

Agilent MassHunter Qualitative Data Analysis

Presenters: Howard Sanford

Stephen Harnos

MassHunter Qualitative Analysis

Chromatogram Functions

MassHunter Qualitative Analysis Software B.07.00

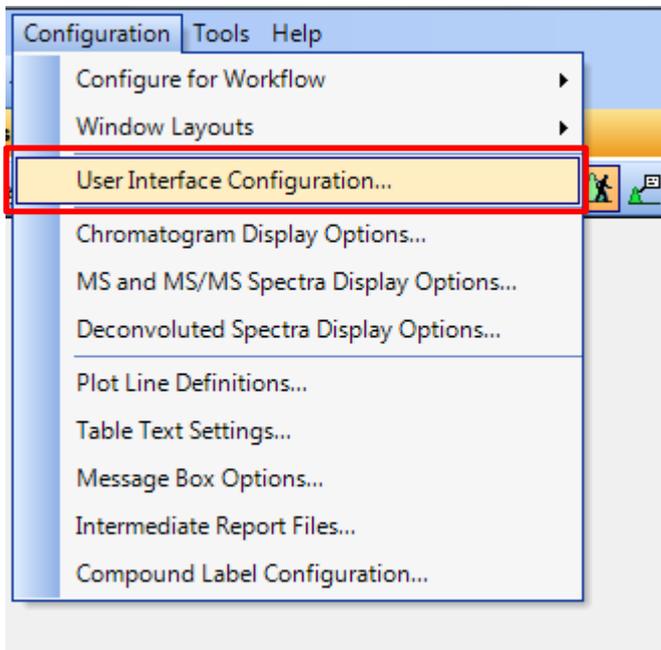
Topics

- User Interface Configuration
- User Workflows
- Views
 - Navigator
 - Compound Details
- Methods
 - Unified Method Concepts
 - Method Explorer
 - Method Editor
- Working with Chromatograms
 - Anchoring and Scaling
 - Chromatogram Functions
 - Integrators
- Training Resources
- Define Qualitative Analysis

MassHunter Qual - Configurable Software

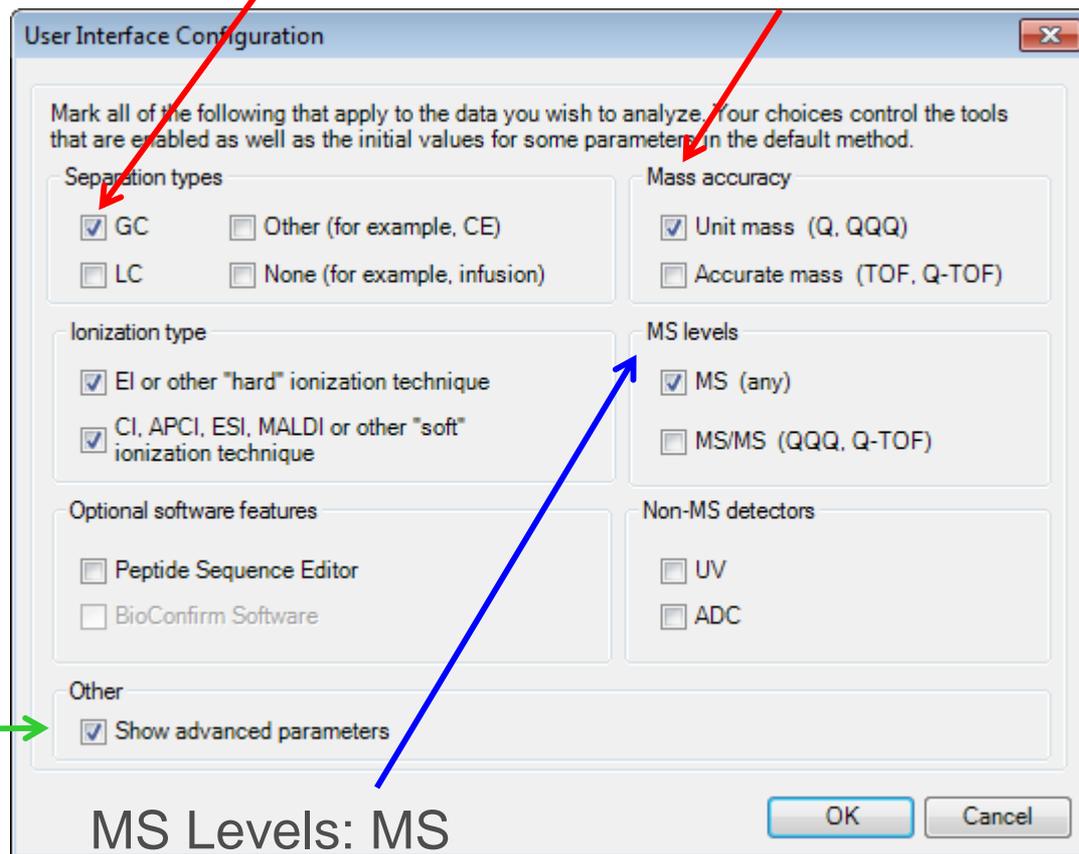
- One program for many instruments and types of data.
 - Single Quad (LC & GC) Unit resolution, Scan, SIM data
 - Triple Quad (LC & GC) Unit Resolution Scan, SIM, MRM (MS/MS) data
 - TOF (LC) High resolution, scan data
 - Q-TOF (LC & GC) High resolution MS/MS data
- Many software features can be used by all data types but many are only useful for a particular instrument type.
- MassHunter Qual **MUST** be configured to reduce complexity and hide unneeded and potentially misused features.
- Even when properly configured some features and parameters for MS/MS and accurate mass are still visible, ignore and avoid them.

User Interface Configuration



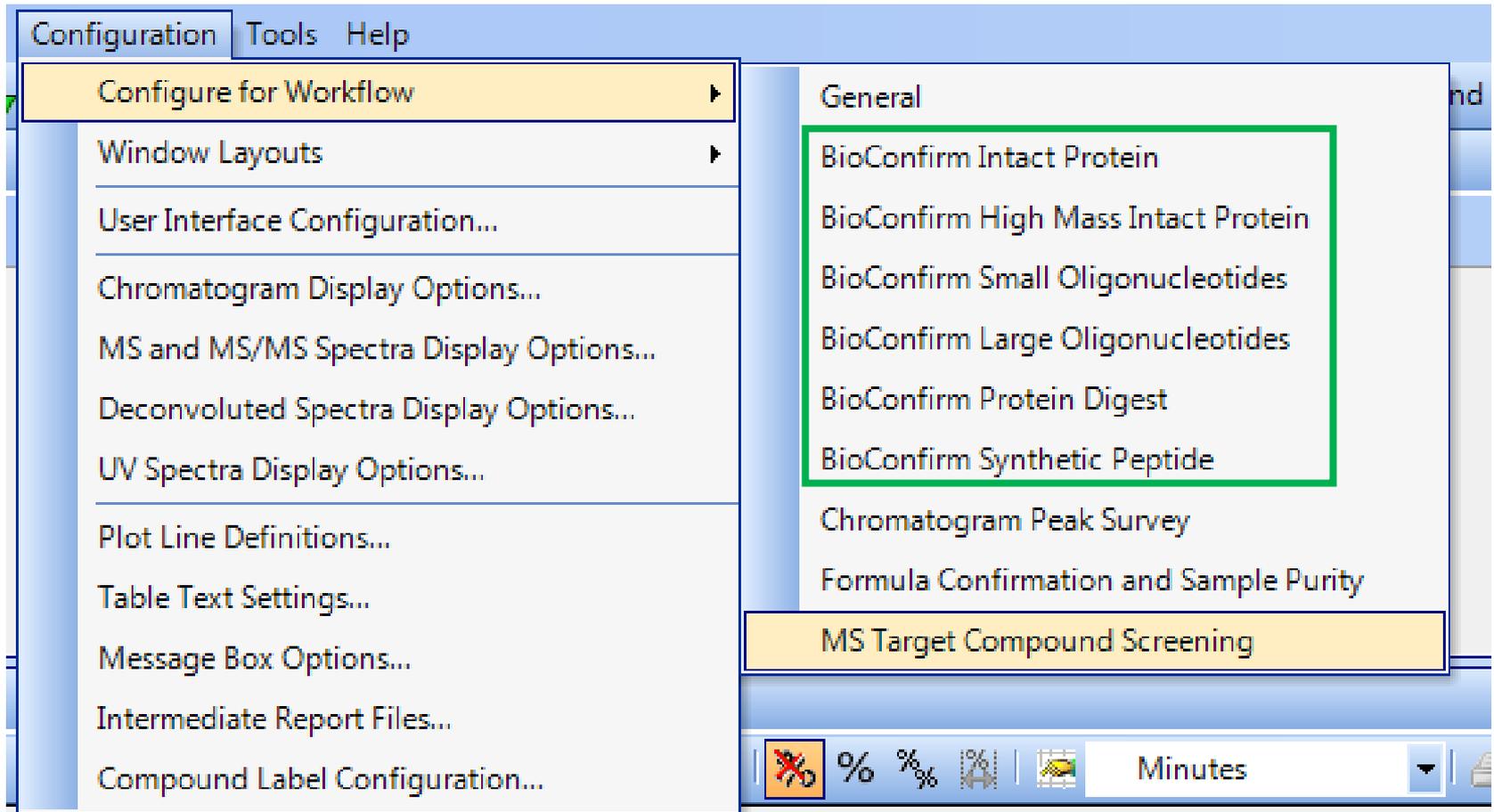
Separation types
(Check GC or LC)

Unit Mass (Q, QQQ)
Accurate Mass
(TOF, QTOF)



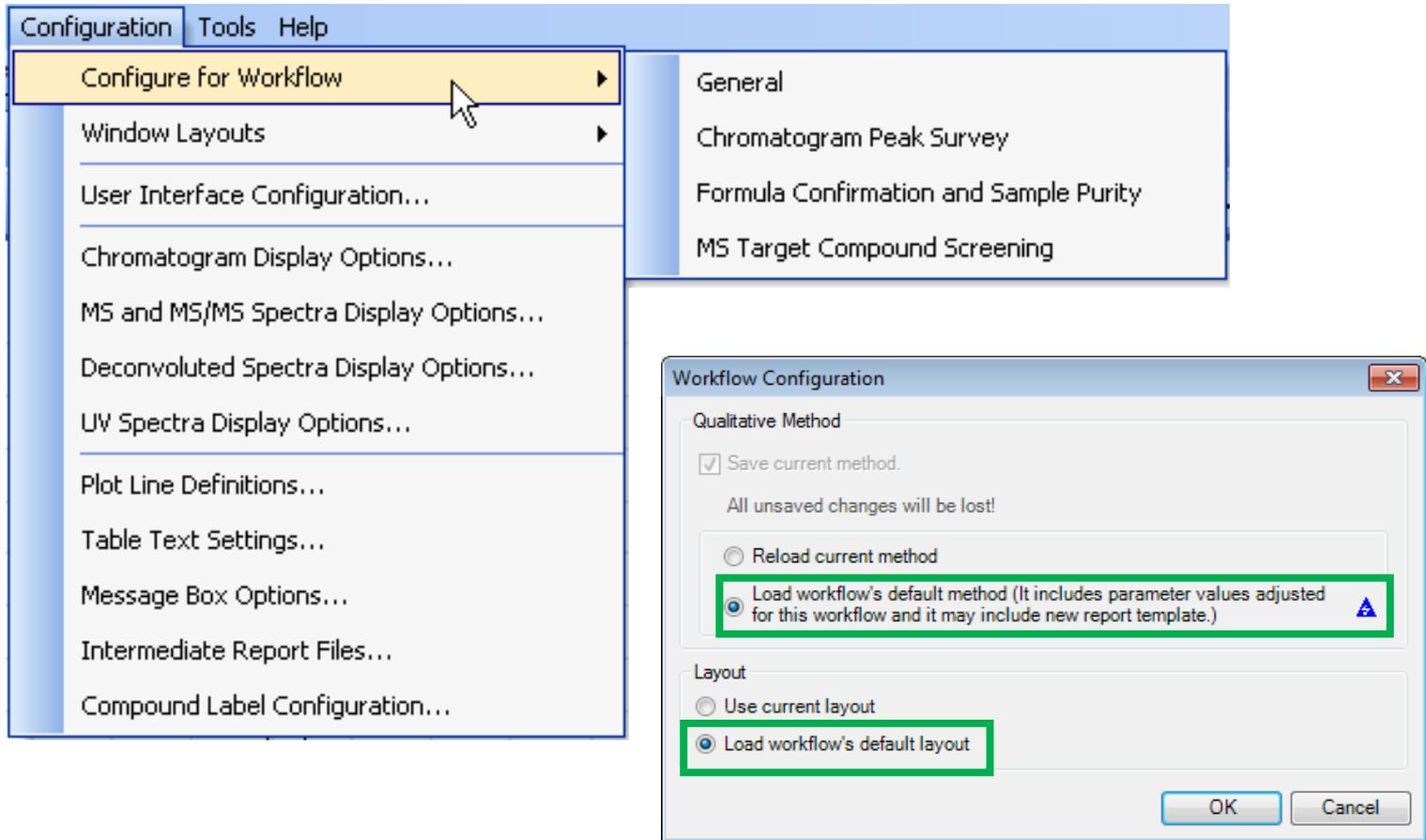
Check Show Advanced
Parameters

MassHunter Qualitative Analysis Workflows



Depends Upon Software Loaded and Configuration Selected

Configure for Workflow

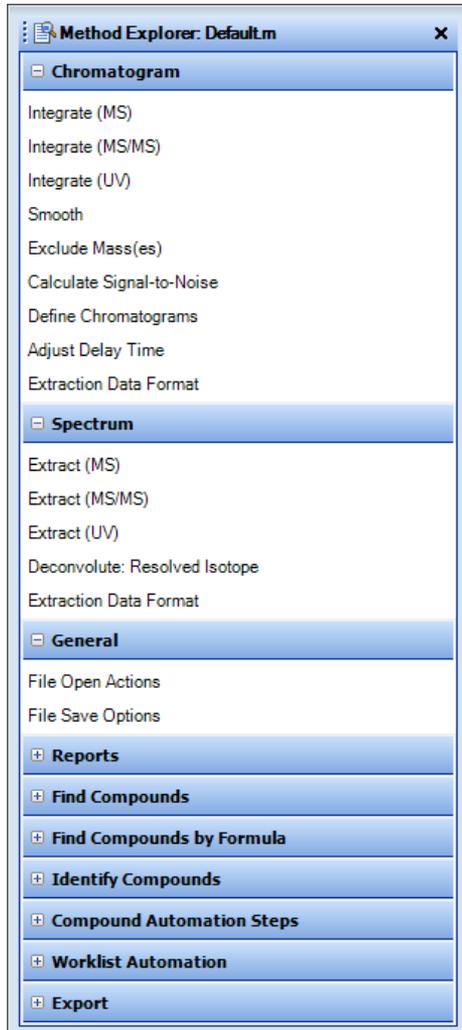


Configuration Changes Graphics, Table, and Method Layouts.

Tip: Load workflow's default method and default layout.

Chromatogram Peak Survey Workflow

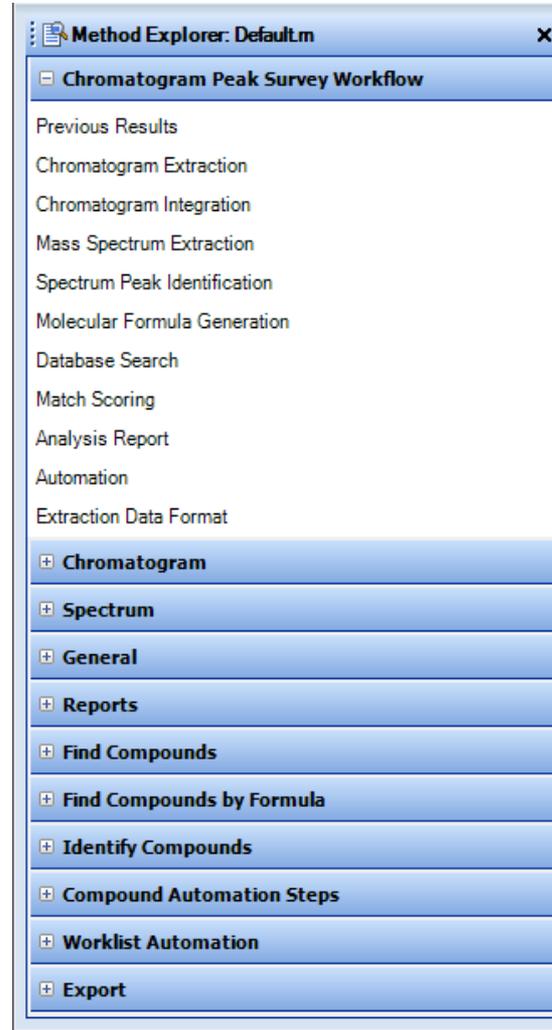
General



Modify settings for chromatogram.

Modify settings for spectral extraction.

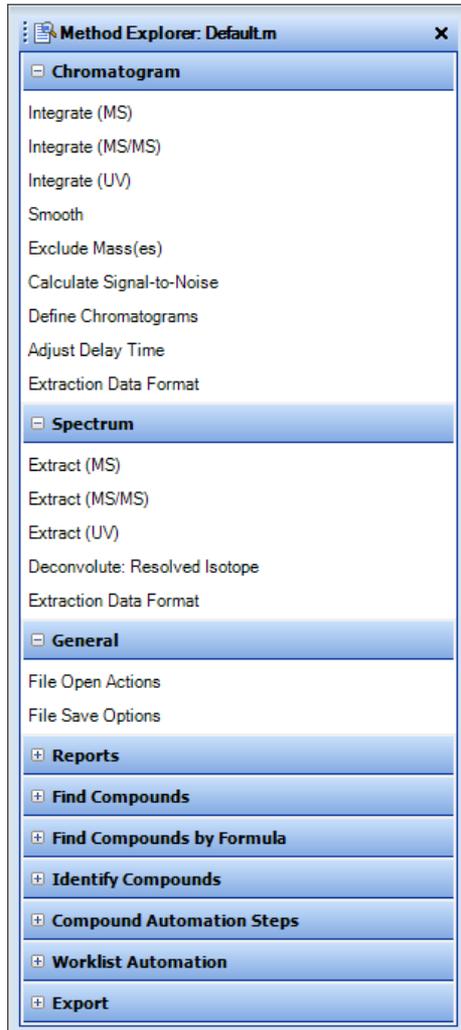
Chromatogram Peak Survey



Specified workflow added.

MS Target Compound Screening Workflow

General



MS Target Compound Screening Workflow



Navigator View

Data Navigator

Navigator View

Chromatogram Results



Method Explorer

Method Editor

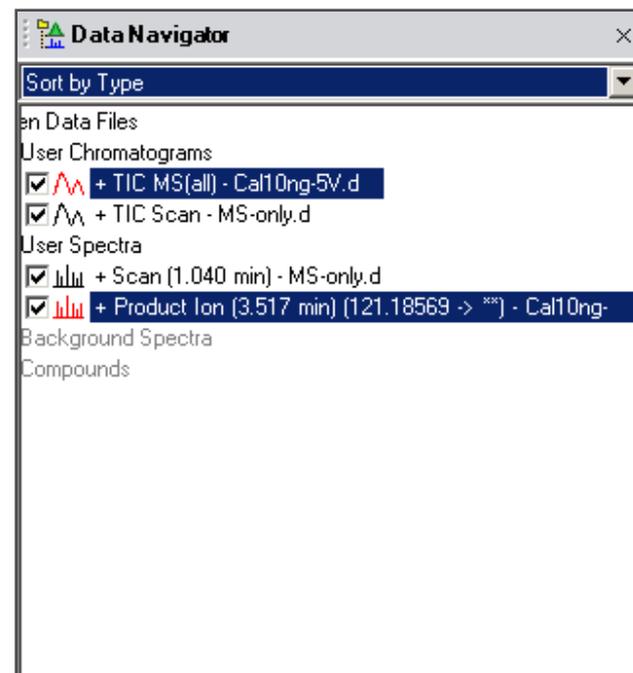
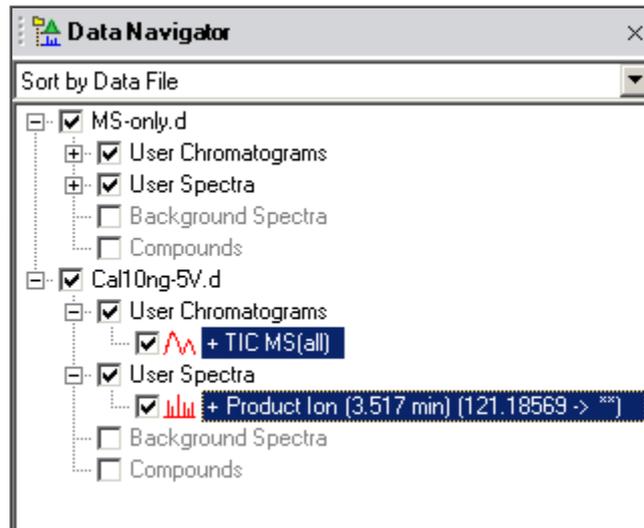
Spectrum Results

Data Navigator

The Data Navigator pane shows the data files which are loaded into Qualitative Analysis.

The user can selectively display the information associated with a data file (i.e. chromatograms, spectra, compounds) by selecting/deselecting a checkbox.

In the top drop-down, the user can choose to sort by Data File or Type (i.e. User Chromatogram, etc.)



Compound Details View

Compound Details View

Compound List

The screenshot displays the Agilent MassHunter Qualitative Analysis interface. The main window is titled "Compound List" and contains a table of identified compounds. A red arrow points to the "Compound Details View" tab, and a blue arrow points to the "Compound List" tab. Below the main table, a detailed view for "Cpd 76: alpha-Ketopantoic acid" is shown, including its chemical formula (C6 H10 O4) and various mass and retention parameters. To the left, the "Compound Chromatogram Results" window shows a chromatogram with a prominent peak at 5.892 minutes, labeled "Cpd 76: alpha-Ketopantoic acid". To the right, the "Compound MS Spectrum Results" window displays the mass spectrum for the peak, with the base peak at m/z 169.0470. A green arrow points from the "Compound MS Spectrum Results" window to the "Compound Fragment Spectrum Results" window, which shows "No Fragment Spectrum available for this compound."

Label	Cpd	Name	Formula	Score	Mass	Avg Mass	Std Dev	Mass (DB)	Mass (MFG)	Diff (MFG, ppm)	Diff (MFG, mDa)	Base Peak	m/z	Polarity	Max Z	Min Z
Cpd 125: C3 H10 N4 O3	125		C3 H10 N4 O3	99.39	150.0753	150.122	0.0006		150.0753	0.23	0.03	151.0825	151.0825	Positive	1	
Cpd 15: isoamyl nitrite	15	isoamyl nitrite	C5 H11 N O2	99.18	117.0788	117.2335		117.079	117.079	1.74	0.2	118.0861	118.0861	Positive	1	
Cpd 17: beta-Alanine	17	beta-Alanine	C3 H7 N O2	98.84	89.0479	89.0778		89.0477	89.0477	-2.73	-0.24	90.0552	90.0552	Positive	1	
Cpd 69: Dimethylglycine	69	Dimethylglycine	C4 H9 N O2	98.79	103.0635	103.1025		103.0633	103.0633	-1.56	-0.16	104.0708	104.0708	Positive	1	
Cpd 1: Proline	1	Proline	C5 H9 N O2	98.28	115.0635	115.1076	0.0002		115.0633	-1.18	-0.14	116.0707	116.0707	Positive	1	
Cpd 73: Quinolinic acid	73	Quinolinic acid	C7 H5 N O4	98.15	167.022	167.0901		167.0219	167.0219	-0.59	-0.1	168.0292	168.0292	Positive	1	
Cpd 27: C6 H4 O4	27		C6 H4 O4	98.02	140.0106	140.0709		140.011	140.011	2.22	0.31	141.0179	141.0179	Positive	1	
Cpd 71: Xanthine	71	Xanthine	C5 H4 N4 O2	97.82	152.0333	152.0895		152.0334	152.0334	0.64	0.1	153.0407	153.0407	Positive	1	
Cpd 76: alpha-Ketopantoic acid	76	alpha-Ketopantoic acid	C6 H10 O4	97.82	146.0578	146.1236	0.0002		146.0579	0.42	0.06	169.047	169.047	Positive	1	

Best	Name	Formula	Score	Mass (DB)	Mass (MFG)	Diff (MFG, ppm)	Diff (abs, ppm)	Diff (mDa)	RT	RT Available (DB)	RT (DB)
	alpha-Ketopantoic acid	C6 H10 O4	97.82	146.0578	146.0579	146.0579	0.42	0.42	5.892	N	
		C7 H6 N4	41.61	146.0579		146.0592	9.25	1.35	5.892		

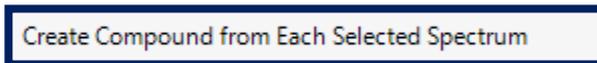
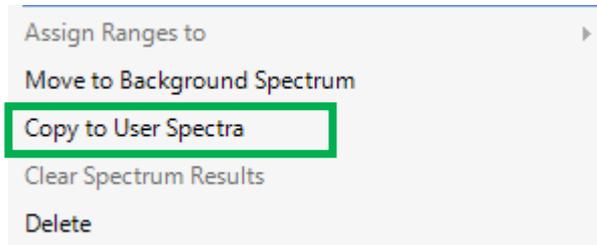
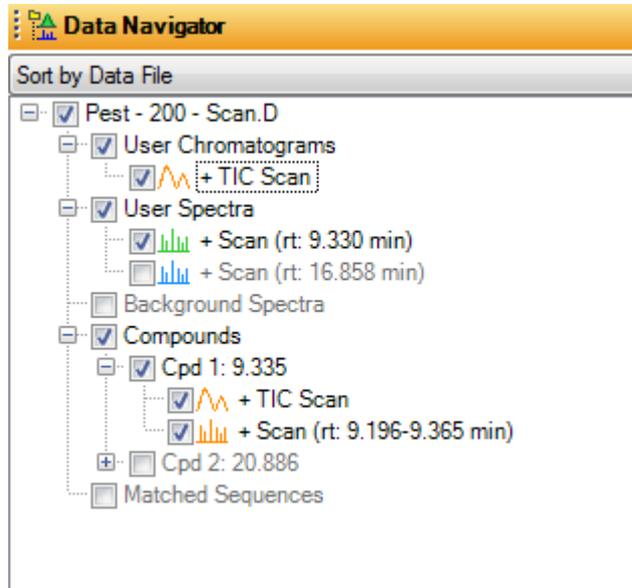
Label	Cpd	Name	Formula	Score	Mass	Avg Mass	Std Dev	Mass (DB)	Mass (MFG)	Diff (MFG, ppm)	Diff (MFG, mDa)	Base Peak	m/z	Polarity	Max Z	Min Z
Cpd 10: C3 H9 N O	10		C3 H9 N O	97.78	75.0688	75.0962	0.0003		75.0684	-5.62	-0.42	76.0761	76.0761	Positive	1	
Cpd 3: Vigabatrin	3	Vigabatrin	C6 H11 N O2	97.57	129.0791	129.1304	0.0003	129.079		-1.31	-0.17	147.1126	147.1126	Positive	1	

Compound Chromatogram Results

Compound Fragment Spectrum Results

Compound MS Spectrum Results

Definitions



User Spectra are mass spectrum that the user creates.

Compounds are generated by one of the 'Find by' algorithms. Compounds are generated by the software.

User Spectra and Compounds are readily interchangeable through the context menu (right click on the User or Compound Spectrum in the MS Spectrum Results window).

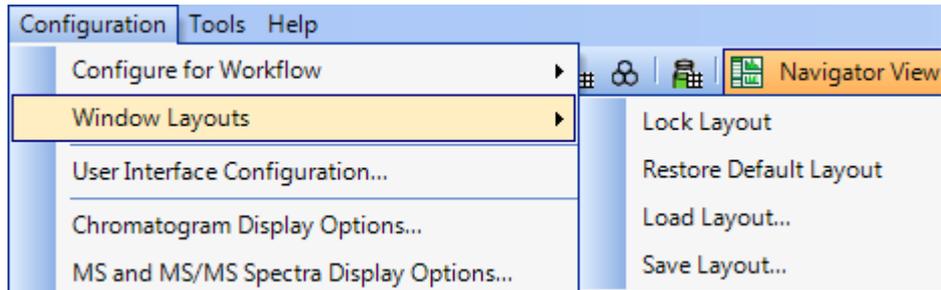
Expose or Hide Windows as Needed

Menu

Toolbar

The screenshot displays the Agilent MassHunter Qualitative Analysis B.06.00 - Default.m interface. The 'View' menu is open, showing options such as Data Navigator, Method Explorer, Method Editor, Chromatogram Results, Spectrum Preview, MS Spectrum Results, Difference Results, Deconvolution Mirror Plot, Integration Peak List, MS Spectrum Peak List 1, MS Spectrum Peak List 2, MS Actuals, Compound List, Compound Identification Results, Spectrum Identification Results, Structure Viewer, Sample Information, Status Bar, and Linked Navigation. The 'Define Chromatograms' option is highlighted. The main workspace contains three windows: 'Chromatogram Results' showing a Total Ion Chromatogram (TIC) for 'pest-20ppm.D' with peaks labeled at retention times (e.g., 4.190, 4.704, 5.057, 5.401, 5.961, 6.766, 7.138, 7.628, 7.811, 7.972, 8.414, 8.772, 8.998, 9.243, 10.519); 'Method Editor: Define Chromatograms' showing the definition of 'BPC (all) MS (Cycle-summed)'; and 'MS Spectrum Results' showing two mass spectra for scans 4.181-4.200 min and 4.694-4.713 min, with peaks labeled at m/z values (e.g., 60.1, 95.0, 130.0, 164.9, 202.9, 236.9, 271.8, 63.1, 89.1, 148.1, 165.1, 205.9).

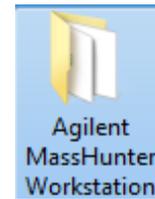
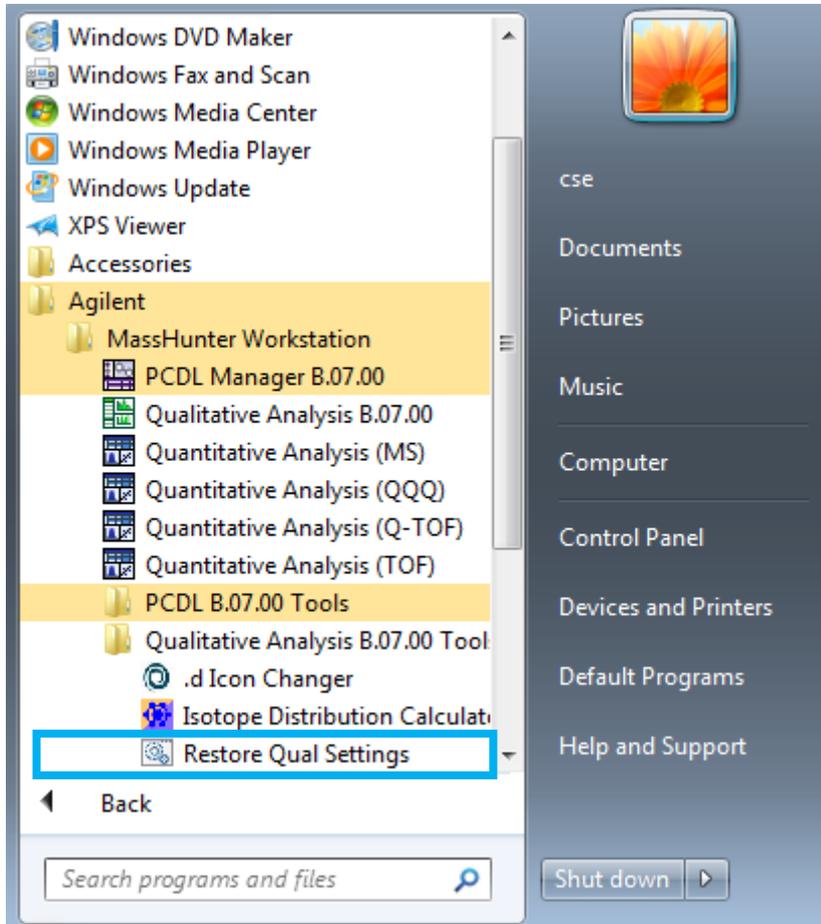
Restore Default Layout



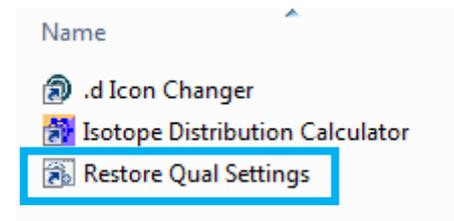
- Complicated windows layouts can be restored to default layout.
- Preferred layouts can be saved and loaded.
- Layouts can be locked.

Restore Qual Setting

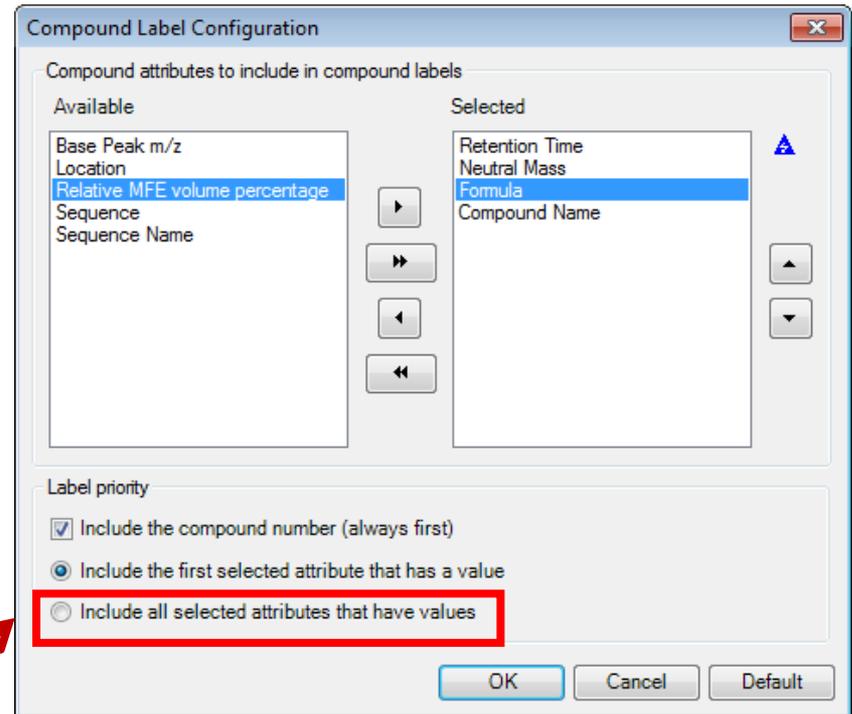
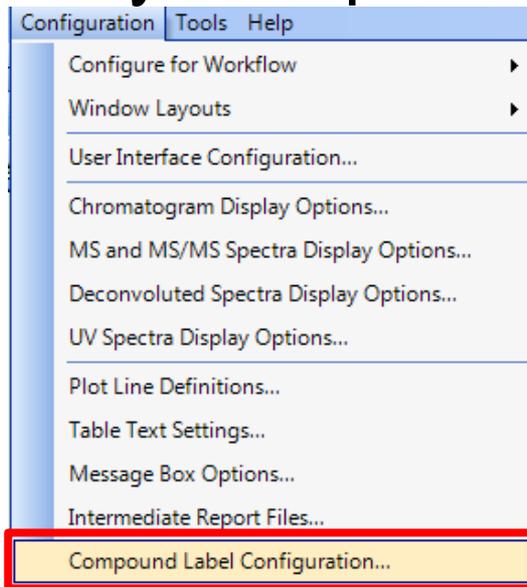
This may be a useful tool to restore the Qualitative Analysis settings if a configuration problem is suspected.



Or Desktop folder



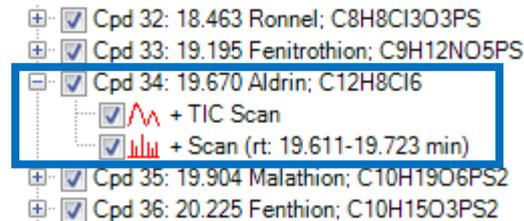
Specify Compound Label Configuration



Configuration > Compound Label Configuration

Tip: Select Include all selected attributes that have values.

In this example, compounds shows the compound number, RT, compound and formula.



Compounds Labels Display in Data Navigator

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

Open Data Files

The screenshot shows the Agilent MassHunter Qualitative Analysis 8.06.00 interface. The 'File' menu is open, highlighting 'Open Data File...'. The 'Open Data File' dialog box is displayed, showing a list of files in the 'Pest' folder. Several files are selected, including 'pest-0.05ppm.D', 'pest-0.1ppm.D', and 'pest-0.2ppm.D'. The 'Options' section at the bottom of the dialog box is also visible, with 'Use current method' selected and 'Load result data' and 'Run 'File Open' actions from selected method' checked.

Select multiple files at once for batch analysis, then click **Open**.

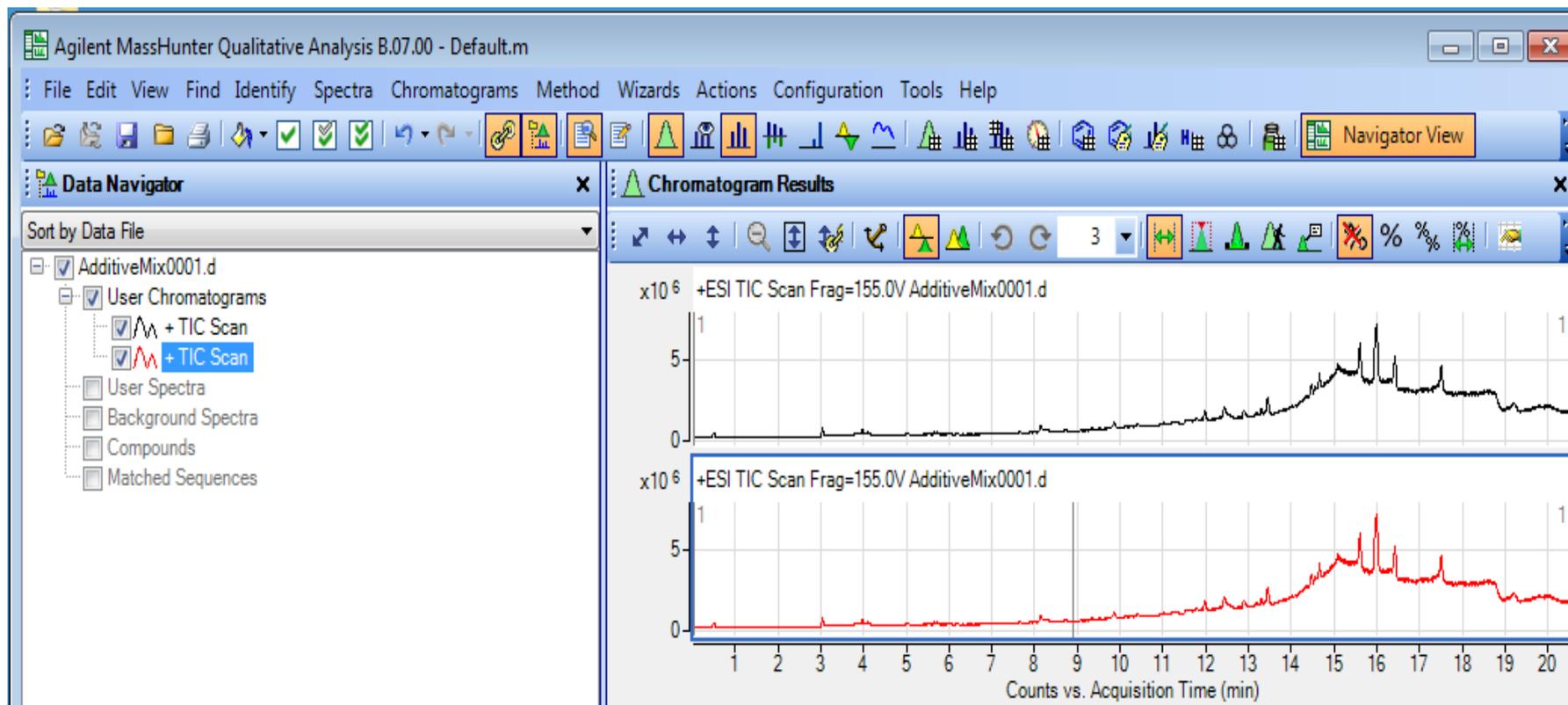
If **Load result data** is checked, the qualitative data manipulations previously saved will be loaded.

If **Run 'File Open' actions from selected method** is checked, automated processing is performed.

If neither **Load result data** or **Run 'File Open' actions from selected method** is checked, then a TIC is automatically extracted from the data files.

Tip

Every time a data file is loaded see 2 TICs.



Refresh Data File

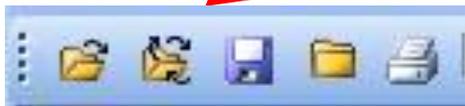
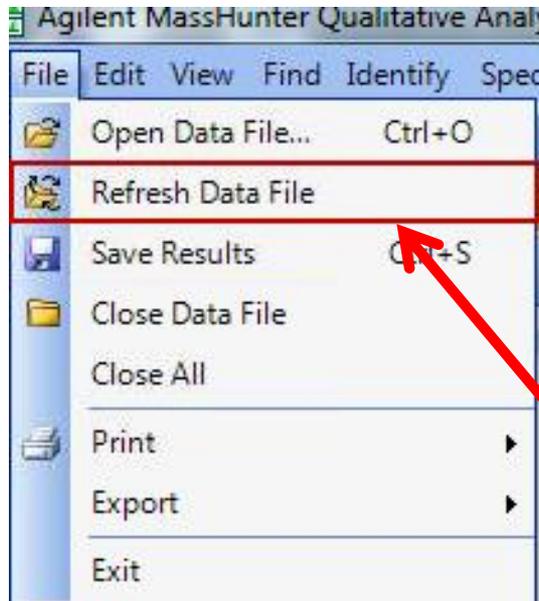
Feature is useful when it is desired to view data as the data file is being acquired.

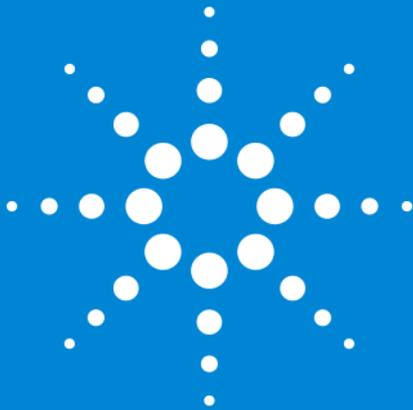
Initially use **Open Data File** as normal to view data file being acquired.

Then use **Refresh Data File** to update the view and add the most recently acquired data.

Refresh Data File is only active if the file is being acquired.

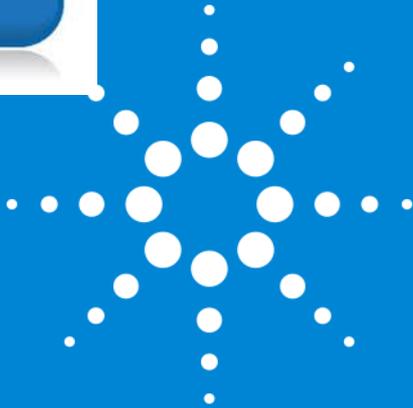
Similar application use for the GC/MSD ChemStation, where it is called SnapShot.





Let's take a moment
for chat questions on
Configuration and
Layouts.

Up Next:
Qualitative Methods



Demo on Configuration and Layouts.

Qualitative Analysis Methods

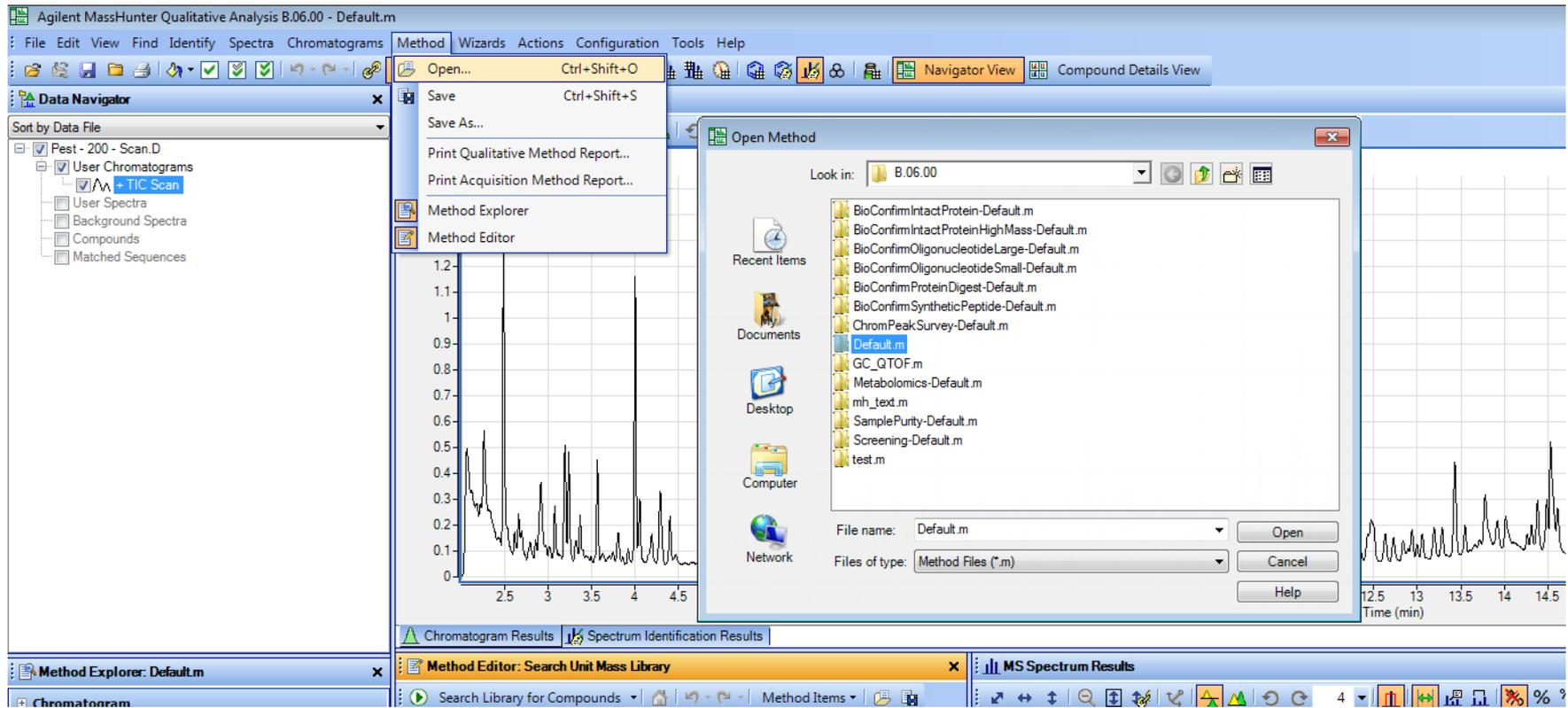
The screenshot displays the Agilent MassHunter Qualitative Analysis B.06.00 interface. The main window shows a chromatogram with a y-axis from 0 to 1.2 and an x-axis from 2.5 to 4.5 minutes. A menu is open, showing options like 'Open...', 'Save', and 'Print Qualitative Method Report...'. An 'Open Method' dialog box is also open, showing a list of method files in the 'B.06.00' folder, with 'Default.m' selected. The 'File name' field is set to 'Default.m' and the 'Files of type' is set to 'Method Files (*.m)'. The bottom status bar shows 'Chromatogram Results', 'Spectrum Identification Results', 'Method Explorer: Default.m', and 'Method Editor: Search Unit Mass Library'.

Qualitative Analysis Methods are stored in a .M folder.

Many application & instrument specific methods, generally use Default.m.

Default.M is read-only, after editing “Save As” to a customized method.

What is a Method? Unified Method Concept



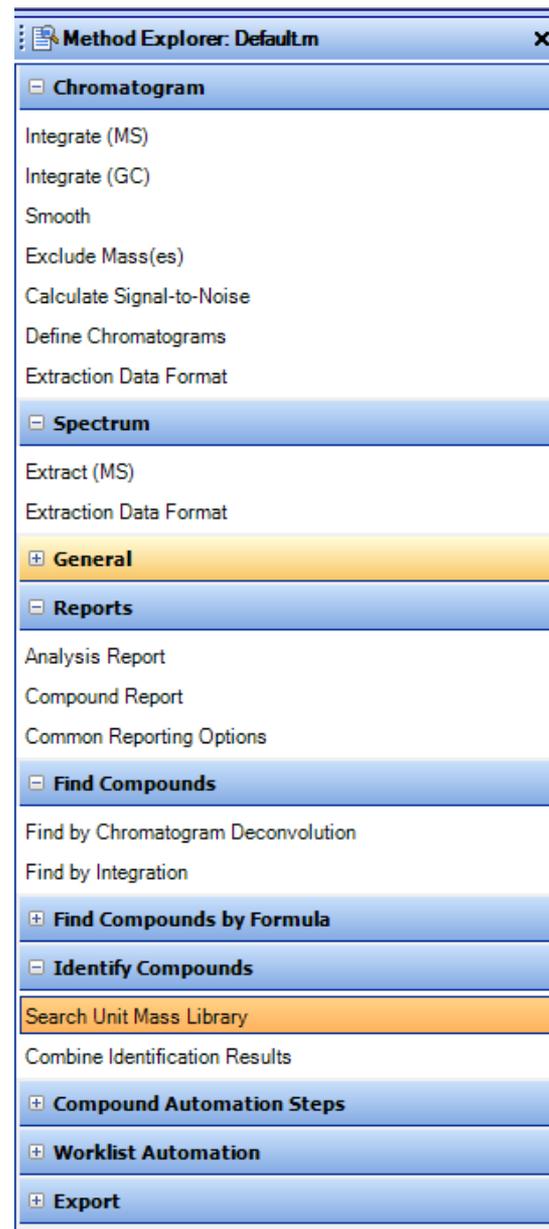
- Qualitative Analysis Methods are stored in a .M folder.
- Quantitative Analysis Methods are stored in a .M folder.
- Quantitative Analysis Reporting Methods are stored in a .M folder.
- Unified method can now be automated to run from the sequence/worklist.

Method Explorer

Acts as a table of contents for the method.

Items in Method Explorer automatically display related Method Editor features.

Items are dynamic and controlled by the User Configuration and Workflow setting.



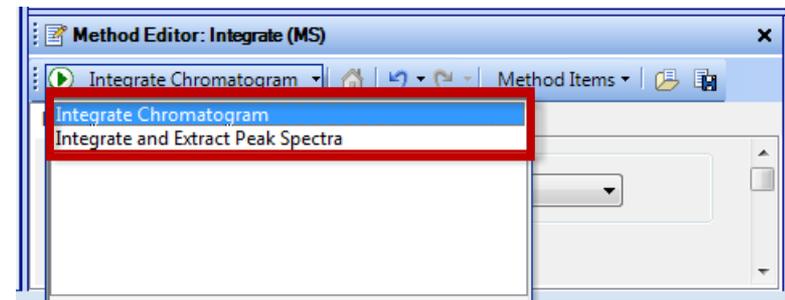
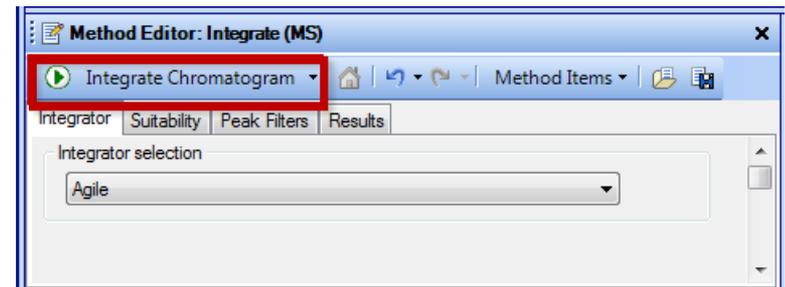
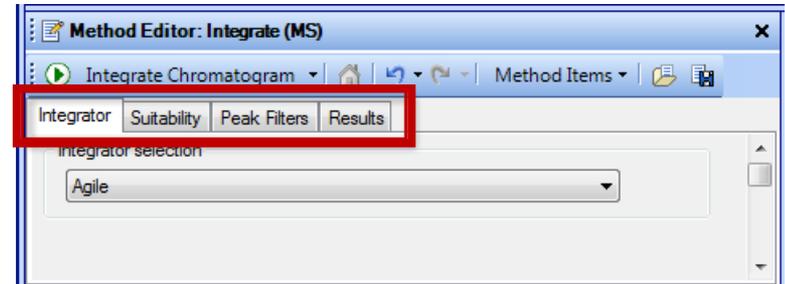
Method Editor

Display and Edit sections of the Method.

Tabs within the Method Editor further organize method parameters.

The “Run” icon executes the function associated with this part of the method.

In some cases the “Run” icon can have different actions, a drop down list will then display them for selection.



Relationship Between Action and Method Editor

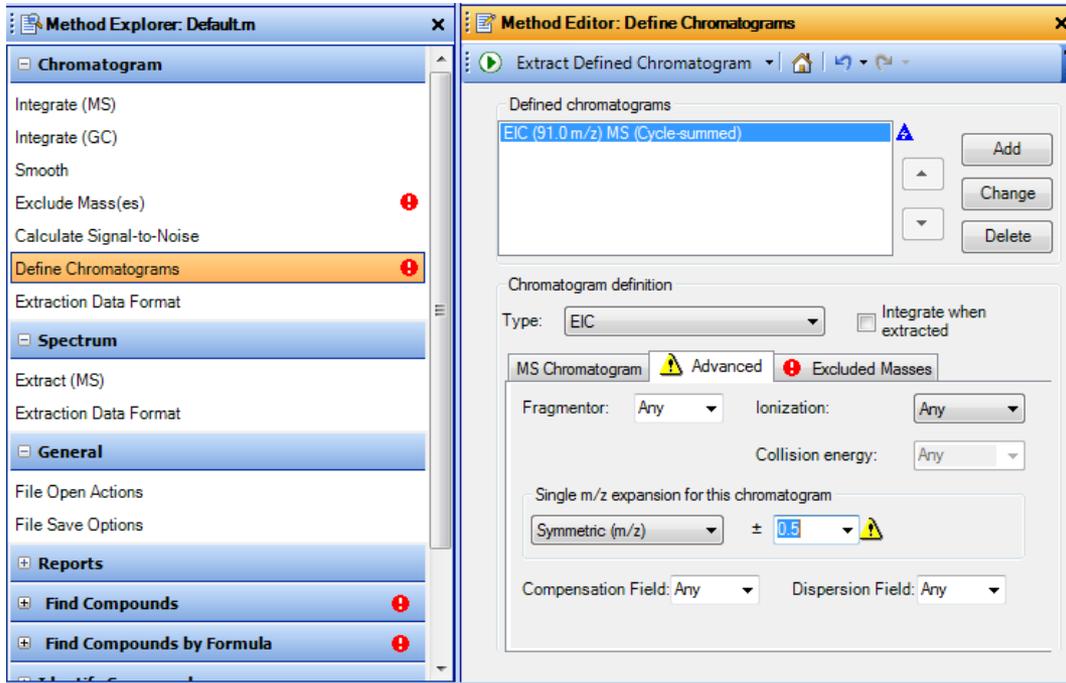
The screenshot displays the Agilent MassHunter Qualitative Analysis B.06.00 - Default.m interface. The **Main Menu** (top) includes options like 'Integrate Chromatogram' and 'Integrate and Extract Peak Spectra'. The **Method Editor: Integrate (MS)** (bottom) shows the configuration for the 'Integrate Chromatogram' action, with a **Run Button** (play icon) to execute the method. The **Right Click Menu** (middle) is shown over a chromatogram plot, offering options like 'Integrate Chromatogram' and 'Integrate and Extract Peak Spectra' for the selected peak. The chromatogram shows a peak at 9.772 minutes. The mass spectrum below shows peaks at 114.1, 126.1, 152.1, 162.1, 177.0, and 188.2 m/z.

Set parameters for action in Method Editor. Then, perform action.
Note : The action will be performed on ALL selected (highlighted) items!

Change and Error Icons



When you make a change to the current method the change is marked. In addition, all other functions that are affected by this change will be marked. Save the **method to remove the icon.**



An invalid value has been entered into a field. The field will reset to the last valid value it contained.



Additional information is required. The error must be fixed before the algorithm will execute.

Working with Chromatograms

- The power of Qualitative analysis is that you can have more than 1 data file open at a time.
- Extract Chromatograms from Data Files.
- Displaying Chromatograms
 - Selecting for display
 - Zooming
 - Scaling
 - Overlay / List mode
 - Anchoring

Define Chromatograms

The screenshot displays the Agilent MassHunter Qualitative Analysis software interface. The main window is titled "Agilent MassHunter Qualitative Analysis B.06.00 - Default.m". The interface is divided into several panes:

- Data Navigator:** Shows a tree view of data files, including "pest-0.05ppm.D", "pest-0.1ppm.D", "pest-0.2ppm.D", and "pest-10ppm.D". Each file has sub-entries for "User Chromatograms", "User Spectra", "Background Spectra", "Compounds", and "Matched Sequences".
- Chromatogram Results:** Displays four stacked Total Ion Chromatograms (TIC) for the different files. The x-axis is labeled "Counts (%) vs. Acquisition Time (min)" and ranges from 4 to 10.5. The y-axis is labeled "x10²".
- Method Explorer: Default.m:** Shows a list of methods, with "Define Chromatograms" selected.
- Method Editor: Define Chromatograms:** Shows the configuration for the selected method. It includes a list of "Defined chromatograms" (currently "BPC (all) MS (Cycle-summed)"), buttons for "Add", "Change", and "Delete", and a "Chromatogram definition" section with a "Type" dropdown set to "BPC" and an "Integrate when extracted" checkbox.
- MS Spectrum Results:** Shows the mass spectrum for the selected method.

Data Loaded & Displayed

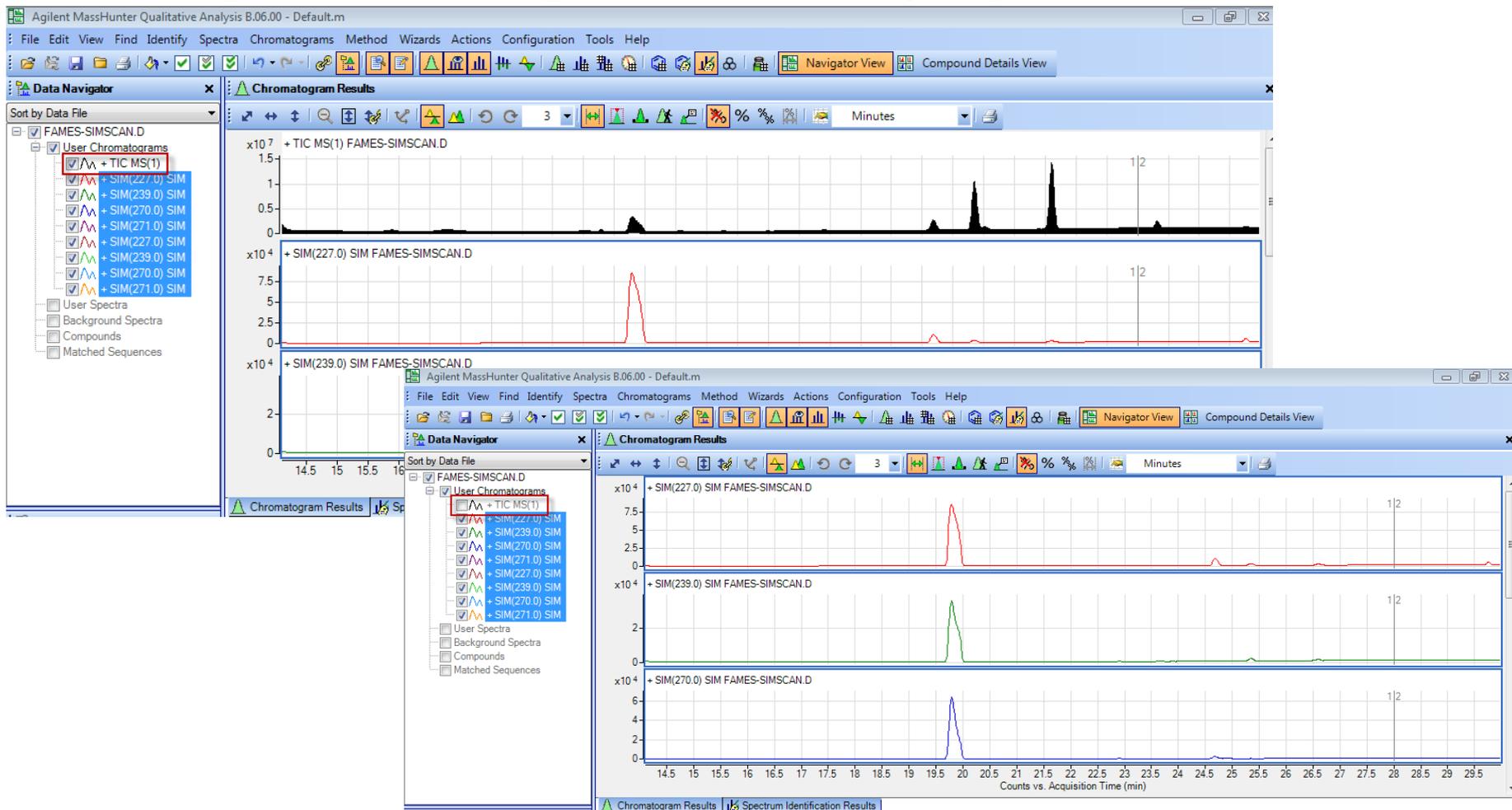
Can Display:
TOF Data
QTOF Data
QQQ Data
SQ Data
UV data
FID Data

Extract Chromatogram

The screenshot displays the Agilent MassHunter Qualitative Analysis software interface. The 'Data Navigator' on the left shows a tree view of data files, including 'pest-0.05ppm.D', 'pest-0.1ppm.D', 'pest-0.2ppm.D', and 'pest-10ppm.D'. A context menu is open over the 'pest-0.05ppm.D' file, with 'Extract Chromatograms...' selected. The 'Extract Chromatograms' dialog box is open, showing a list of opened data files: 'pest-0.05ppm.D', 'pest-0.1ppm.D', 'pest-0.2ppm.D', and 'pest-10ppm.D'. The 'Type' is set to 'EIC'. The 'MS level' is 'All', 'Polarity' is 'Positive', 'Scans' is 'All scan types', and 'm/z of interest' is 'Any'. The 'm/z value(s)' field contains '91.1'. The 'Integrate when extracted' checkbox is unchecked. The 'Merge multiple masses into one chromatogram' checkbox is also unchecked. The background shows a chromatogram plot with a red trace and a zoomed-in view of a peak at 10.5 minutes.

List of Chromatogram types is determined by data in file.

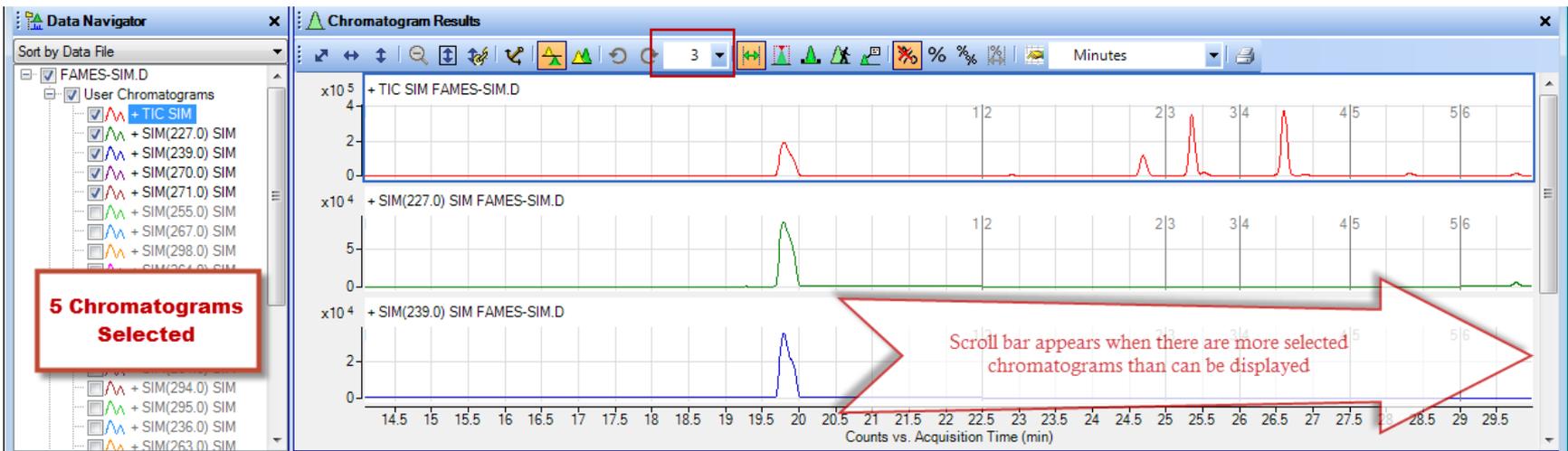
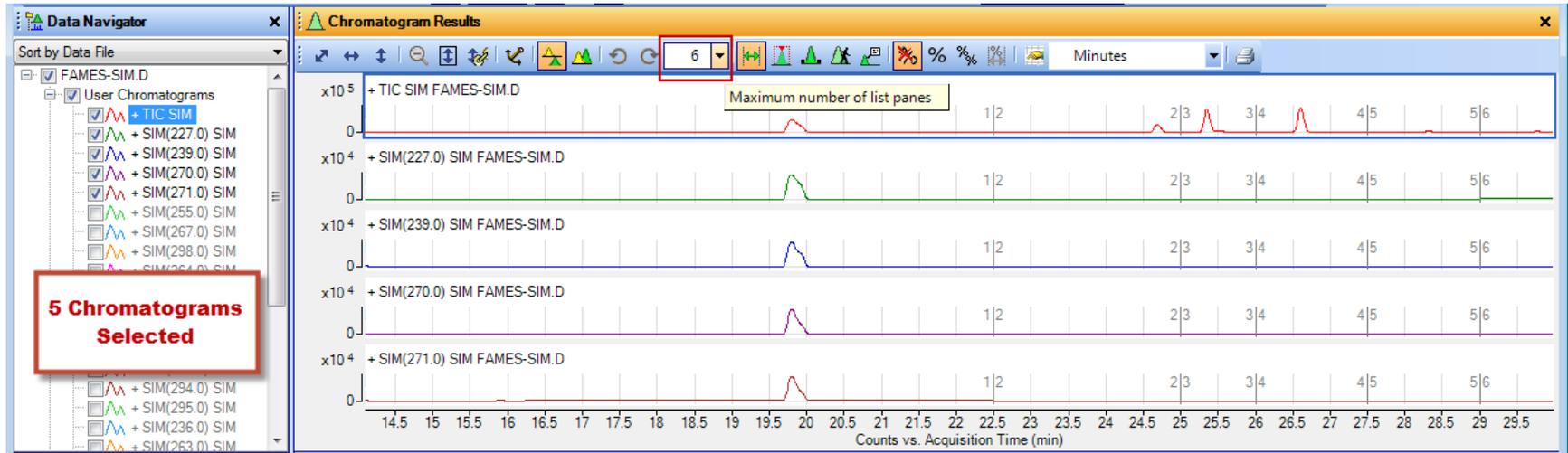
Selecting Chromatograms for Display



Items in the Data Navigator, like Chromatograms, will be displayed if checked and not displayed if unchecked.

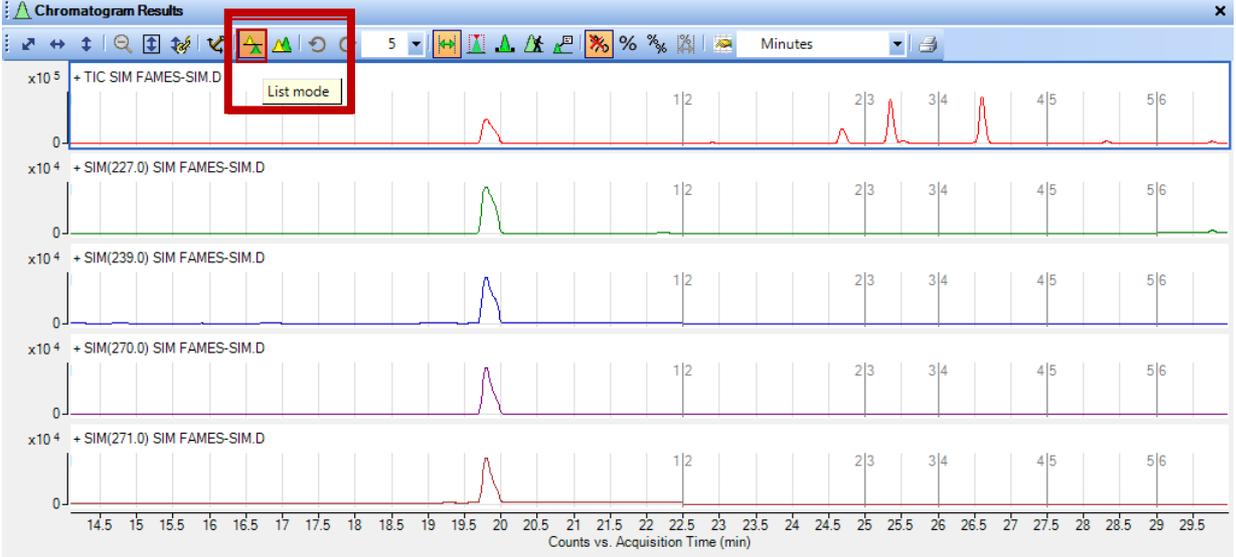
Specify Number of Chromatograms Displayed

Maximum number of chromatograms to display in window, may be fewer.

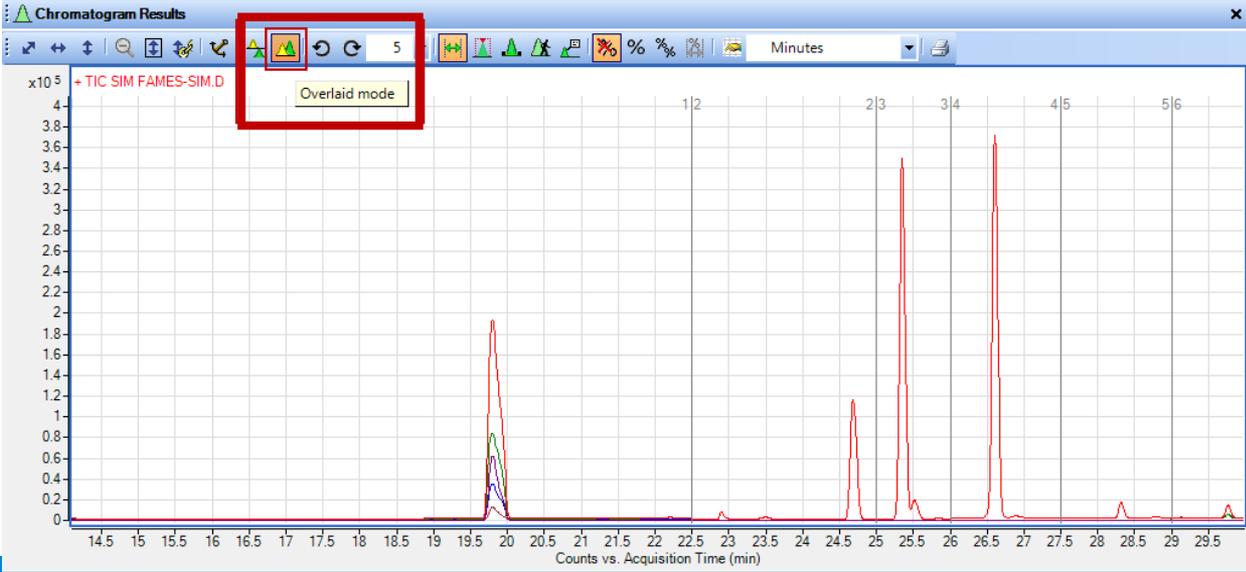


Overlay vs. List Mode Chromatograms

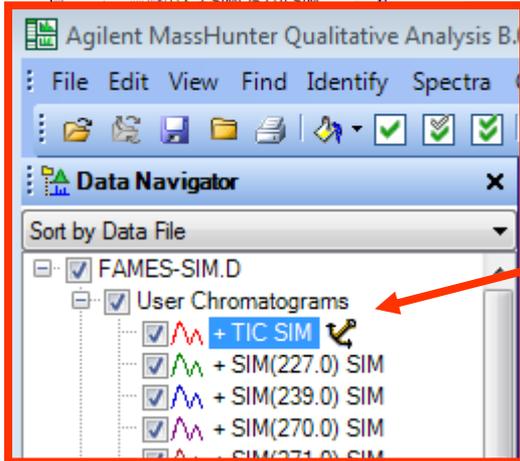
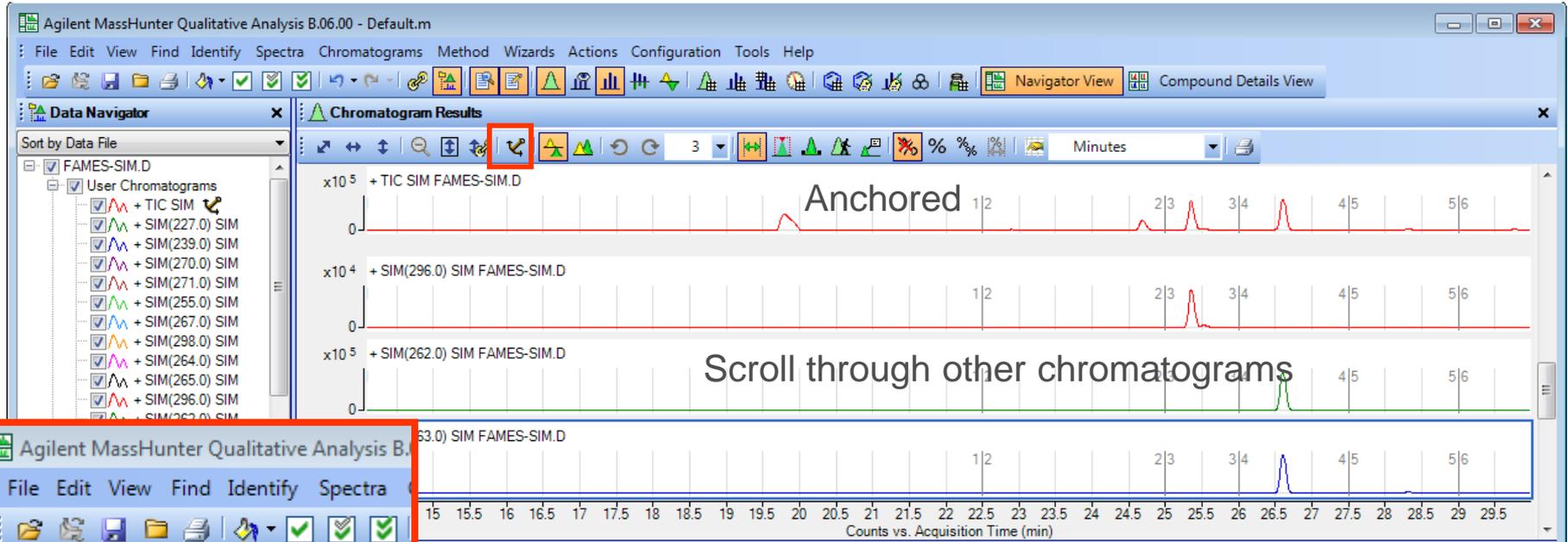
List
(Separated)



Overlaid



Anchoring



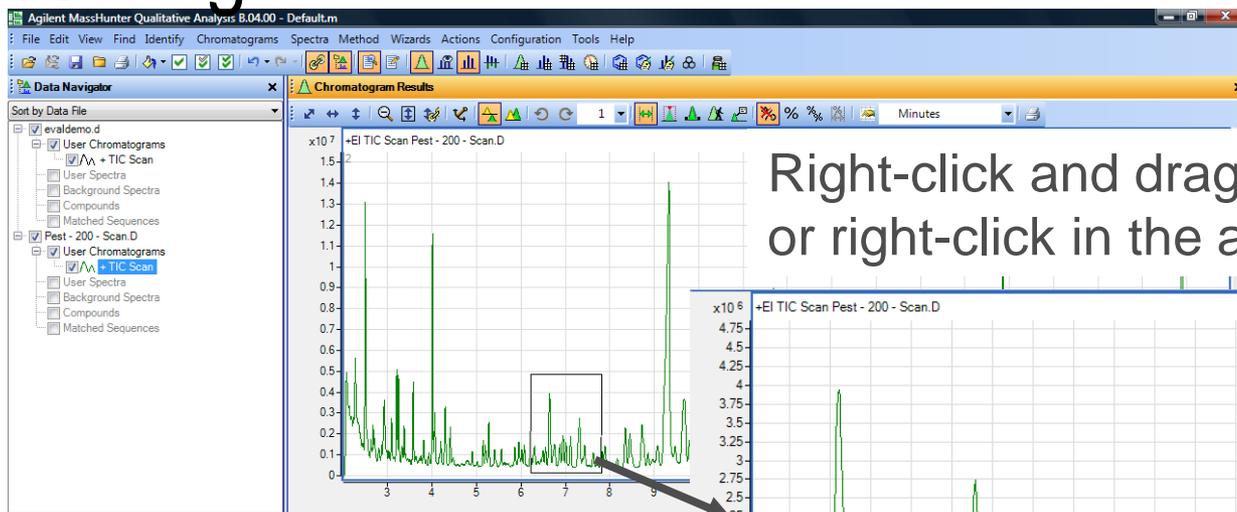
Setting an anchor keeps the anchored chromatogram displayed at all times.

Only one Chromatogram can be anchored at a time.

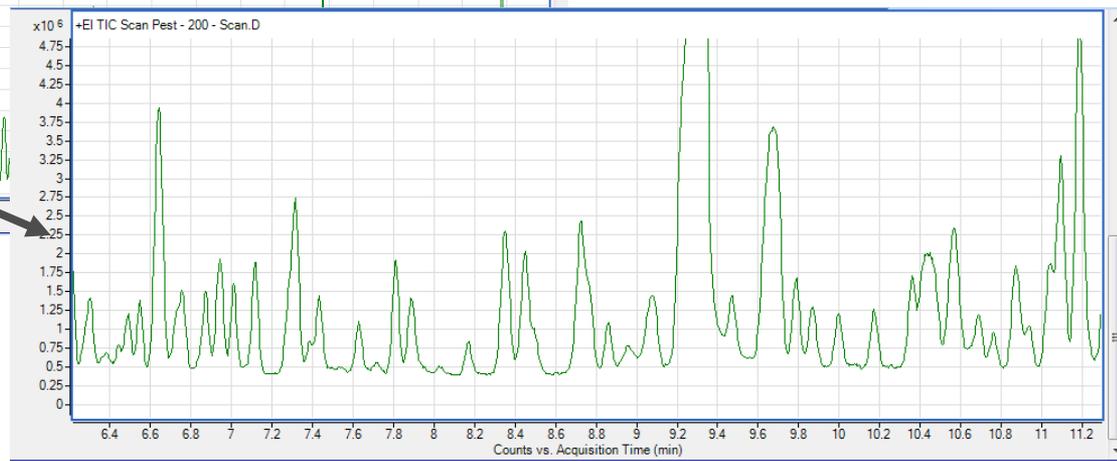
The anchor can be set and cleared from the context menu.

Set Anchor
Clear Anchor

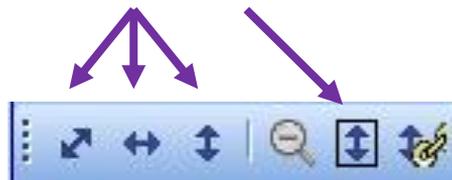
Zooming



Right-click and drag over the desired area or right-click in the axis and drag to zoom.



Autoscale



Unzoom

(multiple levels)

Linked Y-axis

Normalization



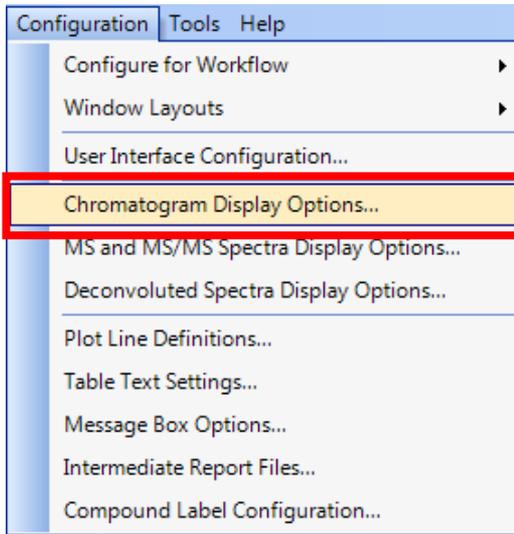
Scale to largest in Each over Selected Range

Scale to largest in Each

Scale to largest in All

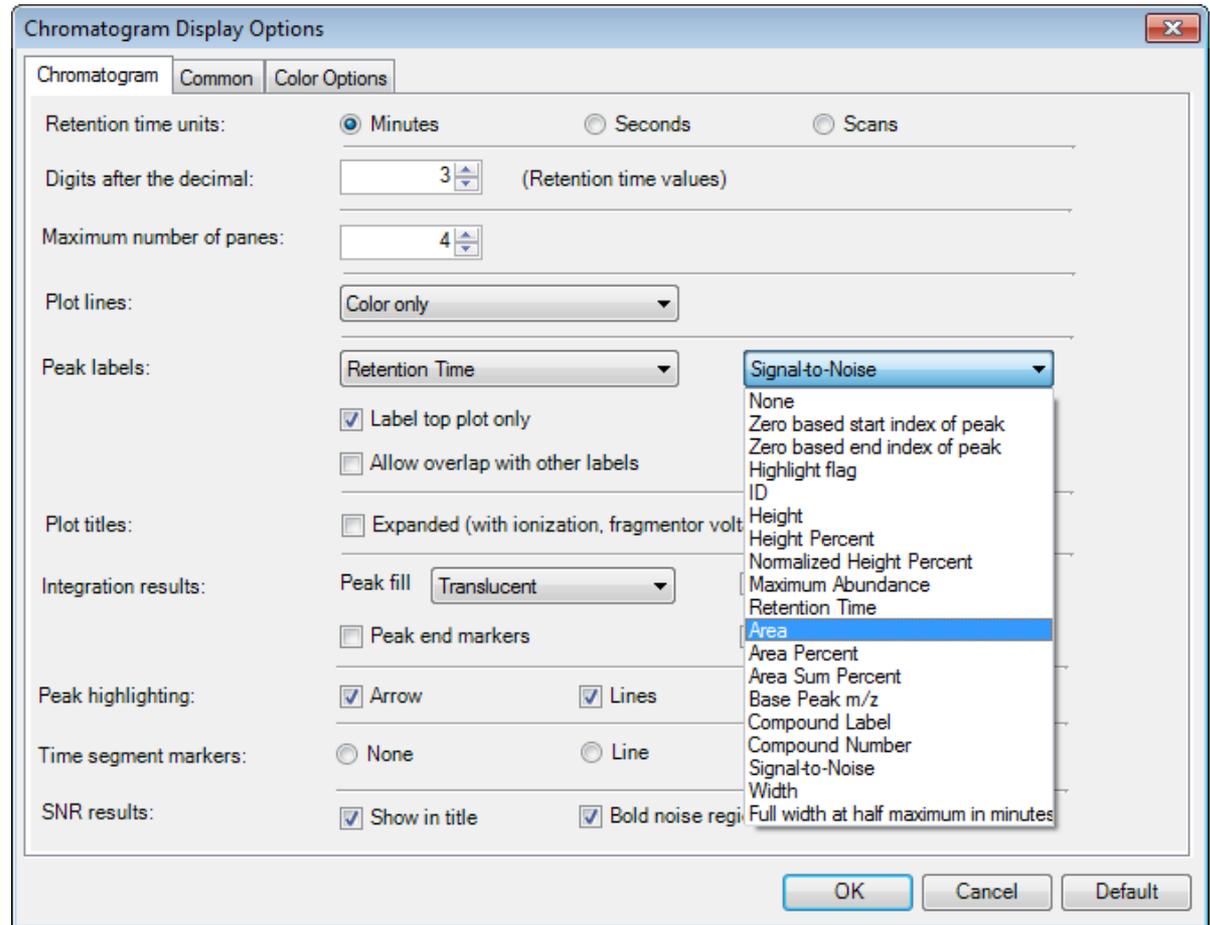
Scale Off

Chromatogram Display Options

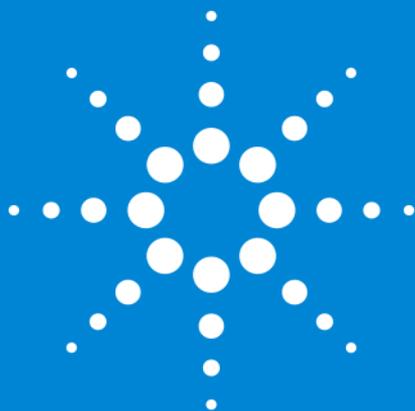


Main Menu

Within Display

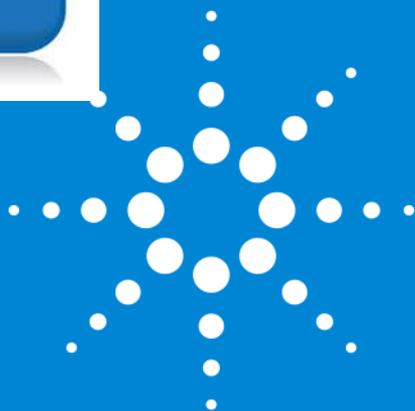


Customize Appearance of Chromatograms



Let's take a moment
for questions on
Chromatogram Display
Options.

Up Next:
Chromatogram Functions



Let's take a moment
for a demo on
Chromatogram Display
Options.

Up Next:
Chromatogram Functions

Chromatogram Functions

Chromatogram

Integrate (MS)

Integrate (GC)

Smooth

Exclude Mass(es)

Calculate Signal-to-Noise

Define Chromatograms

Extraction Data Format

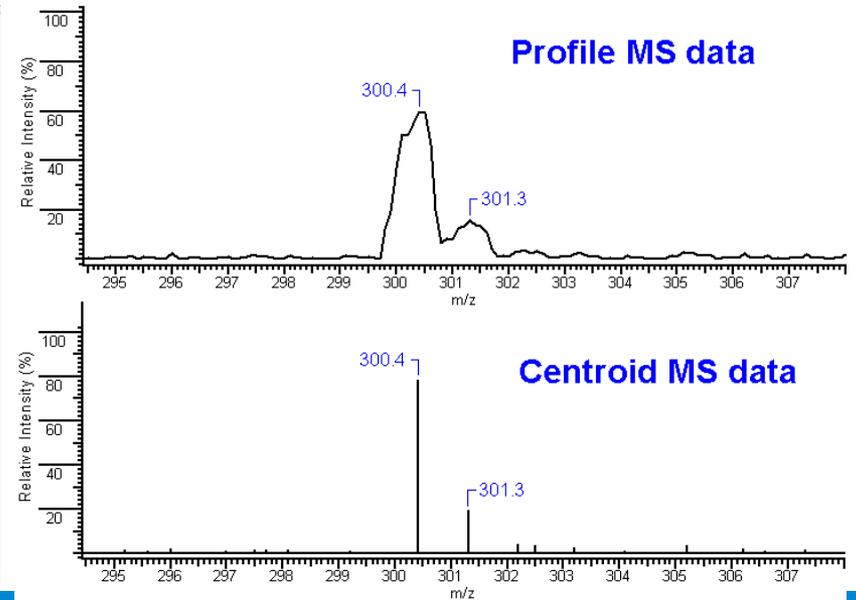
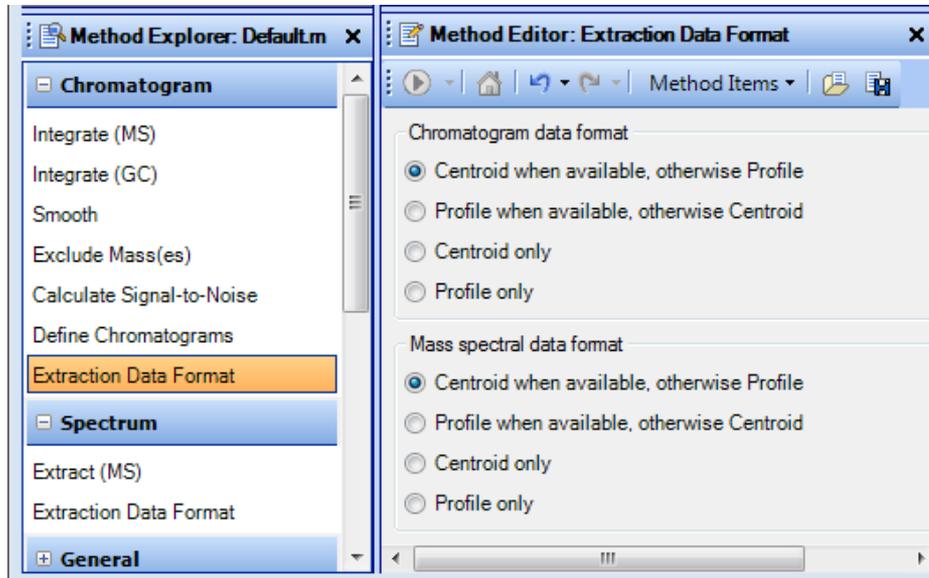
Identify chromatographic peaks for further analysis.

Exclude certain masses when depicting chromatograms.

Extract chromatograms.

Extraction Data Format - Profile and Centroid

- Data files may contain Centroid, Profile (Raw) or both data types.
- Settings determine which type is used to create chromatograms / spectra.
- Centroid data is the most commonly used, ~10 times smaller than Profile
- Profile is useful for mass peak area comparisons such as when optimizing acquisition parameters, i.e. finding the mass defect or center of mass centroid
- How is Profile Data activated?



Extract Defined Chromatogram

The screenshot displays the Agilent MassHunter Qualitative Analysis 8.06.00 interface. The 'Data Navigator' on the left shows a tree view of data files, with a context menu open over the 'pest-0.1ppm.D' file. The 'Extract Defined Chromatograms' option is highlighted in the menu. A red arrow points from this menu item to the 'Extract Defined Chromatograms' dialog box in the foreground. The dialog box shows a list of opened data files: pest-0.05ppm.D, pest-0.1ppm.D, pest-0.2ppm.D, and pest-10ppm.D. Below the list, there are 'Extract' and 'Cancel' buttons. The background shows the 'Chromatogram Results' window with four stacked Total Ion Chromatograms (TIC) for different concentration levels: 0.05ppm.D, 0.1ppm.D, 0.2ppm.D, and 10ppm.D. The x-axis is labeled 'Counts (%) vs. Acquisition Time (Minutes)'.

Software extracts a list of chromatograms which are stored in the Extract Defined Chromatogram section of the method.

List of Chromatogram types is fixed list of all instrument types.

Extract Define Chromatograms

- Select MS Level based on acquisition scan type.

The screenshot displays the Agilent MassHunter Qualitative Analysis software interface. The top panel shows the 'Chromatogram Results' window with a Total Ion Chromatogram (TIC) plot. The y-axis is labeled 'x10⁶ +EI TIC Scan Pest - 200 - Scan.D' and ranges from 0 to 4.75. The x-axis represents time in minutes, ranging from 6.4 to 8.0. The plot shows several peaks, with the most prominent one at approximately 6.6 minutes. The bottom panel shows the 'Method Editor: Define Chromatograms' dialog box. The 'Defined chromatograms' list contains 'BPC (all) MS (Cycle-summed)'. The 'Chromatogram definition' section shows 'Type: BPC' and 'Integrate when extracted' checked. The 'MS Chromatogram' section is expanded, showing 'MS level: MS', 'Polarity: Both', 'Scans: All single stage scan types', 'm/z of interest: Any', and 'm/z value(s):'. A green arrow points to the 'Change' button in the 'Defined chromatograms' list.

Types of Chromatograms

TIC – Total Ion Chromatogram

BPC – Base Peak Chromatogram

EIC – Extracted Ion Chromatogram

SIM – Selected Ion Monitor

Other Chromatograms – GC, DAD, ADC

Instrument Curve (LC) - %Comp., Temps, etc.

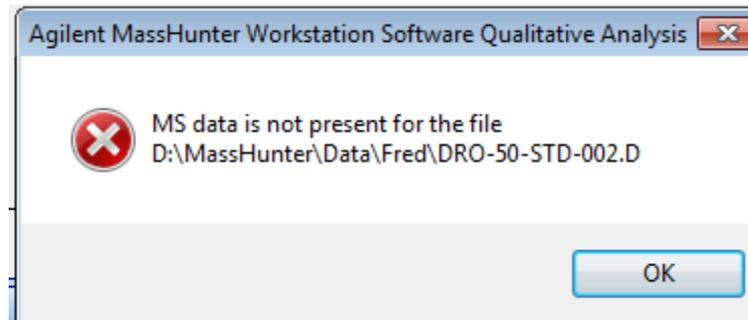
Triple Quad systems only

MRM – Multiple Reaction Monitor

pNLC - Precursor Neutral Loss Chromatogram

Tip: Select Change or Add.

Extracting GC, UV and other Non-MS Signals



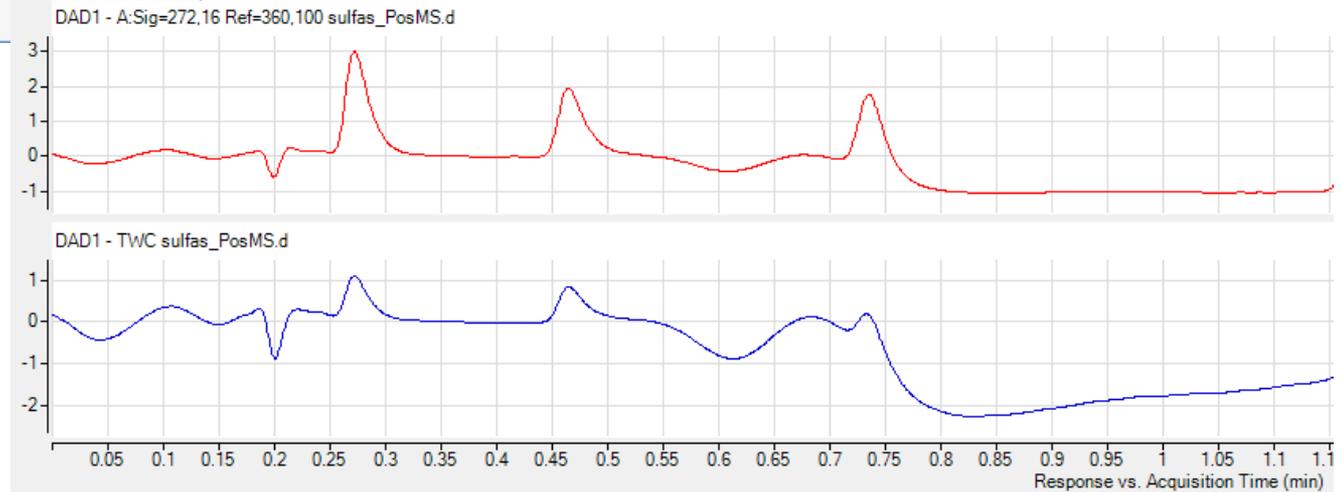
Extract All Non-MS Chromatograms

Actions Configuration Tools Help

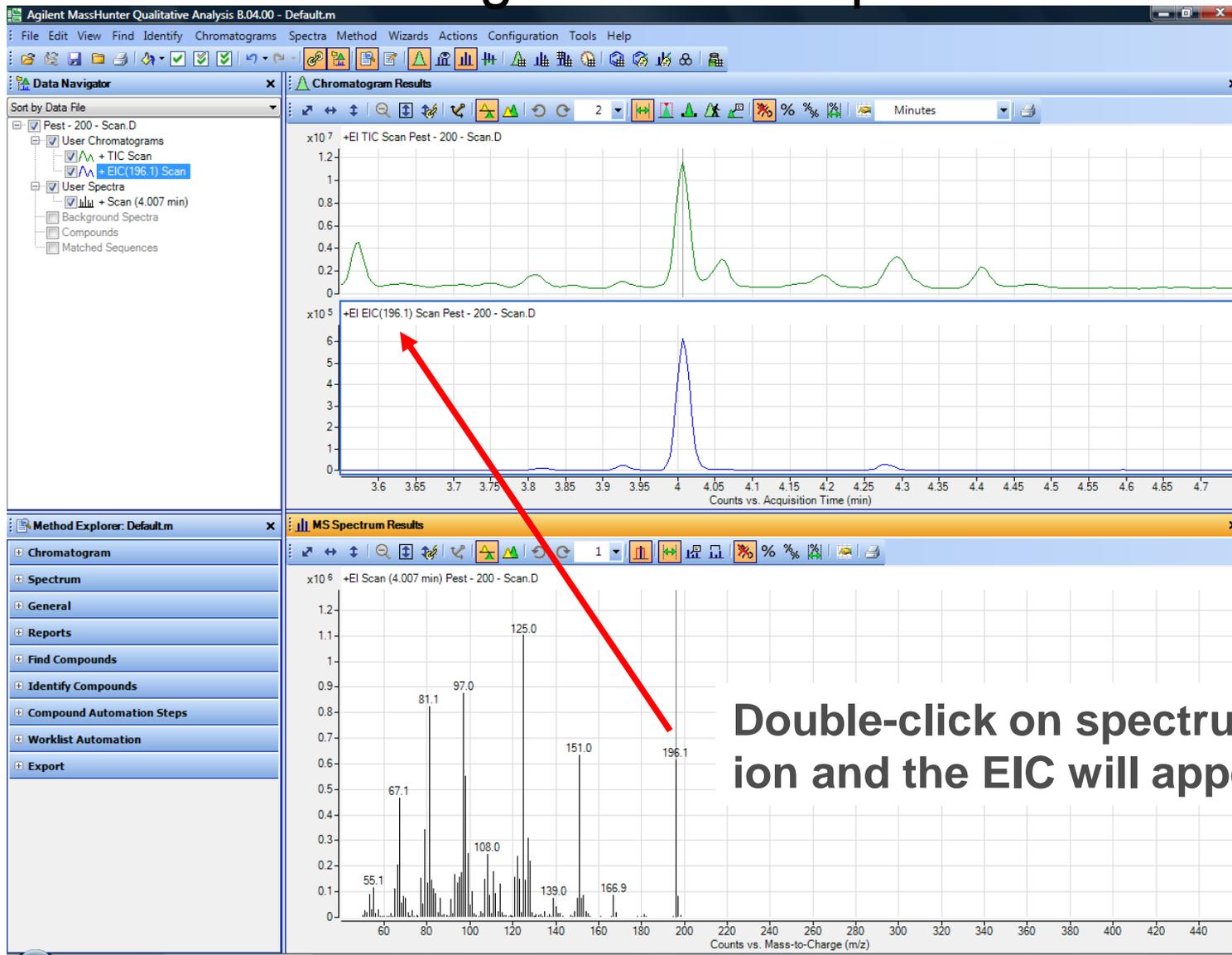
- Run the Worklist Actions
- Run the File Open Actions
- Extract Peak Spectra
- Extract Defined Chromatograms
- Integrate Chromatograms
- Integrate and Extract Peak Spectra
- Smooth Chromatograms

- Correlate TIC with MFE Compounds
- Correlate TIC with Find by Integration
- Extract All Non-MS Chromatograms
- Extract All Instrument Curves

Select **Actions** > **Extract All Non-MS Chromatograms**.



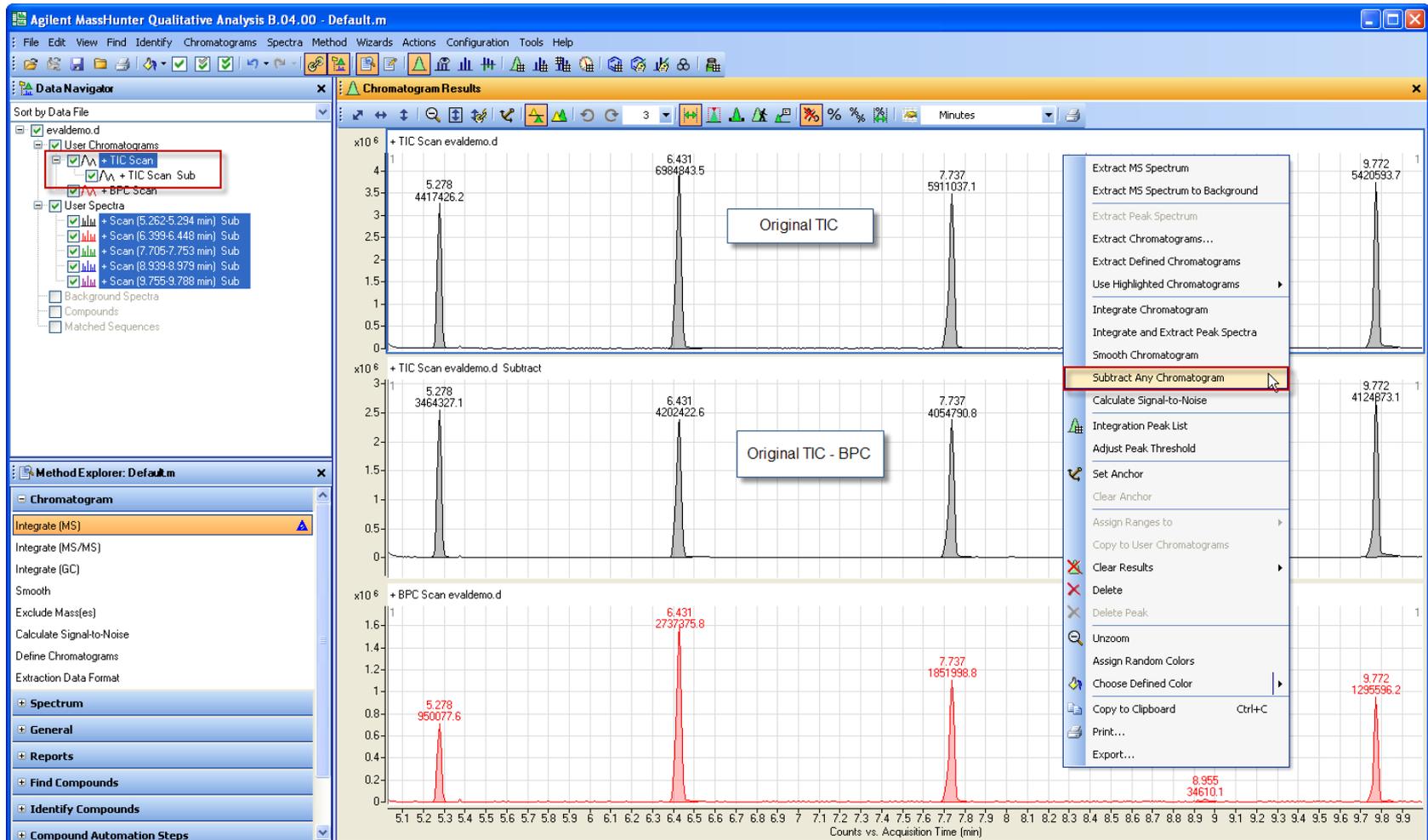
Extract Ion Chromatograms from Spectra



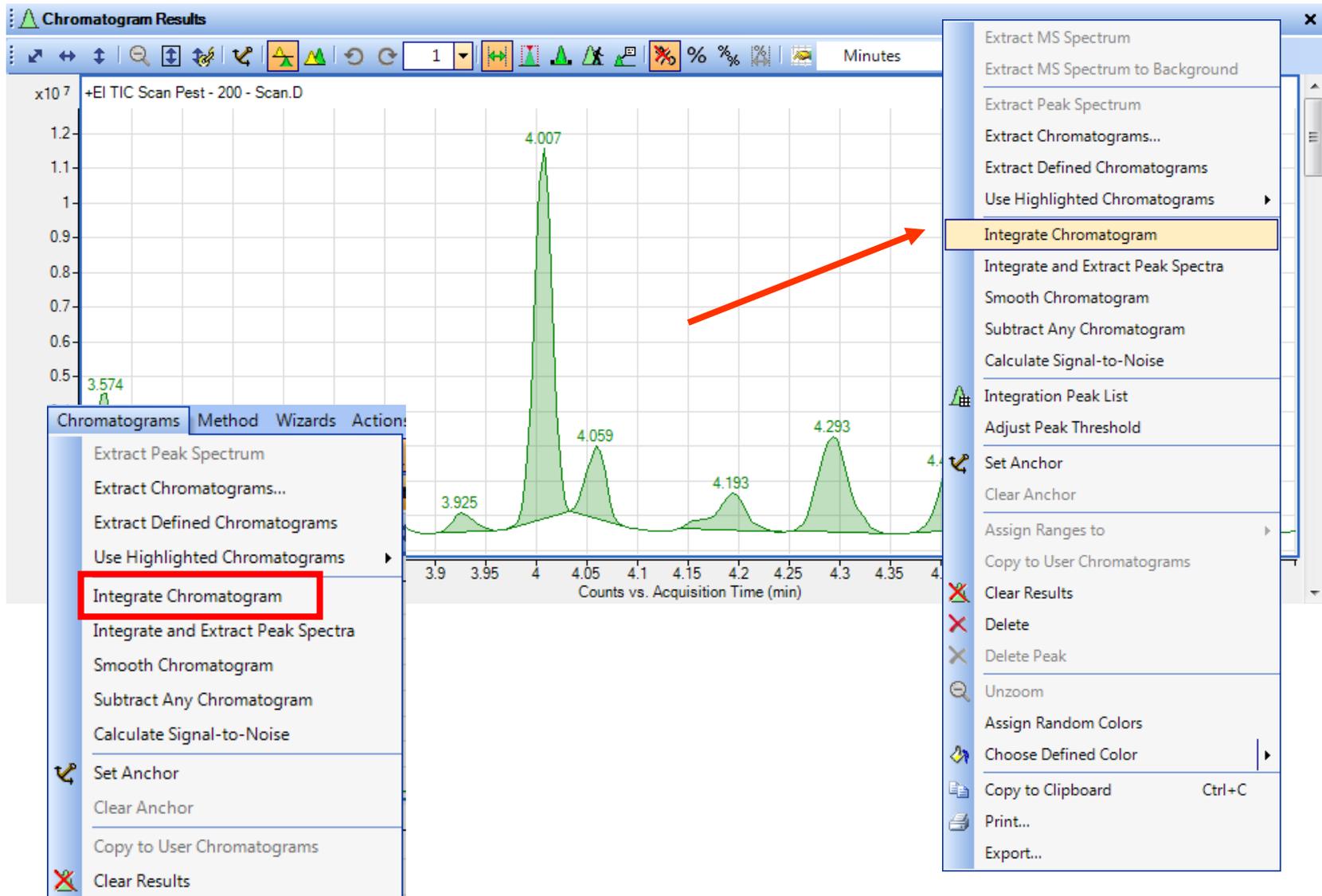
Double-click on spectrum ion and the EIC will appear.

Subtract Any Chromatogram

Right click in Chromatogram, select “Subtract Any Chromatogram”, the next chromatogram you click on will be subtracted from 1st one.



Integrate Chromatogram



Integrate Chromatogram

Independent Integrator for each configuration.

The screenshot displays the Agilent software interface for integrating a chromatogram. On the left, the 'Method Explorer' shows a tree view with 'Chromatogram' expanded, and 'Integrate (MS)' selected. An orange arrow points from the text 'Independent Integrator for each configuration.' to the 'Integrate (MS)' method. The main window is titled 'Method Editor: Integrate (MS)' and shows the 'Integrator' tab with 'Integrate Chromatogram' selected. The 'Integrator selection' list includes 'Agile 2', 'ChemStation', 'General', 'Universal', 'MS/MS', 'MS/MS (GC)', 'Agile', and 'Agile 2'. The 'Results' tab is active, showing 'Filter on' options for 'Peak height' and 'Peak area', with 'Peak area' selected. The 'Area filters' section shows 'Relative area' set to 1.000. The 'Maximum number of peaks' section shows 'Limit (by height) to the largest' set to 100.

Integrator Types

Agile2

- Default Integrator, 3rd generation parameterless integrator
- Better baselines, higher sensitivity to smaller peaks

Agile

- 2nd generation parameterless integrator

Universal

- 1st generation ChemStation integrator
- Familiar to ChemStation users

General (RTE)

- Familiar to MSD ChemStation users
- Areas in Universal are 10 time smaller than seen in ChemStation

MS/MS and MS/MS (GC)

- 1st generation parameterless integrator intended for MS/MS systems, not recommended for SQ. Originally required 64 data points.

ChemStation

- 2nd generation ChemStation
- Intended for UV

Integration Peak List



The screenshot shows the Agilent MassHunter Qualitative Analysis B.06.00 interface. The main window displays a Total Ion Chromatogram (TIC) with several peaks labeled with their retention times: 1.092, 1.729, 2.801, 4.387, 5.862, 7.794, 9.391, 10.330, 12.050, 12.899, and 14.440. A table titled 'Peaks: + TIC Scan' is open, showing the following data:

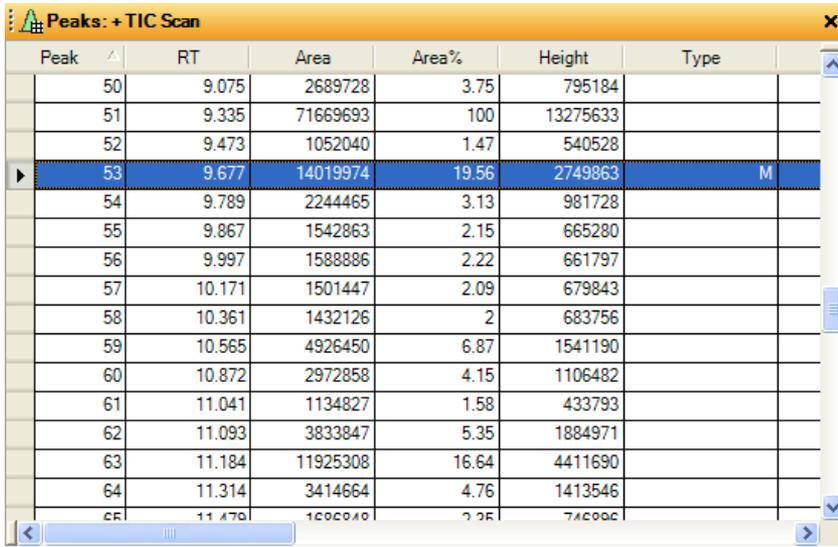
Peak	RT	Area	Height	Type	Width	FWHM	SN
1	1.092	77952859.41	7612918.32		0.413	0.169	
2	1.383	10235578.69	1959827.69		0.112	0.11	
3	1.461	8212983.73	1688114.13		0.134	0.075	
4	1.651	8609082.19	1915739.45		0.112	0.074	
5	1.729	134576403.06	7221652.96		0.447	0.327	
6	2.198	55317944.2	5686861.89		0.503	0.133	
7	2.801	30883808.17	4659114.77		0.257	0.102	
8	3.069	51566225.25	2944294.61		0.503	0.278	
9	3.471	2444509.65	425827.79		0.112	0.123	
10	3.594	23868582.69	2047197.44		0.547	0.154	
11	4.387	37076639.75	4150100.73		0.67	0.14	
12	5.862	18625684.03	1319444.43		0.771	0.235	

An 'Add/Remove Columns' dialog box is open, showing a list of available columns and a list of columns to be displayed. The 'Available Columns' list includes: Area Sum %, Baseline, End, End BL Y, End Y, Height %, Height % (Norm), Start, Start BL Y, and Start Y. The 'Show these columns' list includes: Area, Area %, Base Peak, Cpd, Flags (Tgt), FWHM, Height, k', Label, Max Y, Peak, Plates, Plates/M, Resolution, RT, SNR, Symmetry, Tailing factor, Type, and Width. Buttons for 'Add ->', '<- Remove', 'Add All ->>', '<<- Remove All', 'OK', and 'Cancel' are visible.

Right-click on the Peak List header to Add/Remove Columns.

Tip: Tables can be configured.

Integration Peak Tables (all tables)



Peak	RT	Area	Area%	Height	Type
50	9.075	2689728	3.75	795184	
51	9.335	71669693	100	13275633	
52	9.473	1052040	1.47	540528	
53	9.677	14019974	19.56	2749863	M
54	9.789	2244465	3.13	981728	
55	9.867	1542863	2.15	665280	
56	9.997	1588886	2.22	661797	
57	10.171	1501447	2.09	679843	
58	10.361	1432126	2	683756	
59	10.565	4926450	6.87	1541190	
60	10.872	2972858	4.15	1106482	
61	11.041	1134827	1.58	433793	
62	11.093	3833847	5.35	1884971	
63	11.184	11925308	16.64	4411690	
64	11.314	3414664	4.76	1413546	
65	11.479	1699949	2.35	742896	

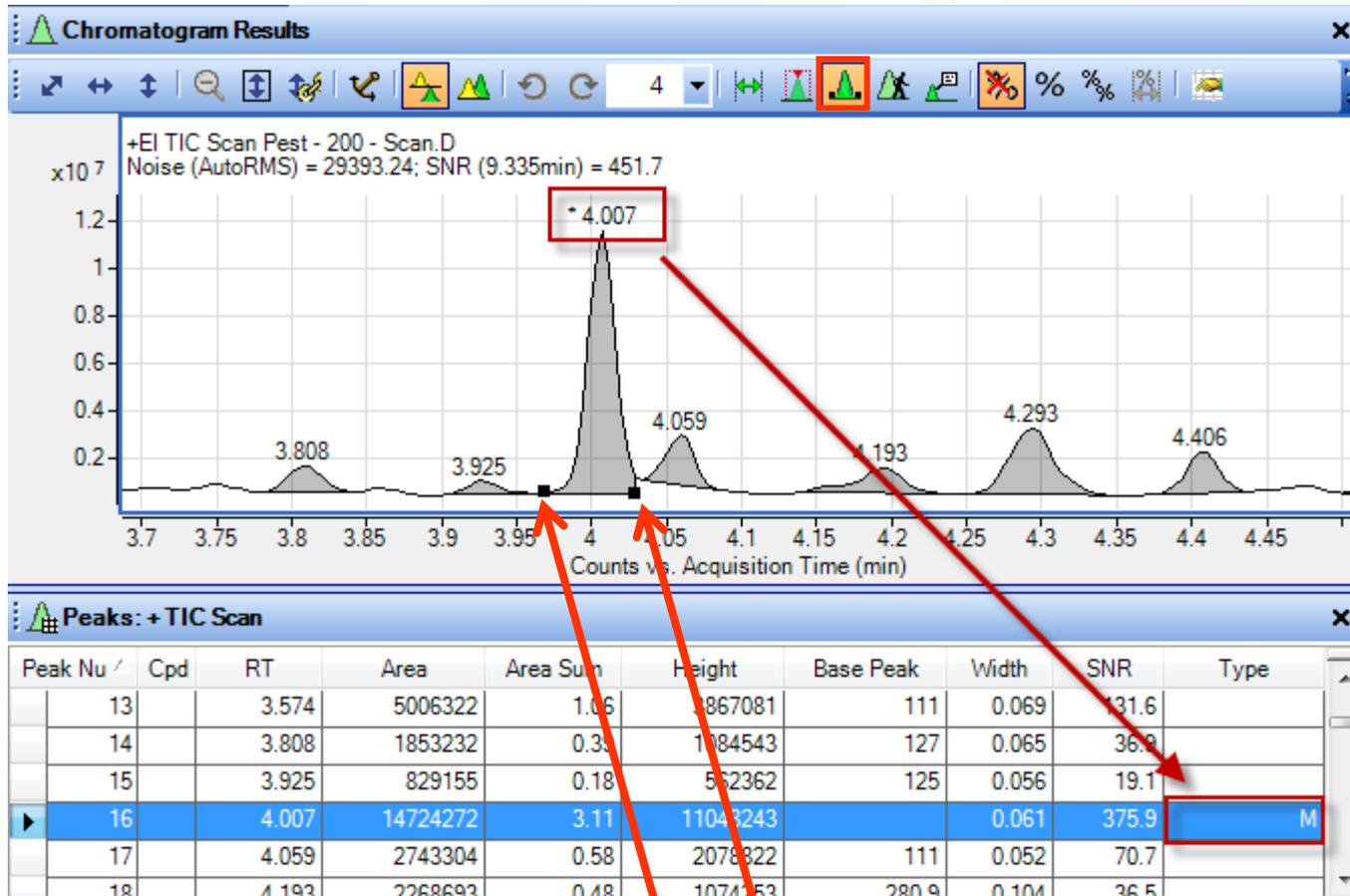
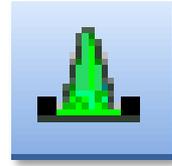
Tables can be moved to different locations.

Tables can be split for easy viewing.

Columns can be added, removed, and moved.

Columns can be moved by Clicking and dragging on column header.

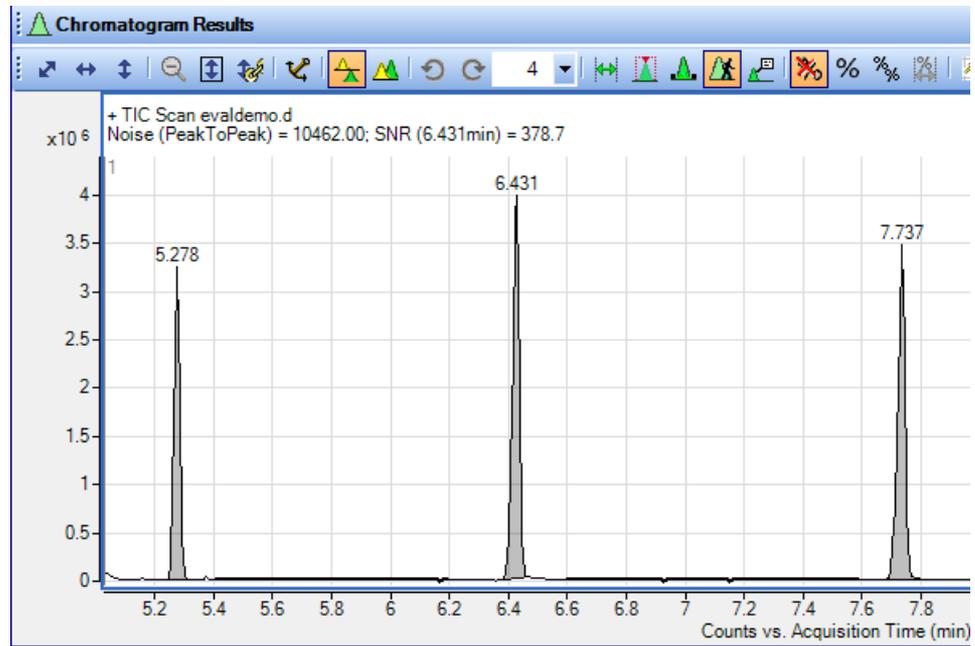
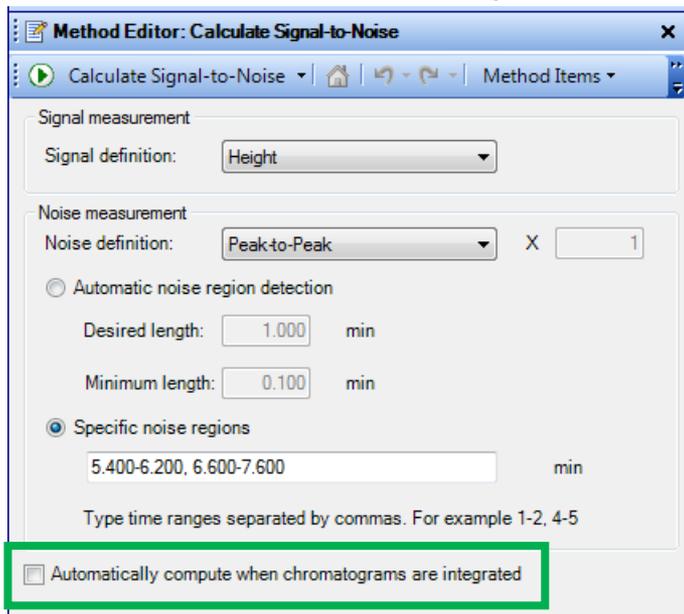
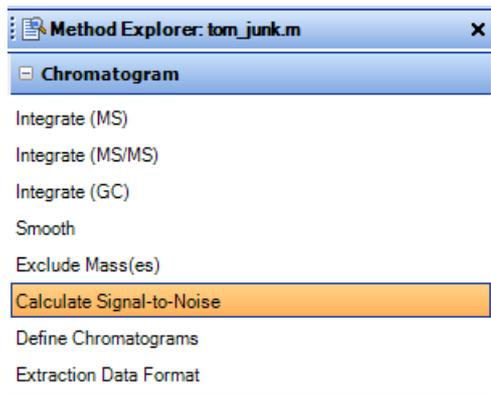
Manual Integration



Use mouse cursor to manually integrate peak.

Calculate Signal-to-Noise Specific Noise Regions

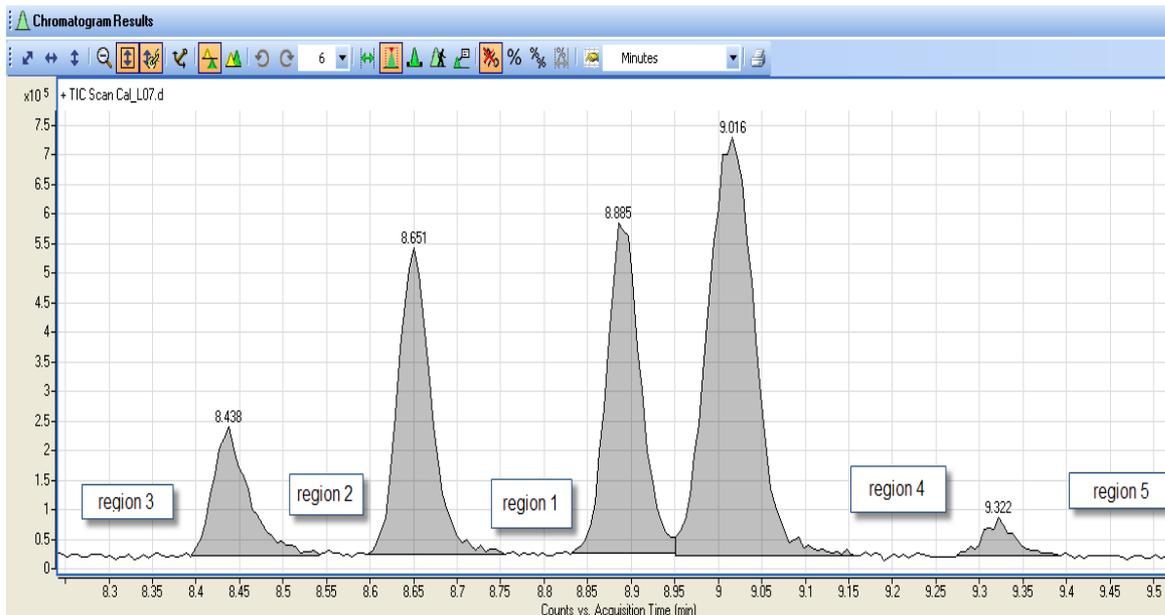
- User defined specific noise regions.
- May be performed automatically when Chromatogram is integrated.



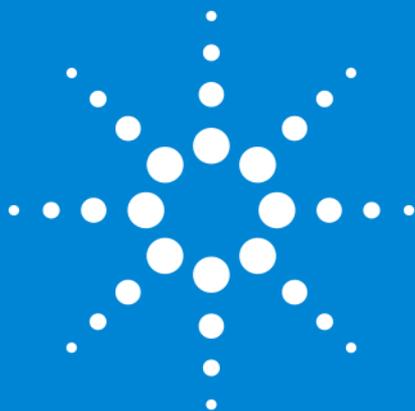
Calculate Signal-to-Noise

Automatic Noise Region Detection

- Alternative to user defined specific noise regions in which the software seeks to locate a “noise region” between the peaks found by the integrator
- User specifies a maximum length (desired) and minimum length of noise region and software locates an acceptable region if one exists



Method Editor: Calculate Signal-to-Noise window. The "Signal measurement" section has "Signal definition" set to "Height". The "Noise measurement" section has "Noise definition" set to "Peak-to-Peak" with a multiplier of 1. The "Automatic noise region detection" option is selected and highlighted with a red box. Below it, "Desired length" is set to 1.000 min and "Minimum length" is set to 0.100 min. The "Specific noise regions" option is unselected. At the bottom, there is a checkbox for "Automatically compute when chromatograms are integrated".



Let's take a few moments for questions on Chromatogram Functions.

Up Next:
Training Resources.



Time for a demo on
Chromatogram
Functions.

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. At the top, the Agilent logo and 'Trusted Answers' are on the left, and navigation links (ABOUT AGILENT, CONTACT US, UNITED STATES, LOGIN) and a search bar are on the right. A red arrow points to the 'TRAINING & EVENTS' menu item. Below the main navigation, a sub-menu for 'Training & Events' is visible, with a red arrow pointing to the 'Education' link. The main content area features a large banner with the text 'AGILENT UNIVERSITY' and a button labeled 'VIEW ALL TRAINING COURSE OFFERINGS >' circled in red. Below the banner, three columns of text describe benefits: 'Increase Tenure and Maximize Productivity', 'Convenient Training', and 'Agilent Training Credits'.

Questions on today's material...

Thank you for your attention.



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