configuration Tools Help

Data Navigator

Sort by Data File

Pest - 200 - Scan.D

- User Chromatograms
 - + TIC Scan
- User Spectra
 - + Scan (11.097 min)
 - + Scan (11.184 min)
 - + Scan (11.318 min)
 - + Scan (11.604 min)
 - + Scan (11.682 min)
 - + Scan (11.912 min)
 - + Scan (11.977 min)
 - + Scan (10.569 min)
- Background Spectra
- Compounds
- Matched Sequences

Chromatogram Results

+EI TIC Scan Pest - 200 - Scan.D

9.4 9.5 9.6 9.7 9.8 9.9 10 10.1 10

Spectrum Preview

+EI Scan (9.655 min) Pest - 200 - Scan.D

8 7.5 7 6.5 6 5.5 5 4.5 4 3.5 3 2.5 2 1.5 1 0.5 0

60 80 100 120 140 160

75.0 111.0 128.1 138.9 152.0 168.0

Extract MS Spectrum

- Extract MS Spectrum to Background
- Extract Peak Spectrum
- Extract Chromatograms...
- Extract Defined Chromatograms
- Use Highlighted Chromatograms
- Integrate Chromatogram
- Integrate and Extract Peak Spectra
- Smooth Chromatogram
- Subtract Any Chromatogram
- Calculate Signal-to-Noise
- Integration Peak List
- Adjust Peak Threshold
- Set Anchor
- Clear Anchor
- Assign Ranges to
- Copy to User Chromatograms
- Clear Results
- Delete
- Delete Peak
- Unzoom
- Assign Random Colors
- Choose Defined Color
- Copy to Clipboard Ctrl+C
- Print...
- Export...

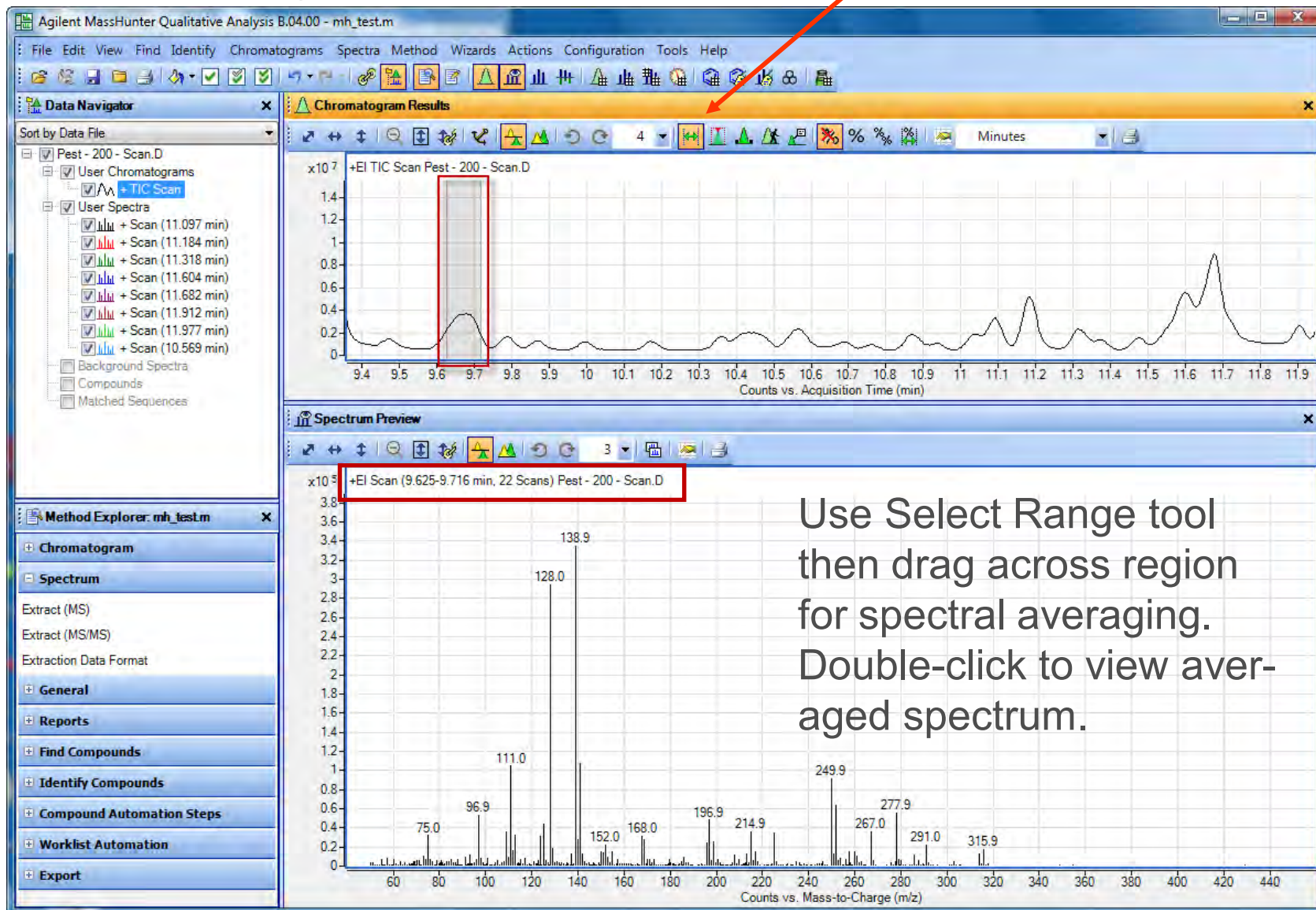
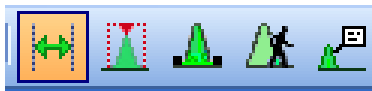
Method Explorer: mh_test.m

- Chromatogram
- Spectrum
 - Extract (MS)
 - Extract (MS/MS)
 - Extraction Data Format
- General
- Reports
- Find Compounds
- Identify Compounds
- Compound Automation Steps
- Worklist Automation
- Export

Extract Spectra

- Double-click on data point.
- Right-click on data point then, **Extract Spectrum**.

Extract Averaged Spectra



Background Subtraction for Manual Spectra

① Use the Ctrl Key to average multiple range selections then Extract Spectrum.

②

③ Change manual spectrum background to **Current background spectrum**.

Agilent MassHunter Qualitative Analysis B.04.00 - mh_test.m

File Edit View Find Identify Chromatograms Spectra Method Wizards Actions Configuration Tools Help

Data Navigator

Sort by Data File

Pest - 200 - Scan.D

User Chromatograms

+ TIC Scan

User Spectra

+ Scan (11.097 min)

+ Scan (11.184 min)

+ Scan (11.318 min)

+ Scan (11.604 min)

+ Scan (11.682 min)

+ Scan (11.912 min)

+ Scan (11.977 min)

+ Scan (10.569 min)

Background Spectra

+ Scan (16.503-16.650 min)

Compounds

Matched Sequences

Method Explorer: mh_test.m

Chromatogram

Spectrum

Extract (MS)

Extract (MS/MS)

Extraction Data Format

General

Reports

Find Compounds

Identify Compounds

Compound Automation Steps

Worklist Automation

Export

Chromatogram Results

+EI TIC Scan Pest - 200 - Scan.D

x10⁷

1.4

1.2

0.8

0.6

0.4

0.2

0

16.5 16.6 16.7 16.8 16.9 17 17.1 17.2 17.3 17.4 17.5 17.6 17.7 17.8 17.9 18 18.1 18.2 18.3 18.4 18.5 18.6 18.7 18.8 18.9

Counts vs. Acquisition Time (min)

Method Editor: Extract (MS)

Extract Peak spectrum

Method Items

Manual Extraction

Peak Spectrum Extraction (MS)

Peak Filters

Manual spectrum background

MS

Current background spectrum

Spectrum Preview

+EI Scan (16.503-16.650, 17.174-17.408 min, 90 Scans) Pest - 200 - Scan.D

x10⁴

1.05

1

0.95

0.9

0.85

0.8

0.75

0.7

0.65

0.6

0.55

0.5

0.45

0.4

0.35

0.3

0.25

0.2

0.15

0.1

0.05

0

60 80 100 120 140 160 180 200 220 440

Counts vs. Mass-to-Charge (m/z)

57.1 81.0 95.1 125.0 181.0 224.0

06.9

Extract EIC

Extract Chromatograms...

MS Spectrum Peak List 1

MS Spectrum Peak List 2

MS Actuals

Assign Ranges to

Move to Background Spectrum

Copy to User Spectra

Unzoom

Assign Random Colors

Choose Defined Color

Copy to Clipboard Ctrl+C

Print...

Export...

Background Subtraction for Manual Spectra

The screenshot displays the Agilent MassHunter Qualitative Analysis software interface. The main window is titled "Agilent MassHunter Qualitative Analysis B.04.00 - mh_test.m". The "Data Navigator" on the left shows a tree view of data files, with "Scan (16.858 min)" selected and a "Sub" button highlighted. The "Chromatogram Results" window shows a Total Ion Chromatogram (TIC) plot of "x10⁷ +EI TIC Scan Pest - 200 - Scan.D" with a prominent peak at approximately 16.858 minutes. A green callout box labeled "Extract Spectrum" points to this peak. The "Method Editor: Extract (MS)" window is open, showing "Manual Extraction" and "Peak Spectrum Extraction (MS)" tabs. The "MS Spectrum Results" window displays the extracted mass spectrum for "x10⁶ +EI Scan (16.858 min) Pest - 200 - Scan.D", with a "Subtract" button highlighted. A green callout box labeled "Description indicates subtraction occurred." points to the "Subtract" button. The mass spectrum shows several peaks, with the base peak at m/z 71.1 and other significant peaks at m/z 57.1, 99.1, 113.1, 127.1, 155.1, 183.1, and 211.2.

Extract Peak Spectrum

Extract an averaged spectrum from a chromatographic peak automatically. Must integrate to define chromatographic peaks.

The screenshot displays the Agilent MassHunter Qualitative Analysis B.04.00 interface. The main window shows a Total Ion Chromatogram (TIC) with several peaks labeled with their retention times: 5.861, 5.952, 6.013, 6.069, and 6.216 minutes. The x-axis is labeled 'Counts vs. Acquisition Time (min)'. A context menu is open over the chromatogram, with 'Integrate Chromatogram' highlighted in a red box. Below the chromatogram, the 'Method Editor: Integrate (MS)' window is visible, with the 'Integrate Chromatogram' button also highlighted in a red box. The 'Options' section shows 'Detector' set to 1, 'Point sampling' at 1, 'Start threshold' at 0.200, 'Smoothing' checked, 'Stop threshold' at 0.0, 'Filtering' set to '5 point', and 'Peak location' set to 'Top'. To the right, the 'MS Spectrum Results' window shows a mass spectrum for the peak at 16.858 minutes, with peaks labeled at m/z 57.1, 71.1, 83.1, and 211.2. The x-axis is labeled 'Counts vs. Mass-to-Charge (m/z)'. In the bottom-left corner, the 'Method Explorer' shows the 'Chromatogram' method with 'Integrate (MS)' selected and highlighted in a red box. A yellow text box in the bottom center contains the text: 'Integrate the chromatogram to locate chromatographic peaks. Four step process.'

Extract Peak Spectrum



③ Enable Peak Select tool.

The screenshot displays the Agilent MassHunter Qualitative Analysis B.04.00 interface. The main window shows a Total Ion Chromatogram (TIC) with several peaks labeled with retention times: 5.861, 5.952, 6.013, 6.069, and 6.307. A red dashed box highlights the peak at 5.952 minutes. A yellow callout box with the number 4 and the text "Double-click on peak." points to this peak. In the bottom-left pane, the "Method Editor: Extract (MS)" window is open, showing the "Peak Spectrum Extraction (MS)" tab. A red arrow points to the "Average scans >" field, which is set to 10. A yellow callout box with the number 2 and the text "Set up Peak Spectra Extraction" points to this field. The bottom-right pane shows the "MS Spectrum Results" window, displaying the mass spectrum for the selected peak. The x-axis is labeled "Counts vs. Mass-to-Charge (m/z)" and the y-axis is labeled "x10⁴". The base peak is at m/z 321.9. Other significant peaks are labeled at m/z 81.0, 96.9, 122.9, 144.9, 173.9, 237.9, 265.9, and 293.9.

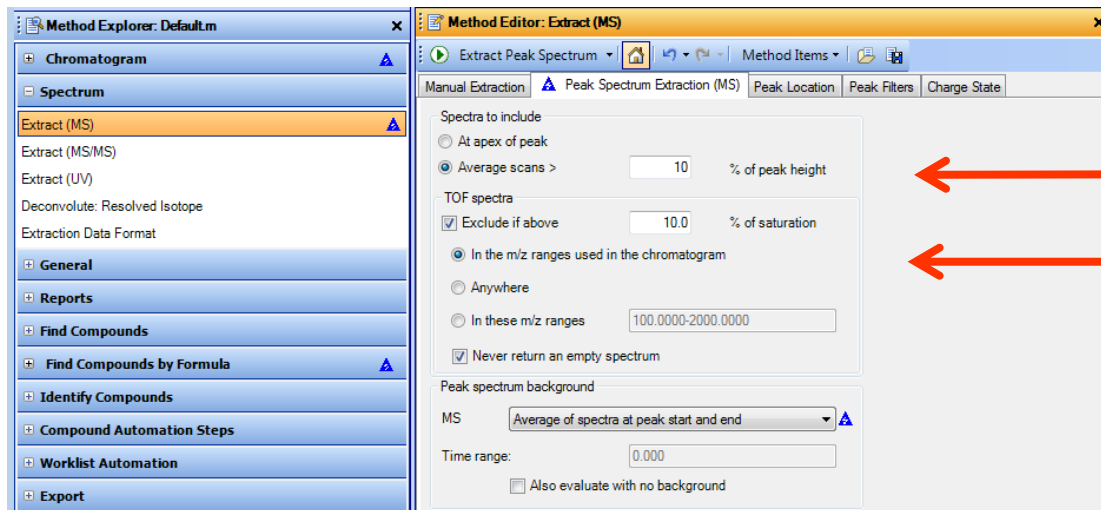
Extract Peak Spectra Automatically

The screenshot displays the Agilent MassHunter Qualitative Analysis B.04.00 interface. The main window shows a Total Ion Chromatogram (TIC) with several peaks labeled with retention times: 5.861, 5.952, 6.013, and 6.069. A yellow callout box at the top right contains the text "Spectra Results from each Integrated Peak". A red arrow points from this callout to the chromatogram. Another red arrow points from the callout to the "Integrate and Extract Peak Spectra" option in a context menu that is open over the chromatogram. The context menu includes options such as "Extract MS Spectrum", "Integrate Chromatogram", and "Integrate and Extract Peak Spectra". The "Method Editor: Extract (MS)" window is also visible, showing extraction parameters like "Average scans" (10) and "Exclude if above" (10.0). A yellow callout box at the bottom center contains the text: "Tip: Set integration parameters and Extraction parameters in the Method Editor first. Select Integrate and Extract Peak Spectra from the menu." The "Method Explorer" on the left shows the "Extract (MS)" method selected.

Spectra Results from each Integrated Peak

Tip: Set integration parameters and Extraction parameters in the Method Editor first. Select Integrate and Extract Peak Spectra from the menu.

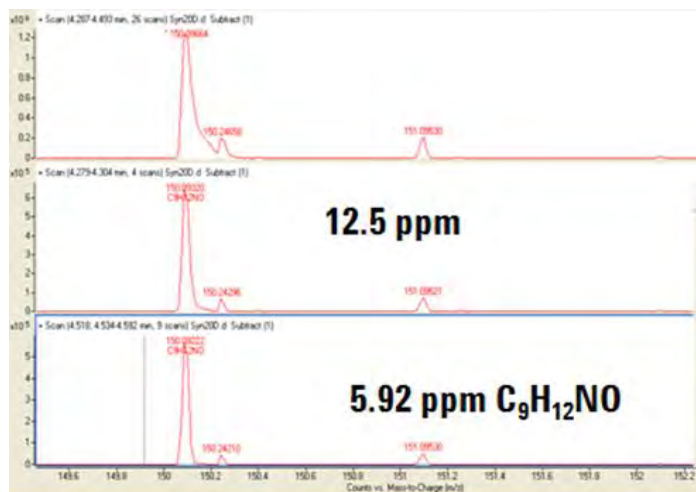
Considerations for Accurate Mass Data Using Extract Peak Parameters – Saturation



Change 5%

Change 20%

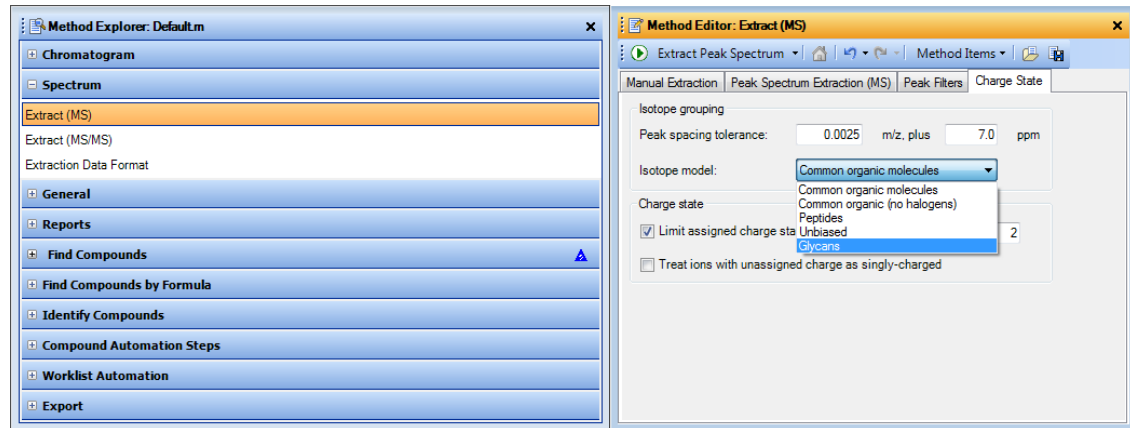
For very narrow chromatographic peaks that are completely saturated you may have to turn this function off or error occurs: No Data Found.



Using Extract Peak Parameters – Isotope Model

**Chose Isotope model that
Corresponds to workflow.**

**Common organic molecules
Peptides
Unbiased
Glycans**

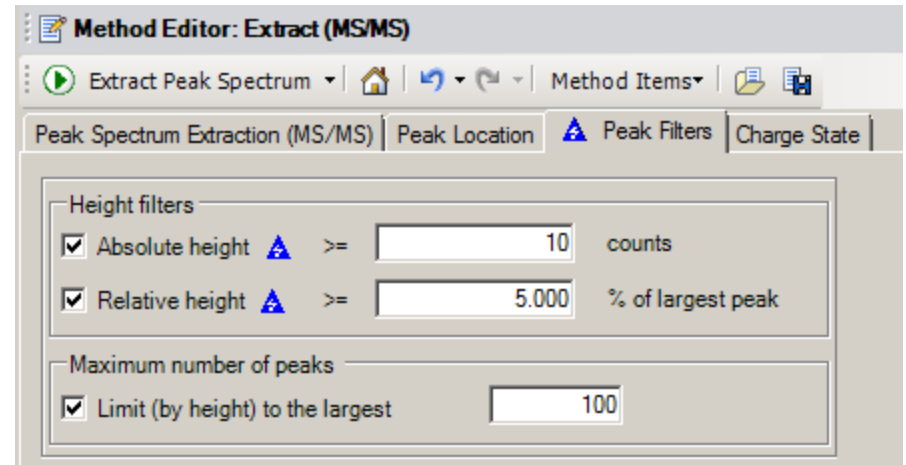
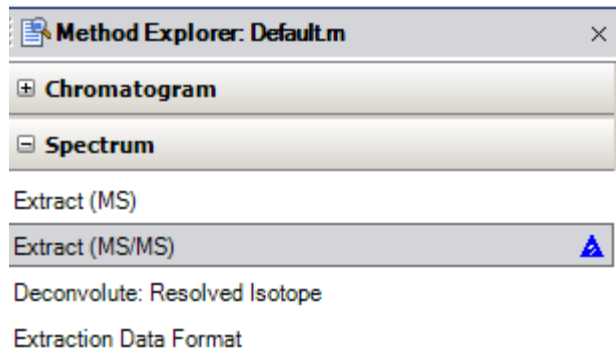


Tip: Check Limit Assigned Charge States Maximum Values.

For Small Molecule Applications: Set to 2

For High Molecular Weight Apps: Uncheck or Max 10

Extract Spectra – Peak Filters



Tip: Always remember to set Peak Filter Limits to reduce noise. Important when library searching.

Context Sensitive Help

?

Height filters

Absolute height ▲ >= counts

Relative height >= % of largest peak

Maximum number of peaks

Limit (by height) to the largest

Peak spectrum background

MS

Time range

- Current background spectrum
- Spectrum at peak start
- Spectrum at peak end
- Average of spectra at peak start and end
- Designated time range(s)

Spectra to include

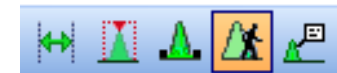
At apex of peak

Average scans > % of peak height

- Common organic molecules
- Common organic (no halogens)
- Peptides
- Unbiased
- Glycans

Tip: Context Sensitive Help is available through the F1 Key.

Walk Chromatogram



The screenshot displays the Agilent MassHunter Qualitative Analysis software interface. The main window shows a Total Ion Chromatogram (TIC) with several peaks labeled with their retention times: 5.861, 5.952, 6.013, 6.069, 6.216, and 6.307. The x-axis is labeled 'Counts vs. Acquisition Time (min)' and ranges from 5.8 to 6.42. The y-axis is labeled 'x10⁶' and ranges from 0 to 4. The software interface includes a menu bar (File, Edit, View, Find, Identify, Chromatograms, Spectra, Method, Wizards, Actions, Configuration, Tools, Help), a toolbar, and a Data Navigator on the left. The Data Navigator shows a tree view of the data files and spectra. The Method Editor: Extract (MS) window is open, showing extraction parameters for the selected peak. The Spectrum Preview window shows the mass spectrum for the selected peak at 5.952 minutes, with the x-axis labeled 'Counts vs. Mass-to-Charge (m/z)' and the y-axis labeled 'x10⁵'. The mass spectrum shows several peaks, with the base peak at 321.9 m/z. Other labeled peaks include 65.0, 96.9, 121.0, 173.9, 201.9, 237.9, and 293.9.

Chromatogram Results

+EI TIC Scan Pest - 200 - Scan.D

5.861 5.952 6.013 6.069 6.216 6.307

Counts vs. Acquisition Time (min)

Method Editor: Extract (MS)

Extract Peak Spectrum | Method Items

Manual Extraction | Peak Spectrum Extraction (MS) | Peak Filters

Spectra to include

- At apex of peak
- Average scans > 10 % of peak height

TOF spectra

- Exclude if above 10.0 % of saturation

Spectrum Preview

+EI Scan (5.952 min) Pest - 200 - Scan.D Subtract

65.0 96.9 121.0 173.9 201.9 237.9 293.9 321.9

Counts vs. Mass-to-Charge (m/z)

Walk Chromatogram
Use left and right arrows on keyboard to step through spectra.

MS Spectrum Peak List One



The screenshot displays the Agilent MassHunter Qualitative Analysis interface. The main window shows a Total Ion Chromatogram (TIC) with several peaks labeled with their retention times: 5.861, 5.952, 6.013, 6.069, 6.216, and 6.307 minutes. The x-axis is labeled 'Counts vs. Acquisition Time (min)' and the y-axis is labeled 'x10⁶ +EI TIC Scan Pest - 200 - Scan.D'. A red box highlights the peak at 6.216 minutes.

Below the chromatogram, the 'MS Spectrum Results' panel shows two mass spectra. The top spectrum is for the selected peak at 6.216 minutes, showing a base peak at m/z 93.0 and other significant peaks at 68.1 and 136.0. The bottom spectrum is for a different scan at 2.253-2.296 minutes, showing a base peak at m/z 93.0 and another peak at 131.0.

To the right of the MS spectrum, the 'MS Peaks One: + Scan (2.041-2.106 min) Sub' table lists the following data:

m/z	Species	Abund	Abund	Abund % (Norm)	Max Abund
53.1		27397.6	9.27		27397.6
67.1		150742.4	51.01		150742.4
68.1		187409.7	63.42		187409.7
77		68352.8	23.13		68352.8
78.1		16252.1	5.5		16252.1
79		117390	39.73		117390
80		45228.3	15.31		45228.3
81		27925.3	9.45		27925.3
91		110364	37.35		110364
92		111613.8	37.77		111613.8
93		295492.2	100		295492.2
94.1		114854	38.87		114854
95.1		33656.4	11.39		33656.4
105		41578.4	14.07		41578.4
105.1		18000.2	6.09		18000.2
107		114399.2	38.71		114399.2
108		39713.3	13.44		39713.3
121		136363.2	46.15		136363.2
134.1		17098	5.79		17098
136		138343.1	46.82		138343.1

A yellow callout box in the bottom left corner contains the following instructions:

- Right-click spectrum.
- **MS Spectrum Peak List One.**
- Tool is also available.

MS Spectrum Peak List Two



Agilent MassHunter Qualitative Analysis B.04.00 - mh_test.m

File Edit View Find Identify Chromatograms Spectra Method Wizards Actions Configuration Tools Help

Data Navigator

Sort by Data File

- Pest - 200 - Scan.D
 - User Chromatograms
 - + TIC Scan
 - User Spectra
 - + Scan (2.041-2.106 min) Sub
 - + Scan (2.253-2.296 min) Sub
 - + Scan (2.478-2.513 min) Sub
 - + Scan (2.604-2.639 min) Sub
 - + Scan (2.656-2.682 min) Sub
 - + Scan (2.768-2.829 min) Sub
 - + Scan (2.890-2.950 min) Sub
 - + Scan (3.063-3.102 min) Sub
 - + Scan (3.180-3.215 min) Sub
 - + Scan (3.228-3.262 min) Sub
 - + Scan (3.301-3.345 min) Sub
 - + Scan (3.358-3.383 min) Sub
 - + Scan (3.557-3.587 min) Sub
 - + Scan (3.786-3.830 min) Sub
 - + Scan (3.912-3.951 min) Sub

Chromatogram Results

+EI TIC Scan Pest - 200 - Scan.D

5.861 5.952 6.013 6.069

Counts vs. Acqui

MS Spectrum Results

+EI Scan (2.041-2.106 min, 16. ...)

93.0 136.0

+EI Scan (2.253-2.296 min, 11. ...)

93.0

+EI Scan (2.478-2.513 min, 9 S. ...)

73.1 192.9 266.9 355.0

Counts vs. Mass-to-Charge (m/z)

MS Peaks One: +Scan (2.041-2.106 min) Sub

m/z	Species	Abund	A
53.1		27397.6	
67.1		150742.4	
68.1		187409.7	
77		68352.8	
78.1		16252.1	
79		117390	
80		45228.3	
81		27925.3	
91		110364	
92		111613.8	
93		295492.2	
94.1		114854	
95.1		33656.4	
105		41578.4	
105.1		18000.2	
107		114399.2	
108		39713.3	
121		136363.2	
134.1		17098	
136		138343.1	

MS Peaks Two: +Scan (2.478-2.513 min) Sub

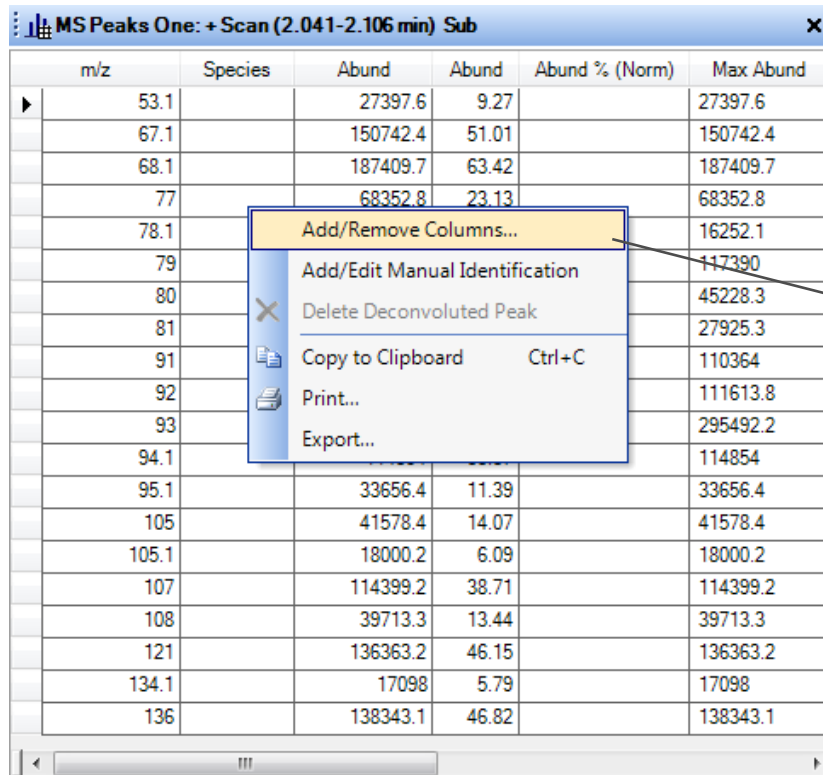
m/z	Species	Abund	Abund	Abund % (Norm)	I
73.1		522338	36.36		52
192.9		77674.7	5.41		77
248.9		72716.6	5.06		72
250.9		127531.8	8.88		12
266.9		1436423.5	100		14
267.9		377111.3	26.25		37
268.9		252688.3	17.59		25
355		1433785.1	99.82		14
356		505299.2	35.18		50
357		330757.8	23.03		33
358		86166.2	6		86

Method Explorer: mh_test.m

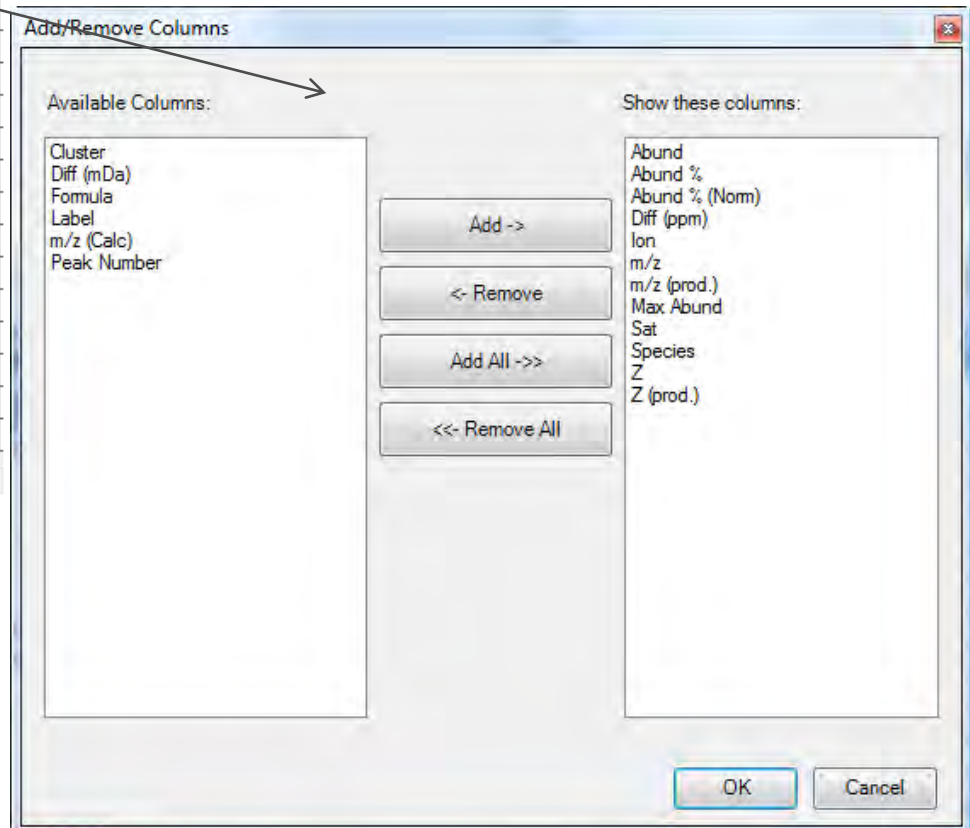
- Chromatogram
- Spectrum
- Extract (MS)
- Extract (MS/MS)
- Extraction Data Format
- General
- Reports
- Find Compounds
- Identify Compounds
- Compound Automation Steps
- Worklist Automation
- Export

- CTRL click at 2nd spectrum
- MS Spectrum Peak List Two
- Tool is also available.

MS Spectrum Peak List



m/z	Species	Abund	Abund	Abund % (Norm)	Max Abund
53.1		27397.6	9.27		27397.6
67.1		150742.4	51.01		150742.4
68.1		187409.7	63.42		187409.7
77		68352.8	23.13		68352.8
78.1					16252.1
79					117390
80					45228.3
81					27925.3
91					110364
92					111613.8
93					295492.2
94.1					114854
95.1		33656.4	11.39		33656.4
105		41578.4	14.07		41578.4
105.1		18000.2	6.09		18000.2
107		114399.2	38.71		114399.2
108		39713.3	13.44		39713.3
121		136363.2	46.15		136363.2
134.1		17098	5.79		17098
136		138343.1	46.82		138343.1



For relative abundance, right-click table header, and **Add/Remove Columns**. Select desired columns.

MS Spectrum Peak Filter

The screenshot displays the Agilent MassHunter Qualitative Analysis software interface. The 'Method Editor: Extract (MS)' window is open, showing the 'Peak Filters' tab. The 'Height filters' section is configured with 'Absolute height' set to ≥ 20000 counts and 'Relative height' set to ≥ 5.000 % of largest peak. The 'Maximum number of peaks' is set to 100. A red arrow points from the 'Relative height' filter to the MS Spectrum Results plot, which shows a mass spectrum with peaks at m/z 69.1, 124.0, 175.9, and 205.9. A horizontal red line is drawn at an abundance of 20000. The 'MS Peaks One: + Scan (6.268-6.329 min) Sub' table is also visible, showing the following data:

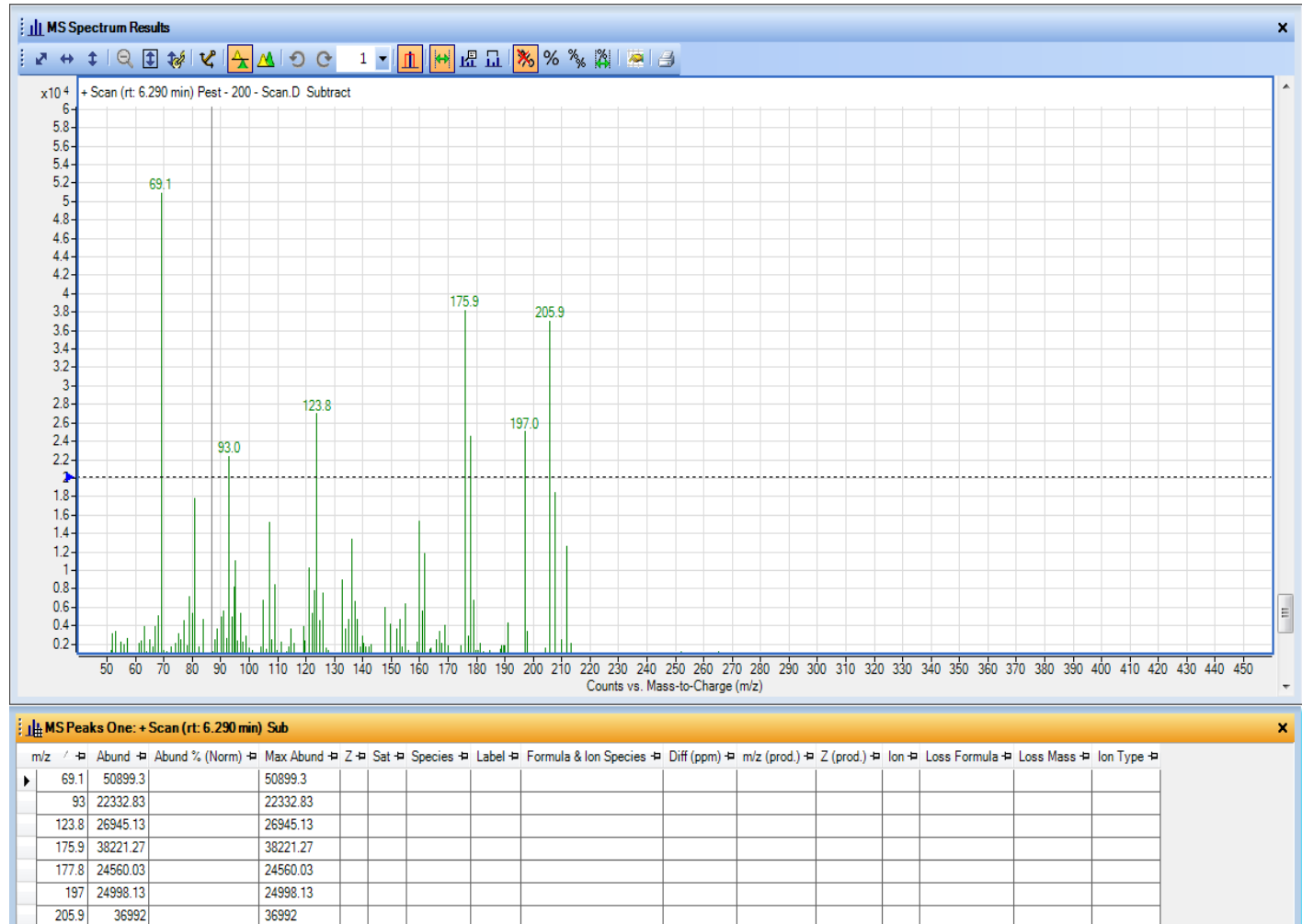
m/z	Species	Abund	Abund	Abund % (Norm)	Max Abund	Z	Sat	m/z (p
205.9		46522.4	100		46522.4			
175.9		42664.9	91.71		42664.9			
69.1		34973.9	75.18		34973.9			
124		29238.1	62.85		29238.1			
207.9		26191.7	56.3		26191.7			

Only affects MS Peaks table.

MS Spectrum Peak Filter Interactive Setup

- Position the cursor at the location for the threshold.
- Right click and select **Adjust Peak Threshold**.

• **Tip: Scale Spectra must be off.**



- MS Spectrum Peak List 1
- MS Spectrum Peak List 2
- MS Actuals
- Adjust Peak Threshold**

Accurate Mass Considerations

How to Recalibrate a Mass Spectrum

Use on **User Spectra** only.


Do not background subtract.

Right-click in MS Spectrum Results window and select **Recalibrate**.

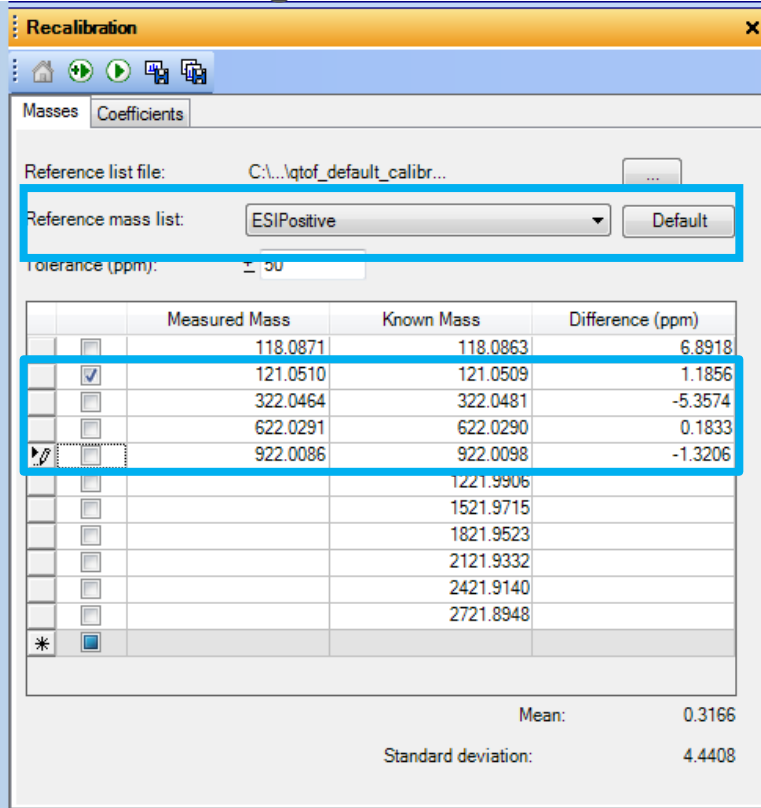
Calculates and applies new calibration to highlighted spectra. 

Select  to apply current recalibration to highlighted spectra.

Saves new calibration to highlighted spectra. 

Save new calibration to whole datafile. 

Restores original calibration. 



	Measured Mass	Known Mass	Difference (ppm)
<input type="checkbox"/>	118.0871	118.0863	6.8918
<input checked="" type="checkbox"/>	121.0510	121.0509	1.1856
<input type="checkbox"/>	322.0464	322.0481	-5.3574
<input type="checkbox"/>	622.0291	622.0290	0.1833
<input checked="" type="checkbox"/>	922.0086	922.0098	-1.3206
<input type="checkbox"/>		1221.9906	
<input type="checkbox"/>		1521.9715	
<input type="checkbox"/>		1821.9523	
<input type="checkbox"/>		2121.9332	
<input type="checkbox"/>		2421.9140	
<input type="checkbox"/>		2721.8948	
*			

Mean: 0.3166
Standard deviation: 4.4408



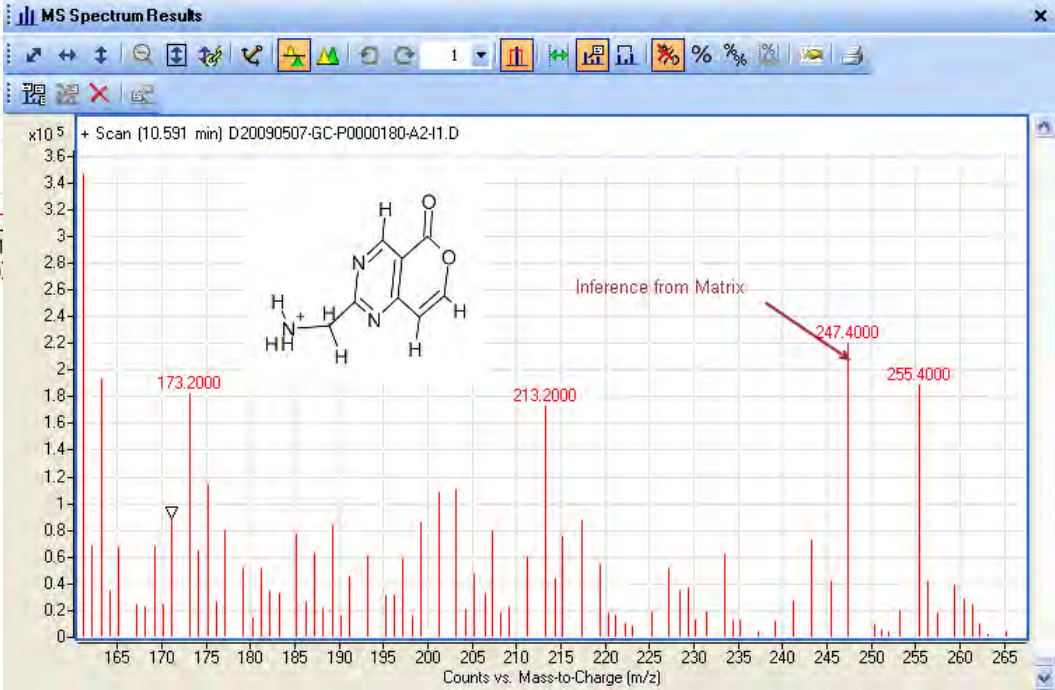
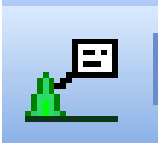
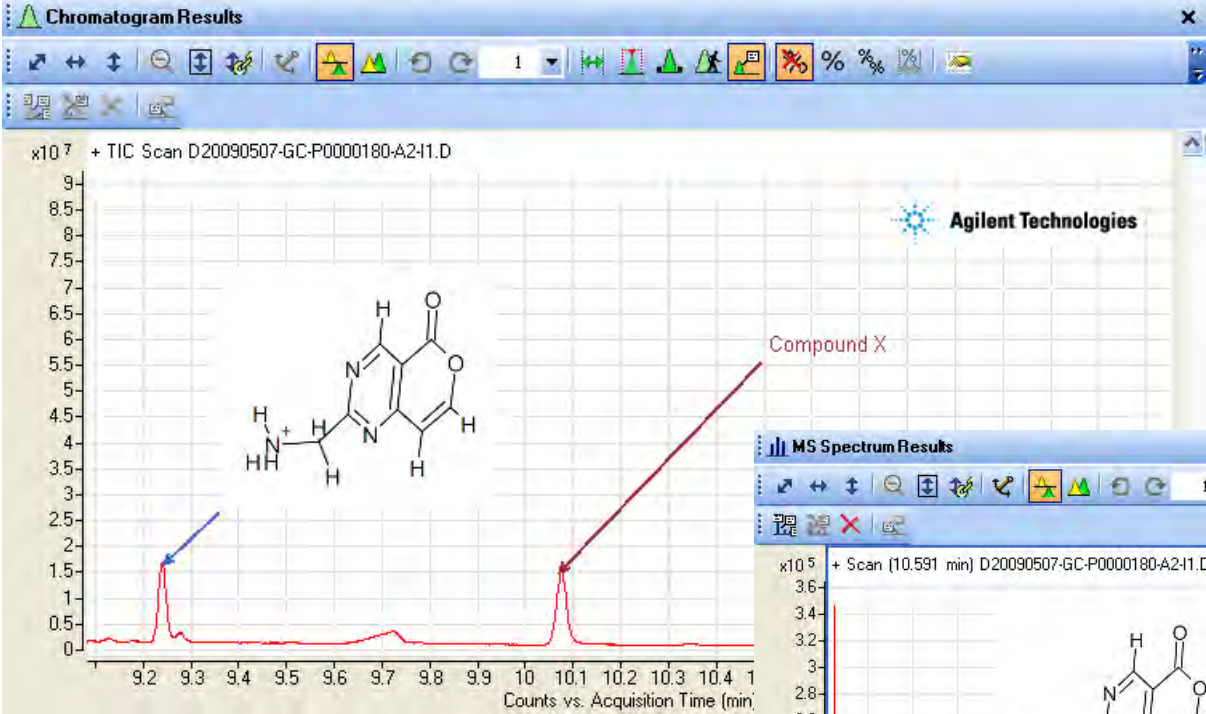
Let's take a moment
for chat questions
on Working with
Mass Spectra

Up Next:
Demo



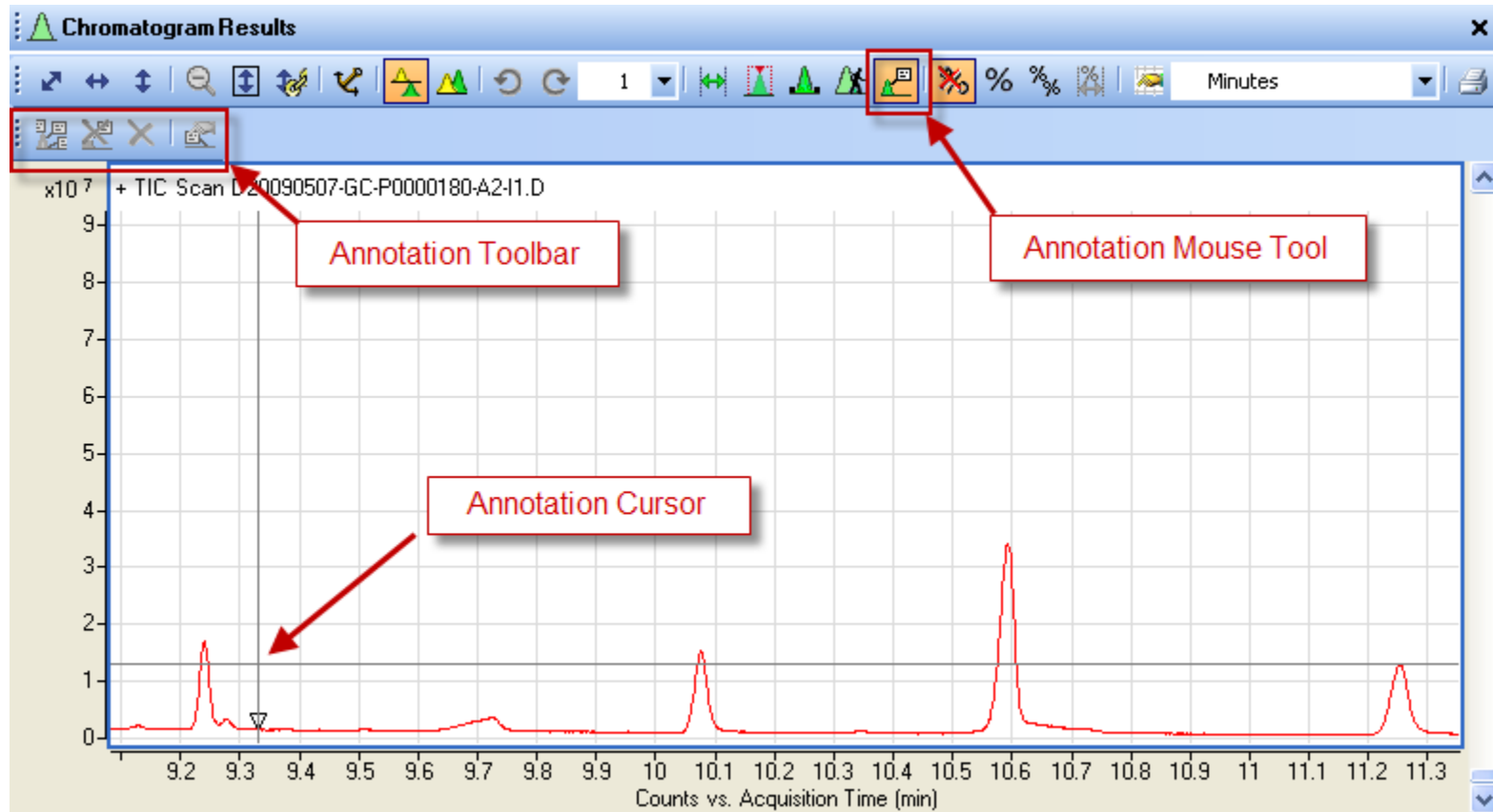
Up Next:
Annotation Functions

Annotation of Chromatograms and Spectra

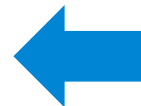
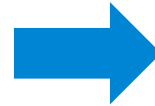
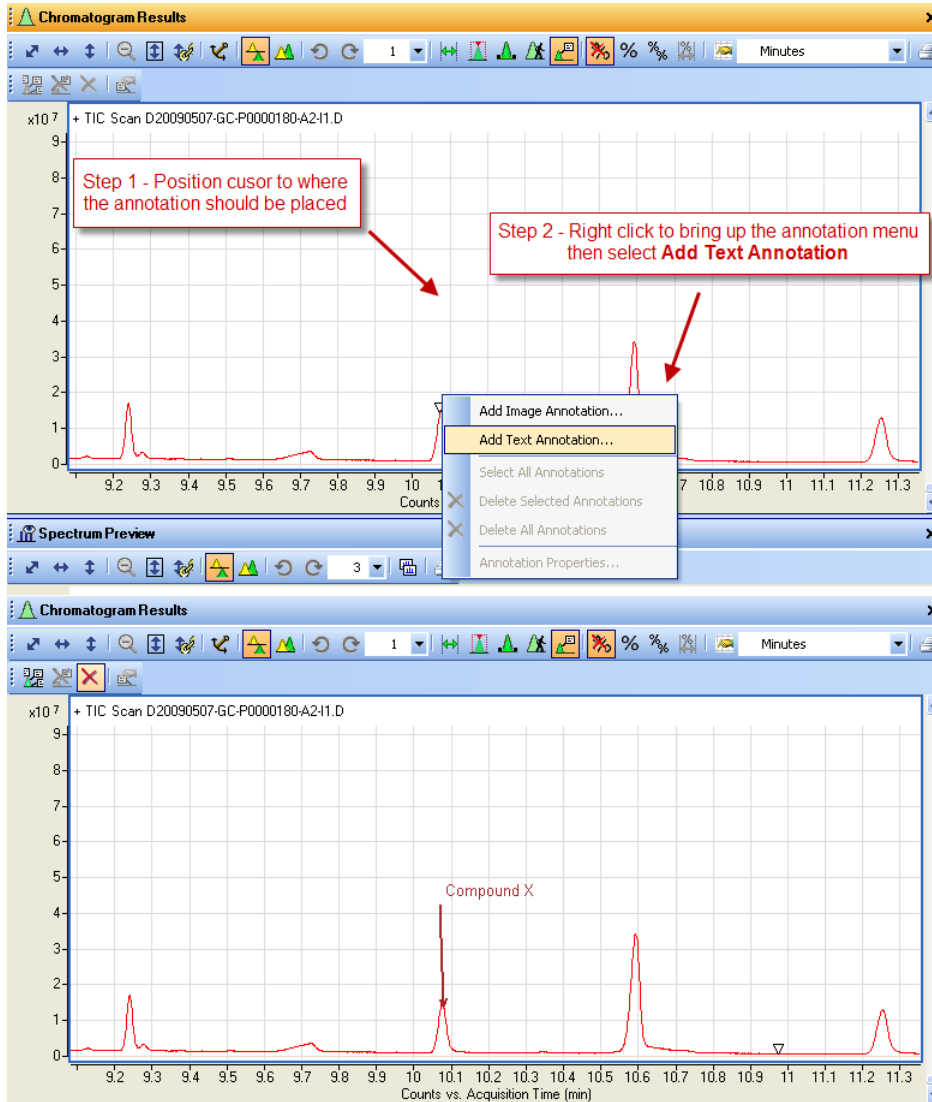


Place Graphic into Annotation Mode

- Click Annotation Mouse Tool
- Annotation Toolbar and Annotation cursor appear



Add a Text Annotation



The 'Add/Edit Text Annotation' dialog box is shown with the following settings:

- Text:** Compound X
- Text color:** Brown
- Orientation:** 0 degrees
- Font style:** Regular
- Font size:** 10
- Annotation type:** Anchored
- Show pointer
- Pointer properties:**
 - Color:** Brown
 - Pattern:** Solid line
 - Weight:** Medium
 - Pointer head:** Arrow
 - Pointer head location (the x, y value using the data displayed):**
 - X: 10.079183333333 min
 - Y: 14256440 (abundance)
 - Upper left corner of the annotation (the x, y value using the data displayed):**
 - X: 10.08 min
 - Y: 49063600.57 (abundance)
- Floating
- Upper left corner of the annotation relative to the upper left corner of the canvas:**
 - Relative X (%): 43.8202247191011 (% calculated using x,y values from the canvas)
 - Relative Y (%): 50.4885933485342

At the bottom, a red box with the text 'Step 4 - Click OK' points to the 'OK' button.

Text and Pointer Can Be Repositioned

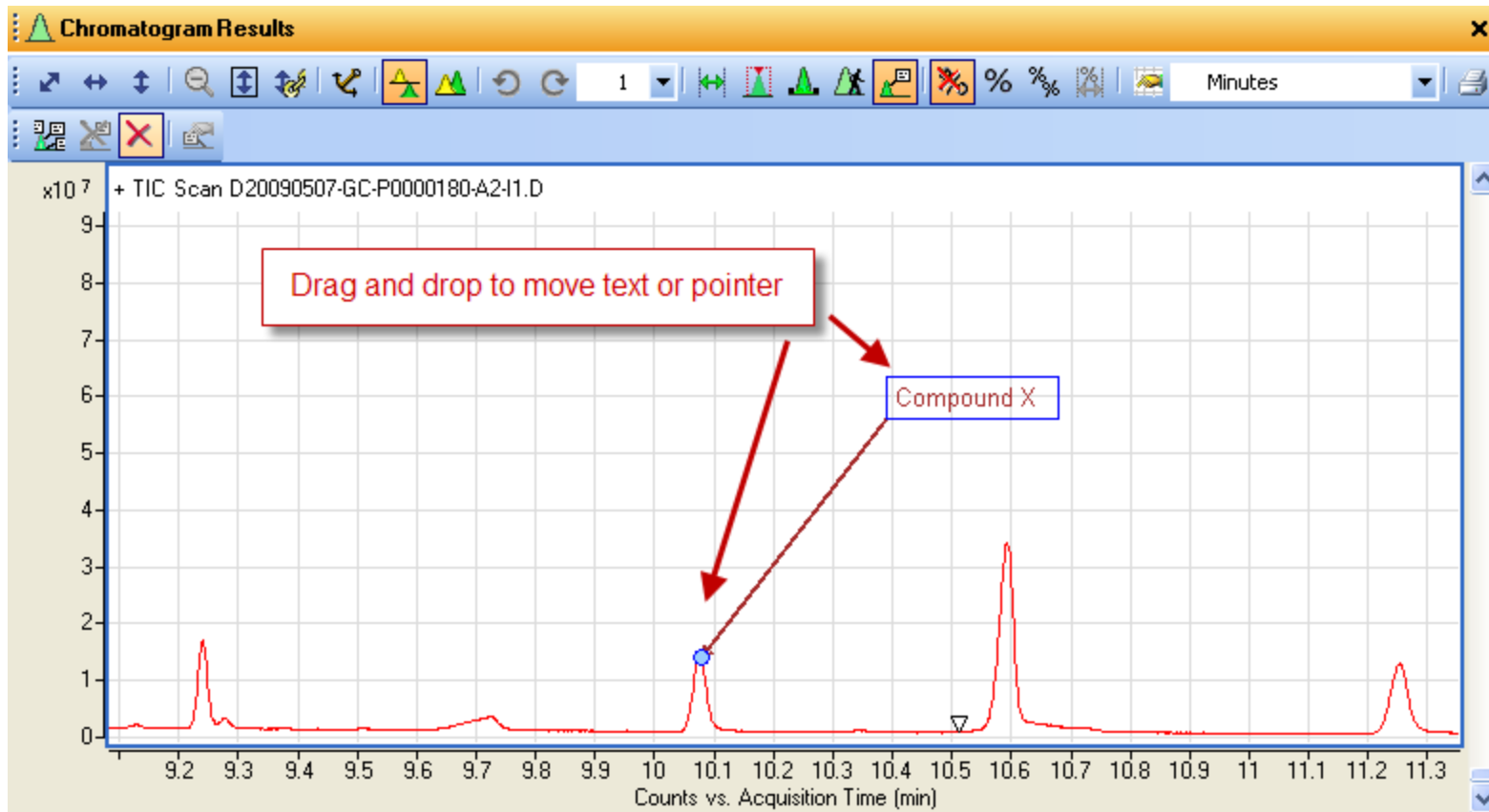
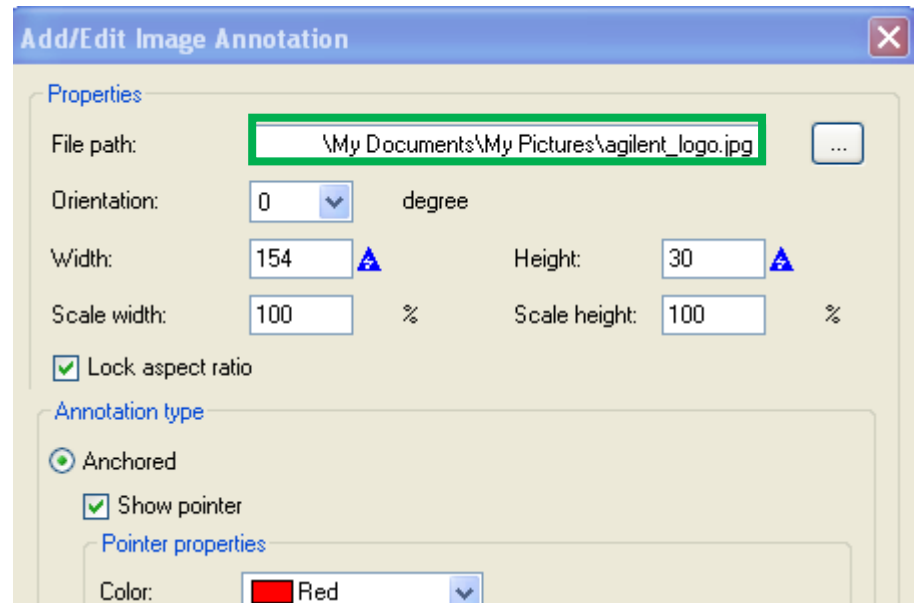
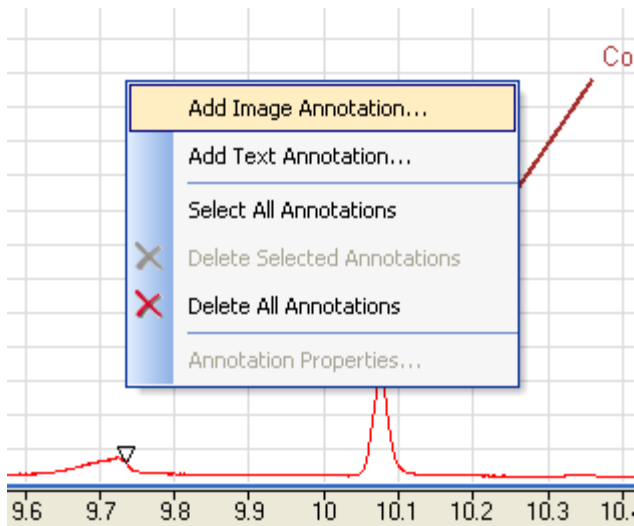
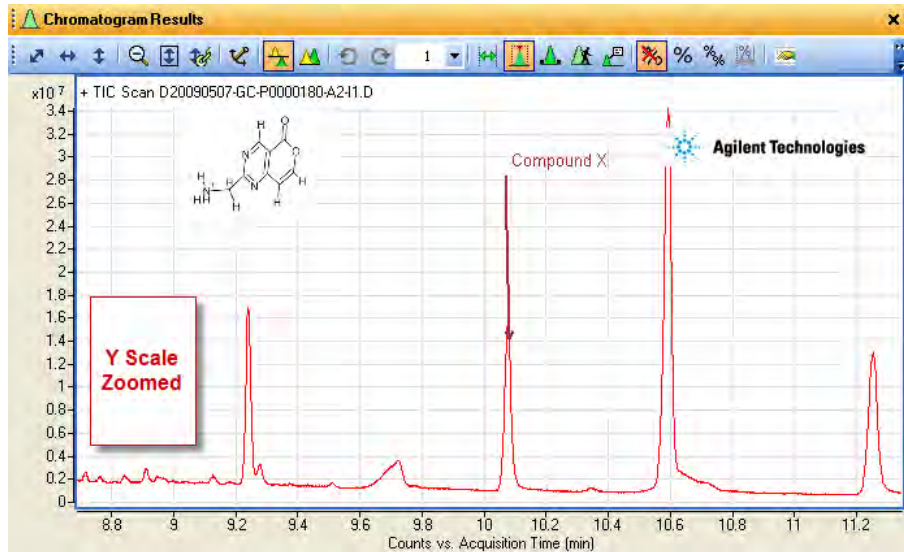
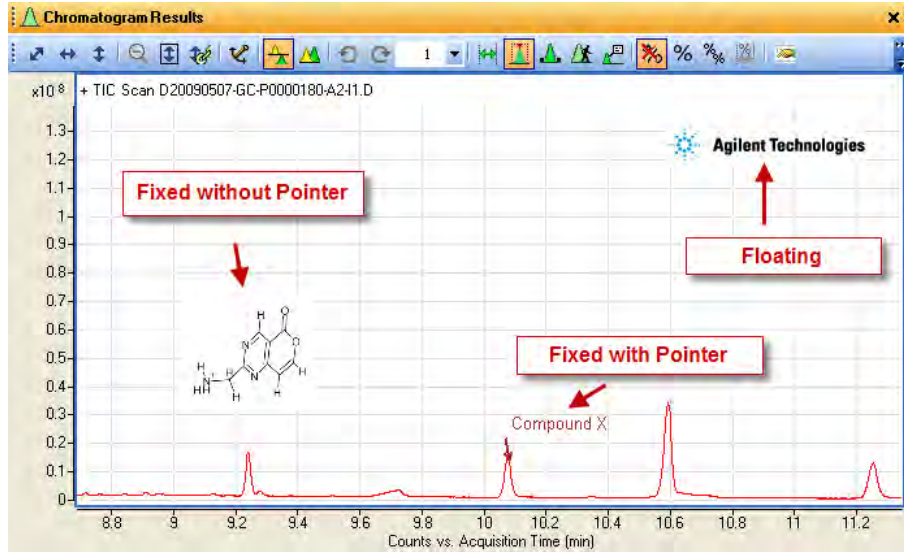


Image Annotation

- Same steps as adding Text
- JPEG and MOL (molecular structure) files are supported
- Image may be scaled and pivoted



Anchored vs. Floating Annotation



Add/Edit Text Annotation dialog box showing properties and annotation type settings.

Properties

Text:

(Press Ctrl+Enter or Alt+Enter to add a new line)

Text color:

Orientation: degrees

Font style: Font size:

Annotation type

Anchored

Show pointer

Pointer properties

Color:

Pattern:

Weight:

Pointer head:

Pointer head location (the x, y value using the data displayed):

X: min

Y: (abundance)

Upper left corner of the annotation (the x, y value using the data displayed):

X: min

Y: (abundance)

Floating

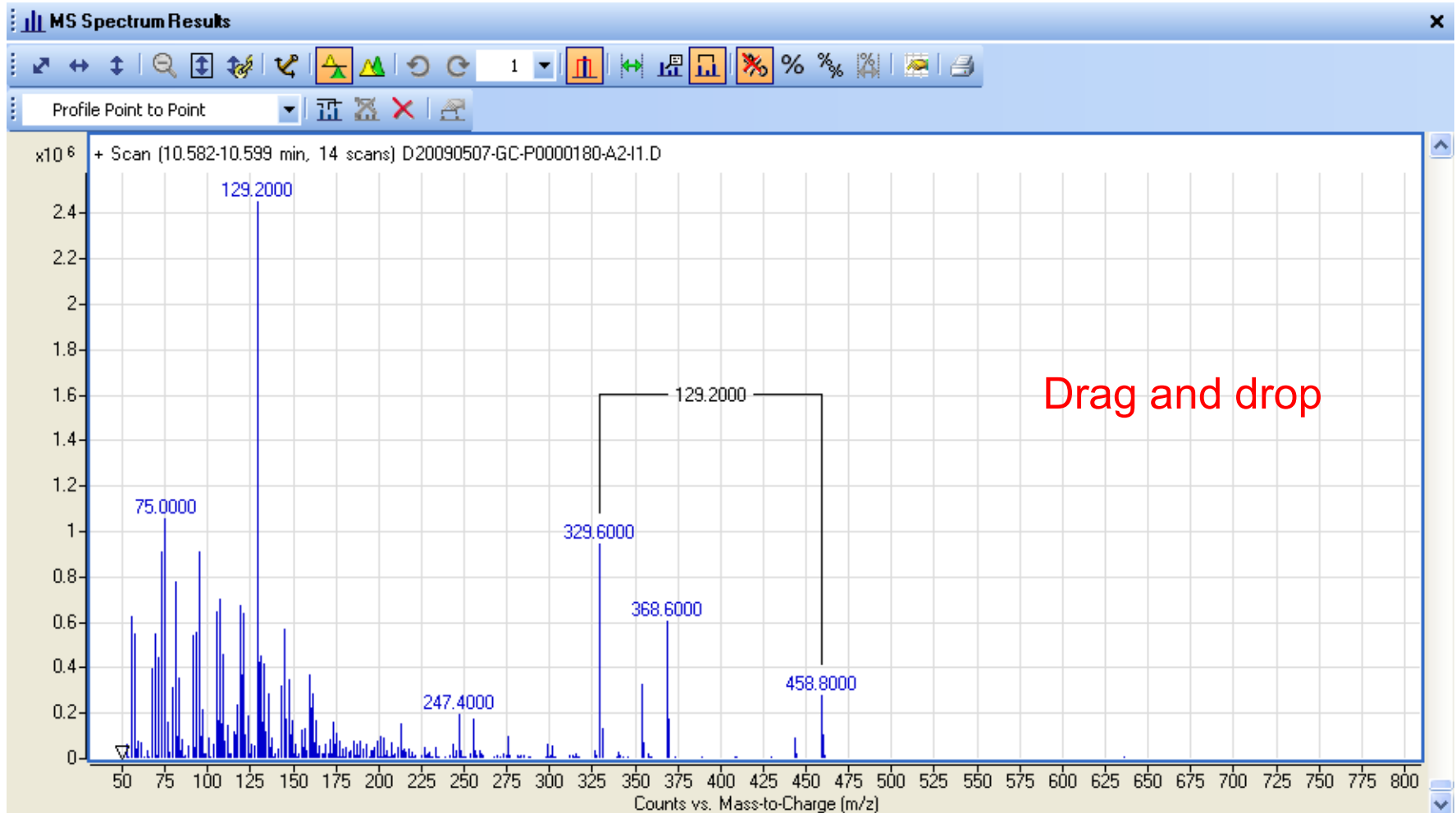
Upper left corner of the annotation relative to the upper left corner of the canvas:

Relative X (%): (% calculated using x,y values from the canvas)

Relative Y (%):

Delta Mass Caliper

- New tool to calculate and display mass differences between two ions.



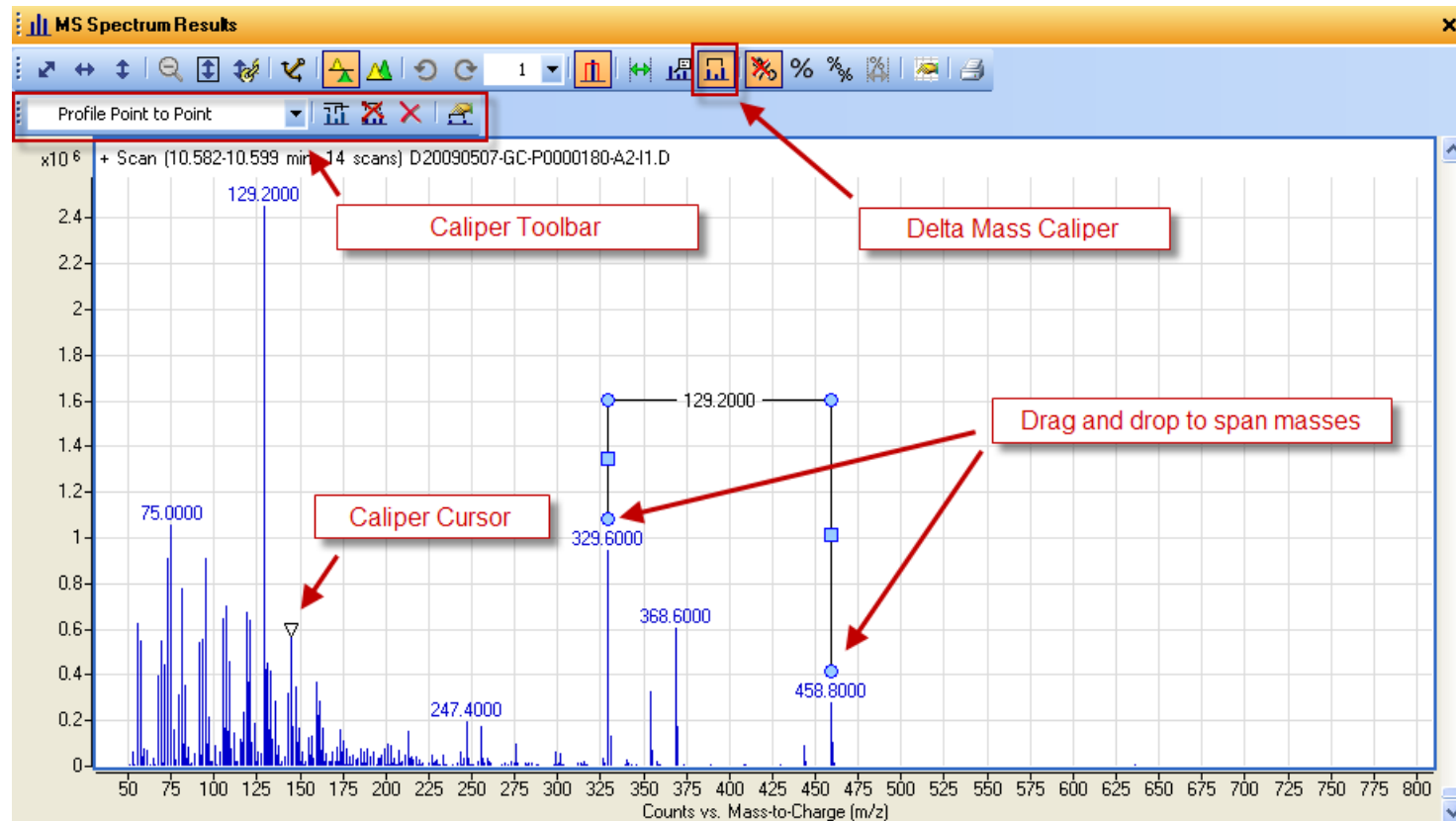
Delta Mass Caliper - Mass Caliper Mode

Click **Delta Mass Caliper Mouse** icon

Caliber Toolbar and Caliper cursor appear

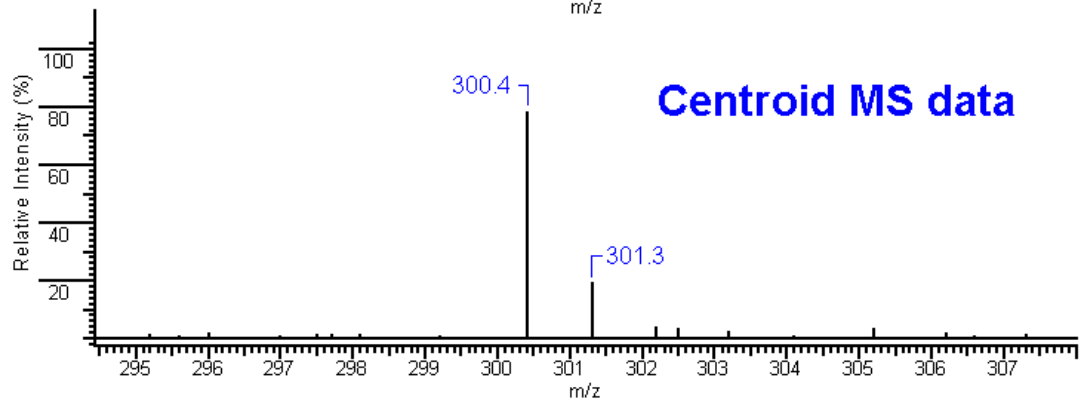
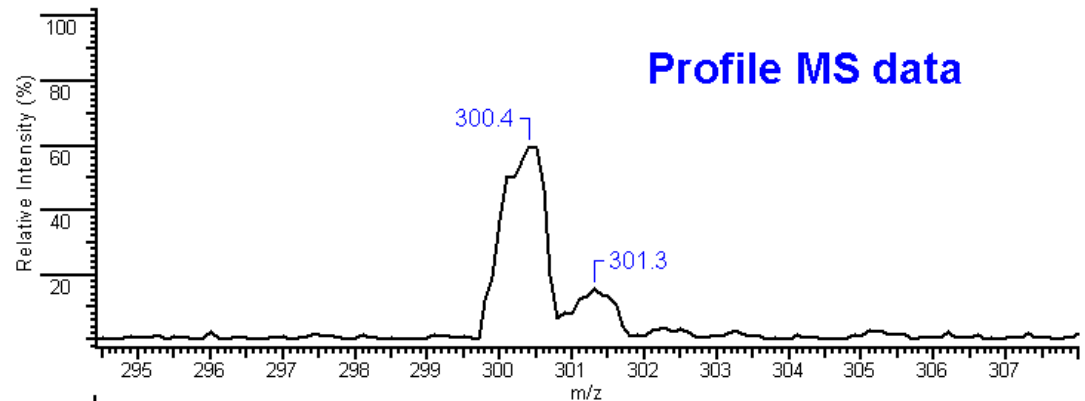
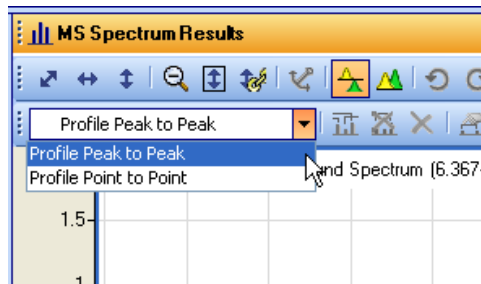
Add or edit Calipers

Calipers can only be placed where there is a signal and “snap” to closest ion



Delta Mass Caliper – Profile Options

- Only used on profile data
- Profile Peak to Peak will “snap” Caliper to profile peak apex
- Profile Point to Point will allow the user to position the Caliper to any point





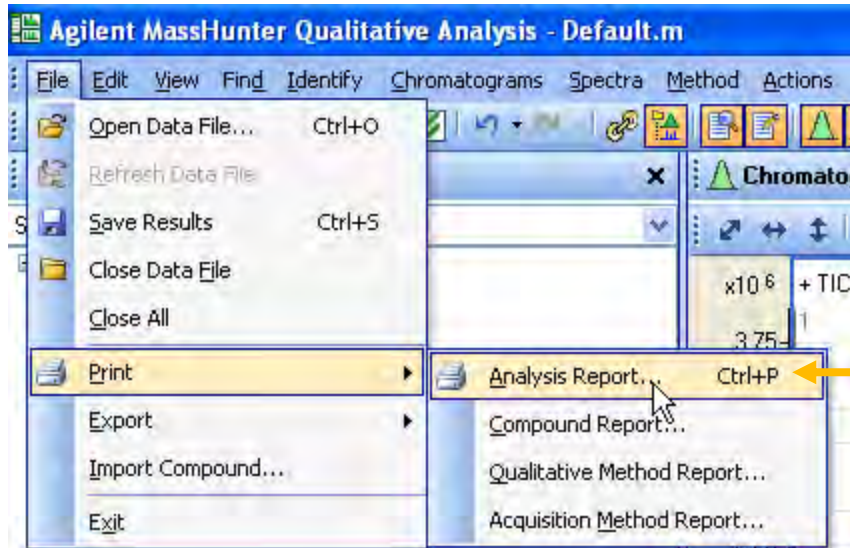
Let's take another
moment for chat
questions on
Annotations

Up Next:
Demo



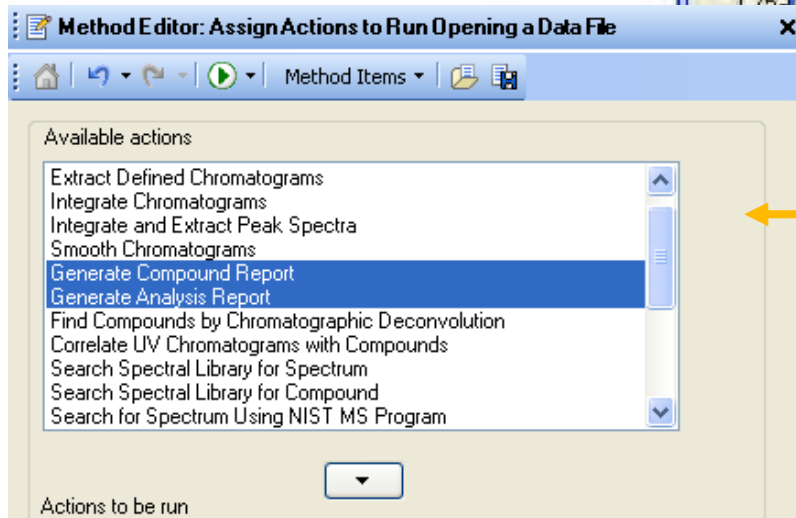
Up Next:
Reporting

Print a Report from Qualitative Analysis



Print Qualitative Reports:

- Directly from menu.
- Indirectly from Automation
 - File Open Actions
 - Worklist Automation
 - Covered in the Familiarization Guides.



Report Generation Options

Agilent MassHunter Qualitative Analysis - Default.m

File Edit View Find Identify Chromatograms Spectra Method Actions Tools Help

Open Data File... Ctrl+O
Refresh Data File
Save Results Ctrl+S
Close Data File
Close All
Print
Export
Exit

Chromatogram Results

x10¹ +EI TIC Scan Pest - 200 - Scan.D

6.95 7 7.05 7.1 7.15 7.2 7.25 7.3 7.35 7.4

Method Explorer: Default.m

- Chromatogram
 - Integrate (MS)
 - Integrate (MS/MS)
 - Smooth
 - Exclude Mass(es)
 - Calculate Signal-to-Noise
 - Define Chromatograms
- Spectrum
 - Extract (MS)
 - Extract (MS/MS)
- General
 - Analysis Report**
 - Compound Report
 - Common Reporting Options
 - File Open Actions
 - Extraction Data Format
- Find Compounds
- Identify Compounds
- Compound Automation Steps

Method Editor: Analysis Report

User chromatograms

- Show user chromatograms
 - With peak tables
 - With signal to noise results

User spectra

- Show user spectra
 - With peak tables
 - With library spectrum
 - With difference spectrum

Compounds

- Show compound chromatograms
 - With peak tables
- Show compound spectra
 - With peak tables

Print Analysis Report

List of opened data files:

- Pest - 200 - Scan.D

Report contents

- All results Separate report per data file
- Only highlighted results

Print report

- Print report Printer name: <Default>
- Print preview

Save report

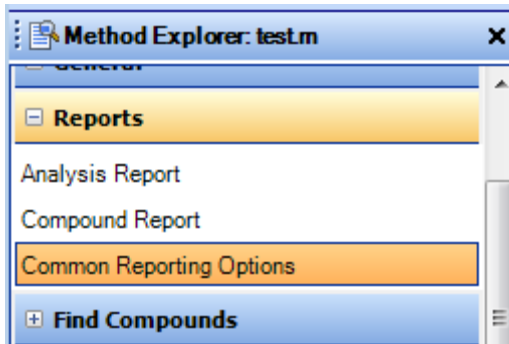
- Save report as Excel file Save report as PDF file
- Inside data file's reports subdirectory
- At specified directory: C:\MassHunter\reports

If report file already exists

- Overwrite existing report
- Auto-generate new report file name

OK Cancel

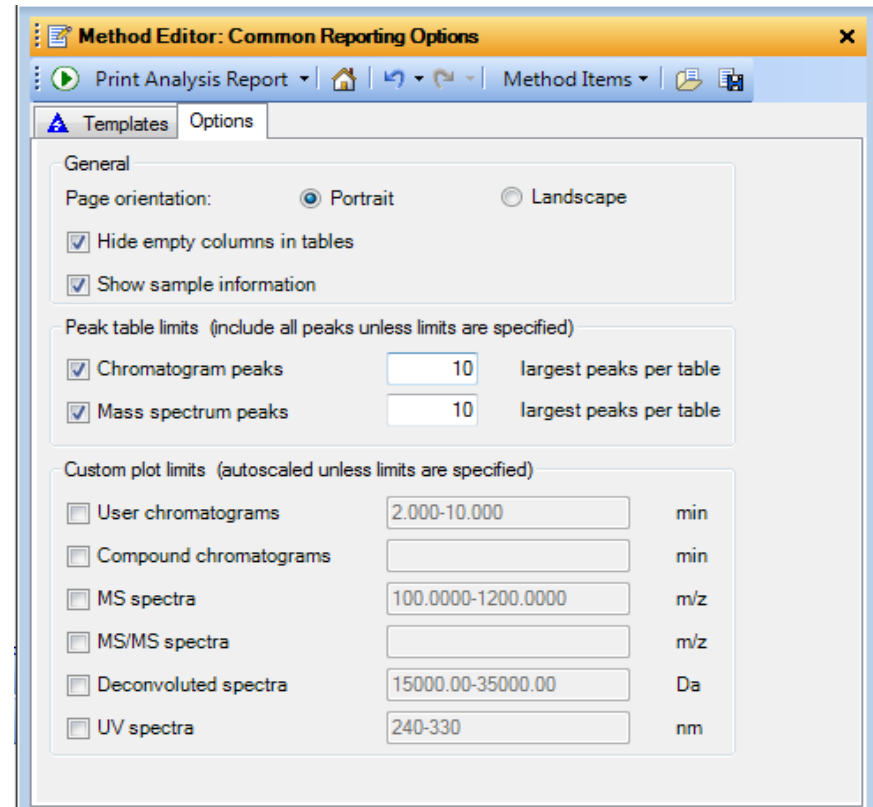
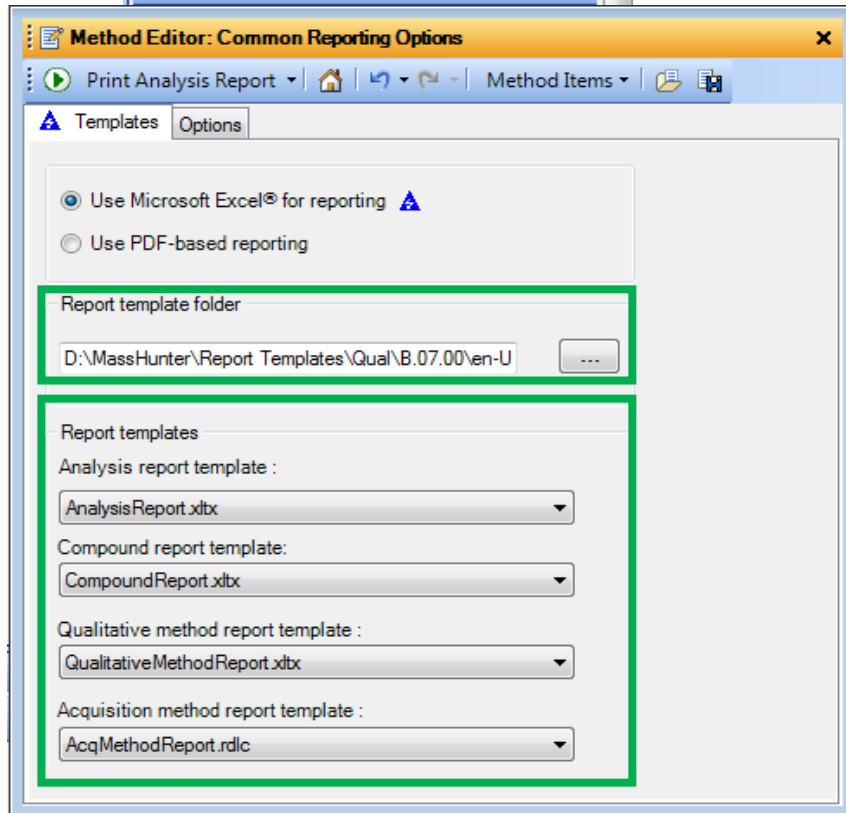
Common Reporting Options



Excel Based Reporting

Uses xlsx files

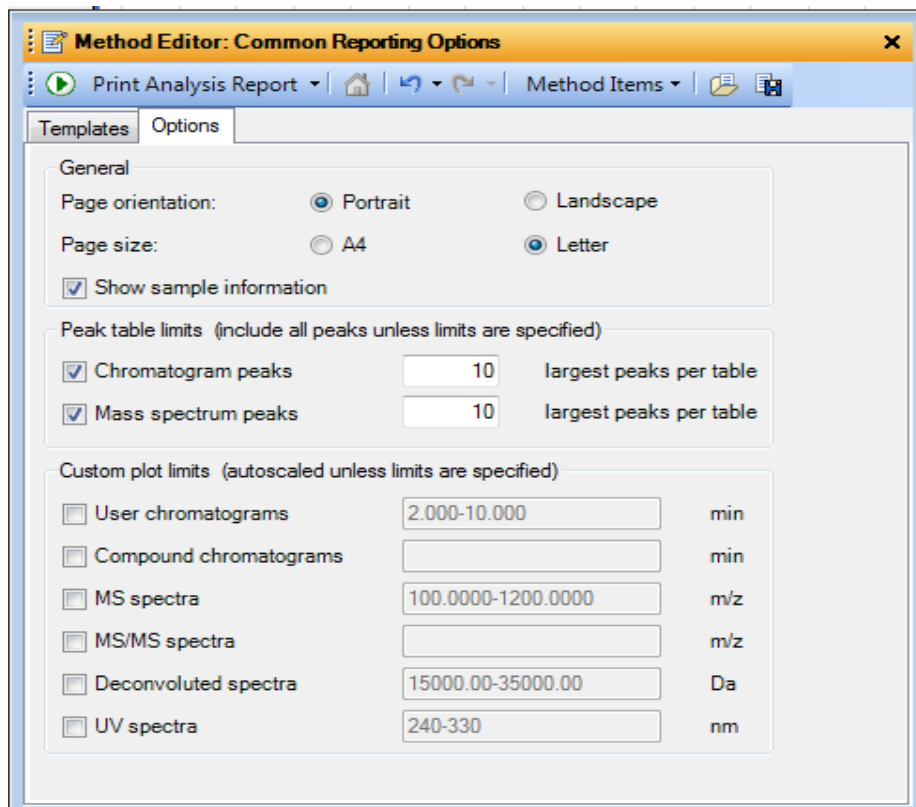
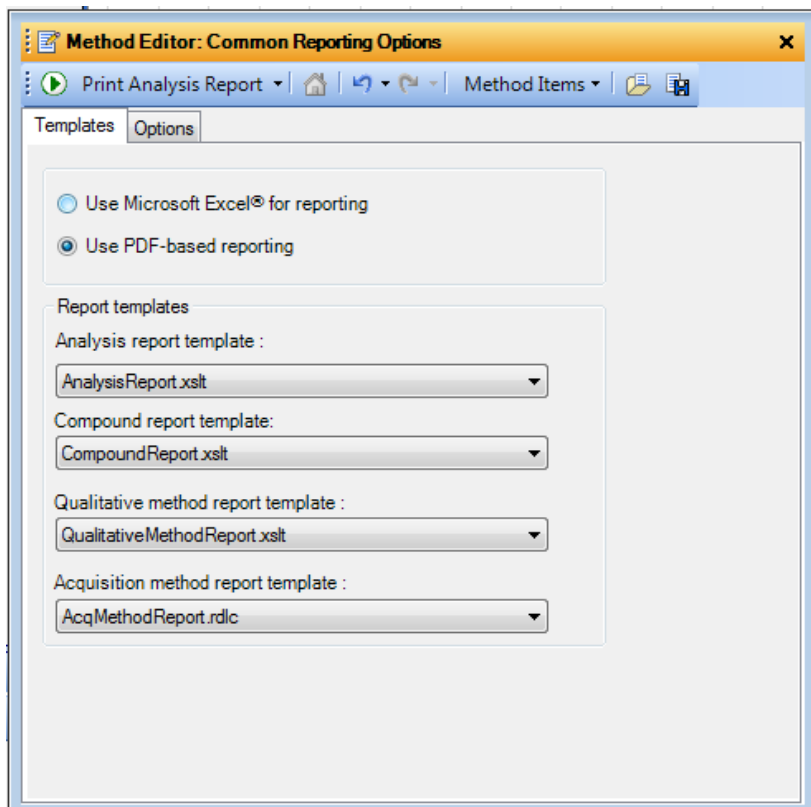
Tip: Review Common Reporting Options first.



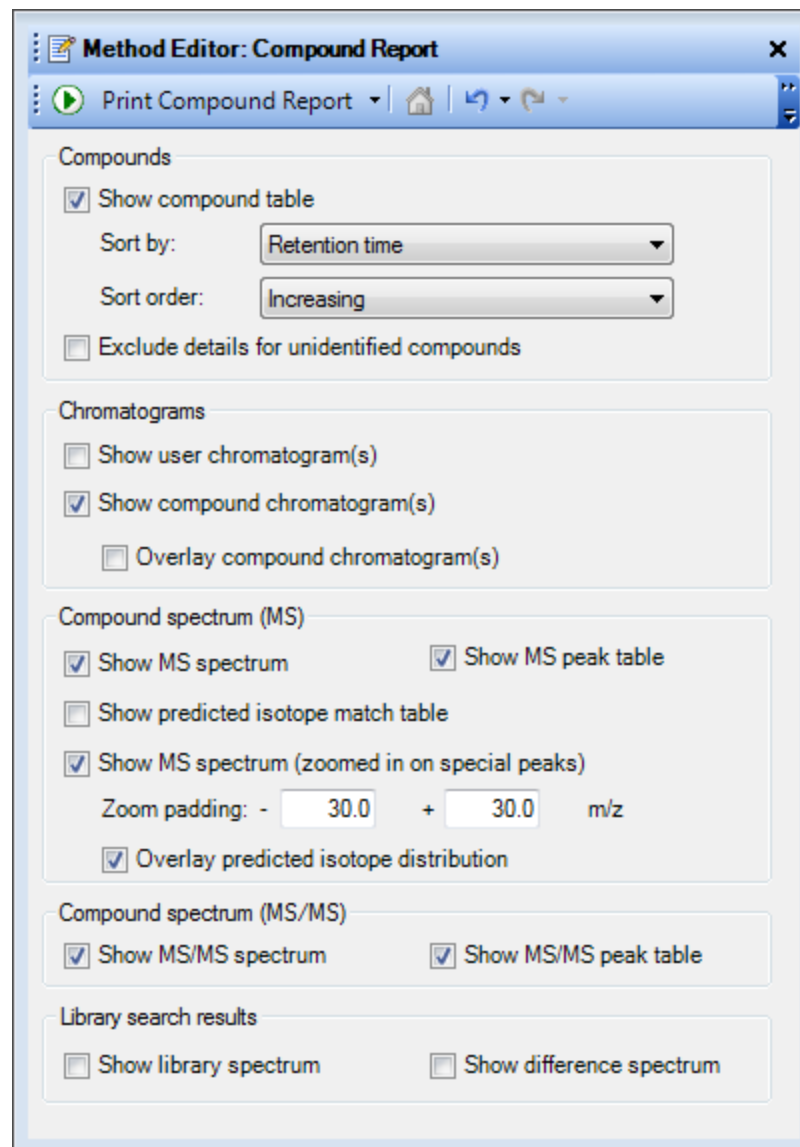
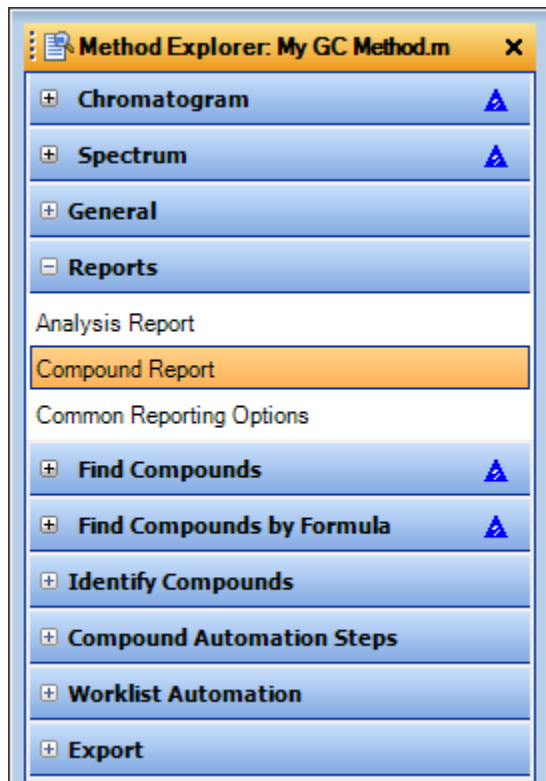
Common Reporting Options

New to Qualitative Analysis
B.07.00 SP1

PDF Based Reporting
Uses xslt files



Compound Report Options



Tools

The screenshot shows the Agilent MassHunter Qualitative Analysis B.04.00 interface. The top menu bar includes File, Edit, View, Find, Identify, Chromatograms, Spectra, Method, Wizards, Actions, Configuration, Tools, and Help. Below the menu is a toolbar with various icons. Annotations with arrows point to specific icons:

- Open data files:** Points to the folder icon in the toolbar.
- Save results to data files:** Points to the floppy disk icon in the toolbar.
- Choose defined color:** Points to the color selection icon in the toolbar.
- Show all items (relates to Data Navigator):** Points to the icon with two green checkmarks in the toolbar.
- Close data file:** Points to the red 'X' icon in the toolbar.
- Print Qualitative Analysis Report:** Points to the printer icon in the toolbar.
- Show all highlighted items:** Points to the icon with a magnifying glass and a checkmark in the toolbar.
- Show only highlighted items:** Points to the icon with a magnifying glass and a checkmark in the toolbar.
- Linked Navigation:** Points to the icon with a key in the toolbar.

The interface also shows a Data Navigator on the left, a Chromatogram Results plot in the center, and a Method Explorer on the bottom left. The chromatogram plot shows a peak at 6.216 minutes. The MS Spectrum plot shows a peak at 69.1 m/z.

Tools

The screenshot displays the Agilent MassHunter Qualitative Analysis software interface. The main window shows a chromatogram with several peaks labeled with retention times: 5.912, 6.013, 6.216, and 6.307. A toolbar at the top contains various icons for data navigation and analysis. Below the chromatogram, there are several panels and toolbars:

- Data Navigator:** Located on the left, it shows a list of data files and scans.
- Method Editor:** Located below the Data Navigator, it shows the current method being used.
- Chromatogram Results:** The main plot area showing the chromatogram with peaks.
- MS Spectrum Results:** A panel showing the mass spectrum of a selected peak, with a peak at 175.9 m/z.
- MS Actuals:** A plot showing the actual mass spectrum of the sample.
- Integration Peak List:** A list of peaks and their retention times.
- Compound List:** A list of identified compounds.
- Structure Viewer:** A panel showing the chemical structure of a selected compound.
- Sample Information:** A panel showing details about the sample being analyzed.

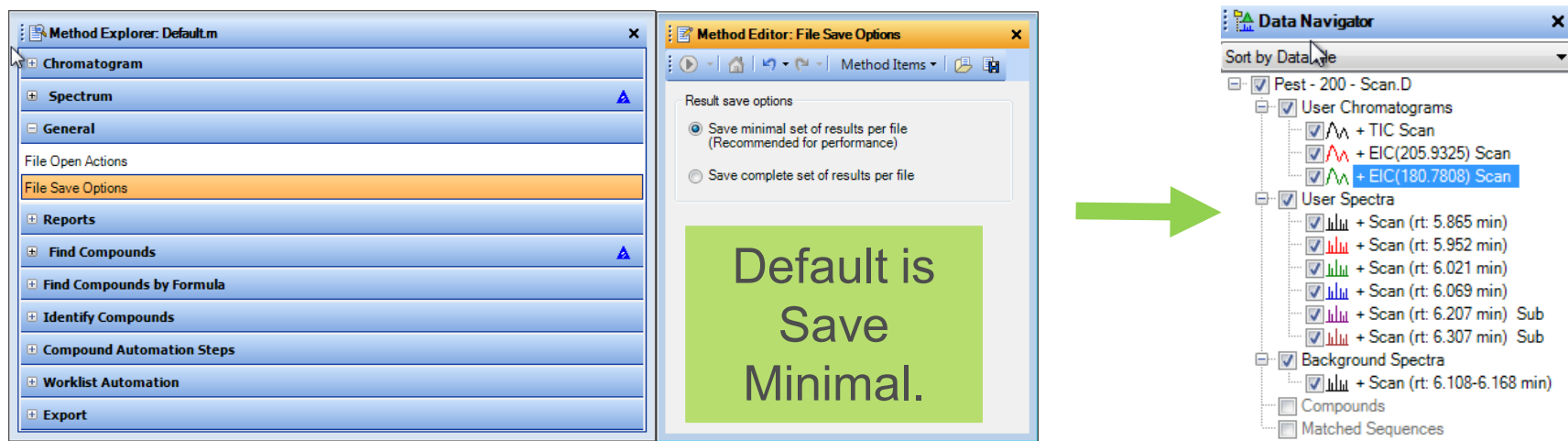
Annotations in the image point to various features:

- Red:** Data Navigator, Difference Results, Compound List, Integration Peak List.
- Blue:** Method Editor, Chromatogram Results, Compound Identification Results.
- Green:** Spectrum Identification Results, MS Spectrum Peak List 1 & 2, MS Actuals, Sample Information.

Saving Data Files and Opening Data Files

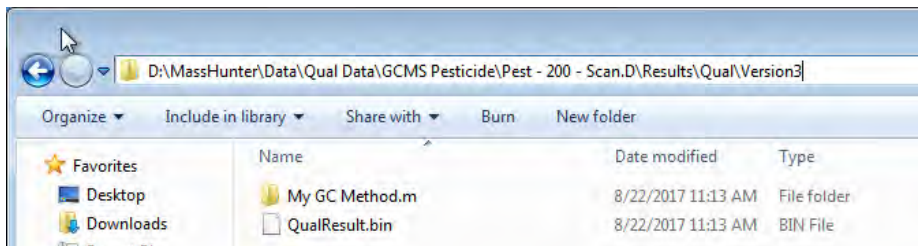
The screenshot displays the Agilent MassHunter Qualitative Analysis B.04.00 - mh_test.m interface. The top menu bar includes File, Edit, View, Find, Identify, Chromatograms, Spectra, Method, Wizards, Actions, Configuration, Tools, and Help. The toolbar contains various icons for file operations, including a red box highlighting the Open, Save, and Save As icons. The Data Navigator on the left shows a tree view of data files, with a red arrow pointing to the Open icon and the text "Open data files". The Chromatogram Results window shows a chromatogram with peaks labeled at 5.926, 6.069, and 6.216 minutes. A blue arrow points to the Save icon and the text "Save results to data files". The Method Editor: Extract (MS) window shows extraction parameters: Absolute height >= 20000 counts, Relative height >= 5.000 % of largest peak, and Maximum number of peaks 100. The MS Spectrum Results window shows a mass spectrum with peaks labeled at 69.1, 124.0, 175.9, and 205.9 m/z.

File Save Options -The Results File

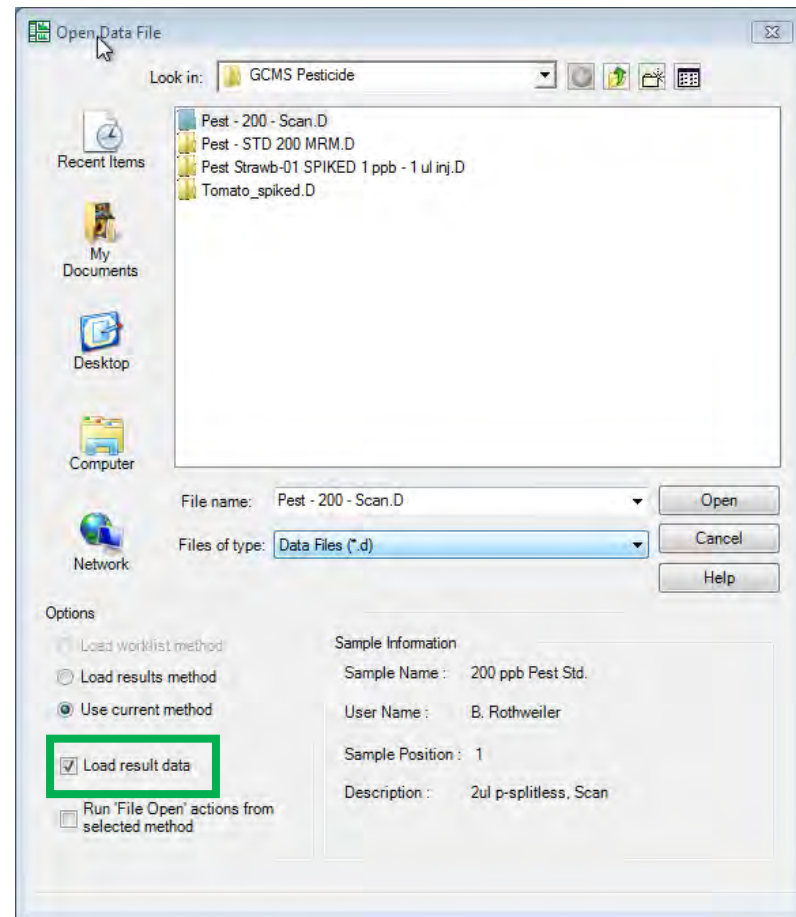


- **Save minimal** – only the compound level nodes are saved. No spectra or compound chromatograms are saved. If you open again, you will need to re-extract the complete result set.
- **Save complete** – all compound results are saved including spectra and chromatograms.
- In this example, all the User Chromatograms, User Spectra and Background Spectra are saved.

The Results File



- The results file is saved within the data file as QualResult.bin.
- A copy of the qualitative analysis method is also saved.
- Only one results file and method can be saved.
- The results file is easily loaded with the data file.
- Complete data archival.





Let's take a few
moments for questions
on Reporting.

Up Next:
Demo on Reporting



Up Next:
Training Resources

Training Resources

Training resources that are available.

Convenient Training

Our team of industry experts delivers a quality learning experience with a high degree of flexibility to fit the needs of your lab – in our classrooms, at your site or online:

- **Classroom Training** – Introductory level to in-depth, hands-on training for lab hardware or software.
- **Customized On-Site Training** – Effective learning environment designed to achieve operational excellence and employee development without the need to travel.
- **Online** – From foundation to expert offerings when and where you need it at your own pace

Introducing Agilent University

Upgraded customer experience:

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

Introduce new eLearning capabilities:

- Recorded and video-based learning
- Virtual online classes

Expanded portfolio:

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

Helping customers:

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

The screenshot shows the Agilent University website. A red arrow points to the 'TRAINING & EVENTS' menu item in the top navigation bar. Another red arrow points to the 'Education' sub-menu item. A red circle highlights the 'VIEW ALL TRAINING COURSE OFFERINGS >' button in the main banner area. The banner also features the 'AGILENT UNIVERSITY' logo and a background image of a person's face.

Agilent Community

community.agilent.com

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Collaborate - Ask and answer questions.

Connect - Interact with other Agilent users.

Discover - Find relevant discussions, documents, and videos

Share - Contribute your insights

Gas Chromatography



Liquid Chromatography



Mass Spectrometry



Software



Consumables



Sample Preparation



Energy and Chemicals



Environmental Applications



Food and Agriculture



Agilent Technologies

Questions on today's material...

Thank you for your attention.



MassHunter Qualitative Analysis

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