Agilent MassHunter Qualitative Data Analysis

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Stephen Harnos

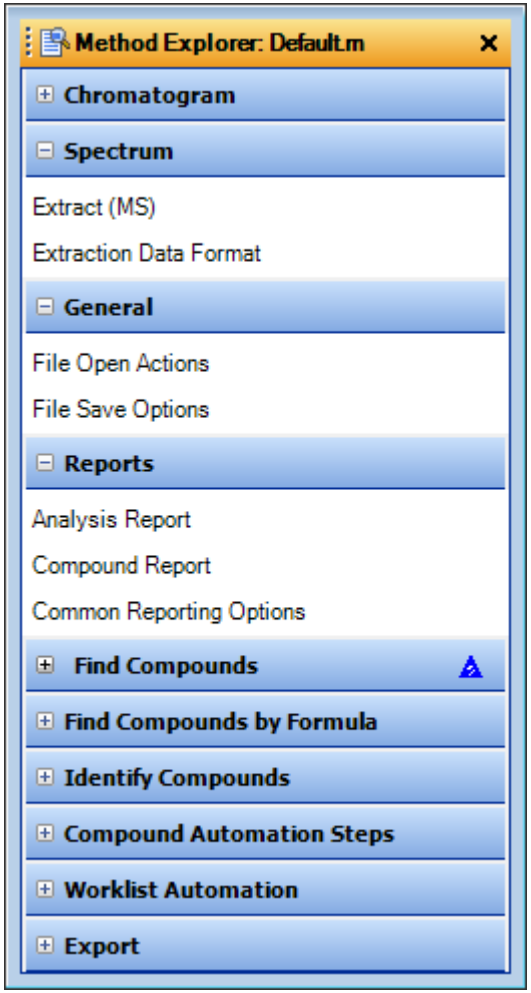
MassHunter Qualitative Analysis

Spectrum Functions

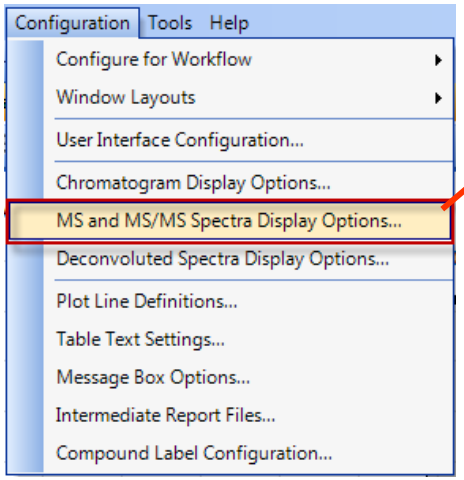
MassHunter Qualitative Analysis Software B.07.00

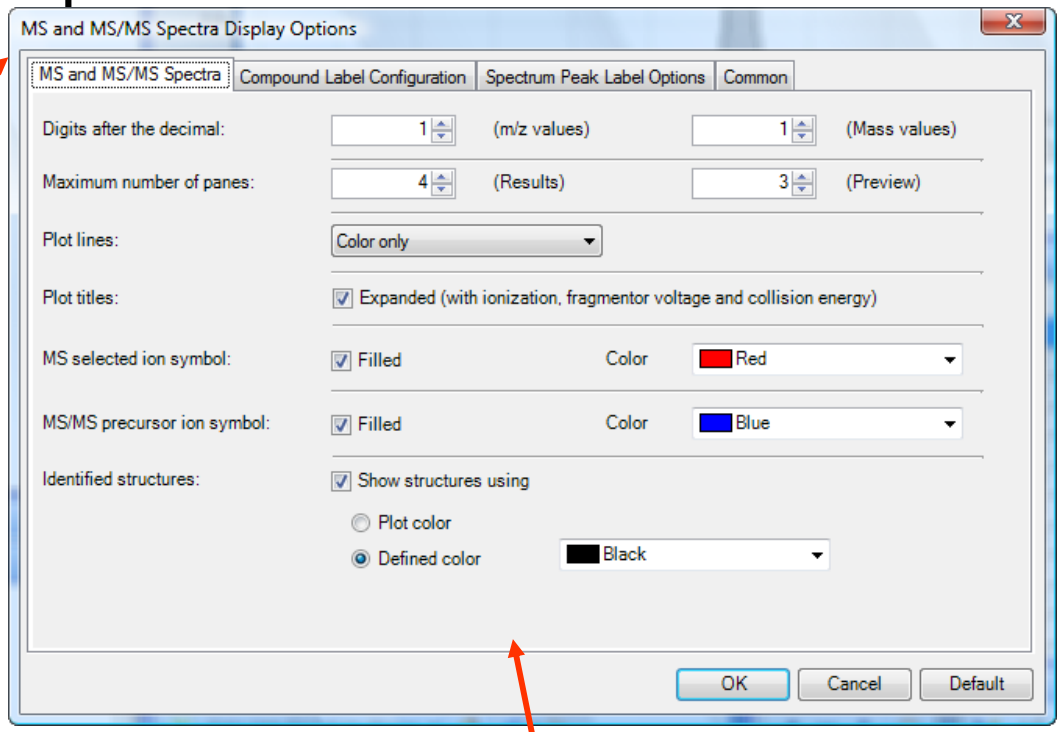
Topics

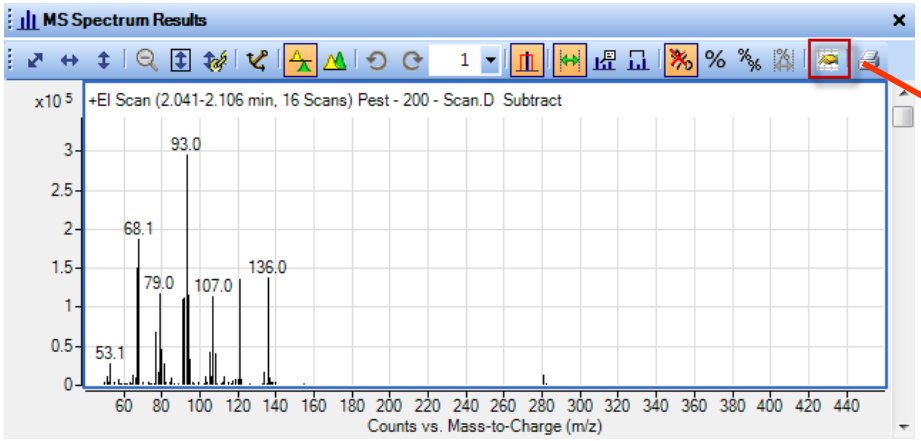
- Review Chromatogram Functions
- Spectrum Functions
  - Spectral Display
  - Extract a Spectrum and Averaging
  - Background Subtraction (MS Spectrum)
- Accurate Mass Considerations
  - Isotopic Model
- Spectrum Peak List
- Annotation
  - Text and Graphics
  - Anchoring and Floating
- Report Generation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



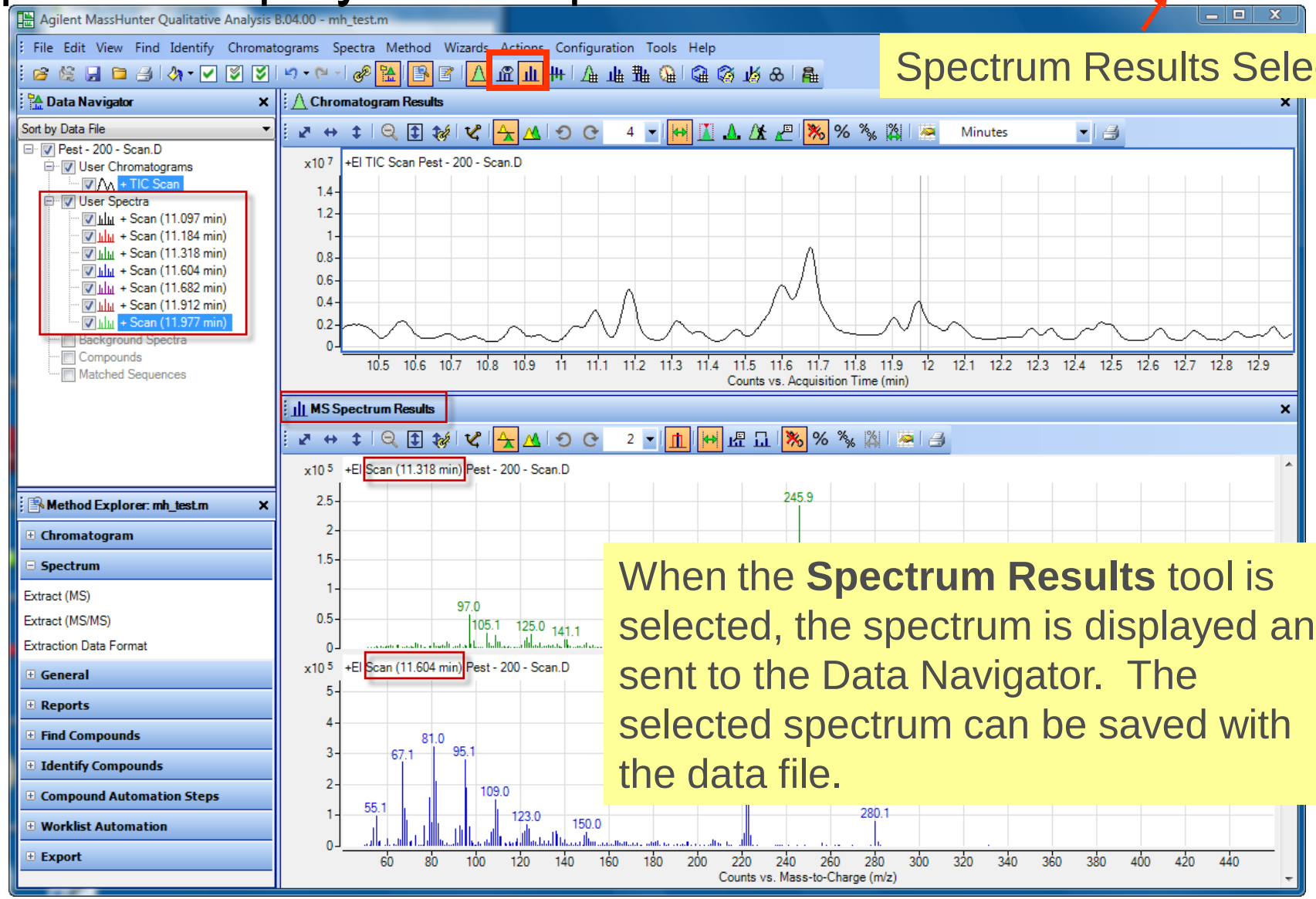
Mass Spectral Display Options







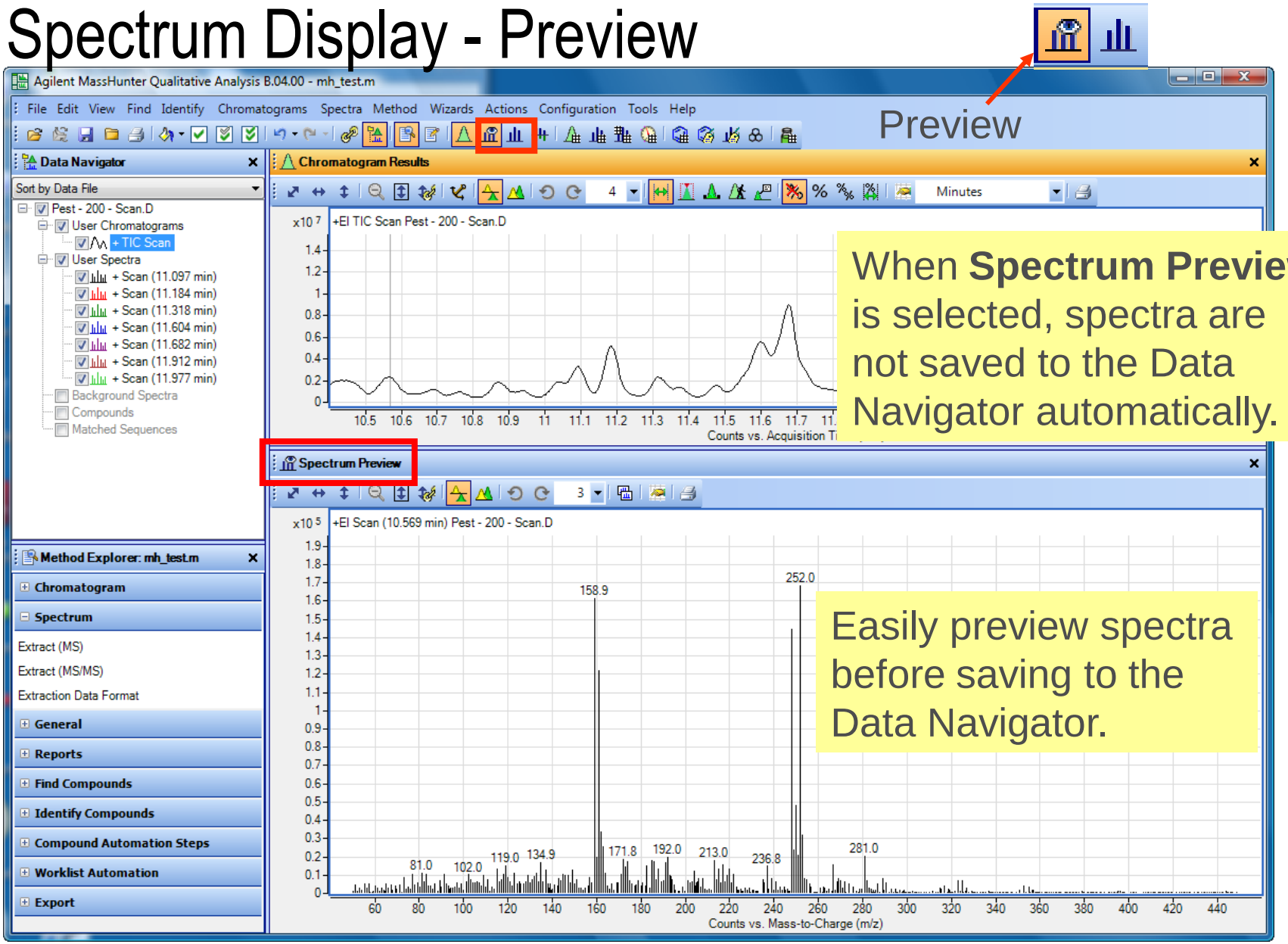
Spectra Display – MS Spectrum Results



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.

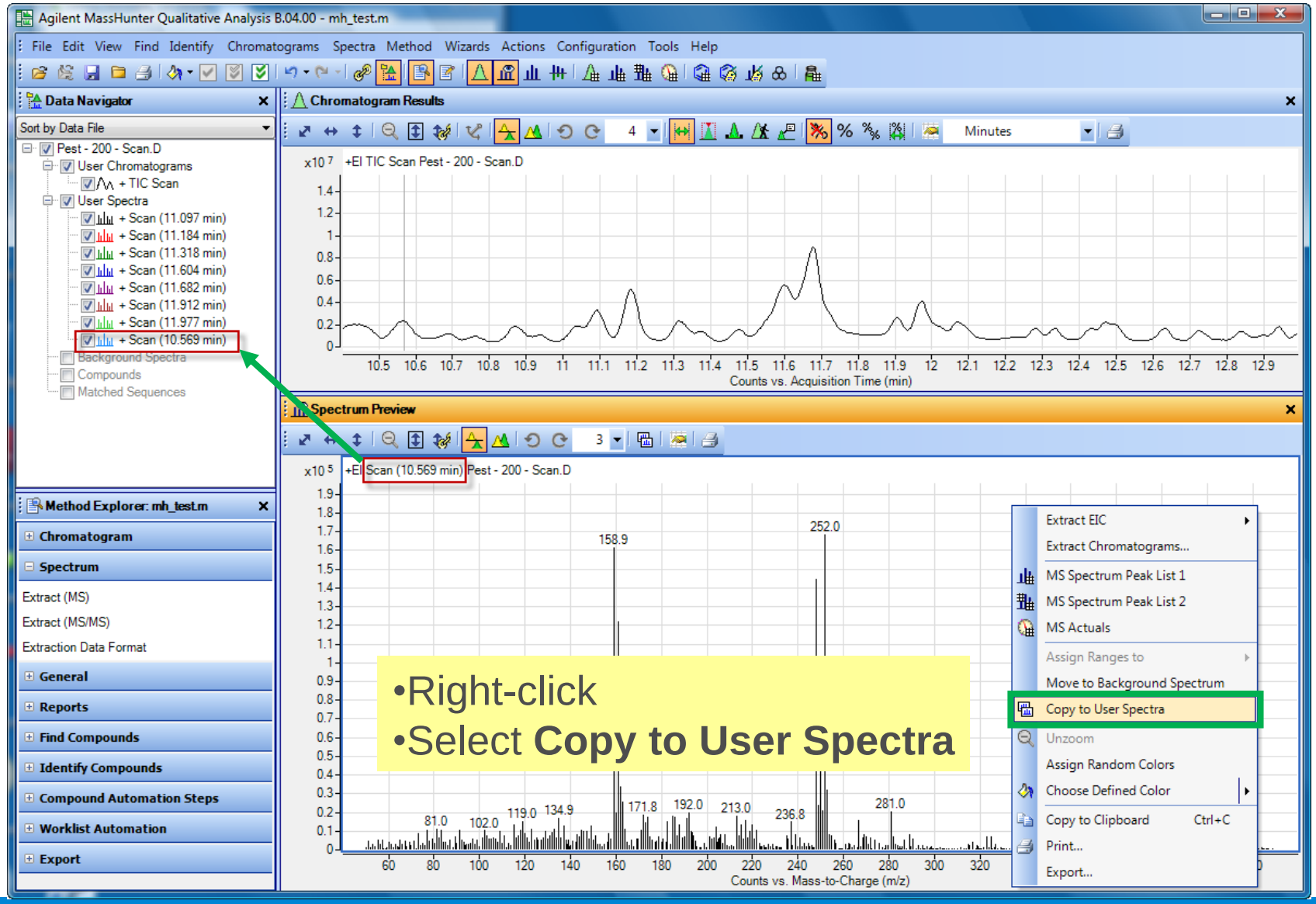
Spectrum Display - Preview



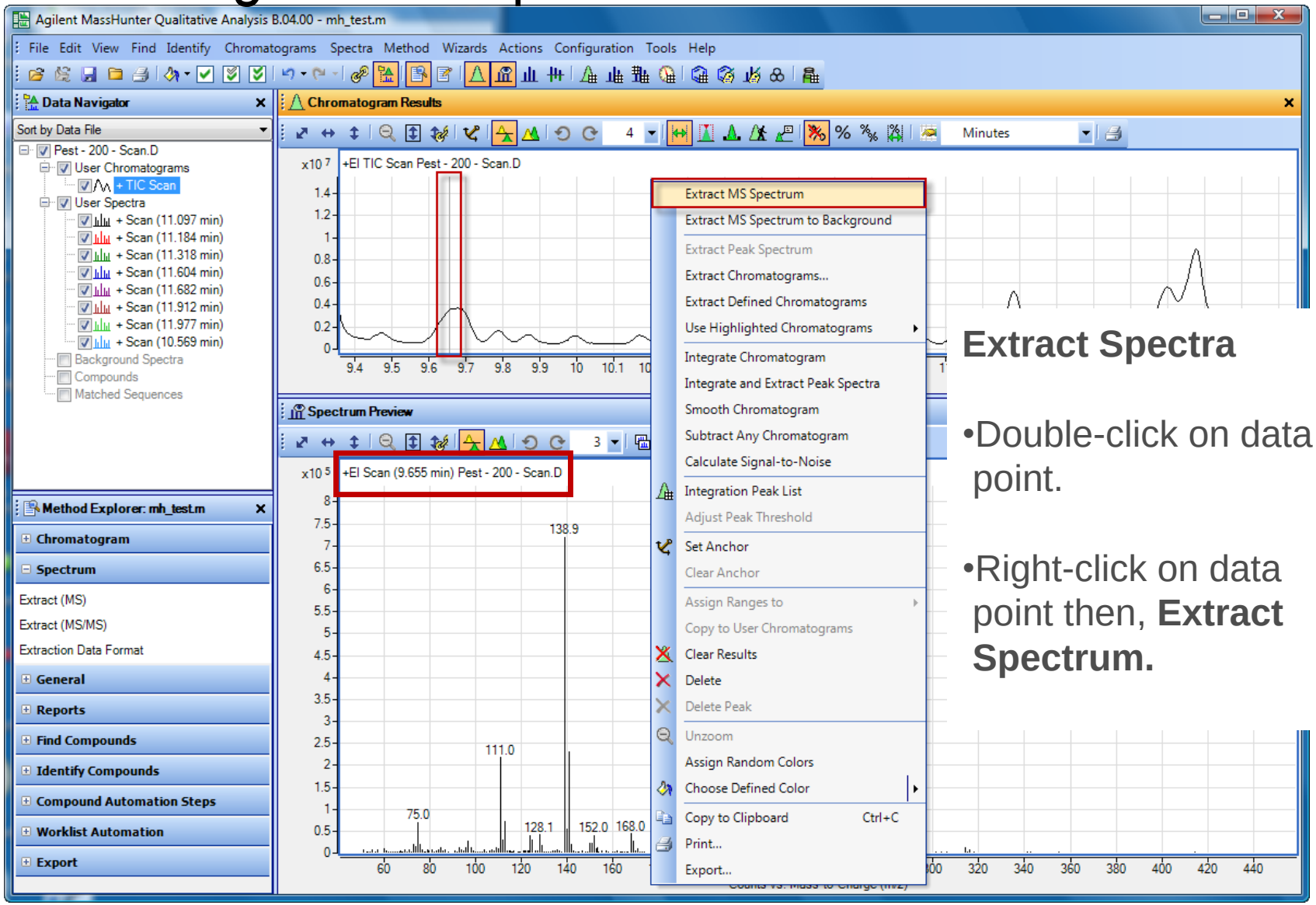
When **Spectrum Preview** is selected, spectra are not saved to the Data Navigator automatically.

Easily preview spectra before saving to the Data Navigator.

Add Preview Spectrum to Results



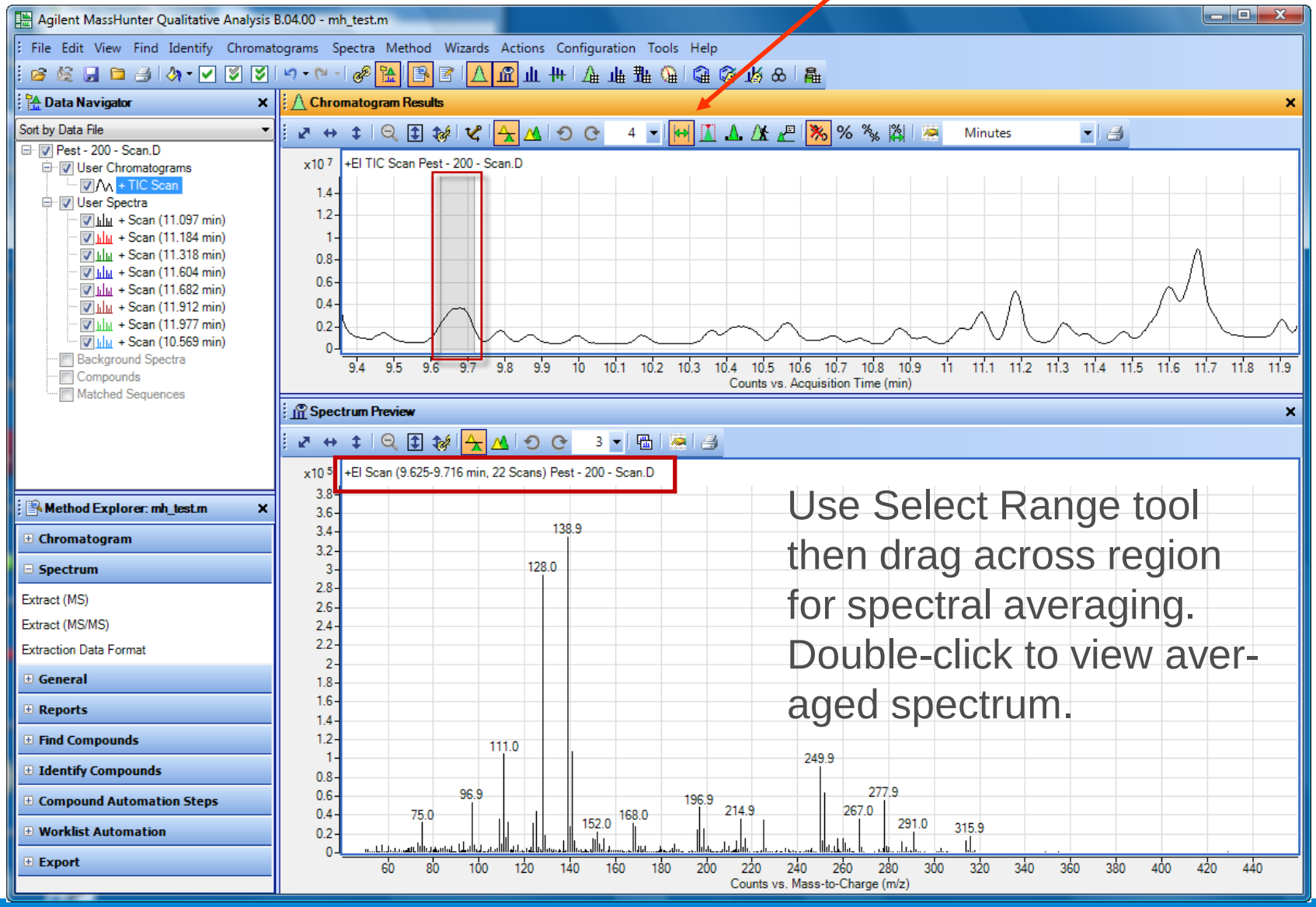
Extract Single Scan Spectrum



Extract Spectra

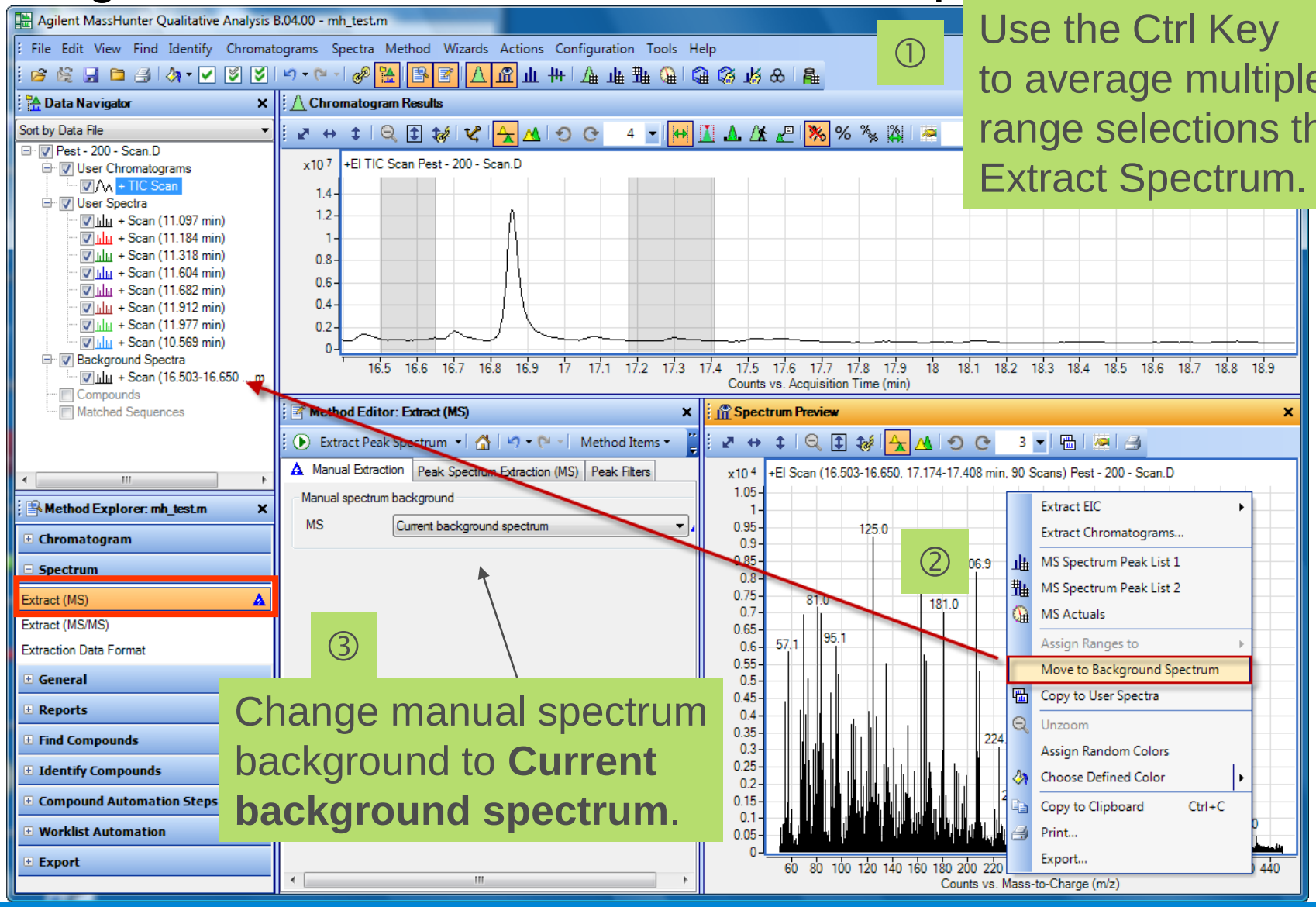
- Double-click on data point.
- Right-click on data point then, **Extract Spectrum.**

Extract Averaged Spectra

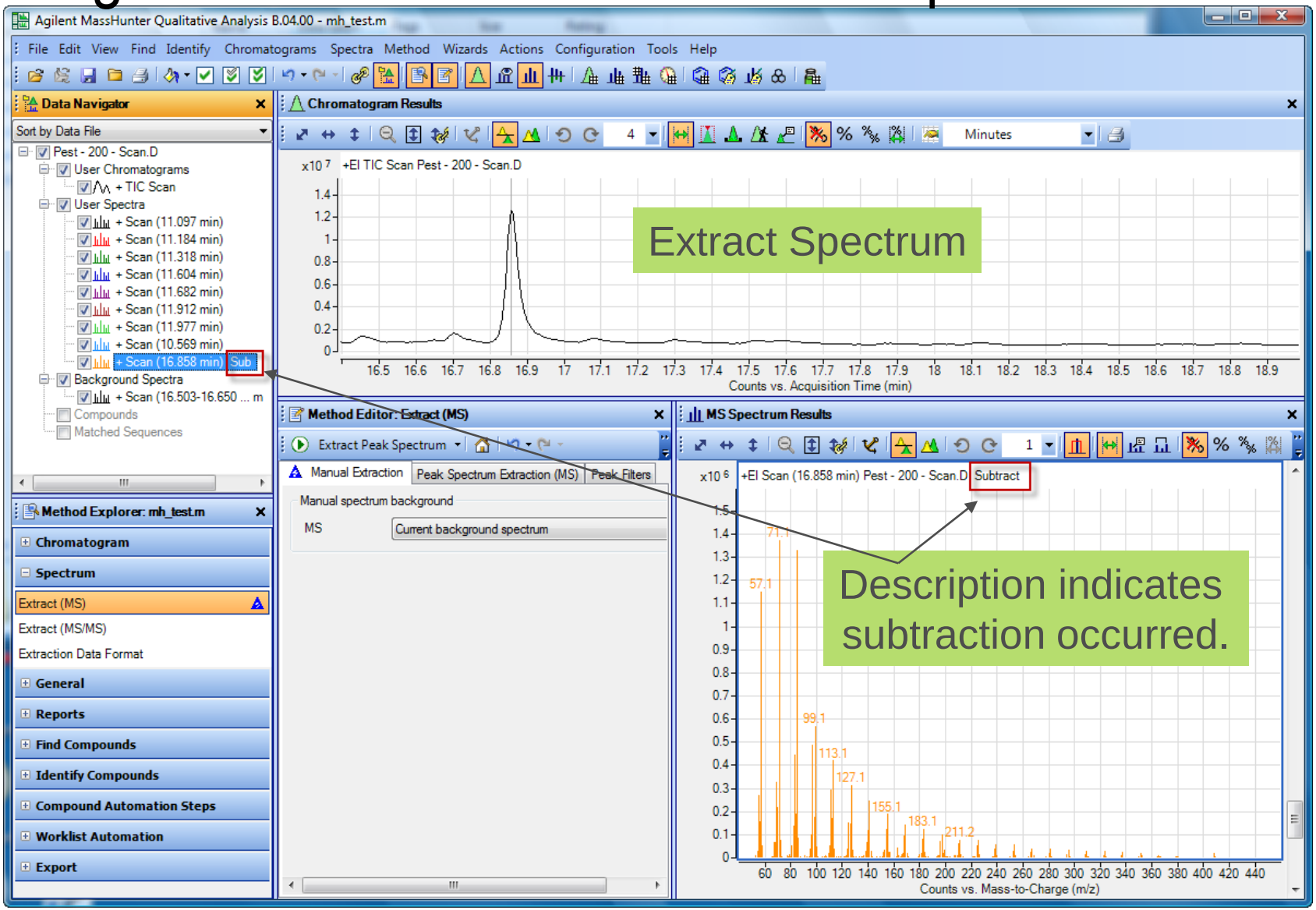


Use Select Range tool then drag across region for spectral averaging. Double-click to view averaged spectrum.

Background Subtraction for Manual Spectra

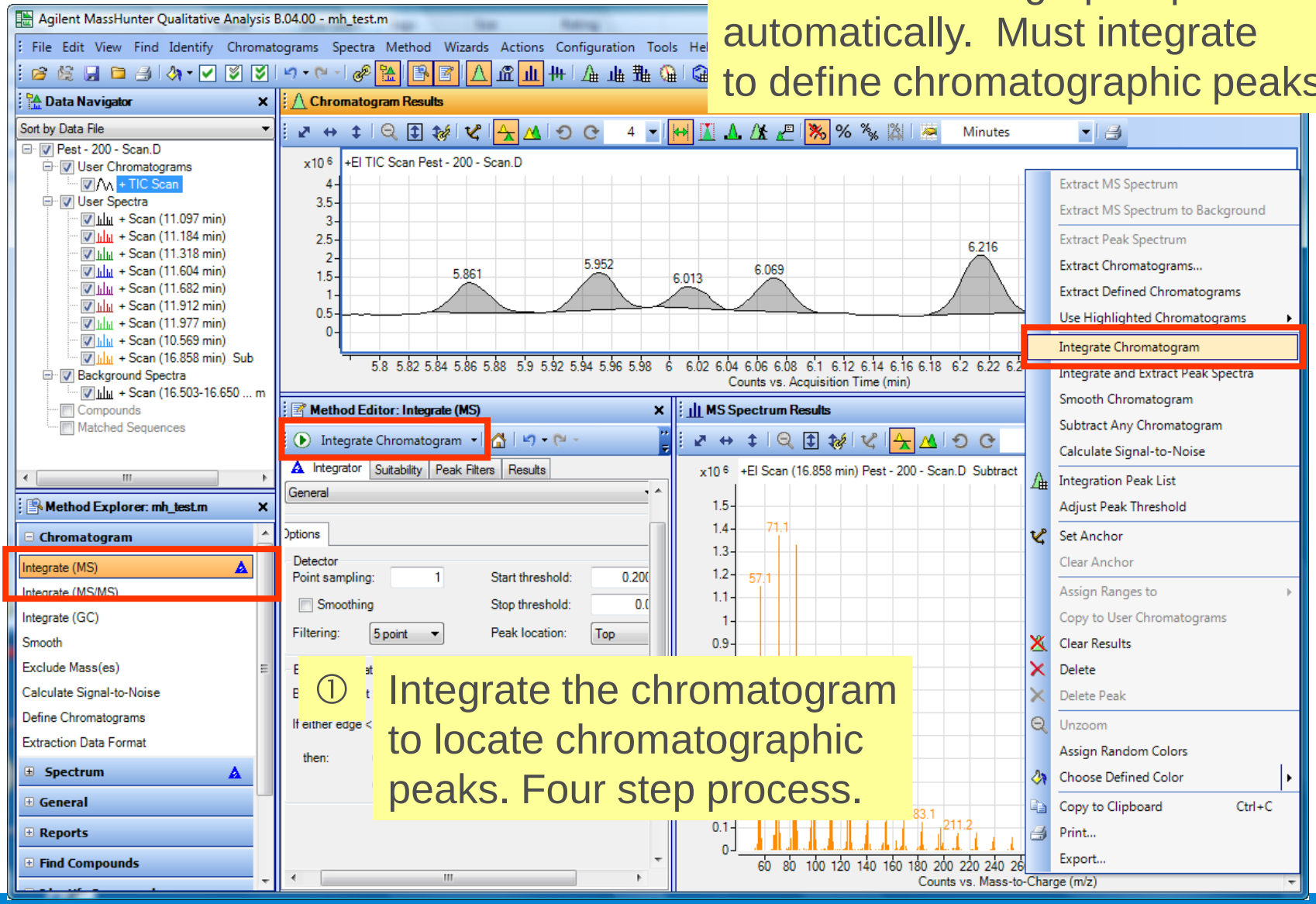


Background Subtraction for Manual Spectra



Extract Peak Spectrum

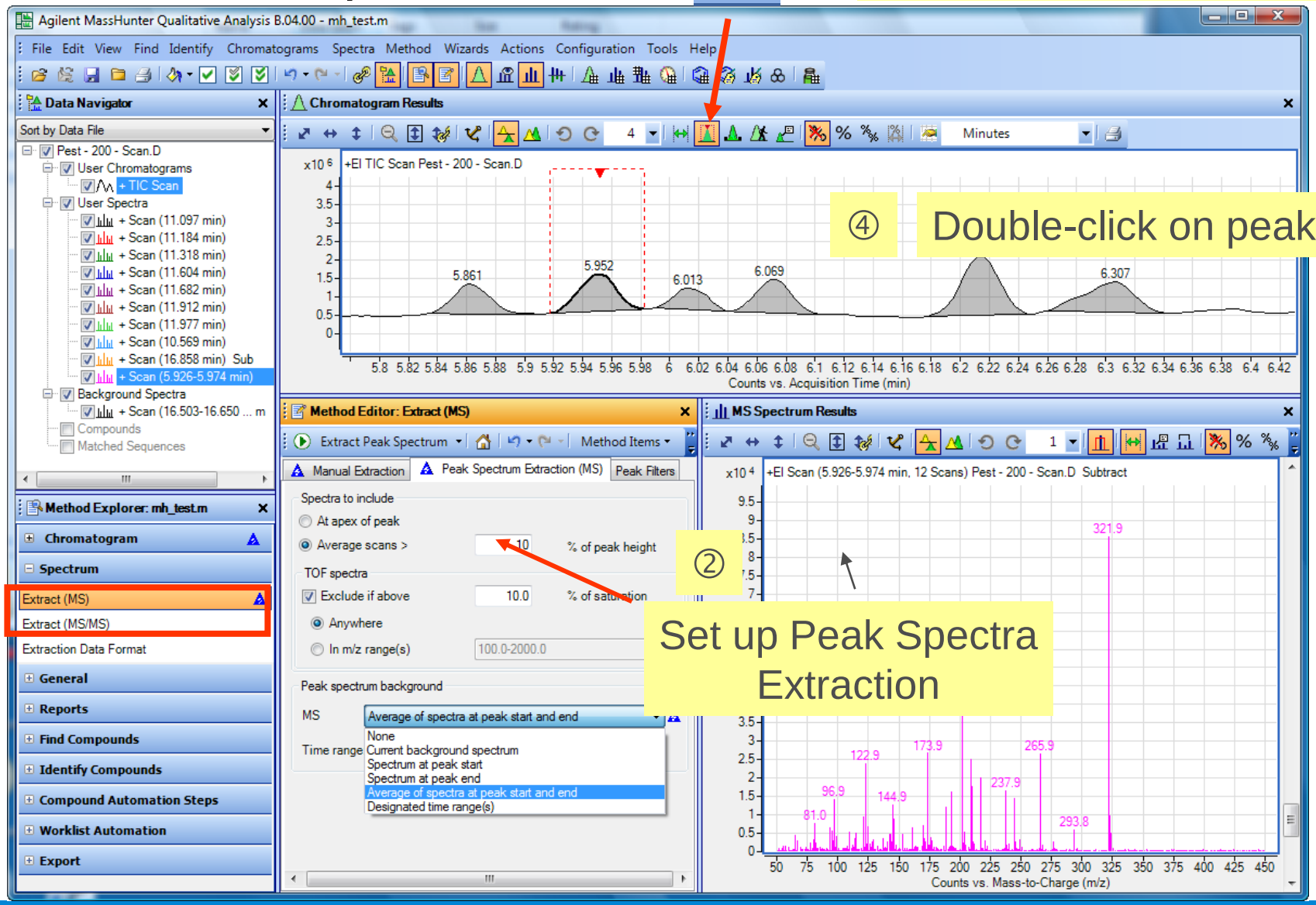
Extract an averaged spectrum from a chromatographic peak automatically. Must integrate to define chromatographic peaks.



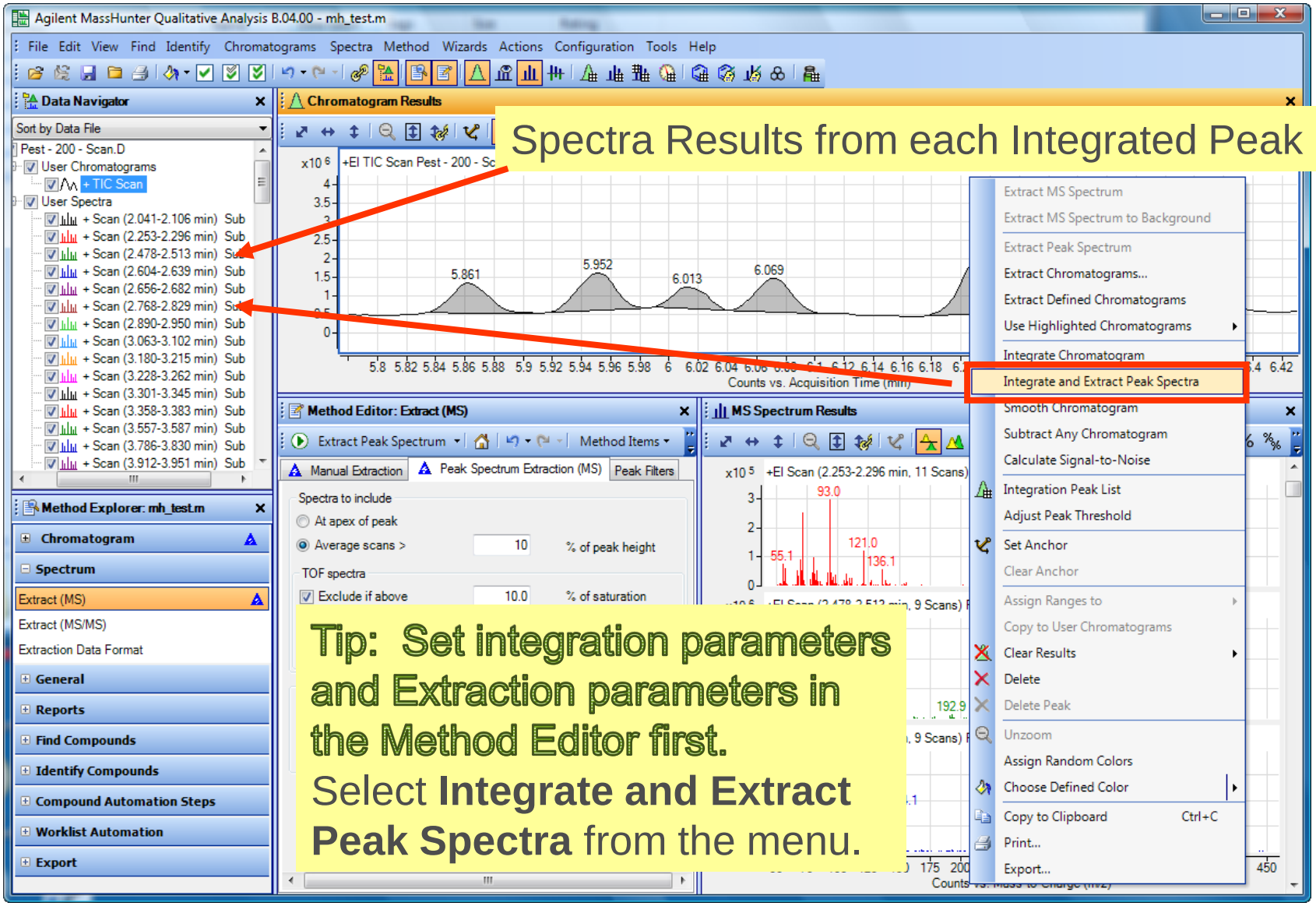
① Integrate the chromatogram to locate chromatographic peaks. Four step process.

Extract Peak Spectrum

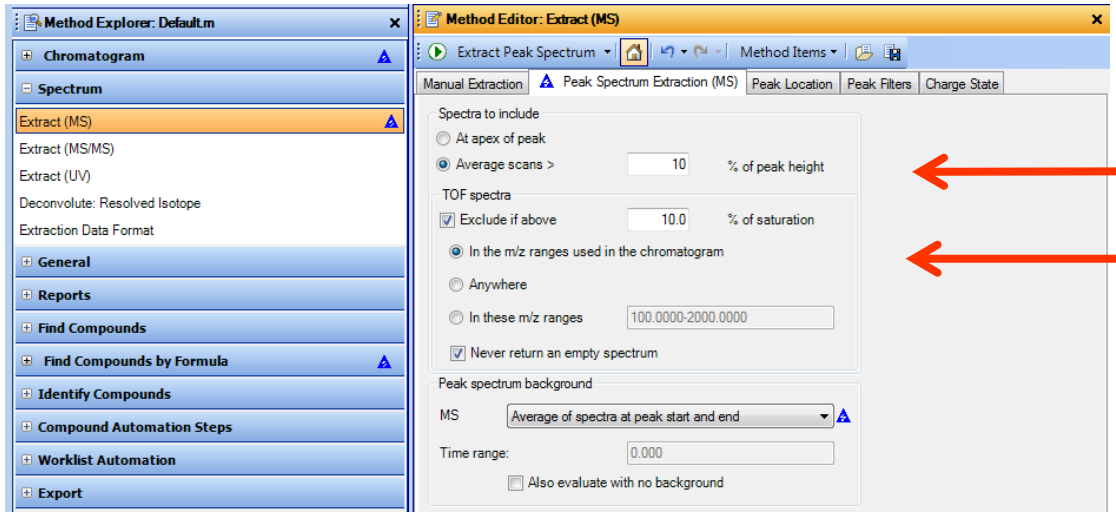
③ Enable Peak Select tool.



Extract Peak Spectra Automatically

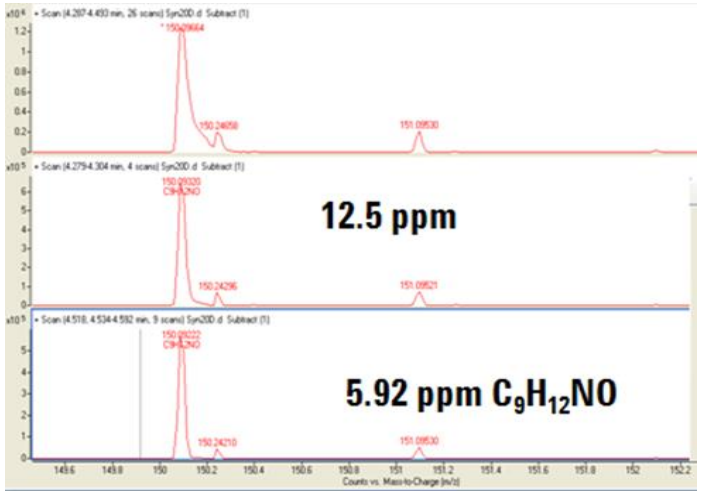


Considerations for Accurate Mass Data Using Extract Peak Parameters – Saturation



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

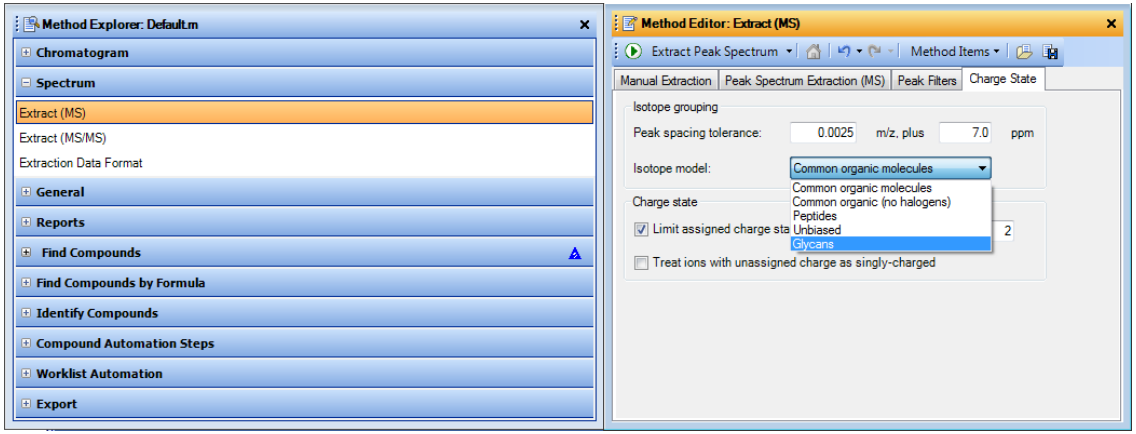
Corresponds to workflow.

Common organic molecules

Peptides

Unbiased

Glycans

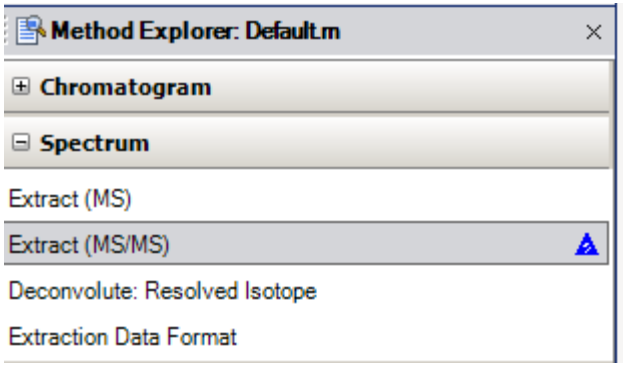


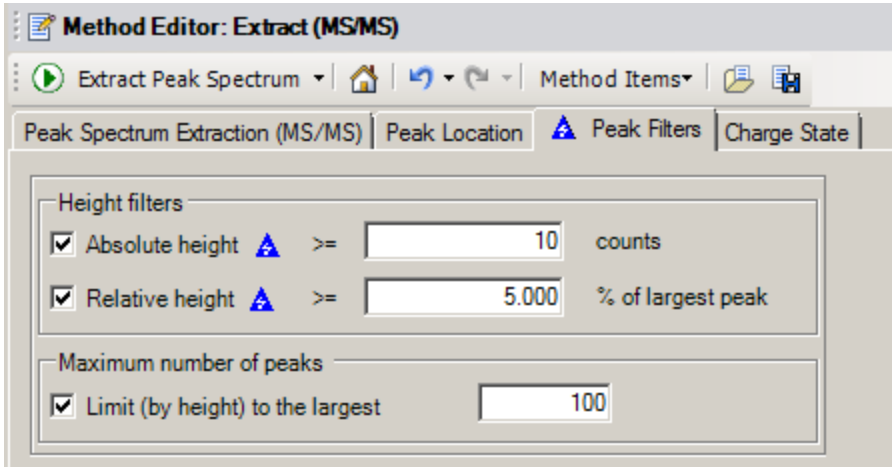
Tip: Check Limit Assigned Charge States Maximum Values.

For Small Molecule Applications: Set to 2

For High Molecular Weight Apps: Uncheck or Max 10

Extract Spectra – Peak Filters

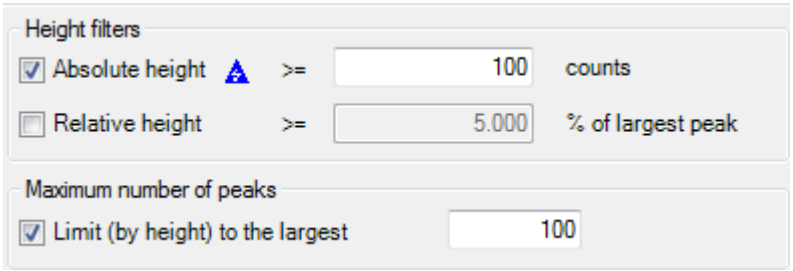


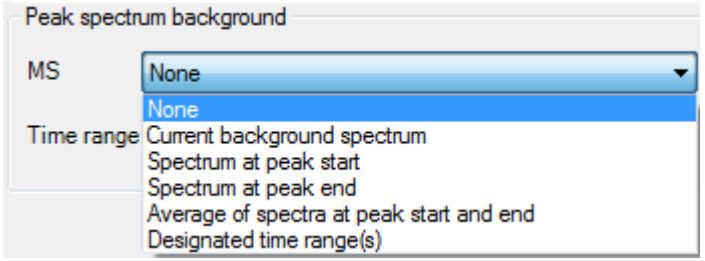


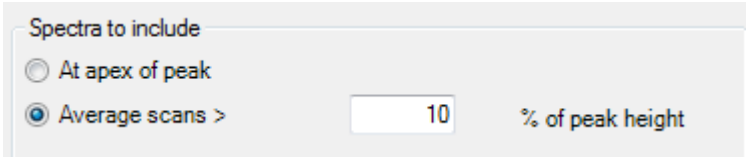
Tip: Always remember to set Peak Filter Limits to reduce noise. Important when library searching.

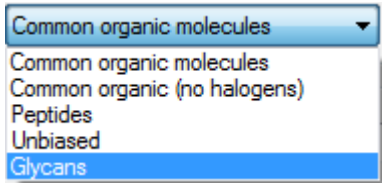
Context Sensitive Help

?



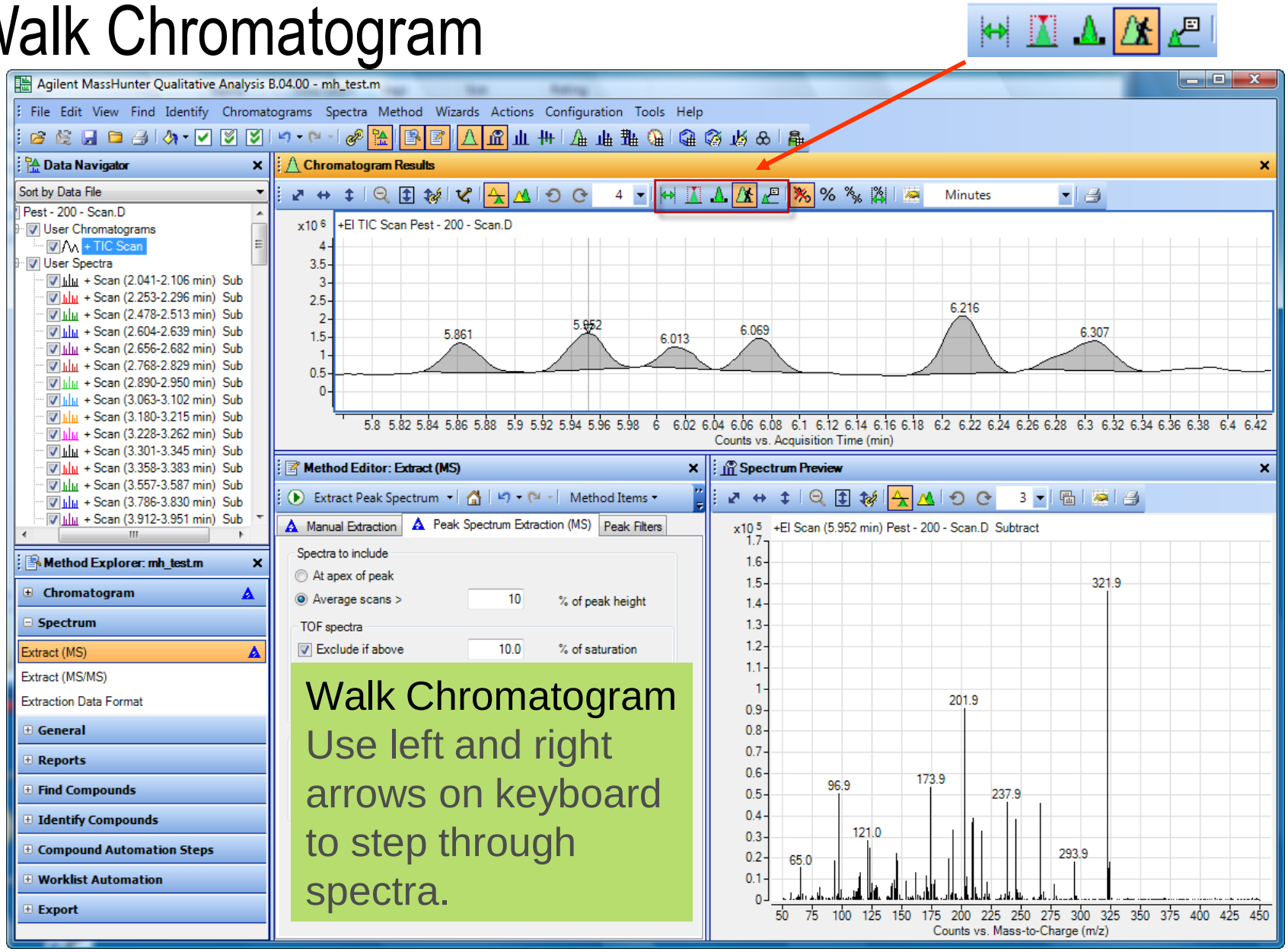




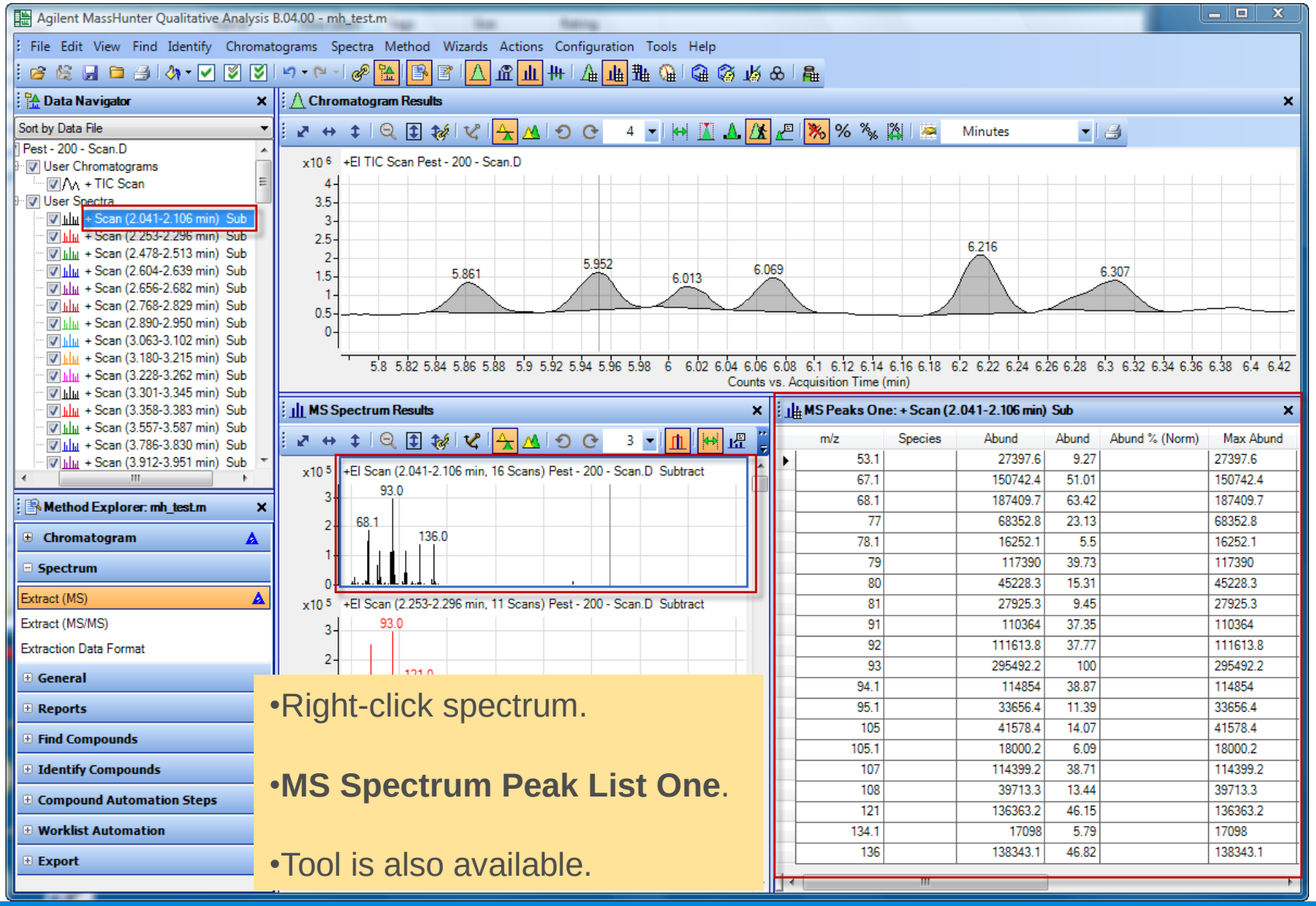


Tip: Context Sensitive Help is available through the F1 Key.

Walk Chromatogram

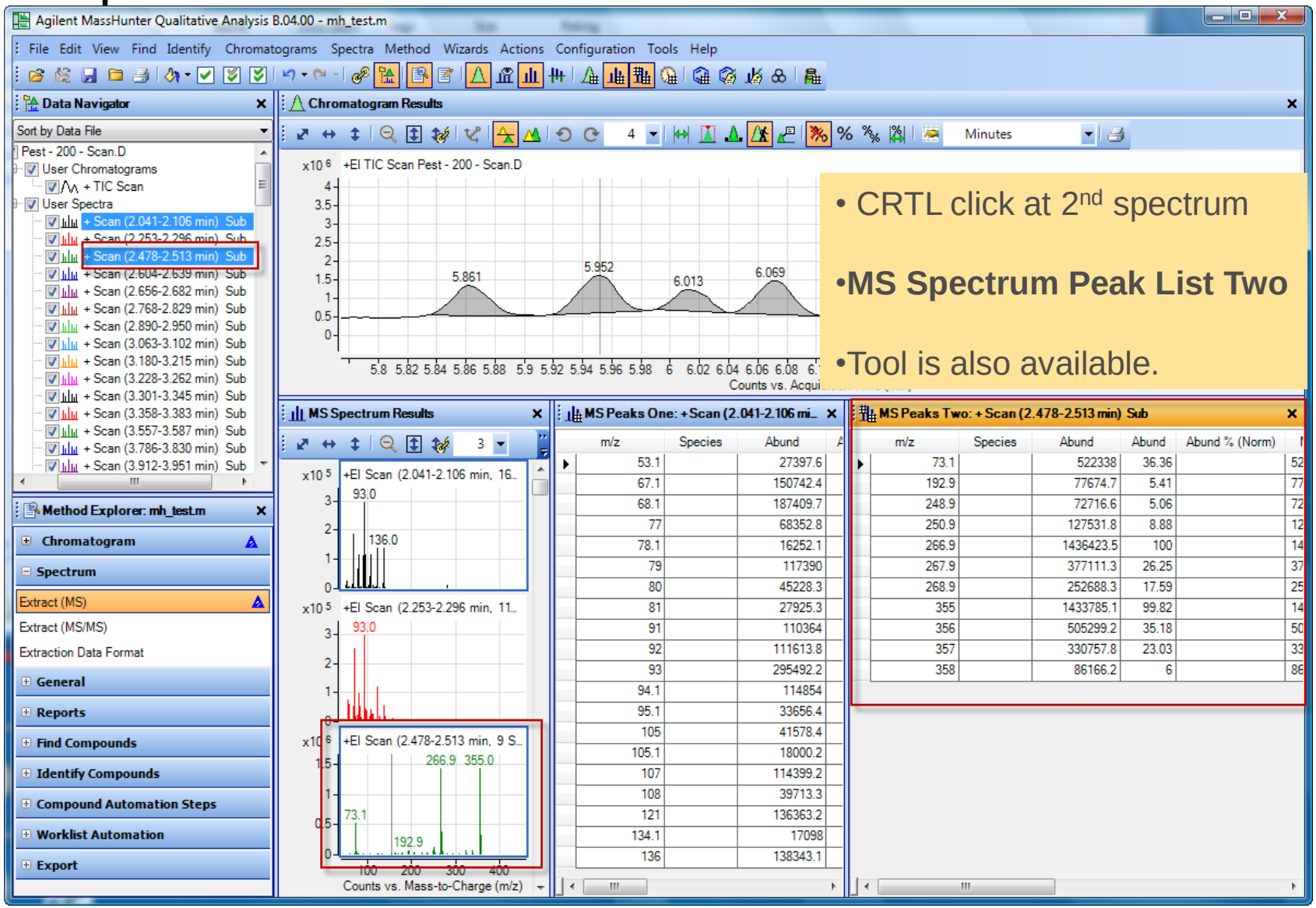


MS Spectrum Peak List One



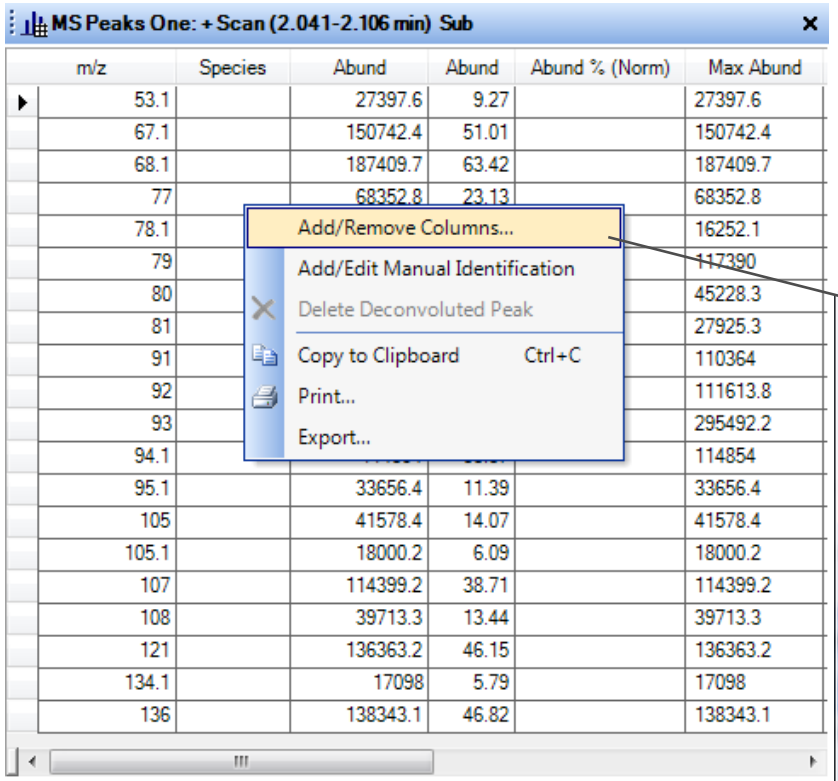
- Right-click spectrum.
- **MS Spectrum Peak List One**.
- Tool is also available.

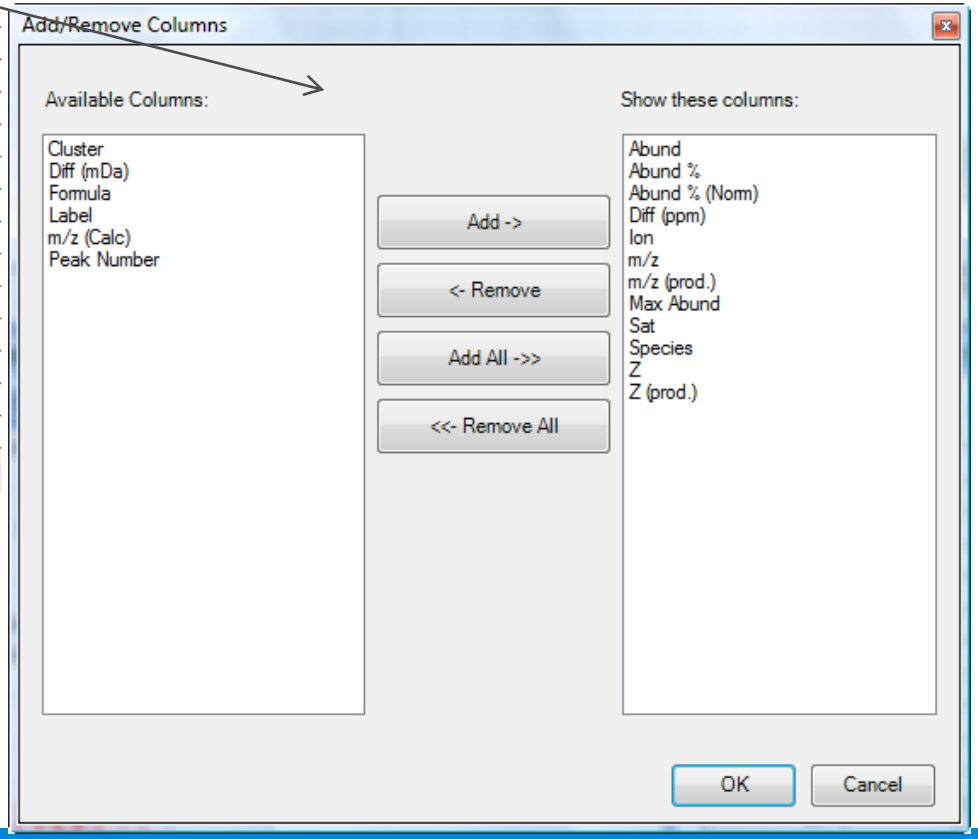
MS Spectrum Peak List Two



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

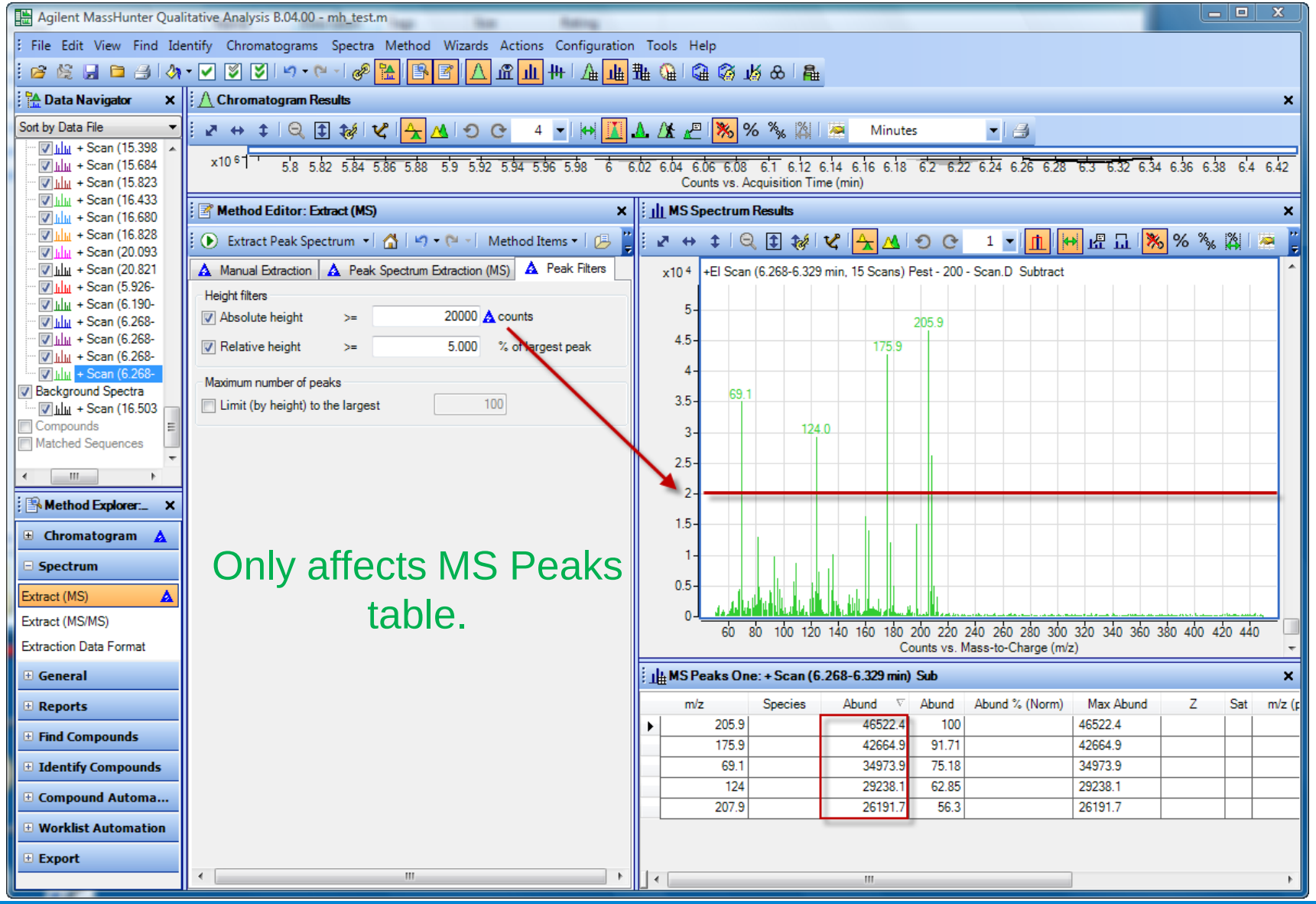
MS Spectrum Peak List





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

MS Spectrum Peak Filter

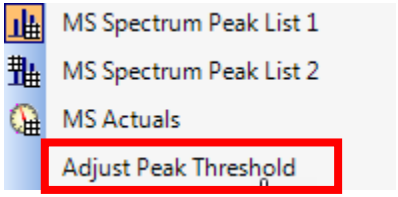


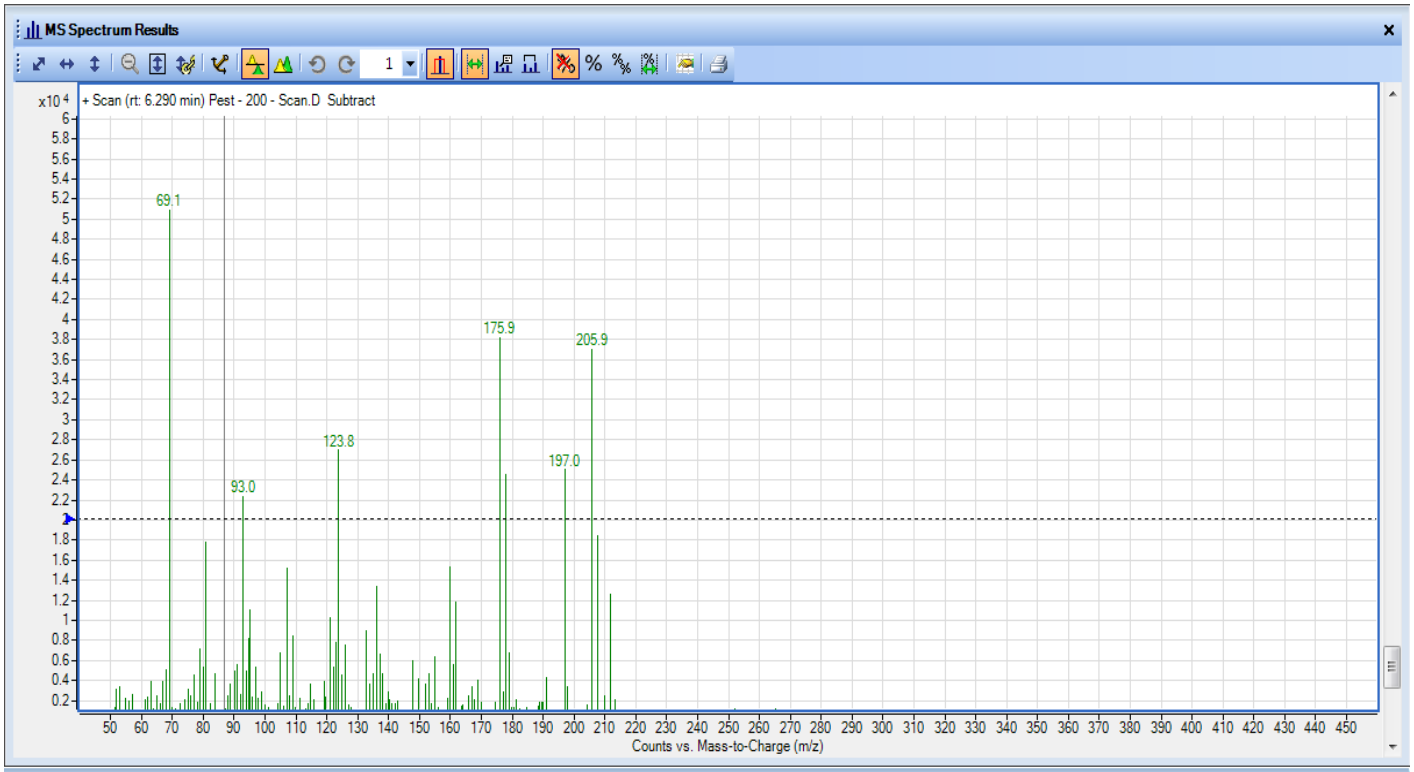
m/z	Species	Abund	Abund	Abund % (Norm)	Max Abund	Z	Sat	m/z (p
205.9		46522.4	100		46522.4			
175.9		42664.9	91.71		42664.9			
69.1		34973.9	75.18		34973.9			
124		29238.1	62.85		29238.1			
207.9		26191.7	56.3		26191.7			

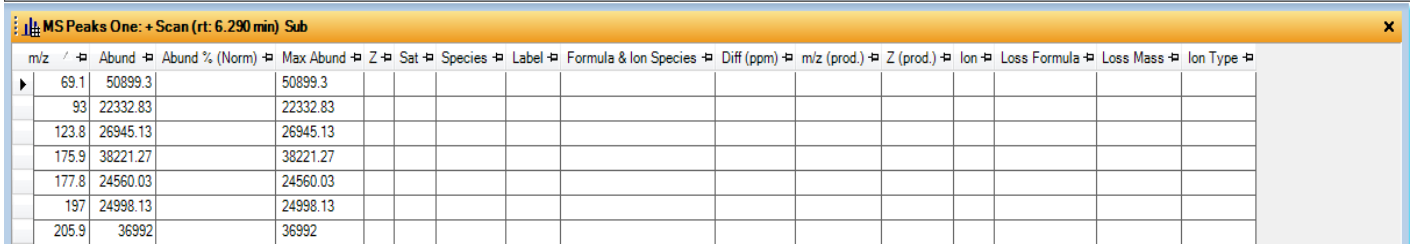
MS Spectrum Peak Filter Interactive Setup

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

- **Tip: Scale Spectra must be off.**







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**.

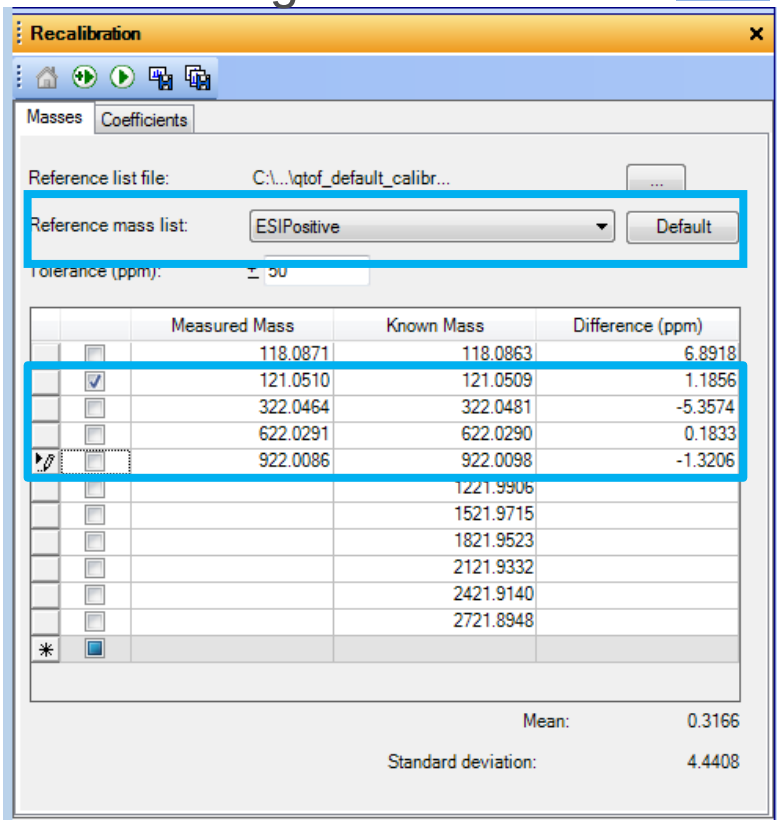
Calculates and applies new calibration to highlighted spectra.

Select to apply current recalibration to highlighted spectra.

Saves new calibration to highlighted spectra.

Save new calibration to whole datafile.

Restores original calibration.

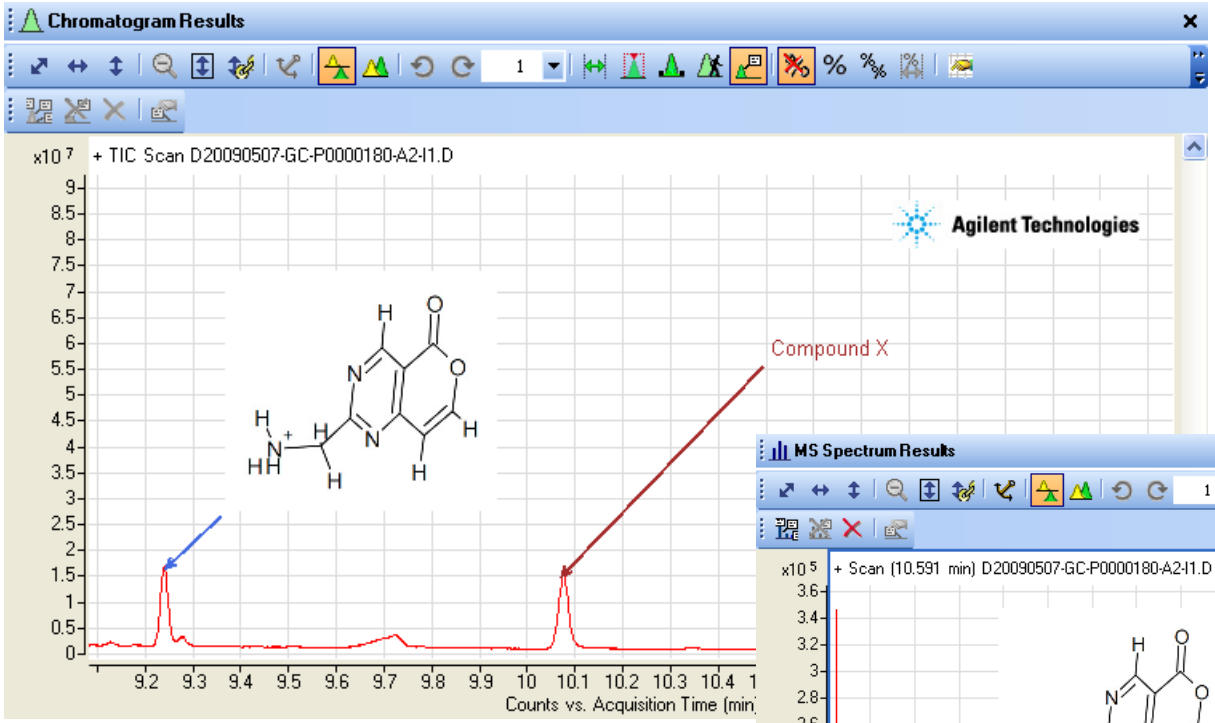


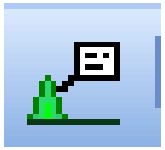
Let’s take a moment for questions on Working with Mass Spectra

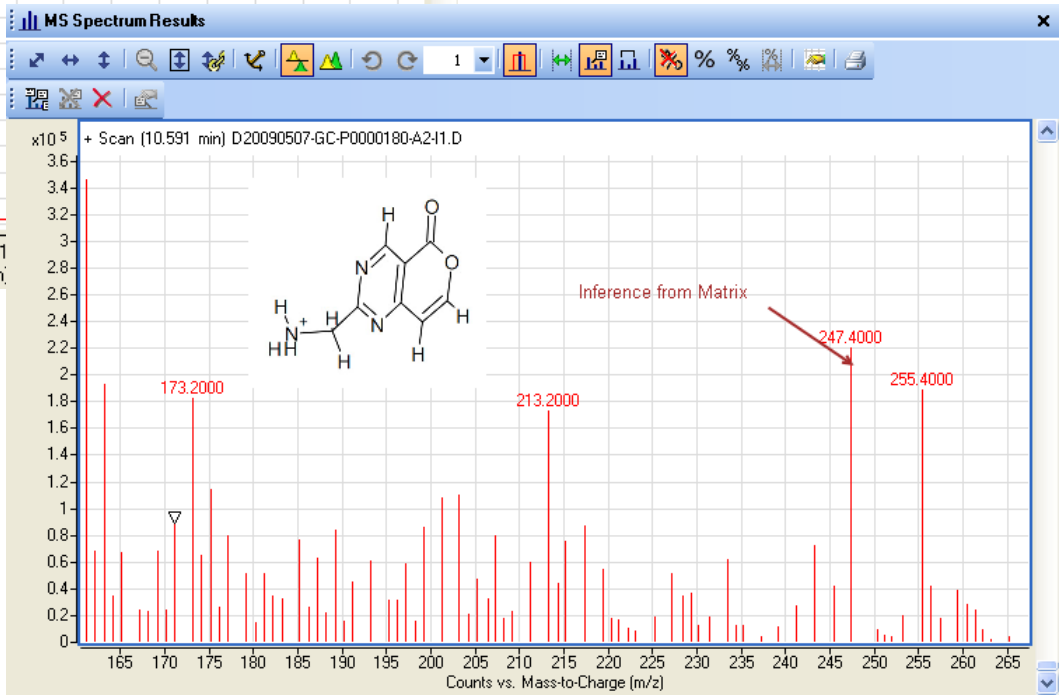
Up Next:

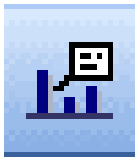
Annotations

Annotation of Chromatograms and Spectra



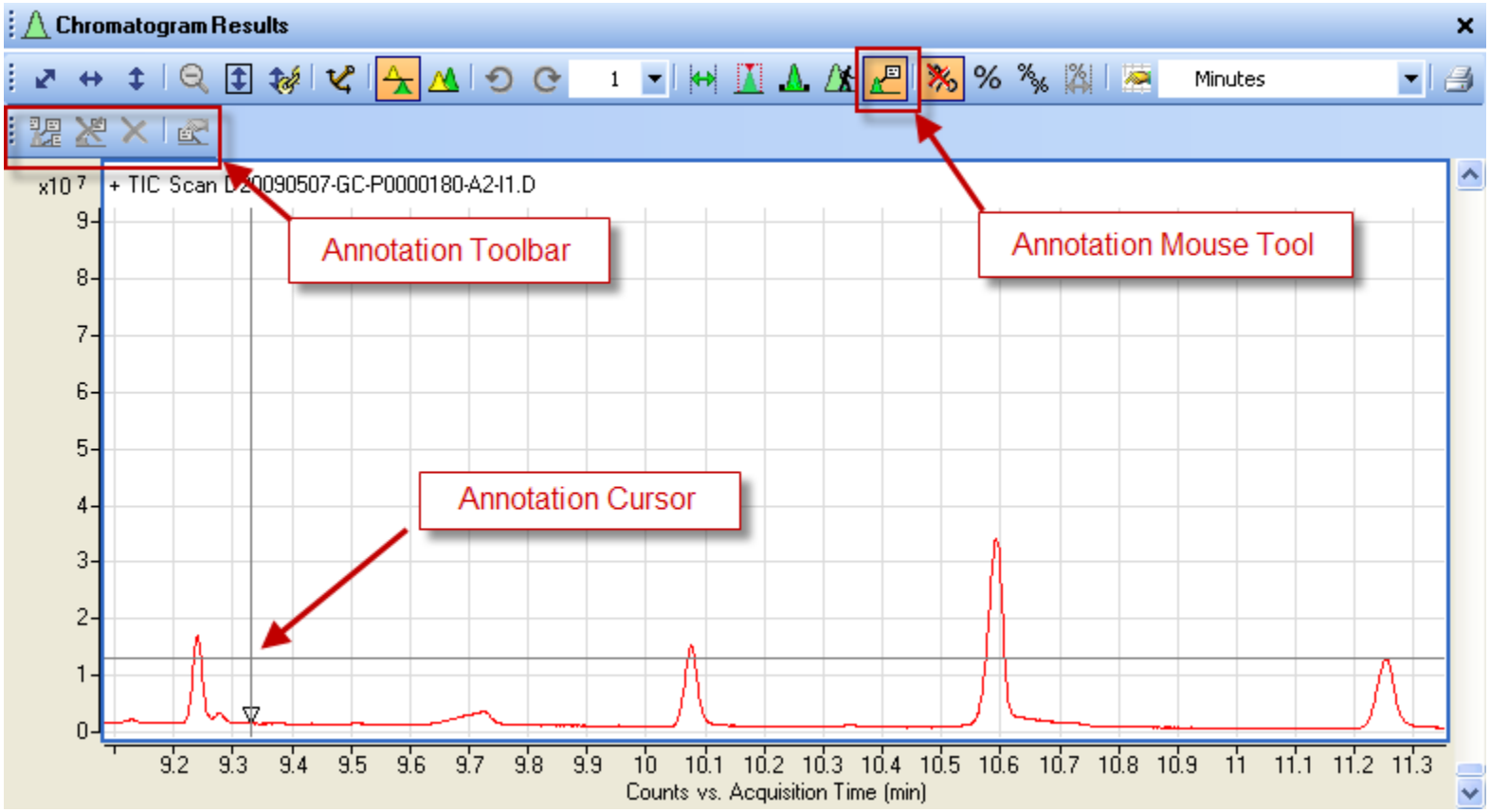




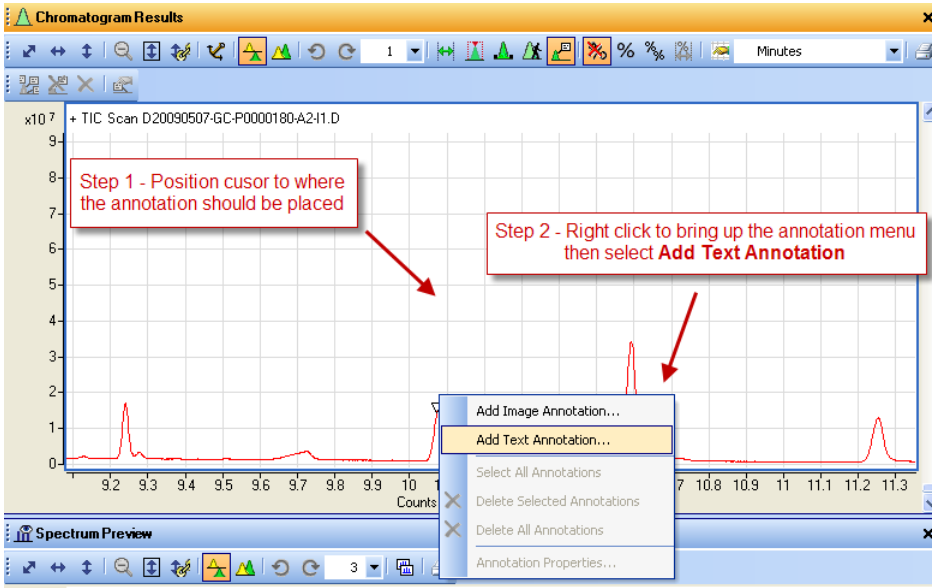


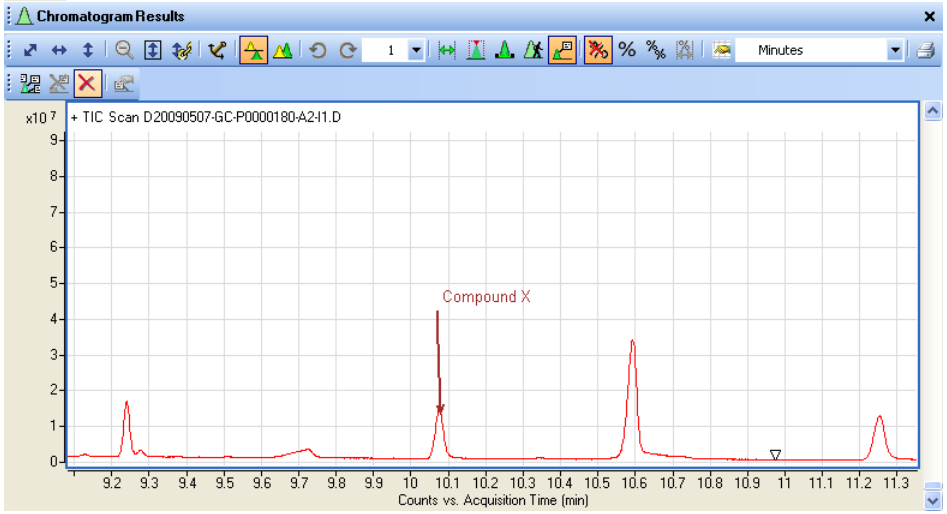
Place Graphic into Annotation Mode

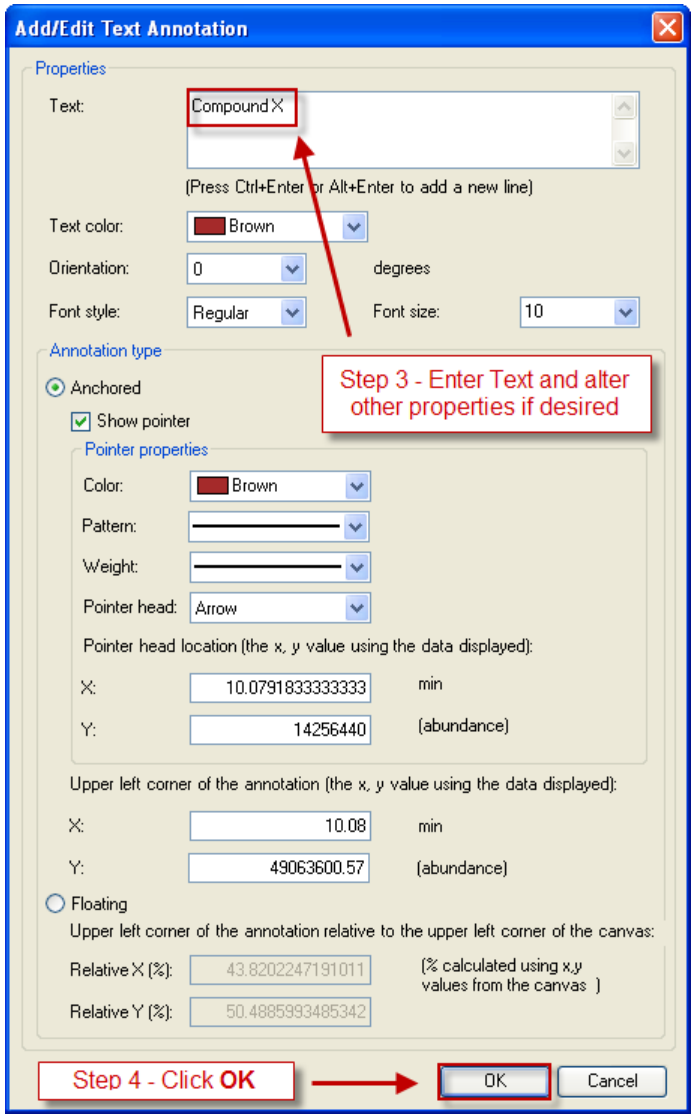
- Click Annotation Mouse Tool
- Annotation Toolbar and Annotation cursor appear



Add a Text Annotation







Text and Pointer Can Be Repositioned

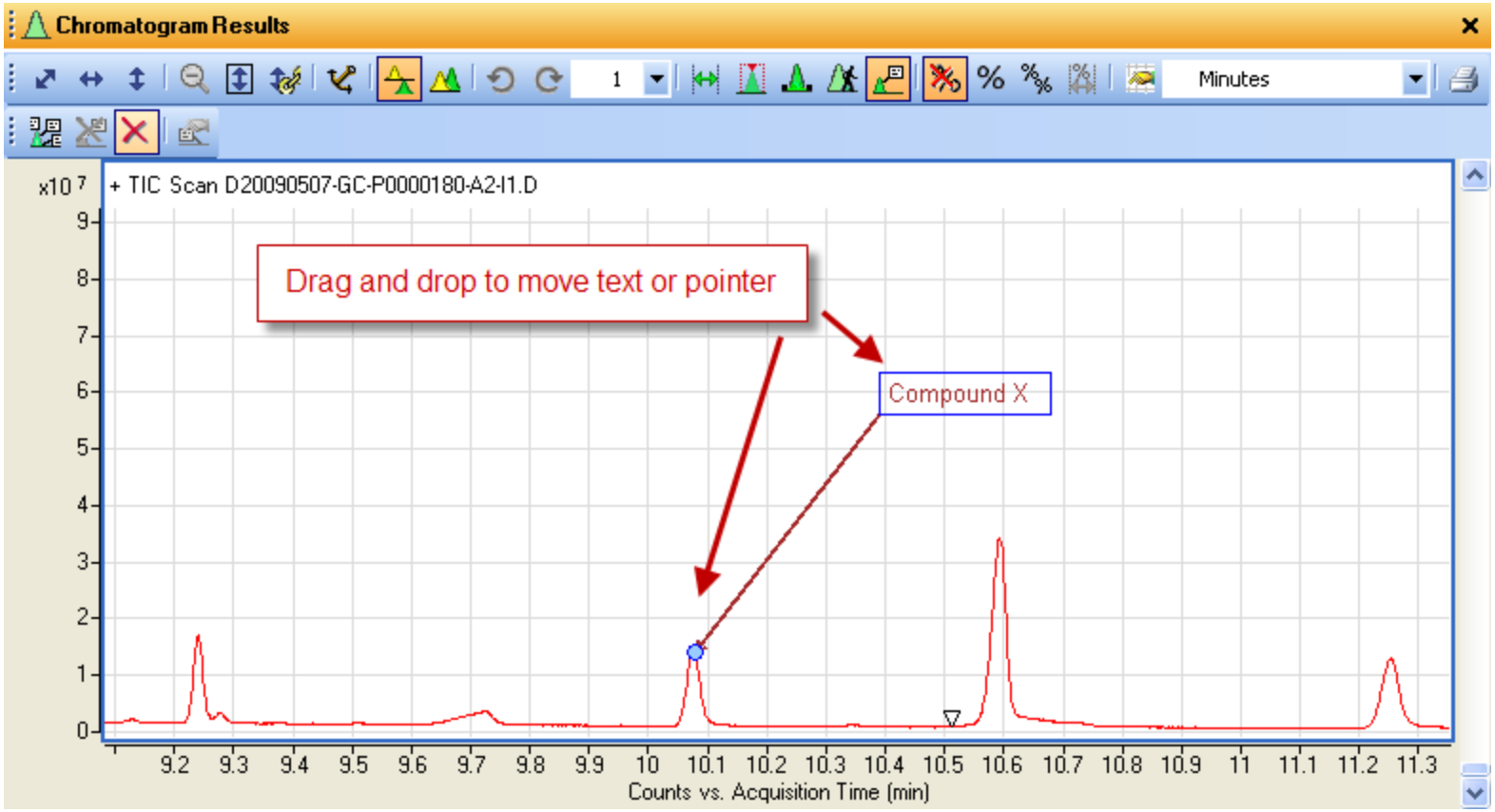
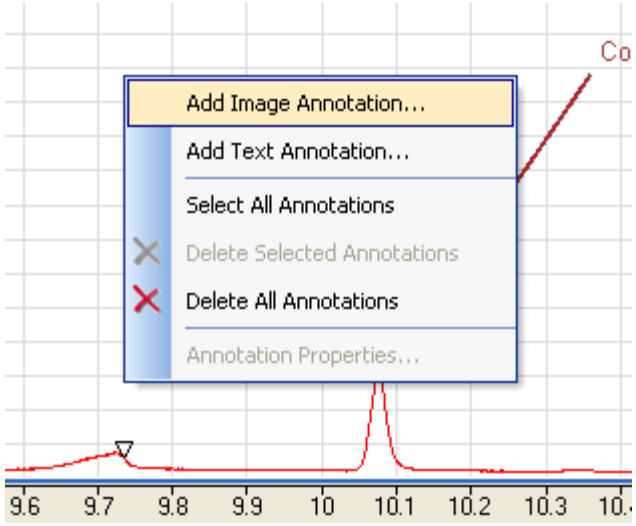
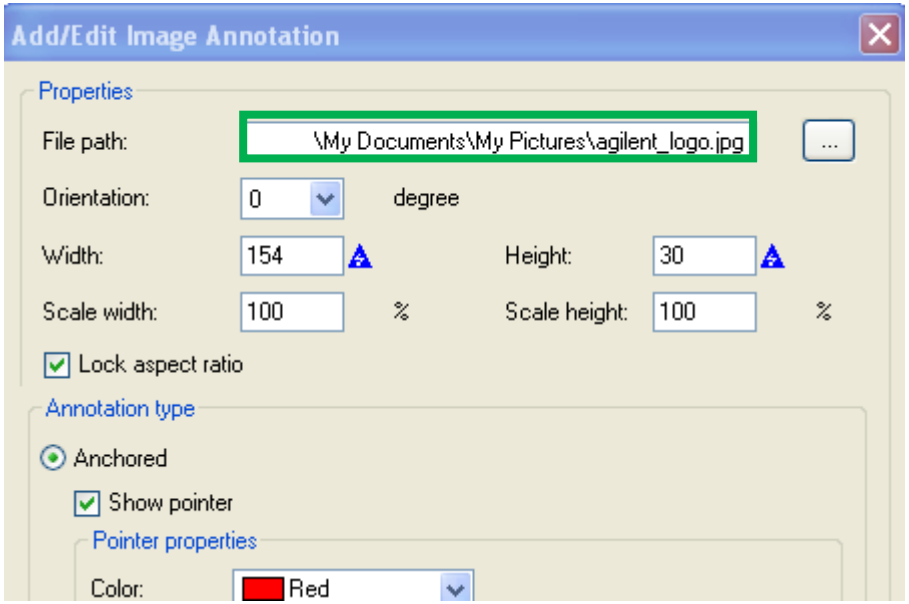


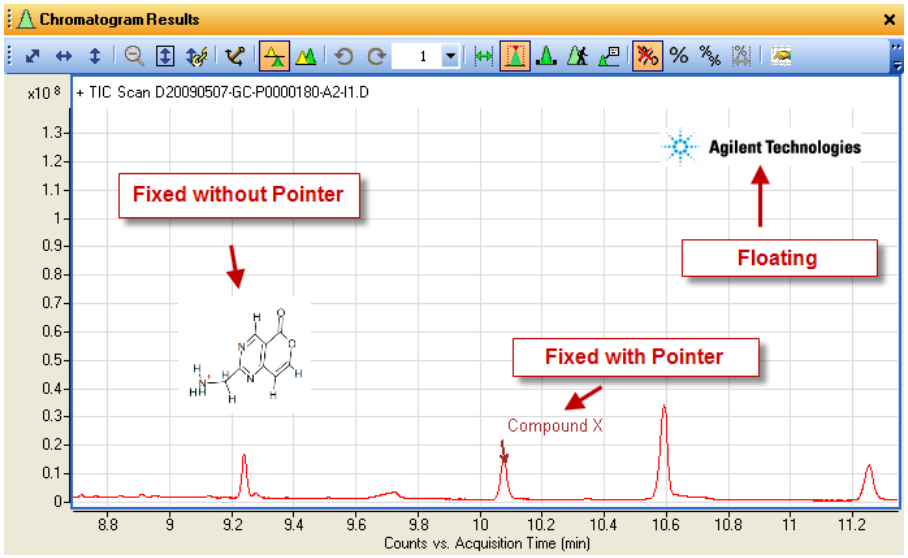
Image Annotation

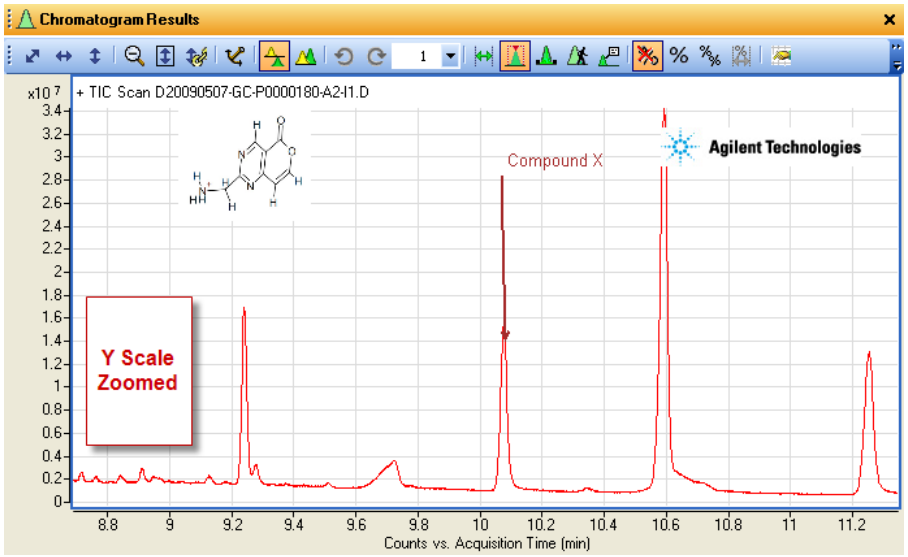
- Same steps as adding Text
- JPEG and MOL (molecular structure) files are supported
- Image may be scaled and pivoted

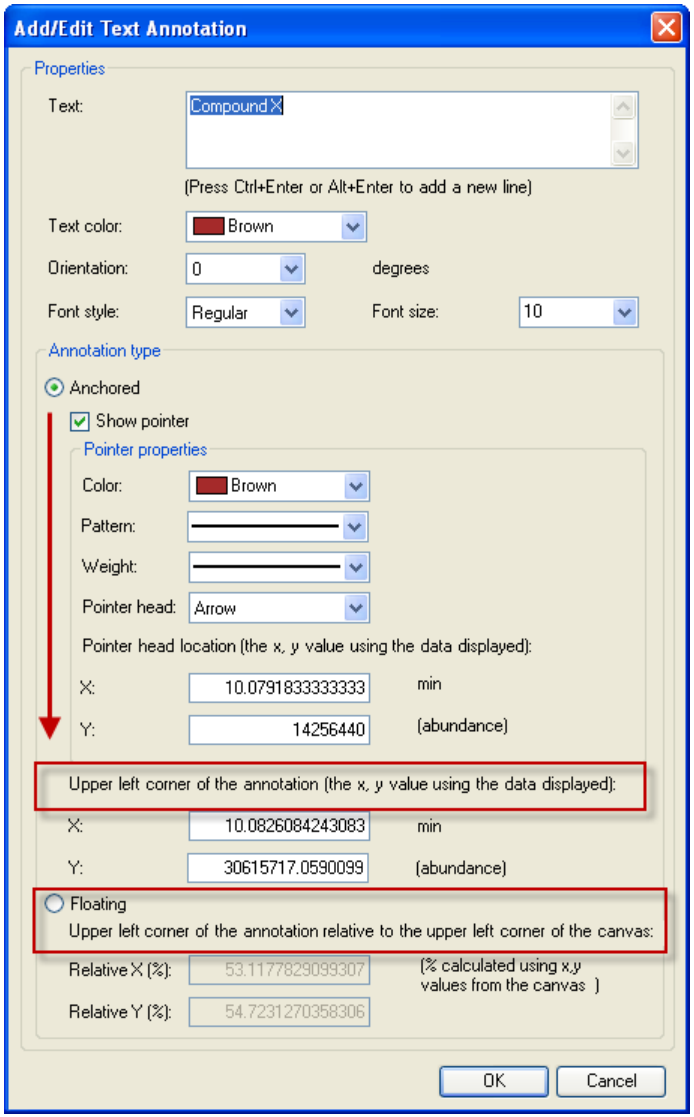




Anchored vs. Floating Annotation

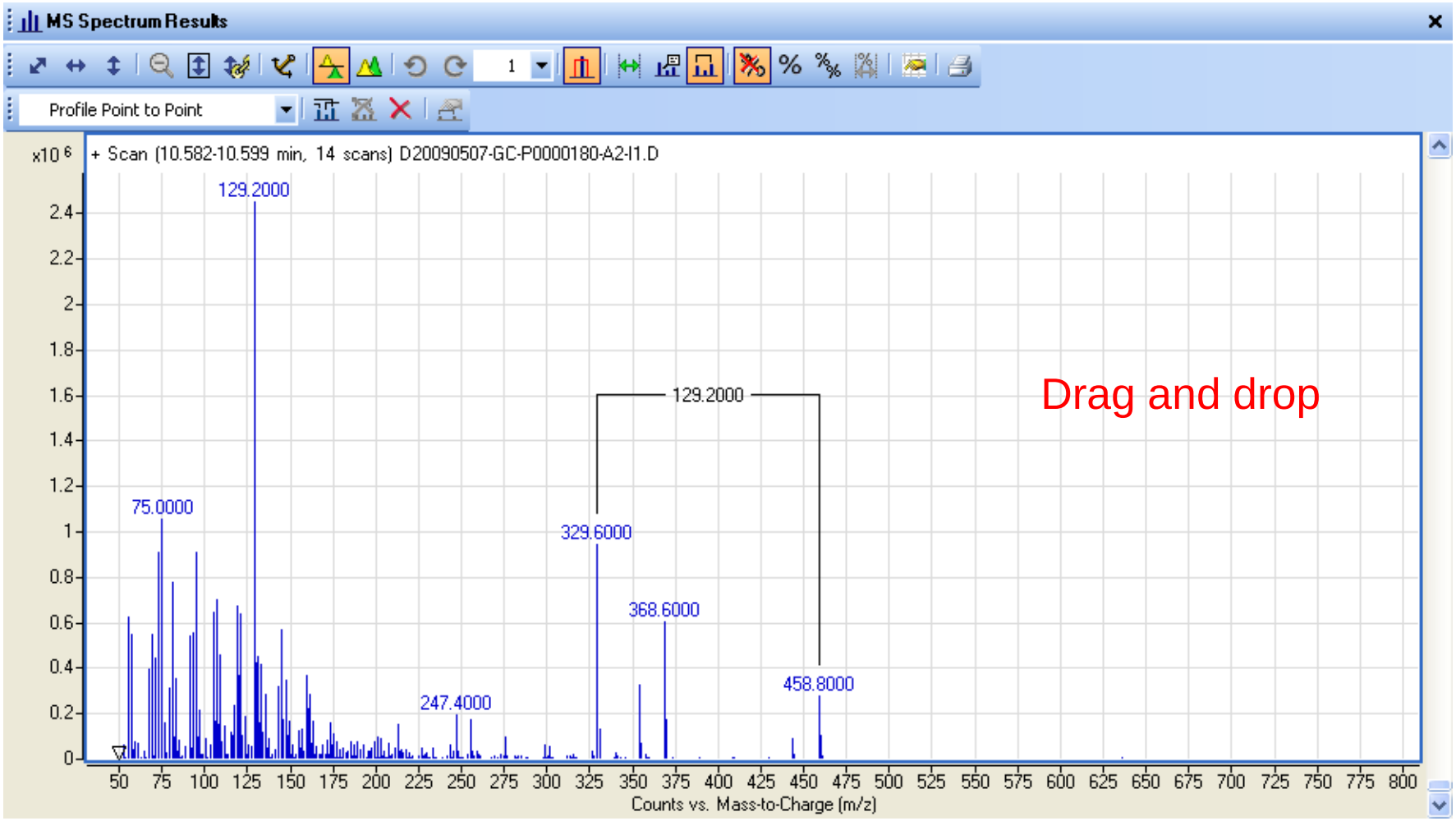






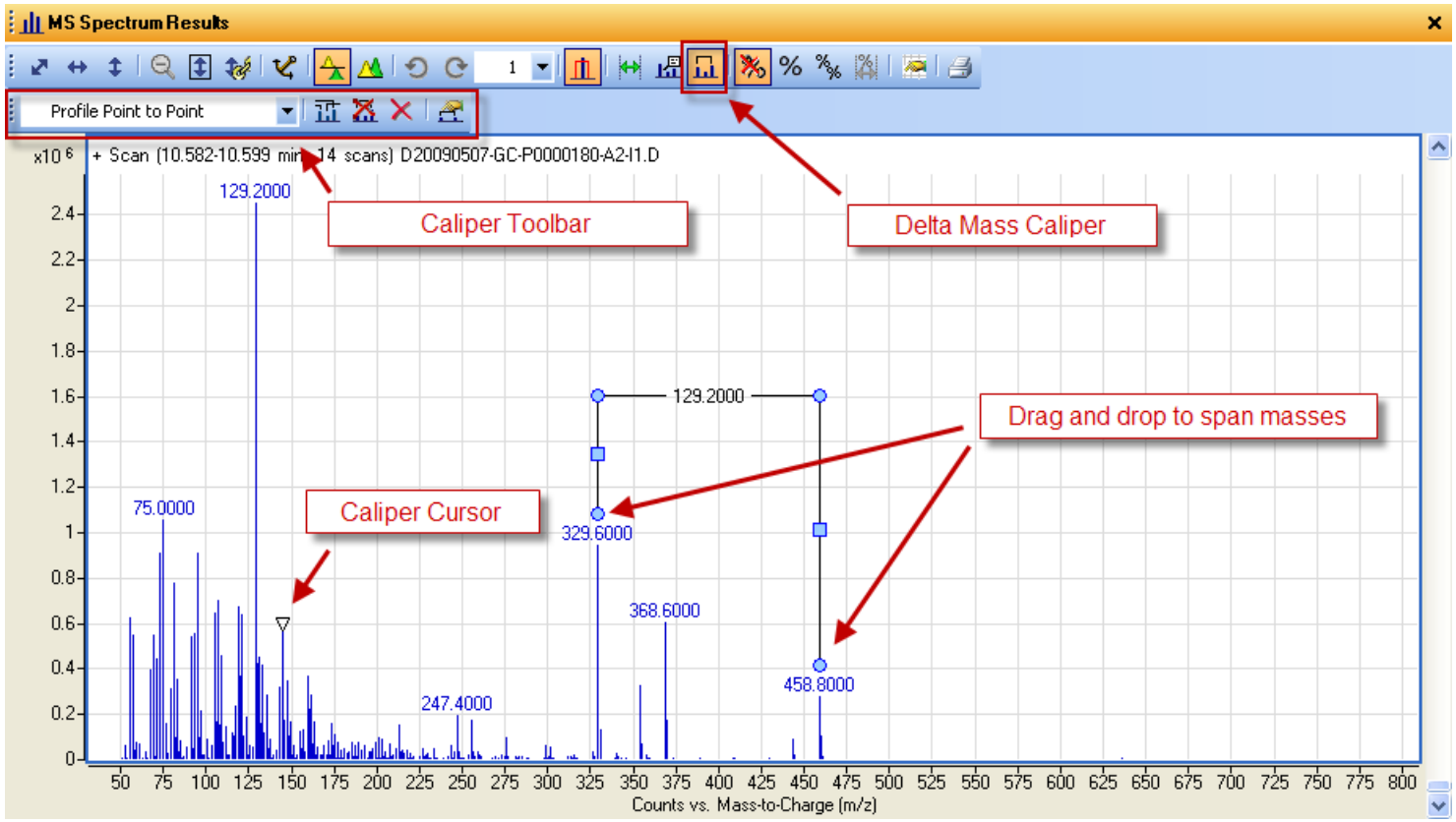
Delta Mass Caliper

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



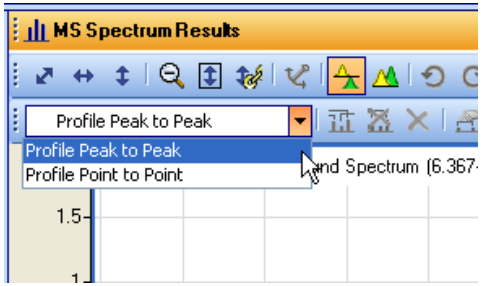
Delta Mass Caliper - Mass Caliper Mode

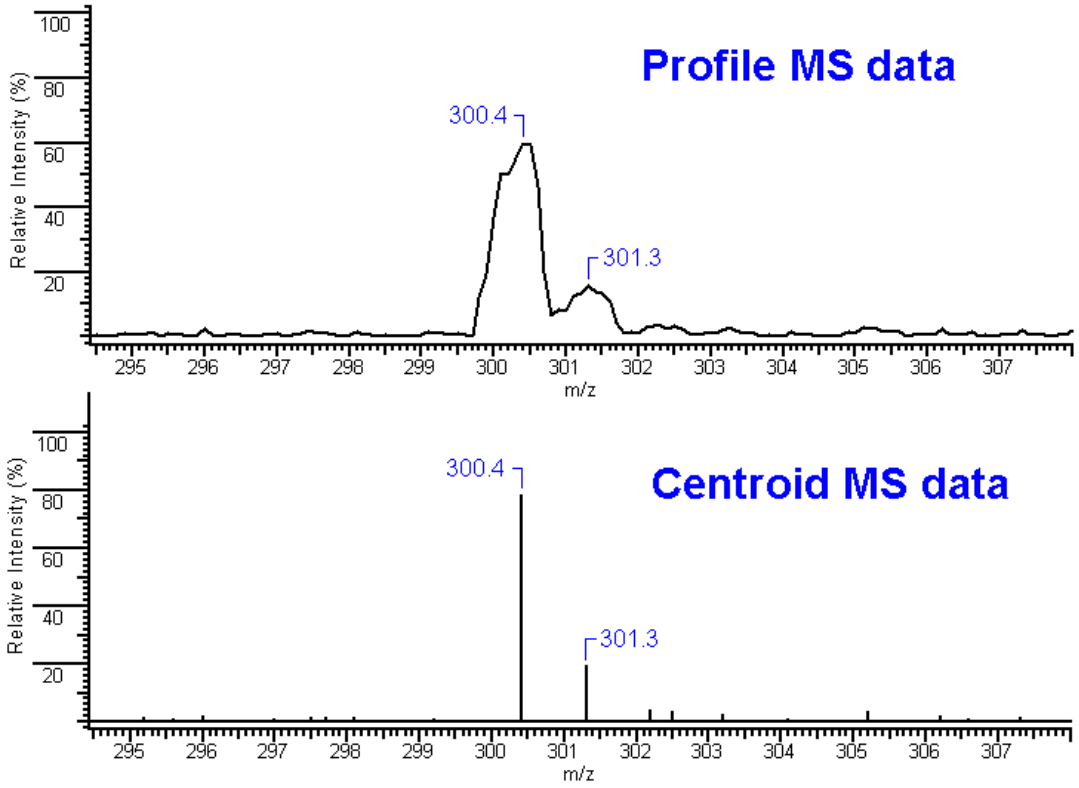
Click **Delta Mass Caliper Mouse** icon
Caliber Toolbar and Caliper cursor appear
Add or edit Calipers
Calipers can only be placed where there is a signal and “snap” to closest ion



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



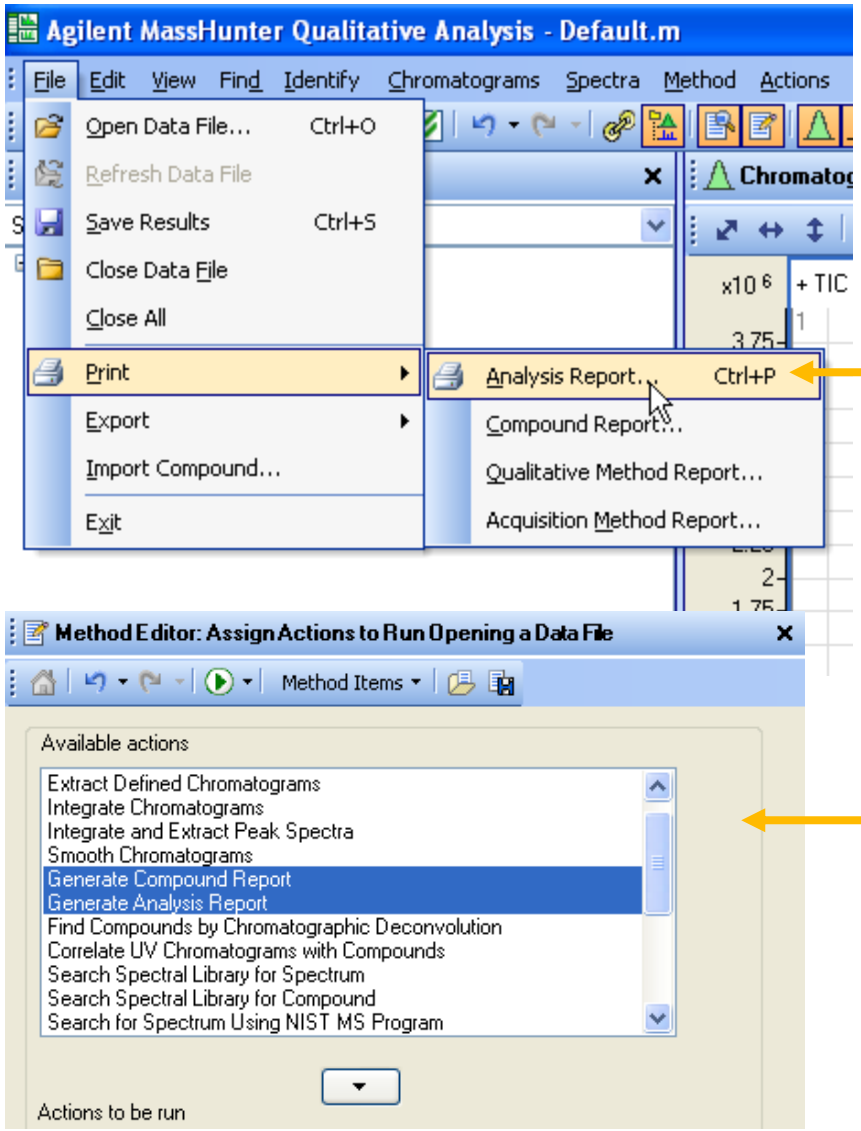


Let’s take another moment for questions on Annotations

Up Next:

Reporting

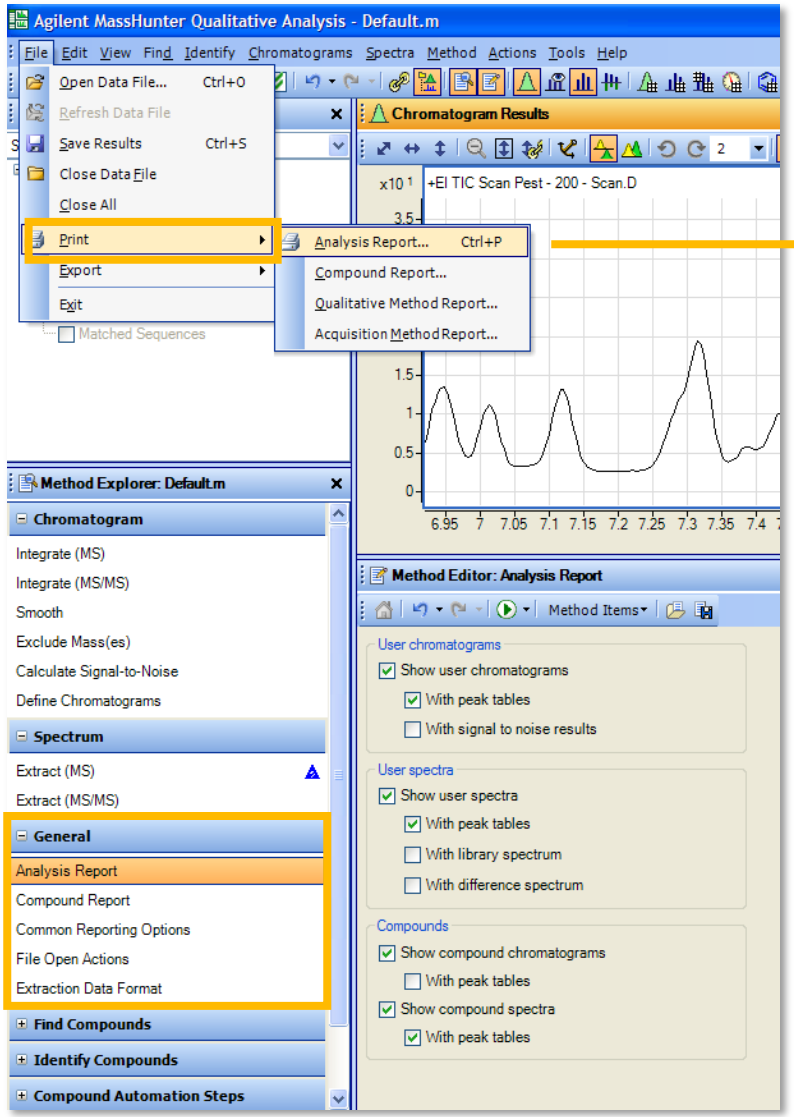
Print a Report from Qualitative Analysis

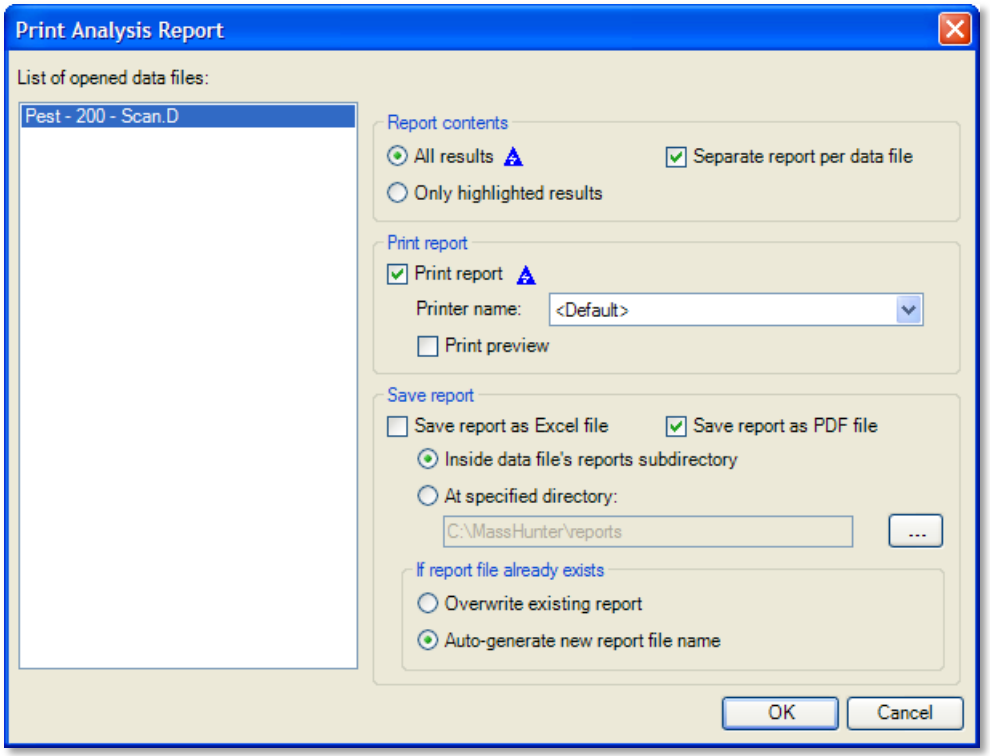


Print Qualitative Reports:

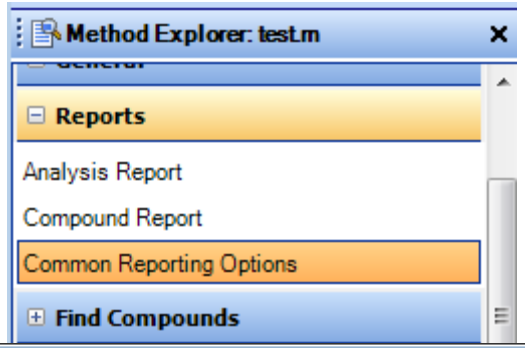
- Directly from menu.
- Indirectly from Automation
  - File Open Actions
  - Worklist Automation
- Covered in the Familiarization Guides.

Report Generation Options





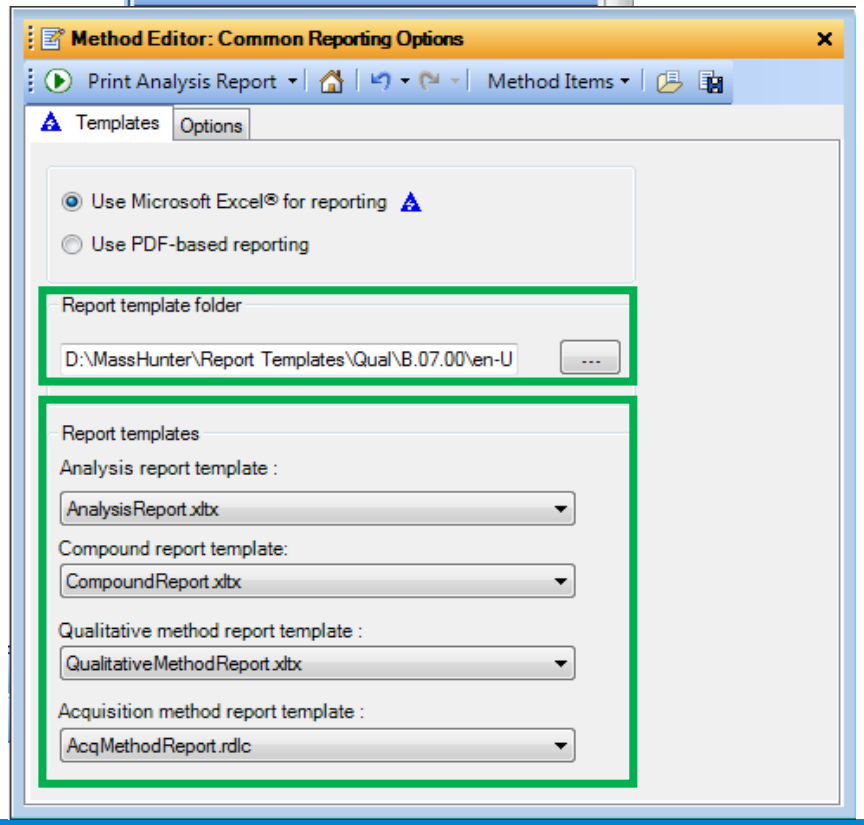
Common Reporting Options

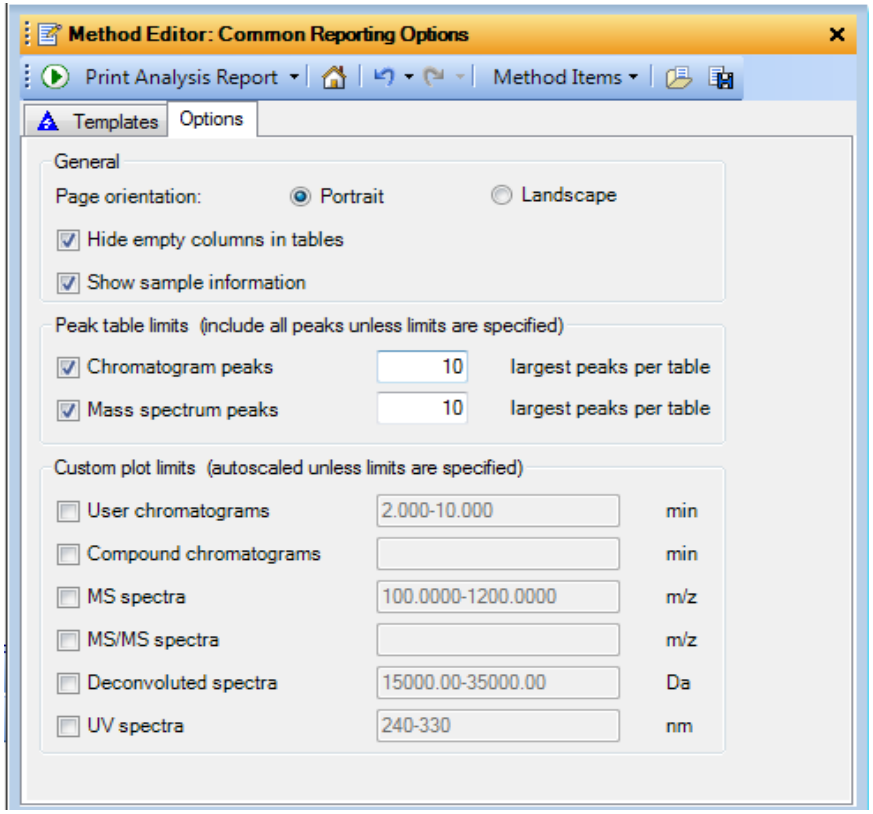


Excel Based Reporting

Uses xltx files

Tip: Review Common Reporting Options first.



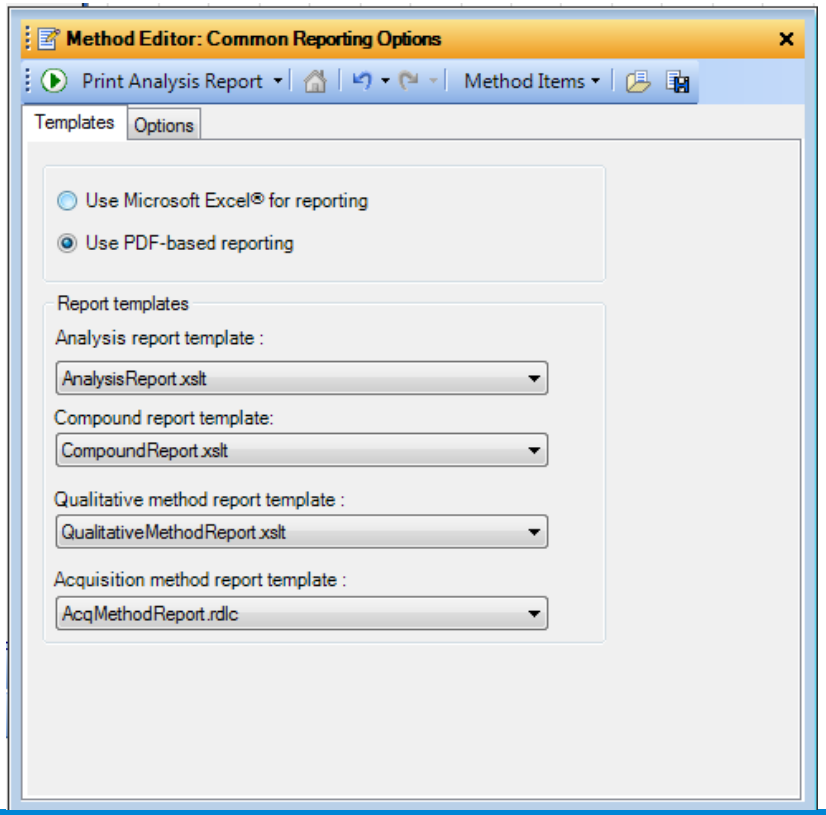


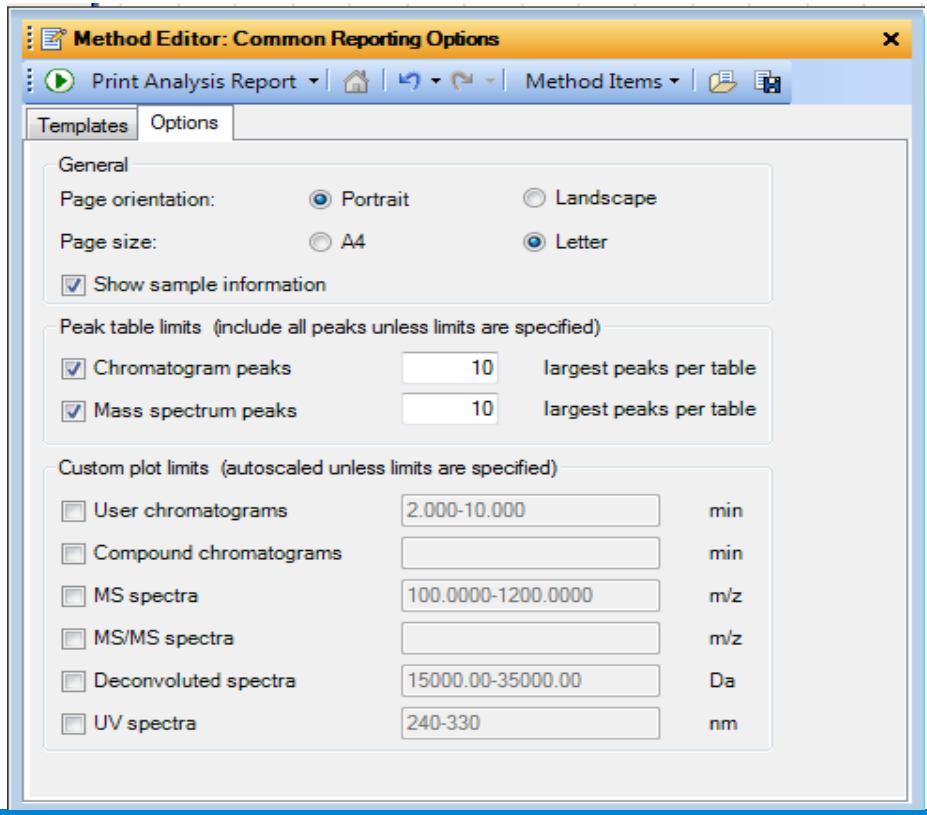
Common Reporting Options

New to Qualitative Analysis B.07.00 SP1

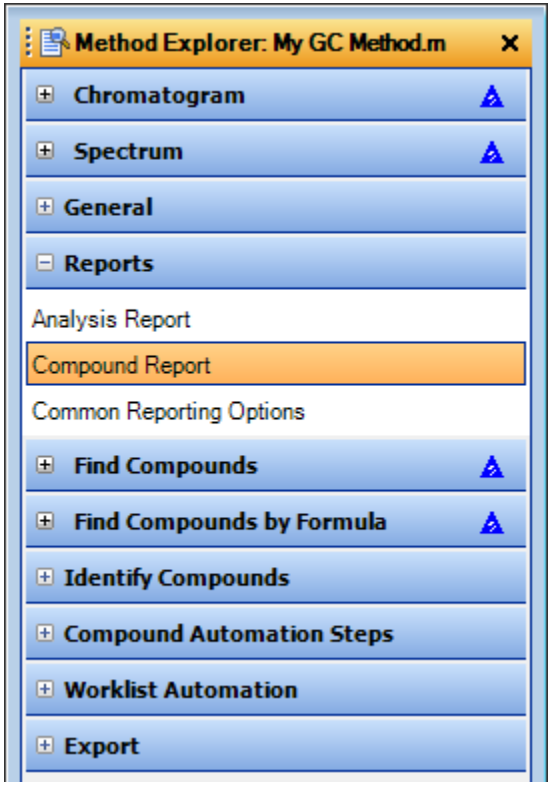
PDF Based Reporting

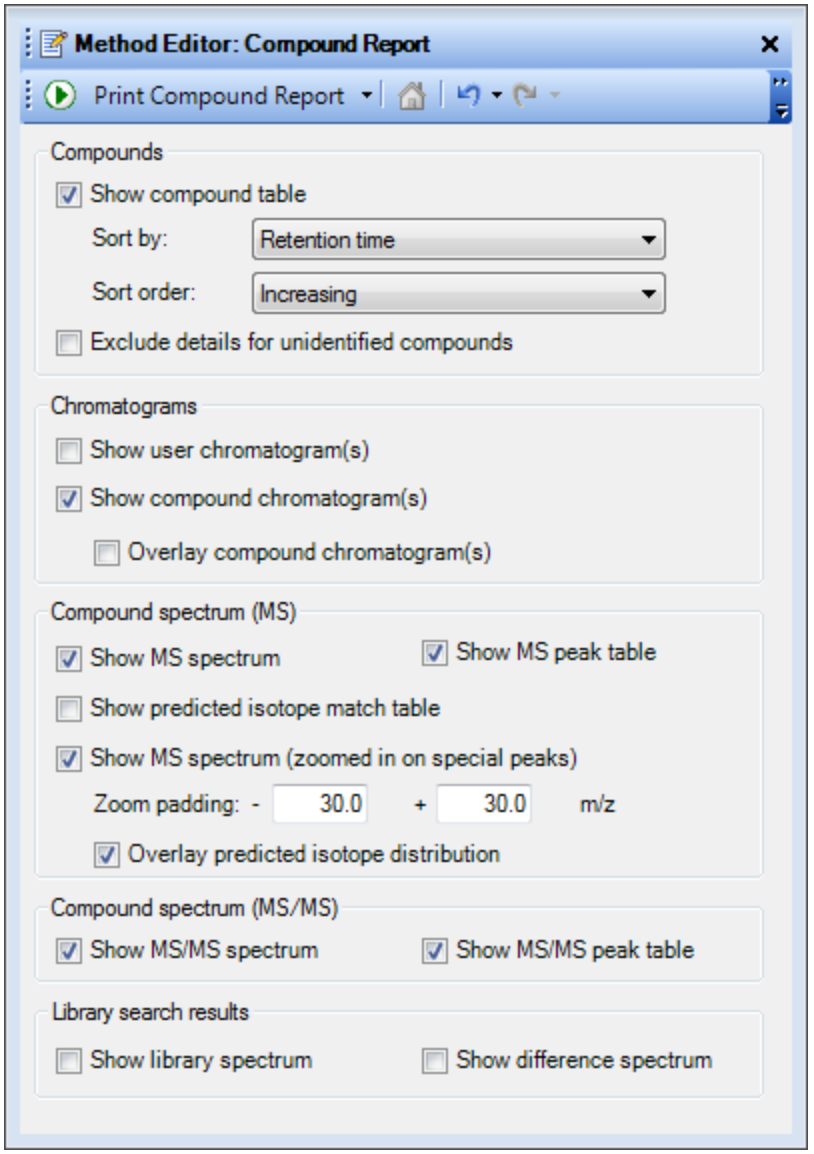
Uses xslt files



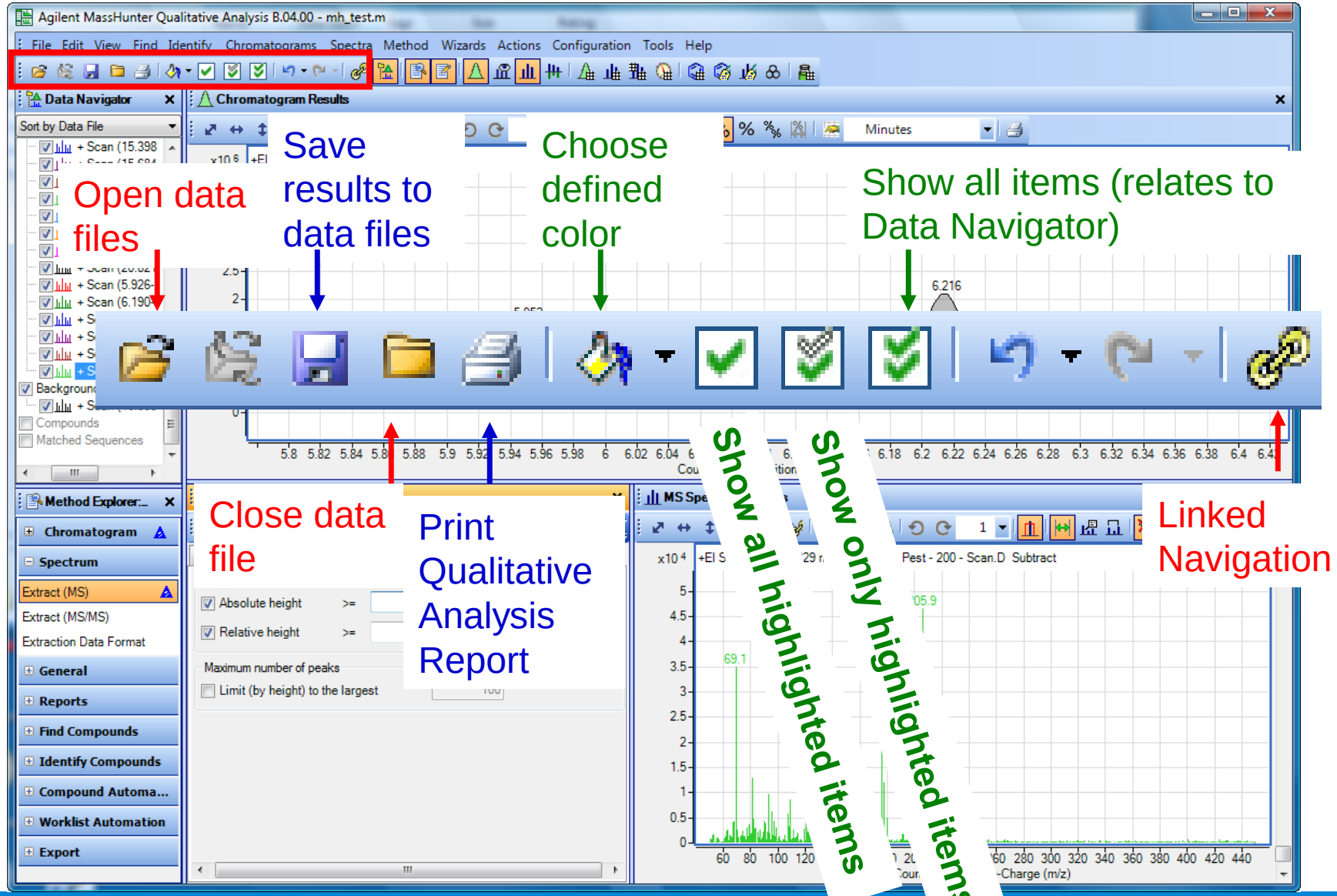


Compound Report Options

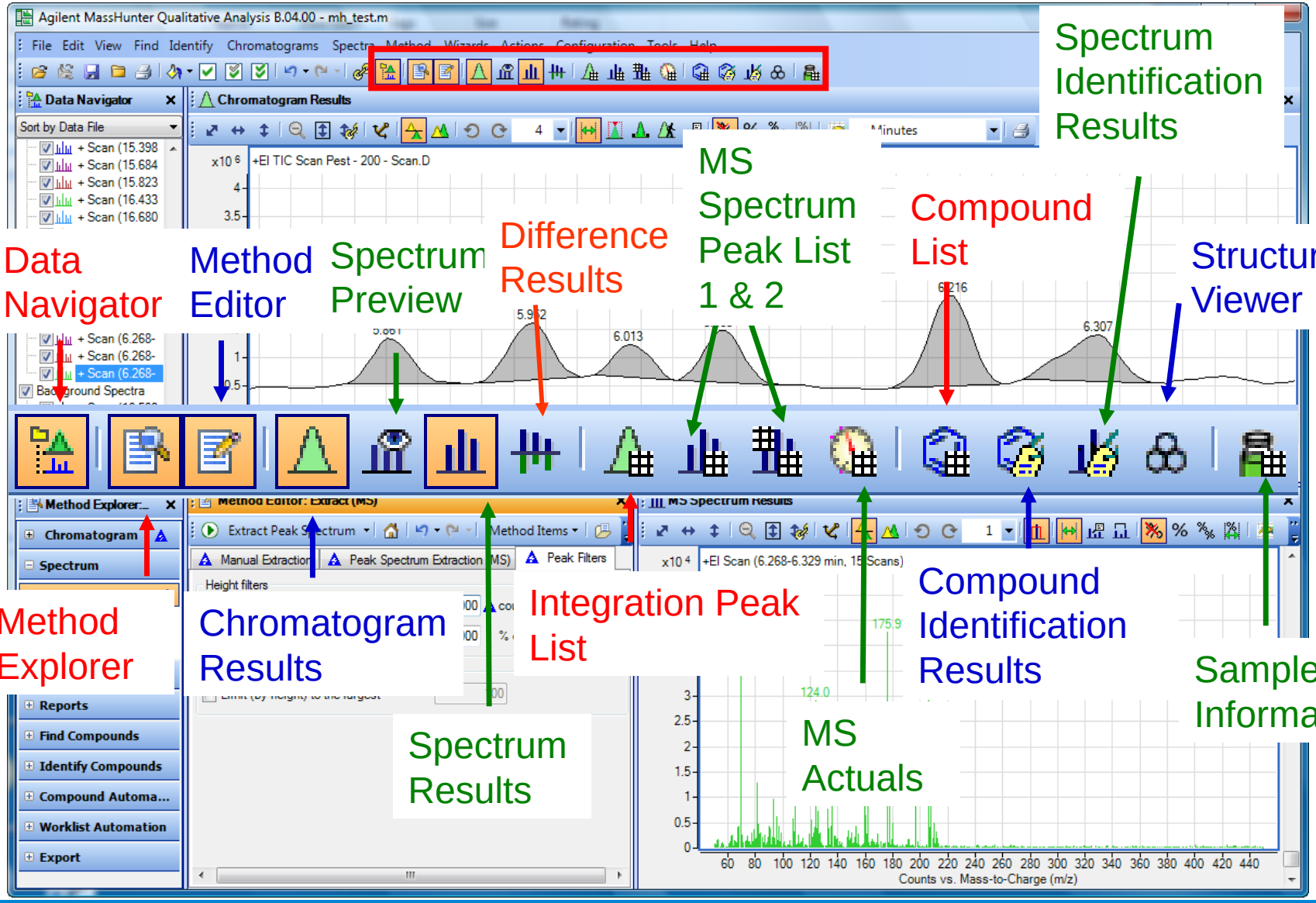




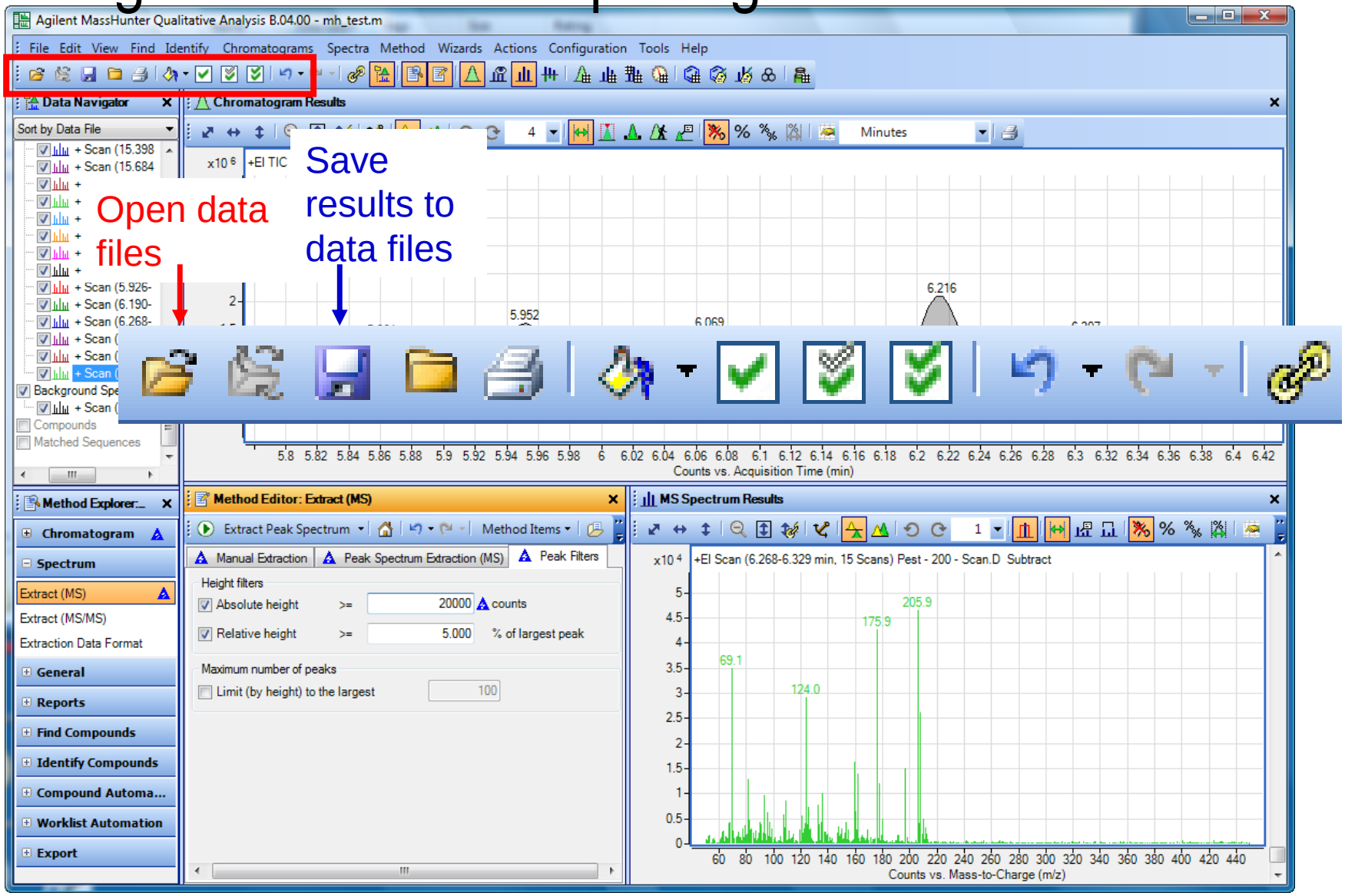
Tools


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
Chromatogram Results
Open data files
Save results to data files
Choose defined color
Show all items (relates to Data Navigator)
Close data file
Print Qualitative Analysis Report
Show all highlighted items
Show only highlighted items
Linked Navigation
Method Explorer
Chromatogram
Spectrum
Extract (MS)
Extract (MS/MS)
Extraction Data Format
General
Reports
Find Compounds
Identify Compounds
Compound Automa...
Worklist Automation
Export
Absolute height
Relative height
Maximum number of peaks
Limit (by height) to the largest
Pest - 200 - Scan.D Subtract

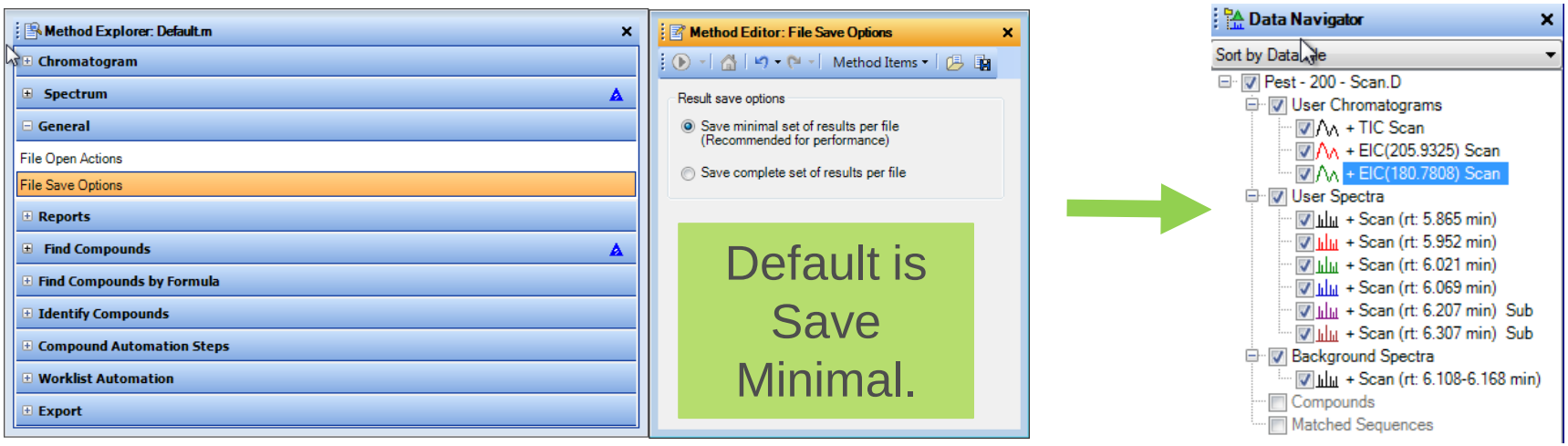
Tools


Agilent MassHunter Qualitative Analysis B.04.00 - mh_test.m
Data Navigator
Chromatogram Results
Spectrum Identification Results
MS Spectrum Peak List 1 & 2
Compound List
Structure Viewer
Data Navigator
Method Editor
Spectrum Preview
Difference Results
Method Explorer
Chromatogram Results
Integration Peak List
Compound Identification Results
Sample Information
Spectrum Results
MS Actuals
Counts vs. Mass-to-Charge (m/z)

Saving Data Files and Opening Data Files



File Save Options -The Results File

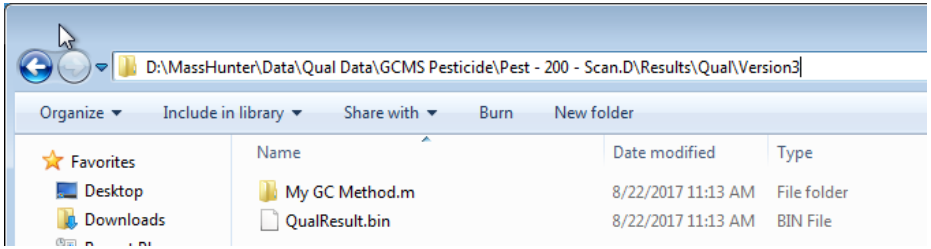


- Save minimal – only the compound level nodes are saved. No spectra or compound chromatograms are saved. If you open again, you will need to re-extract the complete result set.

- Save complete – all compound results are saved including spectra and chromatograms.

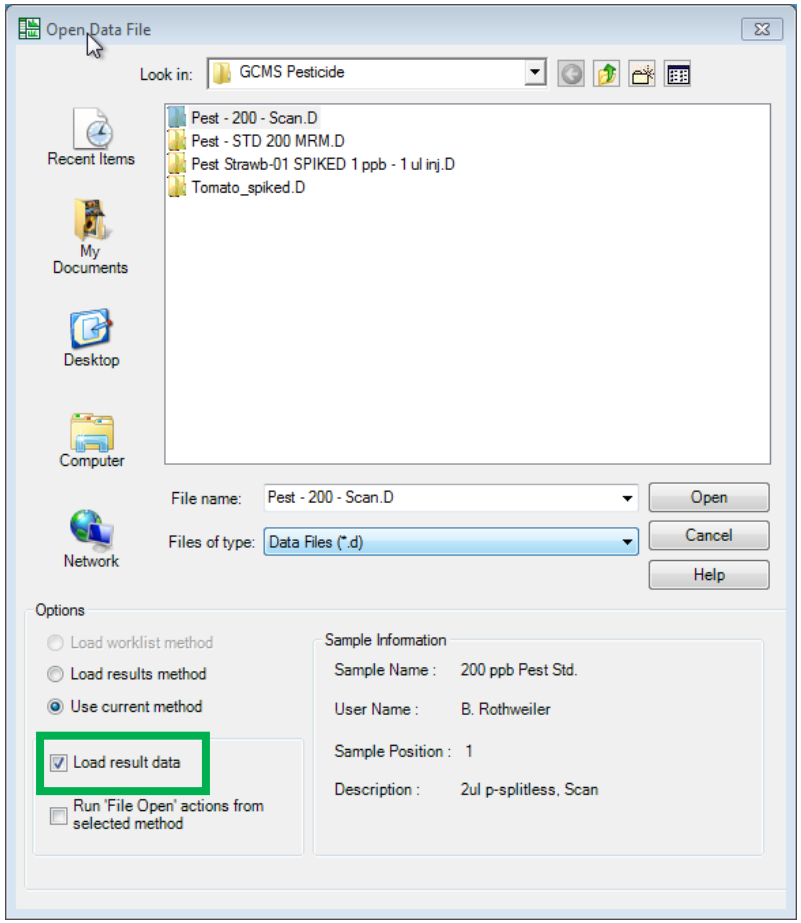
- In this example, all the User Chromatograms, User Spectra and Background Spectra are saved.

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:

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:

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- **Online** – From foundation to expert offerings when and where you need it at your own pace

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- Foundational subjects
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- Advanced subjects
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Helping customers:

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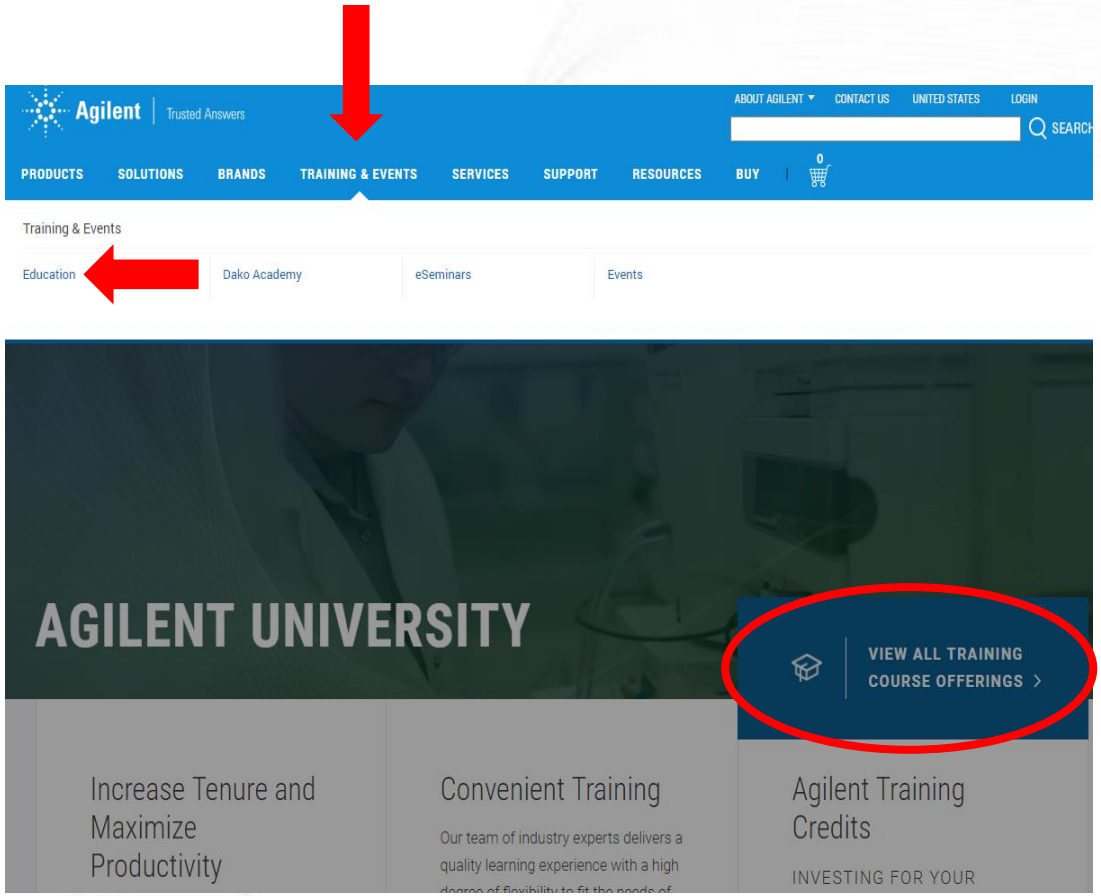

Questions on today's material…

Thank you for your attention.

MassHunter Qualitative Analysis

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