Agilent MassHunter Workstation Software

Qualitative Analysis

Familiarization Guide for GC/MS

Agilent Technologies

Notices

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Software Revision

This guide is valid for B.08.00 and later revisions of the Agilent MassHunter Workstation Software - Qualitative Analysis software, until superseded.

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In This Guide...

This guide contains information to learn to use your Agilent MassHunter Workstation Software - Qualitative Analysis with GC/MS data. Qualitative Analysis has two main programs.

- Qualitative Analysis Navigator - You use this program to examine chromatograms and spectra and identify ions in mass spectra. It is especially well suited to manual, ad-hoc examination of your data.
- Qualitative Analysis Workflows - You use this program's compound mining algorithms to find evidence for compounds in your data. You can also use its identification algorithms to identify unknown compounds based on that evidence.

Different windows are available in each of these programs. The following windows are available in both views:

- Method Editor
- Difference Results
- Structure Viewer
- Formula Calculator
- Mass Calculator

Qualitative Analysis Navigator Program

In this program, you can use the Data Navigator window to interactively select different spectra and chromatograms. You can generate formulas or search a library/database for these spectra.

If you are looking at spectra that you have manually extracted or that are extracted by the **Integrate and Extract Peak Spectra** algorithm, then you want to use this program.

Qualitative Analysis Workflow Program

This program provides a compound centric view of one or more data files. You can look at information on a single compound in different windows. You change the selected compound in the Compound List window. You switch between different data files in the Sample Table.

If you want to use any of the Compound Mining algorithms, you use this program.

If you are using either of these programs and decide that you need to also use the tools available in the other program, that program can be launched using the Launch menu. You can also specify which of the currently open data files should be opened in the launched program.

Before you begin the exercises, please read the instructions in "Before you begin these exercises..." on page 7.

Exercise 1 Learn basics of qualitative analysis

In this exercise, you explore some of the many powerful capabilities of the Qualitative Analysis Navigator program. These tasks are important no matter what data type you are using.

Exercise 2 Find and identify

In these tasks, you find and identify compounds in GC/MS data files. You use the Qualitative Analysis Workflows program to do compound mining. You can also identify those compounds in this program.

Exercise 3 Use workflows, export and print

In these tasks, you learn to set up and run a workflow. Each of these tasks is done using a different workflow.

Reference

In this chapter, you learn some basics about the Qualitative Analysis program.

What's New

in B.08.00

The following features apply to both the Qualitative Analysis Navigator program and the Qualitative Analysis Workflows program.

- Windows 10 and Windows 7 are supported.
- Microsoft Excel 2016 is supported.
- The menus and windows have been simplified.
- The Method Explorer window and the Method Editor window are combined into one window.
- All toolbars have been simplified.
- The user interface configuration is set automatically based on the file or files that are loaded.
- Only relevant menus and windows are available, based on the types of data files loaded.
- Database Search and Library Search are combined and run as a single action. The software automatically runs the correct action based on your data and the database/library selected.
- You select one of four workflows for Method Automation: **Target/Suspect Screening**, **Sample Purity**, **Compound Discovery**, and **Custom**. In the Qualitative Navigator program, you can only run the Custom workflow. In the Qualitative Analysis Workflows program, you can run all of these workflows.
- Additional chromatograms can be extracted when you run a workflow.
- You can run the workflow from the Method menu.
- The gray line that used to show the last location that was clicked is no longer shown in plots. A gray, vertical line shows the current location in the plot, but when the cursor is not in that window, the line is removed.
- Qualitative Analysis uses the latest version of algorithms shared with MassHunter Quantitative Analysis program.

- Qualitative Analysis methods and results are backwards compatible.
- BioConfirm features are removed from the Qualitative Analysis programs.

The following features apply to the Qualitative Analysis Navigator program.

- The Peak Select tool is the default tool for the Chromatogram Results window.
- The Peak Select tool behaves like the Range Select tool in that you can select arbitrary ranges with either tool if the chromatogram is not integrated. However, if the chromatogram is integrated and the range you draw overlaps one or more peaks, then the Peak Select tool selects the RT range of those peaks.
- The Spectrum Preview window is closed automatically.
- You can launch BioConfirm from the Qualitative Analysis Navigator program if BioConfirm is installed.

The following features are available in the Qualitative Analysis Workflows program.

- All features related to finding compounds are in the Qualitative Analysis Workflows software.
- You can select Auto-select compound mining for the Target/Suspect Screening workflow and the Compound Discovery workflow.
- The Compound Discovery workflow automatically runs the Compound Identification workflow.
- The Find by Fragments algorithm runs on GC/TOF or GC/Q-TOF data.
- You can specify a different report template for each workflow.
- The Score (Frag Ratio) column is available in the Compound List window.
- CI is supported for GC/Q-TOF All Ions workflow.
- You can create a CEF file when you run Fragment Confirmation with GC/Q-TOF EI data.

- You can overlay the chromatograms from the selected compounds on the Sample Chromatogram.
- The Extract Chromatograms button is available on the Sample Chromatogram Results window.
- You can extract an EIC when you double-click in the Compound MS or MS/MS spectra.
- When you double-click in the Sample Chromatogram, a compound is extracted and added to the Compound List window, and the Mining Algorithm is Spectrum Extraction.
- The Compound Chromatogram Results window has relative zooming.
- The Sample Table window shows sample information details and Result Summary. You can edit the sample prep parameters.
- The title bar for the Compound List window shows summary details.
- The Compound List groups columns by their column category.
- The Compound List only has one level.
- The Find by Molecular Feature algorithm supports feature finding of GC/MSD and GC/Q-TOF data.
- The Q-Score is included when you create a CEF file with MFE compounds.
- New Qualitative Analysis columns are available in the Agilent Walkup program.
- New Qualitative Analysis columns are available in the Agilent Data Acquisition for TOF/Q-TOF program.

Before you begin these exercises...

- Install the software. See the Installation Guide for instructions.
- Copy the folder named **Data** from your installation disk in uncompressed format to any location on your hard disk.

  This folder contains all the data files needed for these

exercises. You may need to first extract the data files from their .zip format.

NOTE

Do not reuse the example data files already on your system unless you know that you copied them from the originals on the disk and you are the only one using them. If the example data files already on the system do not match the original ones on the disk exactly, then the results obtained during these exercises will not match those shown in the guide.

Contents

Exercise 1
Learn basics of qualitative analysis

In this exercise, you explore some of the many powerful capabilities of the Qualitative Analysis Navigator program for working with GC/Q-TOF and GC/QQQ data. You can do many of these basic tasks in the Qualitative Workflows program, but the actual steps may be different.

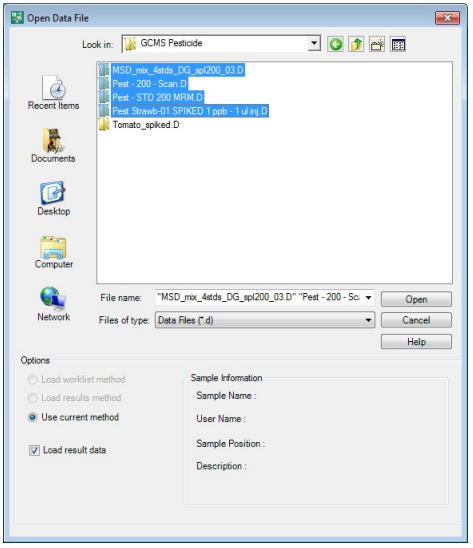
Each exercise is presented in a table with three columns:

- Steps – Use these general instructions to proceed on your own to explore the program.
- Detailed Instructions – Use these if you need help or prefer to use a step-by-step learning process.
- Comments – Read these to learn tips and additional information about each step in the exercise.

Task 1. Open the Qualitative Analysis Navigator program

In this task you open multiple data files in the Qualitative Analysis Navigator program using the current method.

Task 1. Open the Qualitative Analysis program with multiple data files

Steps	Detailed Instructions	Comments
1 Open the Qualitative Analysis program. • Open the data files, **Pest - 200 - Scan.d**, **Pest - STD 200 MRM.d, Pest Strawb-01 SPIKED 1 ppb - 1 ul inj.d** and **MSD_mix_4stds_DG_spl200_03.d** in the folder **\\MassHunter\Data**, or in the folder where you copied them.	**a** Double-click the **Agilent MassHunter Qualitative Analysis Navigator B.08.00** icon  . The system displays the Open Data Files dialog box. **b** Go to the folder **\\MassHunter\Data\GCMS Pesticide** or the folder where the example files are located.	• The Pest - 200 - Scan.d file contains MS data, and the Pest - STD 200 MRM.d and Pest Strawb-01 SPIKED 1 ppb - 1 ul inj.d files contain both MS and MS/MS data (all GC/QQQ). MSD_mix_4stds_DG_spl200_03.d contains GC/Q-TOF data. • You can get help for most windows, dialog boxes, and tabs by pressing the **F1** key when that window is active. • Click **File > Open Data File** if the files are in different folders.
• Make sure that the **Use current method** button is clicked. • Make sure that the **Load result data** check box is clear or grayed out. If the **Load result data** check box is not available, then no results have been saved in the data file. You learn how to save results in "Task 17. Save results" on page 75.	 **Figure 1** Open data files when opening software	

Task 1. Open the Qualitative Analysis program with multiple data files (continued)

Steps	Detailed Instructions	Comments
	c Press and hold the **Shift** key while you click **MSD_mix_4stds_DB_spl200_03.d** and then **Pest Strawb-01 SPIKED 1 ppb - 1 ul inj.d.** **d** Click **Open**. All four data files are displayed in the Data Navigator window, and 1 to 4 chromatograms are displayed in the Chromatogram Results window. **e** In the Chromatogram Results toolbar, click the **List Mode** icon ( ).	• If you press the **Ctrl** key, you can pick files which are not directly next to each other in the list. • What you see in the main window at this point depends on the method, layout, display, and plot settings used before you opened these files. • When you click the List Mode icon, the background of the icon changes to orange.

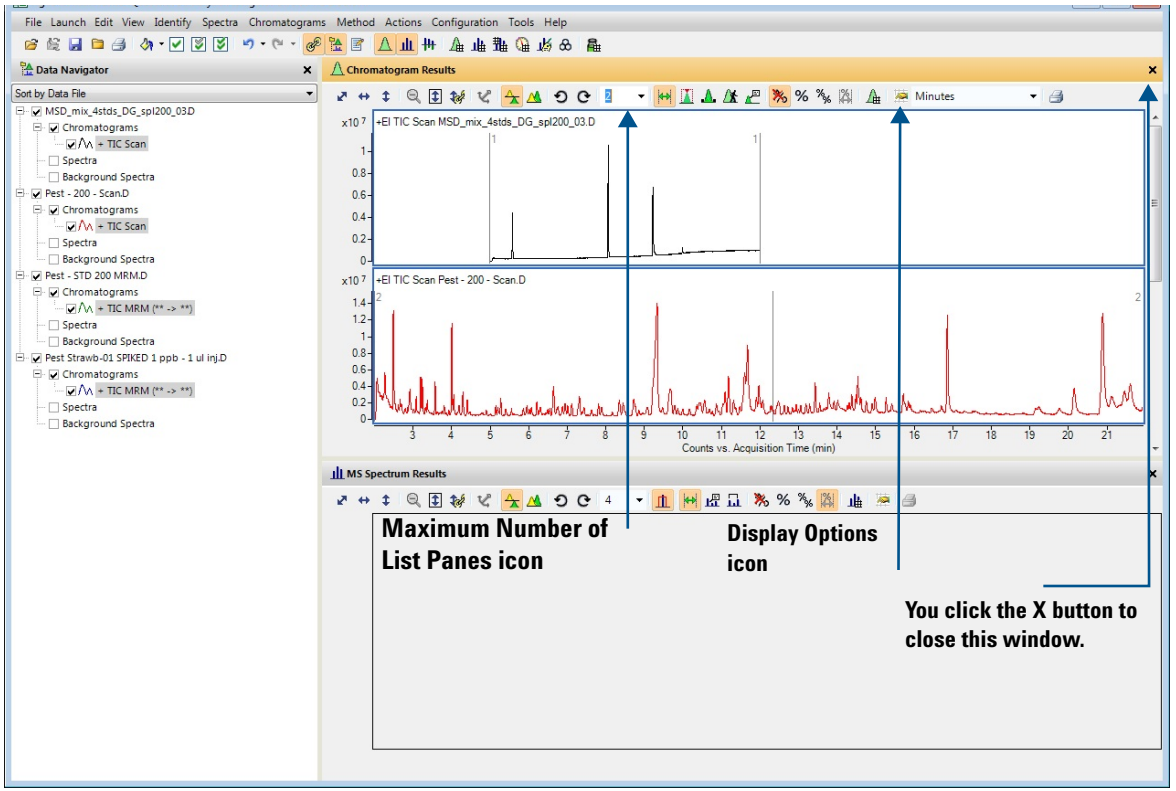


Figure 2 Qualitative Analysis main window

Task 1. Open the Qualitative Analysis program with multiple data files (continued)

Steps	Detailed Instructions	Comments
2 Restore the main window to the default layout and method. • Make sure you can see all four chromatograms.	**a** If necessary, click **Configuration > Window Layouts > Restore Default Layout**. **b** Click the down arrow next to the Maximum Number of List Panes icon in the Chromatogram Results toolbar, and select 4. **c** Click **Method > Open**. **d** Select *default-GCMS.m*. **e** Click **Open**. **f** You may be asked whether or not to save method changes for your current method. Click **Yes** or **No**.	• The Qualitative Navigator program has an adaptive user interface that automatically configures itself based on the type(s) of data file(s) that you open.

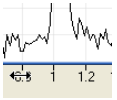
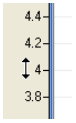
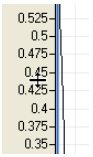
Task 2. Zoom in and out of the chromatogram

In this task, you become familiar with the zoom in and zoom out features of the Qualitative Analysis Navigator program. You can use the zoom features in the Qualitative Analysis Workflows program, also.

Task 2. Zoom in and out of the chromatogram

Steps	Detailed Instructions	Comments
1 Practice zooming in and out of only one of the four chromatograms (both x and y axes). • Hide the others. • Zoom in twice on last peak. • Zoom in one more time autoscaling the y-axis. • Zoom out once to the previous zoom position. • Completely zoom out to the original chromatogram.	**a** Clear the check boxes in the Data Navigator window for the chromatograms you want to hide. **b** Make sure that the **Autoscale Y-axis during Zoom** icon,  , is not selected for the next step. **c** Click the right mouse button and drag over an area on the last peak. **d** Repeat step c. **e** Click the **Autoscale Y-axis during Zoom** icon,  , in the toolbar. **f** Click the right mouse button again and drag over an area of the last peak for the third time. The Qualitative Analysis Navigator program and the Qualitative Analysis Workflows program automatically scale the y-axis to the largest point in the range. **g** Click the **Unzoom** icon  to undo the last zoom operation. You can undo the last fifteen zoom operations. **h** Click the **Autoscale X-axis and Y-axis** icon  to zoom out completely.	• If a line is not checked in the Data Navigator window, that information is not displayed in any other window in the Qualitative Analysis program. You simply mark the check box for that information in the Data Navigator window, and the information is displayed in the other windows again. • A selected icon has an orange background color. • In the Qualitative Analysis Navigator program, you can also use these zoom features on spectra in other plot windows. • In the Qualitative Analysis Workflows program, you can also use these features in the Sample Chromatogram Results window, the Compound Chromatogram Results window, the Compound MS Spectrum Results window, the Compound Fragment Spectrum Results window, and the Spectral Difference Results window.

Task 2. Zoom in and out of the chromatogram (continued)

Steps	Detailed Instructions	Comments
2 Practice zooming in and out on each axis separately. • Zoom in only along the x-axis. Hint: Right-click the x-axis values and move cursor from left to right. • Partially zoom out the x-axis. Hint: Move cursor in opposite direction. • Completely zoom out of the x-axis. • Repeat the previous steps for the y-axis.	**a** To zoom in on the x-axis, move the cursor to the x-axis values until a horizontal double arrow appears. **b** Click the right mouse button and drag the new cursor from left to right across the x-axis values. **c** To zoom out on the x-axis, click the right mouse button and drag from right to left on the x-axis values. **d** Click the **Autoscale X-axis** icon to completely zoom out on the x-axis. **a** To zoom in on the y-axis, move the cursor to the y-axis values until a vertical double arrow appears. **b** Click the right mouse button and drag the new cursor from bottom to top across the y-axis values. **c** To zoom out on the y-axis, click the right mouse button and drag from the top towards the bottom of the y-axis values. **d** Click the **Autoscale Y-axis** icon to completely zoom out on the y-axis.	 **Horizontal Double Arrow**  **New cursor appears when you right-click the x-axis values.**  **Vertical Double Arrow**  **New cursor appears when you right-click the y-axis values.**

Task 3. Anchor a chromatogram

In this task, you anchor a chromatogram. When you anchor a chromatogram, the anchored chromatogram remains permanently on display as you scroll through the other chromatograms to display them.

Task 3. Anchor a chromatogram

Steps	Detailed Instructions	Comments

• Anchor a chromatogram.
  ◦ Show all chromatograms.
  ◦ Make sure the chromatogram viewing list is set to 1.
  ◦ In the Chromatogram Results window, select the second TIC.
  ◦ Anchor this TIC.
  ◦ Scroll through the chromatograms.
  ◦ Clear the anchor.
	a In Data Navigator mark the check boxes for the chromatograms you hid in the previous task.
	b Set the maximum number of panes to 1 in the Chromatogram Results window.
	c In the Chromatogram Results window, scroll if necessary and select the second TIC.
	d Right-click inside the chromatogram, and click **Set Anchor.**
	e Use the scroll bar in the Chromatogram Results window to scroll through the list of chromatograms. The second TIC stays visible always as the first chromatogram.
	f Click **Chromatograms > Clear Anchor.**
		• When you set an anchor for a chromatogram, an anchor icon appears in the Data Navigator window next to the name of the anchored chromatogram.
		• Two chromatograms appear in the Chromatogram Results window after you anchor one even though the viewing list says 1. This now means you view one chromatogram in addition to the anchored chromatogram.
		• You can also right-click the chromatogram and click **Clear Anchor** in the shortcut menu.
		• You cannot anchor a chromatogram or spectrum in the Qualitative Analysis Workflows program.

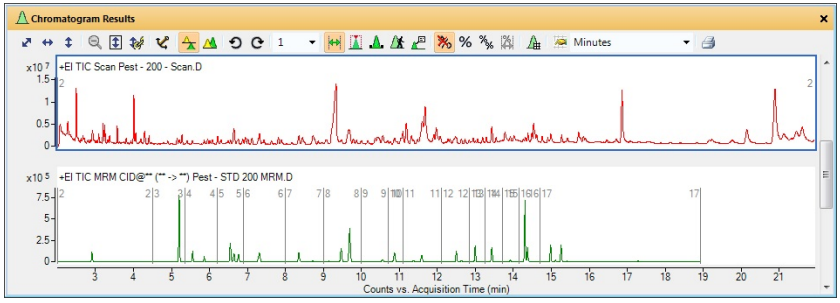


Figure 3 Anchored TIC in the Chromatogram Results window

Task 4. Change window layouts

In this task, you move windows within the main view and create various window layouts. You can save layouts in both the Qualitative Analysis Navigator program and the Qualitative Analysis Workflows program.

Task 4. Change window layout

Steps	Detailed Instructions	Comments
1 Change the window layout: • Change the window size. • Save a window layout. • Unlock the layout. • Change the Chromatogram Results window to be floating. • Move the Chromatogram Results window. • Display the tools for repositioning the windows.	• To change the size of a window, drag the boundary between the windows. • To save a window layout, click **Configuration > Window Layouts > Save Layout**. • To unlock a layout, click **Configuration > Window Layouts > Lock Layout**. • To make a window float, right-click the title bar of the window, and click **Floating** from the shortcut menu. You can instead double-click the title bar of the window to float the window. • To move a window, click the title bar of the window and drag the window to the desired location. • To display the repositioning tools, drag the window over one of the other windows. When one window is overlapped with another, the program displays several layout tools, as shown in Figure 4.	• If the layout is unlocked, the system does not display a check mark next to the Lock Layout menu. • You can only use the repositioning tools when the layout is unlocked. • You can also make a window float by double-clicking the title bar of the window. • The software has many different layouts created. You can also try loading different layouts. • The software has several different workflows. Each workflow loads a different layout. Switching to a different workflow also changes the layout.

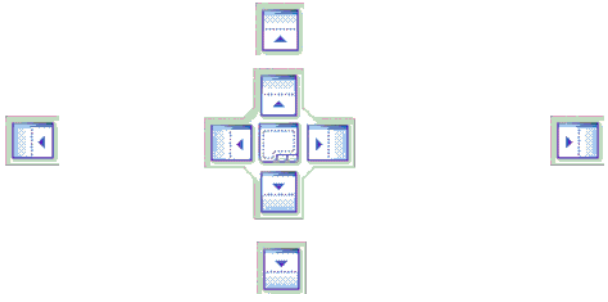


Figure 4 Window repositioning tools

Task 4. Change window layout (continued)

Steps	Detailed Instructions	Comments
2 Reposition the Chromatogram Results window. • Move the window so that it is at the top, to the left, to the right and then at the bottom of the other windows. • Move two windows together so that they are on top of one another and available only through the tabs at the bottom. • Restore the default layout.	• If, while dragging the window by its title bar, you drag the cursor over one of the smaller icons, the window you are dragging will be placed above, to the right, below, or to the left of all of the other windows. • Drag the cursor over the larger icon. The window can also be placed above, to the right, below, or to the left of the other window by dragging the cursor over the edges of the larger icon. • To tab two windows together, drag the cursor over the center of the larger icon. You will see a shadow version of the two windows tabbed together. Stop dragging the mouse. The two windows will be tabbed together. • To restore a floating window to its most recent docked position, you can double-click its title bar or right-click the title bar of the window and click **Floating**. • Click **Configuration > Window Layouts > Restore Default Layout**.	• The cursor must be over one of the arrows in a box in order for repositioning to occur. • Clicking the **Restore Default Layout** command restores the default layout. If you loaded a different layout, then you need to load that layout instead. To load a layout, click **Configuration > Windows Layouts > Load Layout**.

Task 5. Extract chromatograms

In this task, you extract and merge chromatograms from the original TIC using the Qualitative Analysis Navigator program. In the Qualitative Analysis Workflows program, you can extract additional chromatograms when you use the Extract Chromatograms tool on the Sample Chromatogram Results window's toolbar.

Task 5. Extract chromatograms

Steps	Detailed Instructions	Comments
1 Extract extracted ion chromatograms (EICs) from two masses in the **Pest - 200 - Scan.d** data file. • The m/z values are 129.0 and 414.2. • Do not merge the peaks from the individual masses into one chromatogram.	**a** In the Data Navigator window, clear the check boxes for the data files except for **Pest - 200 - Scan.d**. **b** Open the Extract Chromatograms dialog box, using the option below or one of the options to the right: • Click **Chromatograms > Extract Chromatograms**. **c** In the **List of opened data files**, click **Pest - 200 - Scan.d.** **d** In the **Type** list box, select **EIC**. **e** In the **m/z value(s)** box, type `129.0, 414.2` **f** If necessary, clear the **Merge multiple masses into one chromatogram** check box to merge the EICs. **g** If necessary, clear the **Integrate when extracted** check box. **h** Click **OK**. **i** Set the **Maximum number of list panes** to `4` or more in the Chromatogram Results toolbar.	• You can also extract chromatograms in one of the following ways: ◦ Right-click inside the chromatogram, and click **Extract Chromatograms**. ◦ From Data Navigator, highlight the **TIC Scan** for **Pest - 200 - Scan.d**; then, right-click **TIC Scan** and click **Extract Chromatograms**. • You can use an MS level of either **All** or **MS**. • Note that you can also choose to have the extracted chromatogram automatically integrated after extraction. • You can also extract a chromatogram from a mass spectrum. • Only three chromatograms are shown in the Chromatogram Results window because only three chromatograms are available.

Task 5. Extract chromatograms (continued)

Steps	Detailed Instructions	Comments

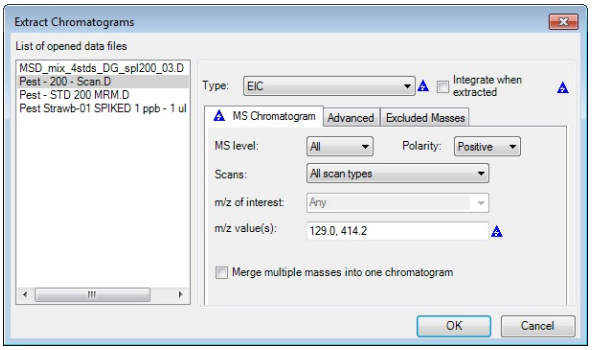


Figure 5 The Extract Chromatograms dialog box

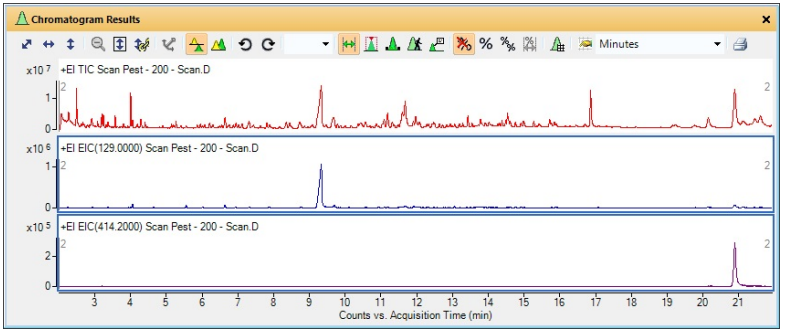


Figure 6 Merged extracted ion chromatograms (EICs) compared to the original TIC

2 Extract extracted ion chromatograms (EICs) from two masses in the **Pest - 200 - Scan.d** data file.
- The m/z values are 129.0 and 414.2.
- Do merge the peaks from the individual masses into one chromatogram.

a Open the Extract Chromatograms dialog box. Click **Chromatograms > Extract Chromatograms**.
b In the **List of opened data files**, click **Pest - 200 - Scan.d.**
c Mark the **Merge multiple masses into one chromatogram** check box to merge the EICs.
d Click **OK**.

- Four chromatograms are automatically shown in the Chromatogram Results window.
- The title for the fourth chromatogram is "+EI EIC(129.0000, 414.2000) Scan Pest - 200 - Scan.D". Both ions are merged in this chromatogram.

Task 5. Extract chromatograms (continued)

Steps	Detailed Instructions	Comments

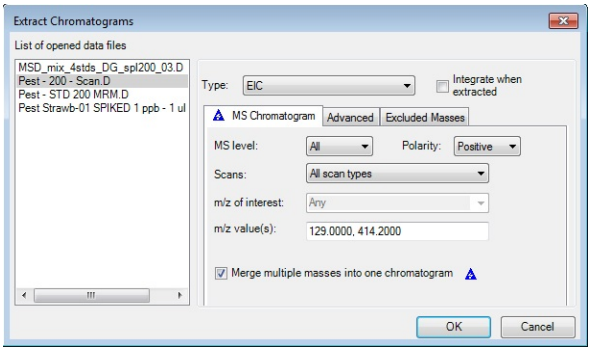


Figure 7 The Extract Chromatograms dialog box with **Merge multiple masses into one chromatogram** marked.

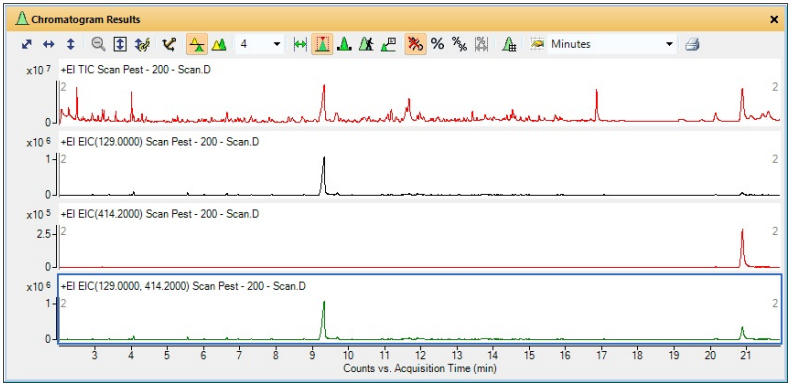


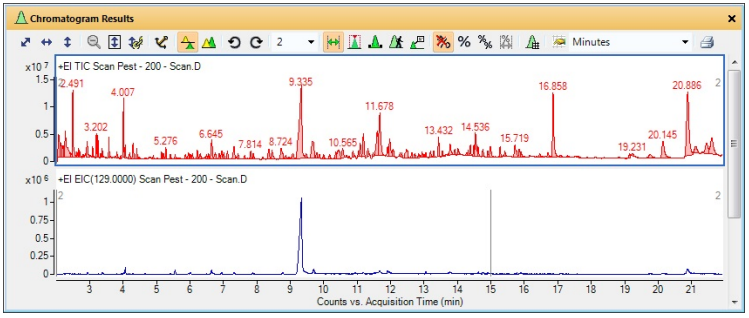
Figure 8 One merged extracted ion chromatogram (EIC) compared to the original TIC and two extracted ion chromatograms.

Task 6. Interactively integrate a GC/MS chromatogram

In this task, you learn different ways to integrate a chromatogram, change integration parameters to modify the results, and calculate the Signal-to-Noise for the integrated peaks for MS/MS data using the Qualitative Analysis Navigator program.

Task 6. Interactively integrate a chromatogram (GC/MS)

Steps	Detailed Instructions	Comments
1 Integrate the TIC Scan chromatogram for the **Pest - 200 - Scan.d** data file, using any of the options listed at right.	**a** Mark the Pest - 200 - Scan.D data file in the Data Navigator window. **b** Highlight the TIC Scan chromatogram, and use one of the following commands: • From the menu bar click **Chromatograms > Integrate Chromatogram**. • Right-click anywhere in the chromatogram window, and click **Integrate Chromatogram**. • In the Data Navigator window, select **Pest - 200 - Scan.D > Chromatograms > TIC Scan;** then, right-click the **TIC Scan**, and click **Integrate Chromatogram**.	• Note that the program integrated practically all the peaks in the chromatogram. • You select the integrator to use for MS data, MS/MS data, and GC data in the Method Editor window. • This chromatogram is an MS chromatogram, so the values that are set in the Integrate (MS) section of the Method Editor are used when integrating this chromatogram.
2 Display only two chromatograms at the same time.	• Select **2** in the **Maximum number of list panes** box in the Chromatogram Results Toolbar.	

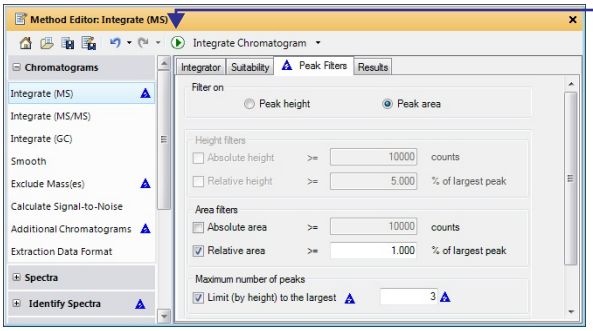


Many small peaks are integrated.

Figure 9 Integrated TIC Scan Chromatogram with many small peaks

Task 6. Interactively integrate a chromatogram (GC/MS) (continued)

Steps	Detailed Instructions	Comments
3 Change the threshold to integrate fewer peaks. • Change the threshold to retain only the three largest peaks.	**a** Click **View > Method Editor**. **b** In the Method Editor window, click **Chromatograms > Integrate (MS)** **c** Click the Integrator tab. **d** Review the parameters. **e** Click the **Peak Filters** tab. **f** Under Maximum number of peaks, mark **Limit (by height) to the largest,** and type 3.	• Note the blue triangle that appears when you change a setting from the value saved in the current method. When you save the method, the triangles disappear.



The Run button is labeled Integrate Chromatogram. The label changes depending on which tab is visible in the Method Editor and which action is selected.

Figure 10 Peak Filters tab with **Limit (by height) to the largest** marked

4 Reintegrate the chromatogram	**g** Click  on the Method Editor toolbar to integrate using the new setting.	• Note that only the three peaks with the highest height are integrated now.

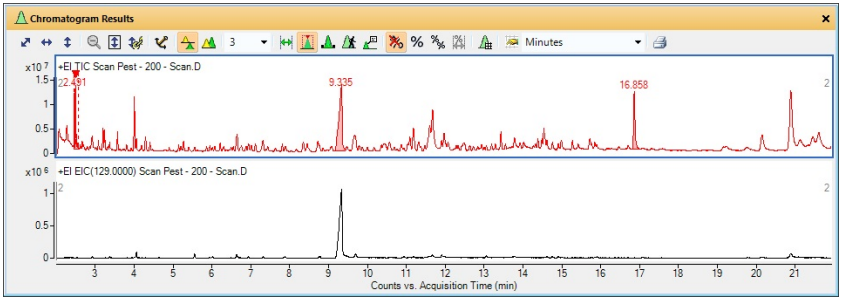


Figure 11 Integrated TIC Scan chromatogram when limiting the number of peaks

Task 6. Interactively integrate a chromatogram (GC/MS) (continued)

Steps	Detailed Instructions	Comments
5 Integrate the TIC MRM chromatogram for the **Pest - STD 200 MRM.D** data file.	**a** In the Data Navigator window, mark the Pest - STD 200 MRM.d data file. **b** In the Data Navigator window, select the **TIC MRM** for the Pest - STD 200 MRM.d data file. **c** Use one of the following commands to integrate the chromatograms. • From the menu bar click **Chromatograms > Integrate Chromatogram**. • Right-click anywhere in the chromatogram window, and click **Integrate Chromatogram**. • In the Data Navigator window, right-click the highlighted chromatogram and click **Integrate Chromatogram**. **d** Click the **Auto-scale Y-axis during Zoom** icon in the Chromatogram Results toolbar. **e** Zoom in from 5.8 to 8.5 minutes. **f** Set the **Maximum number of list panes** to 2.	• Note that the program integrated practically all the peaks in the chromatogram. • These chromatograms are MS/MS chromatograms, so the values that are set in the Integrate (MS/MS) section of the Method Editor window are used when integrating this chromatogram. You can select one integrator to use to integrate MS chromatograms and a different integrator to use to integrate MS/MS chromatograms.

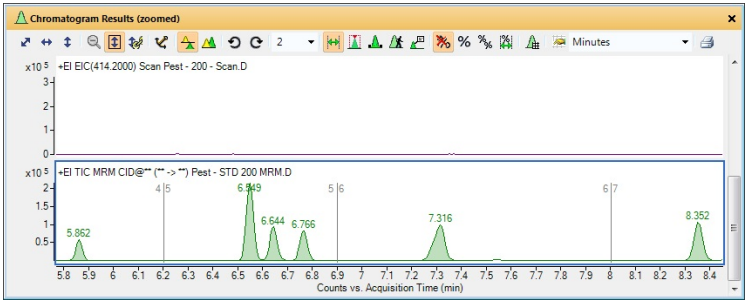


Figure 12 Integrated MRM chromatograms

Task 6. Interactively integrate a chromatogram (GC/MS) (continued)

Steps	Detailed Instructions	Comments
6 Select the **MS/MS (GC)** integrator. Change the filter to only accept peaks with an absolute height greater or equal to 60,000.	**a** From the Method Editor window, select **Chromatograms > Integrate (MS/MS)**. **b** Click the **Peak Filters** tab. **c** Under **Filter on**, click **Peak height**. **d** Under Height filters, mark the **Absolute height** check box. **e** Type 60000 as the **Absolute height**.	• Note the blue triangle that appears when you change a setting from the value saved in the current method. When you save the method, the triangles disappear.

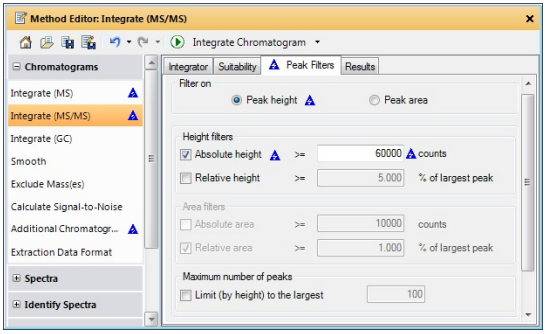
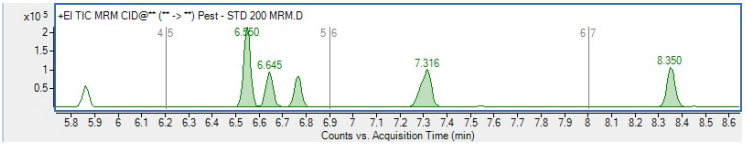


Figure 13 Peak Filters tab with **Absolute height** marked

7 Reintegrate the chromatogram	**f** Click the ▶ button on the Method Editor toolbar.	• Note that only the largest peaks are now integrated.



The smaller peak at 5.8 minutes is not included in the integration results any longer because the absolute height for this peak is lower than 60000

Figure 14 Integrated TIC chromatogram with higher threshold setting

Task 6. Interactively integrate a chromatogram (GC/MS) (continued)

Steps	Detailed Instructions	Comments
8 Restore the settings that are saved for the current method and close Method Editor.	**a** Select the Chromatogram > Integrate (MS/MS) section in the Method Editor. **b** Click the  icon in the Method Editor. **c** Select the Chromatogram > Integrate (MS) section. **d** Click the  . icon in the Method Editor. **e** Close the **Method Editor** window.	• To cancel your changes and restore the values from the method that is loaded, click the **Restore to last saved values from file** icon  on the Method Editor toolbar.
9 Delete all chromatograms except the original. Delete the integration results from the original chromatogram.	**a** Under Chromatograms in the Data Navigator window, highlight all the chromatograms except the original. **b** Right-click the highlighted chromatograms, and click **Delete**. **c** Select all of the TIC chromatograms. **d** Click **Chromatograms >Clear Results**.	• When you use the **Clear Results** command, the chromatograms are not deleted; the results that are connected to the chromatograms are removed. In this case, the integration values are cleared. • Press the **Ctrl** key to highlight more than one chromatogram in the Data Navigator window.

Task 7. Calculate System Suitability values

In this task, you learn different ways to interactively integrate a chromatogram, change integration parameters to modify the results and view the signal-to-noise ratio for each peak. You also learn how to enable System Suitability calculations.

Task 7. Interactively integrate a chromatogram (MS)

Steps	Detailed Instructions	Comments
1 Integrate the **MSD_mix_4stds_DB_spl200_03.d** and **Pest - 200 - Scan.d** chromatogram and using any of the options listed at right.	**a** Mark the check box next to the MSD_mix_4stds_DB_spl200_03.d data file in the Data Navigator window. **b** Mark the check box next to the Pest - 200 - Scan.d data file in the Data Navigator window. **c** Highlight both TICs. **d** Zoom out in the Chromatogram Results window. Click the  . icon in Chromatogram Results. **e** Integrate the **TIC Scan** for these two files, using any of the following options. • From the main menu, click **Chromatograms > Integrate Chromatogram**. • Highlight the chromatograms. Then, right-click the chromatogram, and click **Integrate Chromatogram**. • In Data Navigator, highlight the **TIC Scan** for both data files. Then, right-click either chromatogram and click **Integrate Chromatogram**.	• You can change the integrator in the Chromatogram > Integrate (MS) > Integrator tab. • Note that the integration with default parameters is detecting very small peaks.

Task 7. Interactively integrate a chromatogram (MS) (continued)

Steps	Detailed Instructions	Comments

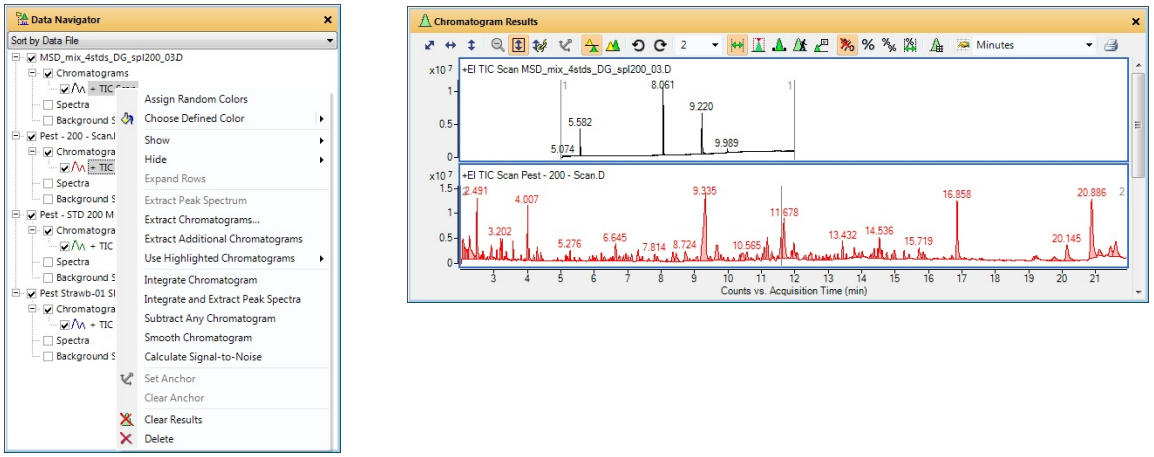


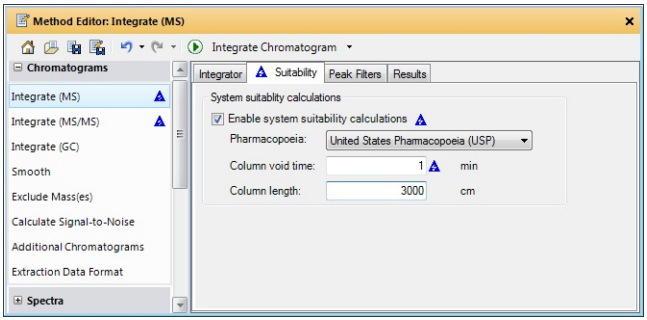
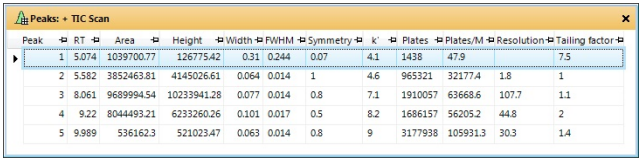
Figure 15 One of the shortcut menus in the Data Navigator and the integrated chromatograms

2 Enable system suitability calculations for the MS chromatograms.

a In the Method Editor, select **Chromatograms > Integrate (MS)** to display the Integrator tab.
b Click the **Suitability** tab.
c Mark **Enable system suitability calculations**.
d Select the **United States Pharmacopoeia (USP)**.
e In the **Column void time** box, type `1`.
f In the **Column length** box, type `3000`.

- Note the blue triangle that appears when you change a setting from the value that is saved in the current method. When you save the method, the triangles disappear.
- The algorithms that are used to set several of the columns in the Integration Peak List change, depending on the selected pharmacopoeia. See the online Help for more information.

Task 7. Interactively integrate a chromatogram (MS) (continued)

Steps	Detailed Instructions	Comments
	 **The actual column void time and column length for these data files is different** **Figure 16** Chromatograms > Integrate (MS) Suitability tab	
3 Reintegrate the chromatogram.	• Click the **Integrate Chromatogram** icon on the Method Editor toolbar to integrate using the new setting.	
4 View the system suitability calculations. • Open the Integration Peak List window. • Review the values for system suitability.	**a** Click **View > Integration Peak List**. **b** Right-click the header of the Peaks window and click **Floating**. **c** Right-click the column header of any column that you do not want to see and click **Remove Column**. **d** Right-click any column header and click **Add/Remove Columns** to change the columns that are visible.	• The system suitability calculations are included in the Integration Peak List table. • These values include k', Tailing factor, Plates, Plates/M, and Symmetry. • You can also enable system suitability calculations for an MS, an MS/MS and a GC chromatogram.
	 **Figure 17** Integrated Peaks table with system suitability values	

Task 7. Interactively integrate a chromatogram (MS) (continued)

Steps	Detailed Instructions	Comments
5 Restore the settings for the default method, and close the Method Editor window and the Integration Peak List window.	**a** To cancel your changes and restore the values from the default method, click the **Restore to last saved values from file** icon  on the Method Editor toolbar. **b** Close the **Method Editor** window. **c** Right-click the title of the Integration Peak List window and click **Floating**. **d** Click **View > Integration Peak List**.	• When you click the **Floating** command in the shortcut menu the second time, the Integration Peak List window is docked where it was originally.

Task 8. Extract spectra from a chromatogram

In this task, you extract a spectrum from exactly where you specify in the chromatogram. The Qualitative Analysis Navigator program extracts a spectrum from a specific data point or extract an average spectrum from an average of multiple data points or ranges.

Task 8. Extract spectra from a chromatogram

Steps	Detailed Instructions	Comments
1 Walk a chromatogram to view the precursor ion and product ion for the last few peaks of **Pest - STD 200 MRM.d**. • Zoom in on the region between 13 and 16 minutes. • Use the Walk Chromatogram icon. • Review the spectra starting at about 13 minutes, and move the arrow to the right.	**a** Mark the **Pest - STD 200 - MRM.D** line in the Data Navigator window. **b** Close the Method Editor window. **c** Click the **TIC MRM** chromatogram in the Data Navigator window. **d** Click the **Autoscale Y-axis during Zoom** icon in the Chromatogram Results toolbar. **e** Select **1** for the Maximum number of list panes. **f** To zoom in on a few peaks, right-click the mouse above the peak at 13 minutes and drag it to 16 minutes, and then release. **g** Click the **Walk Chromatogram** icon in the Chromatogram Results toolbar. **h** Move the Walk Chromatogram cursor to above the X axis at about 13 minutes, and click.	• The Spectrum Preview window is only opened when you click the Walk Chromatogram icon ( ). • The Walk Chromatogram tool is particularly useful on MS/MS data for identifying precursor and product ions.

Task 8. Extract spectra from a chromatogram

Steps	Detailed Instructions	Comments
	i To navigate from spectrum to spectrum, click the chromatogram or press the right and left arrow keys on your keyboard. You can also press and hold one of those arrow keys to rapidly scan a retention time range.	• The spectrum for each point you click in the Chromatogram Results window is automatically displayed in the Spectrum Preview window, which is opened automatically. • Sometimes, multiple spectra are displayed in the Spectrum Preview window. For example, two spectra are shown in the Spectrum Preview window for each point you click near the peak at 13.431 minutes.

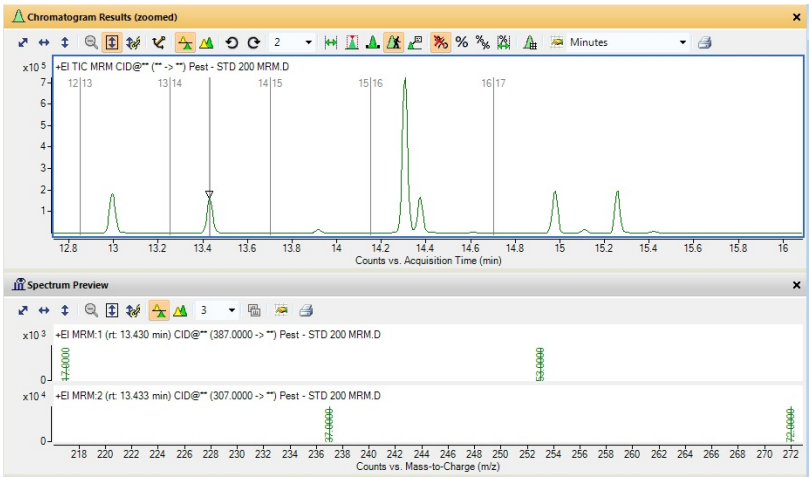


Figure 18 Walk chromatogram to view the two MRM spectra for the peak at 13. 43 minutes

Task 8. Extract spectra from a chromatogram

Steps	Detailed Instructions	Comments

2 Extract spectra on specific data points for the peak at 5.2 minutes and the peak at 14.3 minutes of the **Pest - STD 200 MRM.d** data file.
• Extract a spectrum from the peak at or near 5.2 min. and then one of the valleys, using any one of the options described under Comments.
• Extract a spectrum from the peak at or near 14.3 minutes. (not the valley yet)
	a Click the **Range Select** icon from the Chromatogram Results toolbar.
	b Click the **Zoom Out** icon, , in the Chromatogram Results toolbar.
	c To zoom in to the peak at 5.2 minutes, right-click the mouse above the peak at 4.0 min. and drag it to 6.0 min., then release.
	d On a peak near 5.2 min. extract a spectrum in any of the ways listed in the Comments column.
	e On a valley near 5.1 min., extract the spectrum.
	f Click the **Zoom Out** icon, , in the Chromatogram Results toolbar.
	g Zoom into the region between 14 and 15 min.
	h On a peak near 14.3 minutes, extract a spectrum in any of the ways listed in the Comments column. (Do not extract the valley spectrum yet.)
		• When you zoom, make sure the AutoScale Y-axis during Zoom icon, has an orange background.
		• You can extract a spectrum in any of the following ways:
		  • Double-click the data point in the chromatogram.
		  • Click the data point in the chromatogram; then, right-click anywhere in the chromatogram. Click **Extract MS Spectrum**. The **Extract Spectrum** dialog box is displayed. Make sure the **Pest - STD 200 MRM.d** file is selected, and click **Extract** in the Extract Spectrum dialog box.
		• Note that when you first extract a spectrum, the MS Spectrum Results window appears containing the spectrum, and the type of spectrum and retention time appear under Spectra. All subsequent extracted spectra appear in both places as well.
		• When you extract an MS spectrum from the peak near 14.3 minutes, two spectra are extracted because two transitions occur at that peak.

Task 8. Extract spectra from a chromatogram

Steps	Detailed Instructions	Comments
• Change the display to show at least four spectra.	i If necessary, select 4 in the **Maximum number of list panes** icon in the MS Spectrum Results toolbar.	• Note that when you first extract a spectrum, the MS Spectrum Results window appears containing the spectrum, and the type of spectrum and retention time appear under Spectra. All subsequent extracted spectra appear in both places as well. • When you extract an MS spectrum from the peak near 14.3 minutes, two spectra are extracted because two transitions occur at that peak.

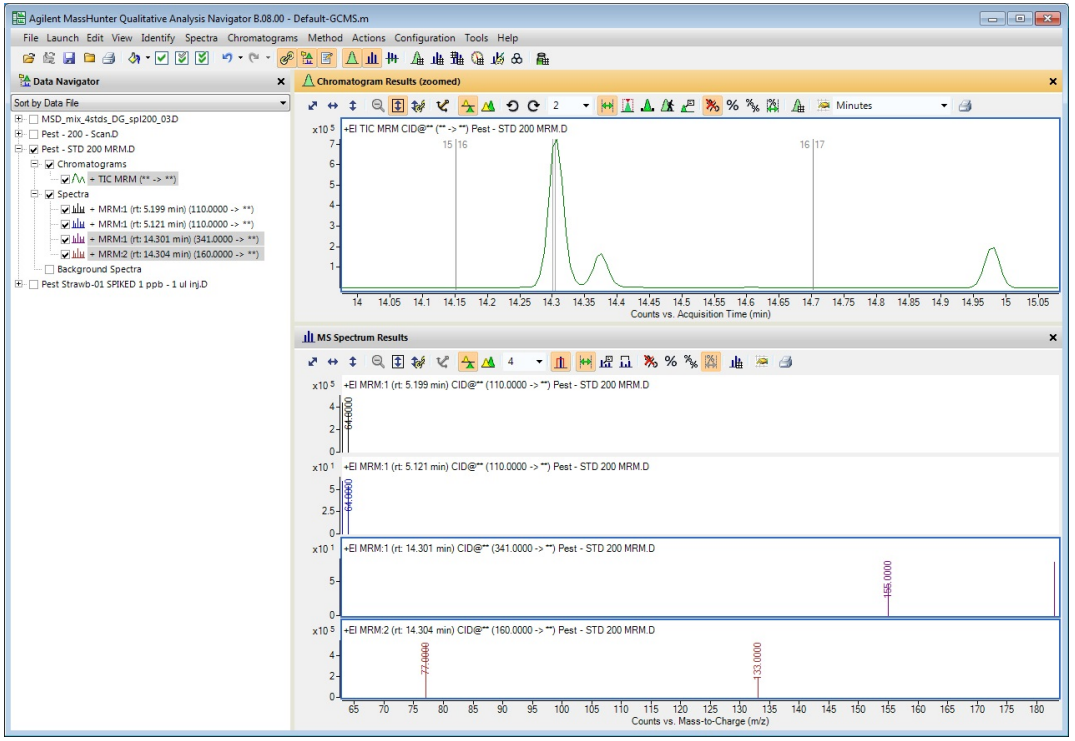


Figure 19 Main window with two MRM spectra from the peak at 5.2 minutes and two MRM spectra from the peak at 14.3 minutes

Task 8. Extract spectra from a chromatogram

Steps	Detailed Instructions	Comments
3 Extract an MS Spectrum for the valley at 14.35 minutes of the **Pest - STD 200 MRM.d** data file. • Bring up Spectrum Preview. • Extract a spectrum from the valley at RT 14.3 minutes. • Copy this spectrum to the User Spectra folder. • Change the display to show 6 spectra. • Turn off Spectrum Preview.	**a** Click the **Walk Chromatogram** icon in Chromatogram Results. **b** On a valley near 14.3 minutes extract a spectrum. **c** Select both spectra in the Spectrum Preview window. **d** Right-click the spectra in the Spectrum Preview window, and click **Copy to Spectra**. The spectra are copied to the Spectra section in the Data Navigator and are shown in the MS Spectrum Results window. **e** Click the **Range Select** icon on the Chromatogram toolbar. **f** Click the down arrow next to the spectrum pane list, and select **6**.	• When Walk Chromatogram is selected, the system displays any manually-selected spectrum in the Spectrum Preview window but not in the Spectra section of Data Navigator. • With Walk Chromatogram on, Qualitative Analysis Navigator overwrites the previous spectrum when you extract a new spectrum. • Walk Chromatogram mode is useful when you quickly want to review the spectra in your chromatogram and save only a few of the spectra.

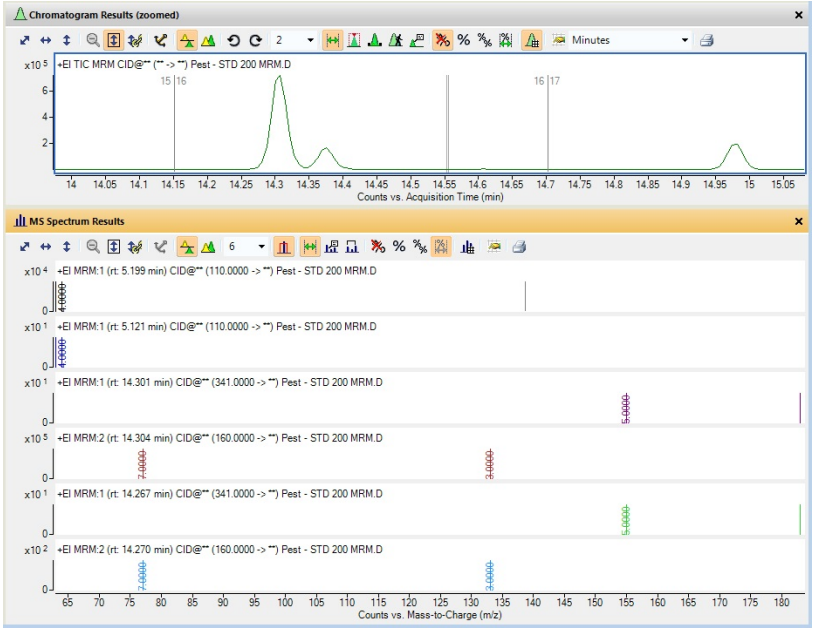


Figure 20 Chromatogram Results and MS Spectrum Results windows

Task 8. Extract spectra from a chromatogram

Steps	Detailed Instructions	Comments
4 Extract a spectrum that averages all points within a specified range for the peak at 14.3 minutes for the **Pest - STD 200 MRM.d** data file: • Zoom out. • Use the Range Select icon on the Chromatogram toolbar. • Set the range across the entire peak. • Extract the spectrum, using any of the options listed.	**a** Click at the left side of the base of the peak at 14.3 minutes and drag to the base of that peak on the right. **b** Select **2** in the Maximum number of list panes in the MS Spectrum Results window. **c** Extract the average spectrum using one of the options on the right.	• You can extract an average spectrum by double-clicking the selected range in the chromatogram. • Or, right-click anywhere in the chromatogram, and click **Extract MS Spectrum** from the shortcut menu. • Note that two averaged MRM spectra appear.

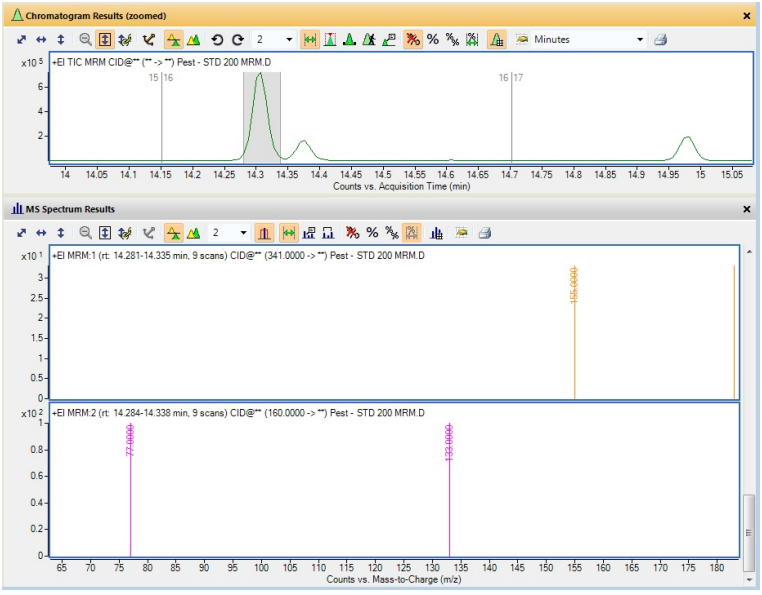
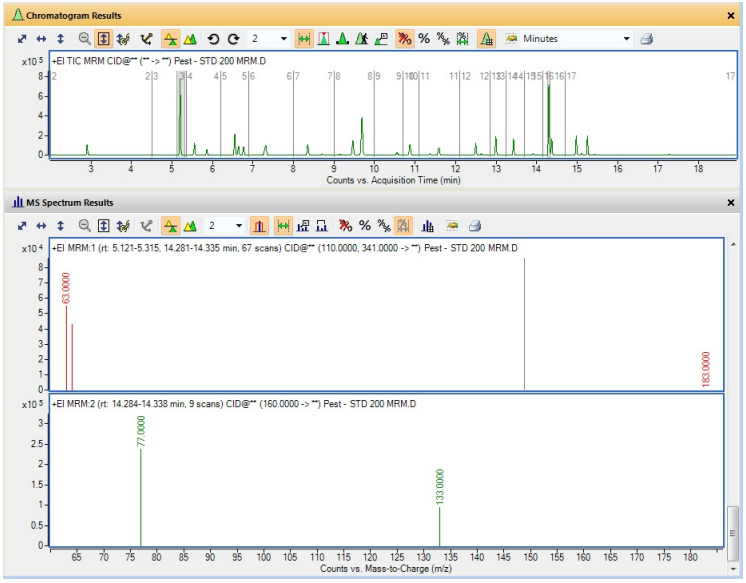


Figure 21 Chromatogram Results and MS Spectrum Results showing two averaged spectra

Task 8. Extract spectra from a chromatogram

Steps	Detailed Instructions	Comments
5 Extract spectra that average the ranges of peaks at 5.2 minutes and at 14.3 minutes together for the **Pest - STD 200 MRM.d** data file. • Hint: Use the Range Select icon and the **Ctrl** key to select the Peak 1 range taken from the halfway point. • Extract the spectra, using any of the options on the right.	**a** Click the **Zoom Out** icon, , in the Chromatogram Results toolbar. **b** Press the **Ctrl** key. **c** Click at the left side of the peak at 5.2 minutes and drag to the right of that peak, and release the mouse. **d** Release the **Ctrl** key. **e** Extract the averaged spectra using this option or the one on the right: • Double-click inside the selected range in either peak.	• Remember that the second peak already has a range selected from step 4. • To extract spectra, you can also right-click anywhere in the chromatogram and click **Extract MS Spectrum**. The Extract Spectrum dialog box is shown. Click **Extract**.



The first spectrum has transitions from both time ranges. The second spectrum only has one time range because the 160.00 -> ** transition is not present in the peak at 5.2 minutes.

Figure 22 Two averaged spectra from two different ranges in the chromatogram

Task 8. Extract spectra from a chromatogram

Steps	Detailed Instructions	Comments
6 Subtract a background spectrum every time you extract a peak spectrum from **Pest - STD 200 MRM.d**. • Delete any scans under User Spectra in Data Navigator. • Extract a background spectrum that is the average of a spectrum at the start of the peak and a spectrum at the end of the peak. • Extract a peak spectrum from the integrated peaks.	**a** Click the Spectra line in the Data Navigator. Right-click the Spectra line, and click **Delete**. **b** Click **Yes**. **c** In Method Editor, select **Spectra > Extract (MS/MS)**. **d** Click the **Peak Spectrum Extraction (MS/MS)** tab, if not visible. **e** In the **Peak spectrum background MS/MS** box, select **Average of spectra at peak start and end**. **f** In the Chromatogram Results toolbar, click the **Peak Select** icon,  . **g** Click the **Chromatograms > Integrate** command. **h** Select the peak near 5.2 minutes. **i** Right-click and click **Extract Peak Spectrum** from the shortcut menu.	• Note that at the end of this process, all extracted peak spectra will automatically have the designated background spectrum subtracted.

Task 8. Extract spectra from a chromatogram

Steps	Detailed Instructions	Comments
		• If you extract a peak spectrum and it has no points, the Extraction Data Format may need to be changed. In the Method Editor window, click **Spectra > Extraction Data Format**. For Mass spectral data format, click an option that can extract either format. For these examples, click **Profile when available, otherwise Centroid**.

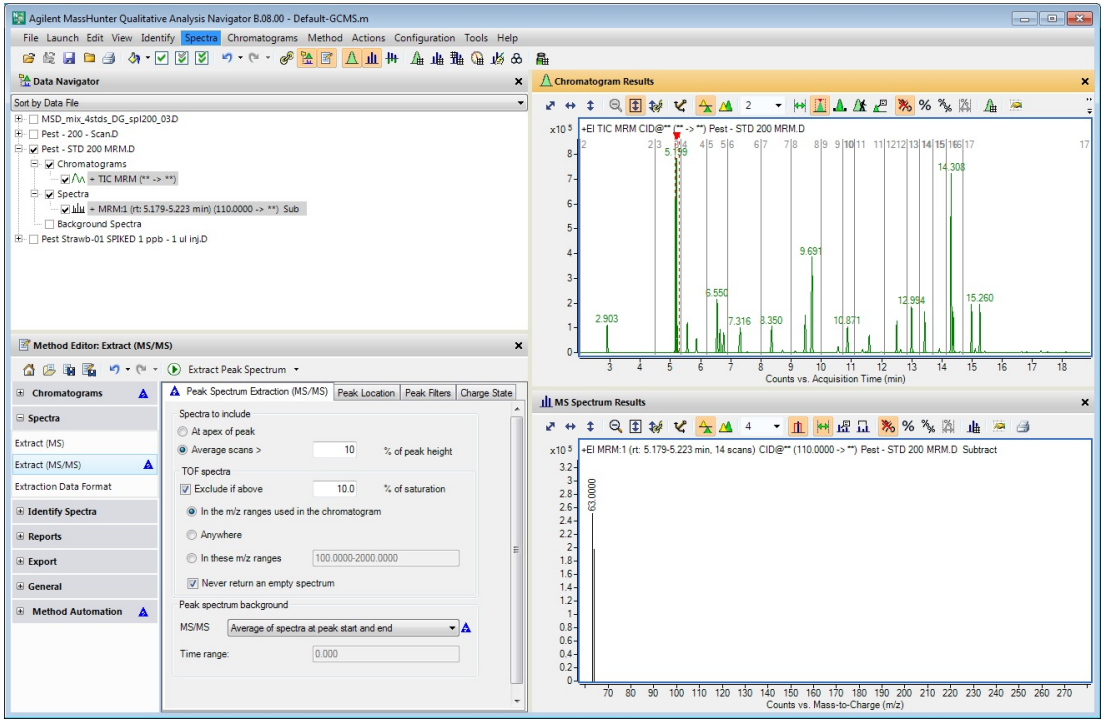


Figure 23 Peak spectrum with a background peak spectrum subtracted

Task 8. Extract spectra from a chromatogram

Steps	Detailed Instructions	Comments
7 Integrate and extract peak spectra from the Pest - STD 200 MRM.d data file.	**a** Click the TIC MRM chromatogram in the Data Navigator window. **b** Click **Chromatograms > Integrate and Extract Peak Spectra**.	• The peak spectra that you extracted manually in the previous step is deleted automatically because by default the **Clear previous peak spectra** check box is marked in the Chromatograms > Integrate (MS/MS) > Results tab.

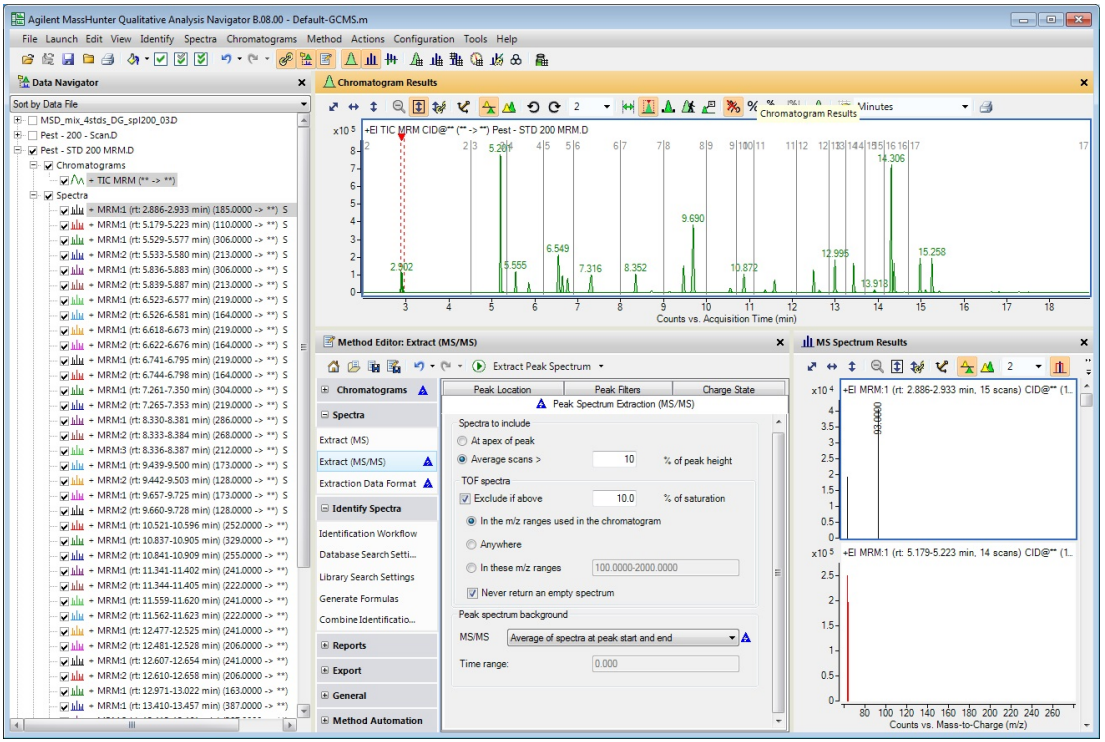


Figure 24 Integrate and Extract Peak Spectra

8 Remove the integration results and the peak spectra.	**a** Select the Pest - Std 200 MRM.d data file. **b** Click **Chromatograms > Clear Results > Include Peak Spectra**.	• You can instead click **Chromatograms > Clear Results > Only Chromatograms** if you do not want to delete the peak spectra.

Task 9. Add annotations

You can add an image annotation or a text annotation to the following graphics windows in the Qualitative Analysis Navigator window:

- Chromatogram Results window
- MS Spectrum Results window
- UV Spectrum Results window

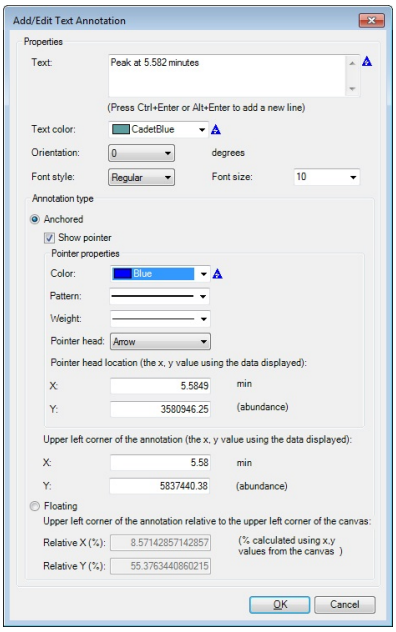
You can add annotations to windows in the Qualitative Analysis Workflows program. If you save the results for the data file, annotations are also saved.

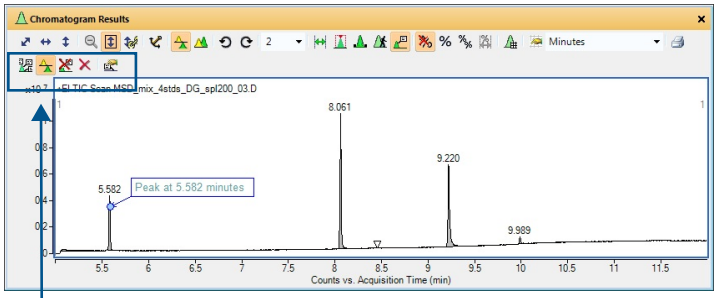
Task 9. Add an annotation

Steps	Detailed Instructions	Comments
1 Select the MSD_mix_4stds_DG_spl200_03.d data file. Hide the other chromatograms.	**a** Mark the check box next to MSD_mix_4stds_DG_spl200_03.D in the Data Navigator window. **b** Click **Edit > Show > Only Highlighted**.	• The chromatograms for the other data files are automatically hidden.
2 Select the location in the chromatogram to add a text annotation.	**a** In the Chromatogram Results window, click the **Annotation** tool ()in the toolbar. **b** Move the cursor to the location in the chromatogram pane where you want to add the annotation. **c** Right-click and then click **Add Text Annotation**.	• The cursor changes to a cross-hair. You use this cursor to select the location to add the annotation. • The Annotate toolbar is available in the Chromatogram Results window. • You can also add annotations to the MS Spectrum Results window, and the UV Spectrum Results window.
3 Add the information about the text annotation in the Add/Edit Text Annotation dialog box.	**a** Type the **Text** for the annotation. **b** Select the **Text color**. **c** Select the **Orientation**. **d** Select the **Font style** and **Font size**. **e** Click either **Anchored** or **Floating**. If you click **Anchored**, select the options for the pointer to the text annotation. If you click **Floating**, you can change the relative position. It is easier to change the position interactively in the graphics window. **f** Click **OK**.	• You can add multiple annotations to a chromatogram or spectrum. • You can use the icons in the Annotate toolbar to select all of the annotations, delete annotations and edit annotations.

Task 9. Add an annotation (continued)

Steps	Detailed Instructions	Comments





The Annotate Toolbar is only available when the Annotate tool is selected.

You can move the annotation to a new location when you click and drag the annotation.

Figure 25 Add/Edit Text Annotation dialog box and the Chromatogram Results window

4 Select the location in the chromatogram to add the image annotation.	**a** Move the cursor to the location in the chromatogram pane where you want to add the annotation. **b** Right-click and then click **Add Image Annotation**.	• You can add a JPG or a MOL image file.

Task 9. Add an annotation (continued)

Steps	Detailed Instructions	Comments
5 Add the information about the text annotation in the Add/Edit Text Annotation dialog box.	**a** Select the image annotation. **b** Type 50 for the Scale width. **c** Mark the **Lock aspect ratio** check box. **d** Click **Floating**. You can change the relative position. It is easier to change the position interactively in the graphics window. **e** Click **OK**. **f** Move the image to the upper, right corner of the chromatogram.	• The Agilent_Logo.tif file is included in the \\MassHunter\Report Templates\Qual\B.08.00\en-US\ Letter folder. You need to convert it to a JPG file. • You can add multiple annotations to a chromatogram or spectrum.

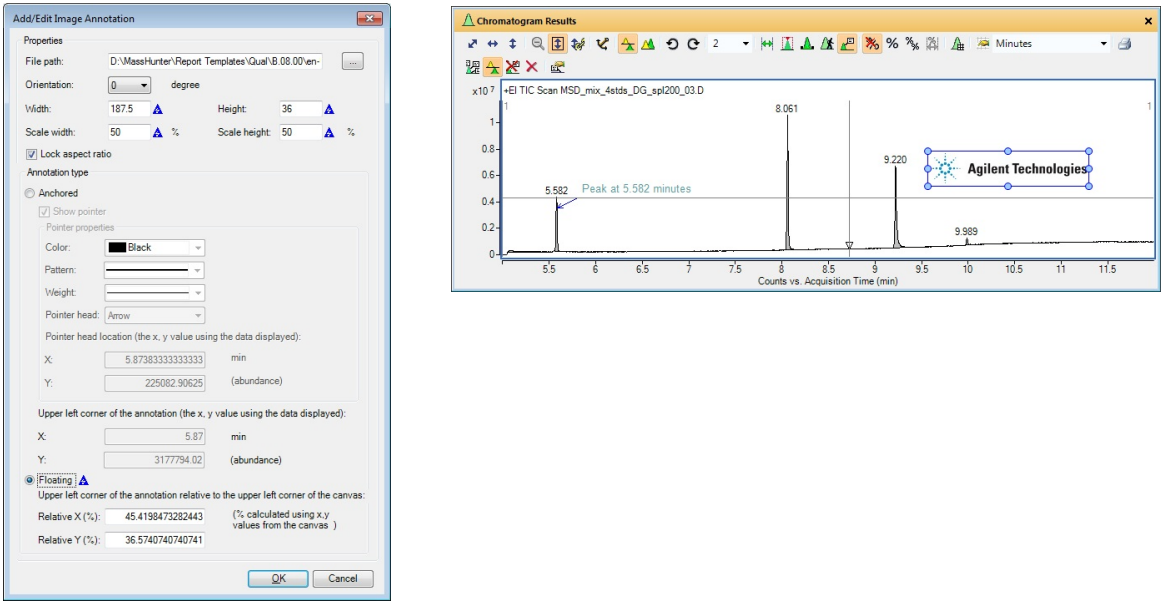
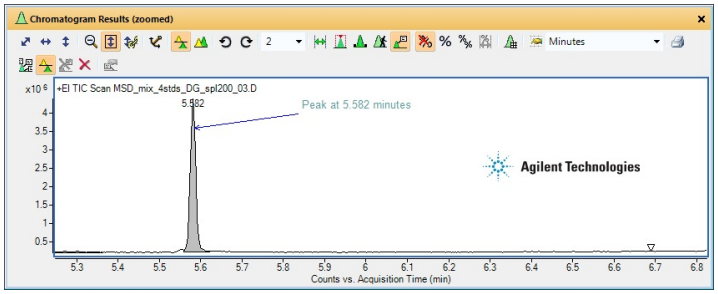


Figure 26 Add/Edit Image Annotation dialog box and the Chromatogram Results window

Task 9. Add an annotation (continued)

Steps	Detailed Instructions	Comments
6 Zoom in to the first peak.	• Zoom to an area around the first peak at 5.5 minutes	



If an annotation is anchored, it stays attached at the position where it is anchored. If you zoom into a different peak, an anchored annotation may not be visible. If an annotation is floating, then the annotation is always shown in the same position relative to the upper left corner of the window.

Figure 27 Anchored and floating annotations in the Chromatogram Results window

7 Switch back to the Range Select tool in the Chromatogram Results window. Delete the annotation first.	**a** Click the icon to remove all annotations. **b** Click the (Range Select) icon in the Chromatogram Results toolbar.	• If you want to save the annotations with the data file results, see "Task 17. Save results" on page 75. • You can switch between five different tools in the Chromatogram Results toolbar. Refer to the online Help for more information. The five tools are: ◦ Range Select ◦ Peak Select ◦ Manual Integration ◦ Walk Chromatogram ◦ Annotation Mouse

Task 10. Add a mass caliper

A caliper shows the difference between two points in a spectrum. You can add a caliper to the MS Spectrum Results window.

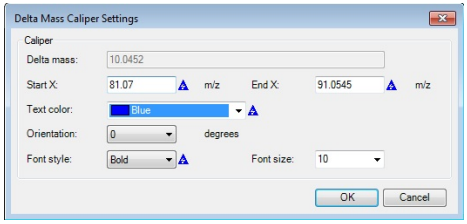
If you save the results for the data file, calipers are also saved.

Task 10. Add a mass caliper

Steps	Detailed Instructions	Comments
1 Integrate and extract peak spectra from MSD_mix_4stds_DG_spl200_03.d.	**a** Mark the check box next to MSD_mix_4stds_DG_spl200_03.D in the Data Navigator window. **b** Click **Edit > Show > Only Highlighted**. **c** Click **Chromatograms > Integrate and Extract Peak Spectra**.	• You can instead click the Show only the highlighted ( ) button in the main toolbar.
2 Add the caliper to the peak spectrum created in the previous task.	**a** In the MS Spectrum Results window, click the **Delta Mass Caliper** tool ( )in the toolbar. **b** (optional) Select **Profile Point to Point** for the type of caliper in the Caliper toolbar. **c** Zoom in from 79 to 99 *m/z*. **d** Move the cursor to the location in the spectrum pane where you want to add the caliper. **e** Drag the cursor to the end point of caliper in the spectrum. As you drag the cursor, the value of the delta mass changes. When you release the mouse button, the caliper is added.	• The cursor changes to an arrow. You use this cursor to select the start and end point of the caliper. • You cannot select the type of caliper if the spectrum is centroided because **Profile Point to Point** has no effect on centroid data. • The "triangle" cursor is set to the point that is selected, or to the top of the peak if you are using **Profile Peak to Peak**.
3 Modify the caliper to use a different color.	**a** Click the caliper created in the previous step. **b** Click the Caliper Properties button ( ) in the MS Spectrum Results Caliper toolbar. **c** (optional) Type the **Start X** and **Start Y** values. **d** Select the **Text color**. **e** Select the **Font style** and **Font size**. **f** Click **OK**.	• You can add multiple calipers to a spectrum. • You can use the icons in the Caliper toolbar to select all of the calipers, delete calipers and edit calipers.

Task 10. Add a mass caliper (continued)

Steps	Detailed Instructions	Comments



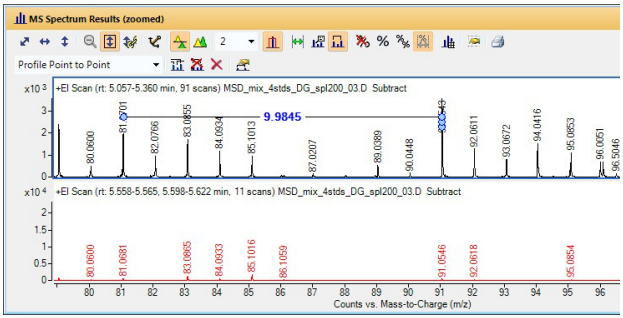


Figure 28 Delta Mass Caliper Settings dialog box and the MS Spectrum Results window

4 Delete integration results and spectra.	**a** Click **Chromatograms > Clear Results > Include Peak Spectra**. **b** Click the **Range Select** tool in the MS Spectrum Results window.	• If you want to save the calipers with the data file results, see "Task 17. Save results" on page 75.

Exercise 2
Find and identify

In these tasks, you find and identify compounds in GC/MS data files. You use the Qualitative Analysis Workflows program to do compound mining. You can also identify those compounds in this program.

Each exercise is presented in a table with three columns:

- Steps – Use these general instructions to proceed on your own to explore the program.
- Detailed Instructions – Use these if you need help or prefer to use a step-by-step learning process.
- Comments – Read these to learn tips and additional information about each step in the exercise.

Task 11. Find Compounds by Chromatogram Deconvolution

This compound mining algorithm identifies compounds in GC/MS data and creates a cleaned MS spectrum for each compound. This functionality is an easy way to "mine" information from complex data. You can only use the Find by Chromatogram Deconvolution algorithm on GC/MS sample data acquired in Scan, Product Ion scan, or Neutral Loss scan mode.

This task shows finding compounds by chromatogram deconvolution with accurate mass data. You can also find compounds by chromatogram deconvolution with unit mass data after you first change the extraction window.

Task 11. Find compounds using Chromatogram Deconvolution (GC/MS)

Step	Detailed Instructions	Comments
1 Open the TIC for the **MSD_mix_4stds_DG_spl200_03.d** data file.	**a** If the program is not open, double-click the **MassHunter Qualitative Workflows** icon  . Otherwise, click **File** > **Open Data File**. **b** Click the **MSD_mix_4stds_DG_spl200_03.d** data file in the **GC** example data file folder. **c** Clear the **Load result data** check box and click **Open**.	• The Find Compounds by Chromatogram Deconvolution algorithm works with both GC/QQQ and GC/Q-TOF data files. • The user interface is updated automatically depending on the type of data files that are loaded.

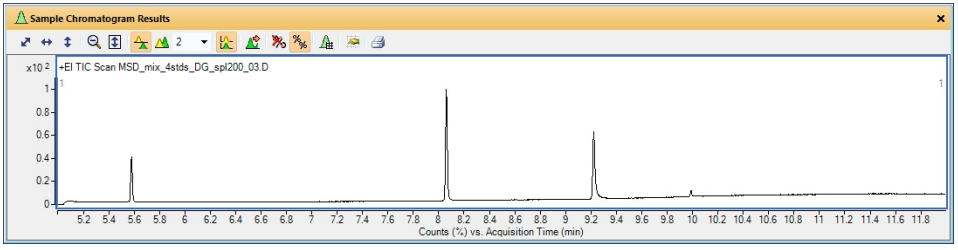


Figure 29 TIC chromatogram from MSD_mix_4stds_DG_spl200_03.d

Task 11. Find compounds using Chromatogram Deconvolution (GC/MS)

Step	Detailed Instructions	Comments
2 Configure the user interface.	**a** Click **Configuration > Window Layouts > Restore Default Layout**. **b** Click **Method > Open**. **c** Select Default-GCMS.m. **d** Click **OK**.	• For these examples, start from the Default-GCMS.m method.
3 Find compounds using the chromatogram deconvolution algorithm. • Select the Agile integrator. • Enter an SNR threshold of 20. • Enter 100 ppm for the **Left m/z delta** and **Right m/z delta** values.	**a** In the Method Editor window, select **Compound Discovery > Find by Chromatogram Deconvolution.** **b** On the Settings tab under Peak filter, type `20` for the **SNR threshold**. **c** Review the parameters for the **m/z delta units**, **Left m/z delta**, and the **Right m/z delta**.	• If you have unit mass data, you enter `0.3` AMU for the **Left m/z delta** value and `0.7` AMU for the **Right m/z delta** value.

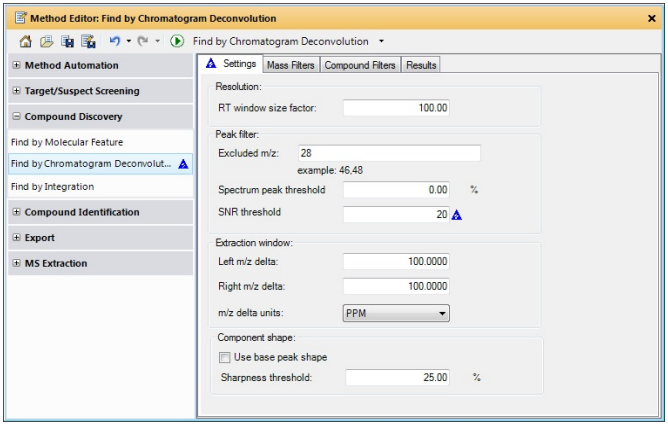


Figure 30 Settings tab in the Find by Chromatogram Deconvolution section

Task 11. Find compounds using Chromatogram Deconvolution (GC/MS)

Step	Detailed Instructions	Comments
• Select to extract EIC, MS spectra and MS/MS spectra.	**d** Click  to run the **Find Compounds by Chromatogram Deconvolution** algorithm on the data file. **e** If necessary, click the **View > Compound List** command. **f** Close the Method Editor window, and the Structure Viewer window.	• The Qualitative Analysis Workflows program finds 5 compounds under these conditions. • You can instead click **Find > Find by Chromatogram Deconvolution**. • If the data file is not indexed, it can take a long time when you run this algorithm.

Task 11. Find compounds using Chromatogram Deconvolution (GC/MS)

Step	Detailed Instructions	Comments
4 Examine the compounds. See Figure 31.	**a** Click the **Hide Empty Columns** icon in the Compound List window. **b** Click the first compound in the Compound List window. **c** When the Compound List window is selected, use the arrow keys to switch compounds.	• Showing both spectra is a convenient way to display all the information for a single compound. • Note that both the cleaned spectrum and the raw spectrum are shown.

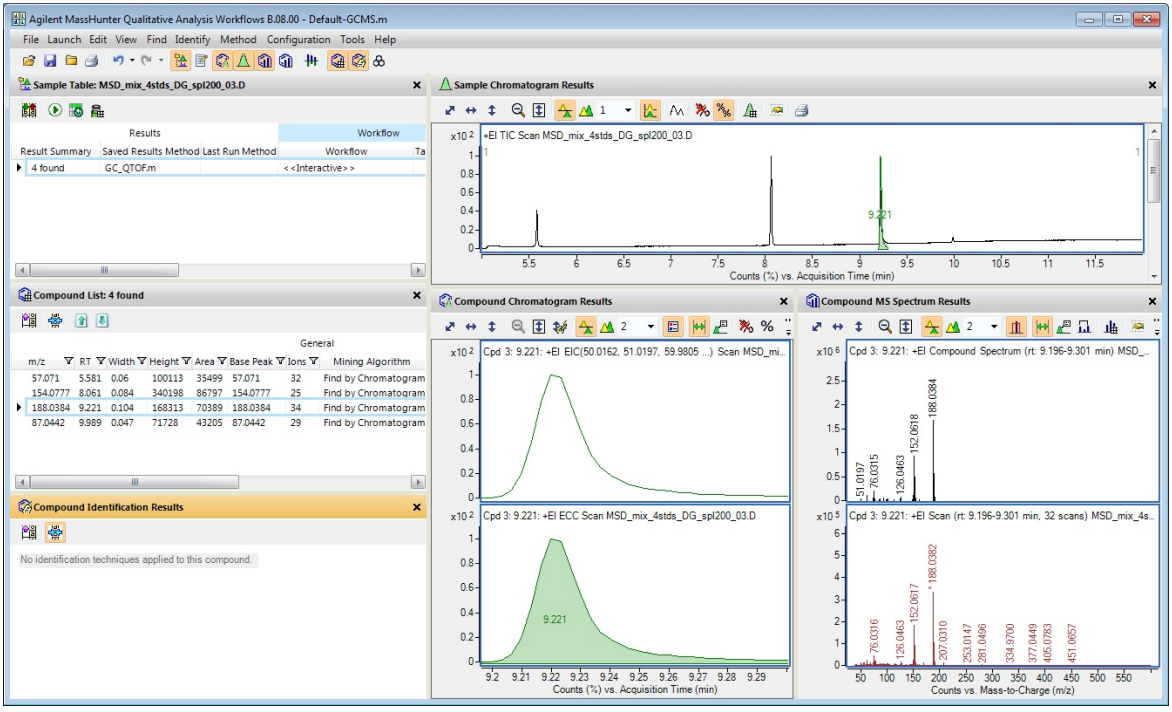


Figure 31 Find Compounds by Chromatogram Deconvolution results

Task 12. Identify compounds using the Search Library/Database search algorithm

In this task, you identify and generate formulas for the compounds found in "Task 11. Find Compounds by Chromatogram Deconvolution" on page 50. You can do this task if you have purchased the *NIST11.l* library (or a later version) or if you use the *demo.l* library. If you have two libraries, you can even select both libraries.

Task 12. Identify compounds using the Search Library algorithm

Step	Detailed Instructions	Comments
1 Do a library /database search of all of the compounds in the MSD_mix_4stds_DG_spl200_03.d data file.	**a** Click **View > Method Editor**. **b** In the Method Editor window, click **Compound Identification > Identification Workflow**. **c** Note that the **Identify by - Library / Database search** check box is marked. **d** (optional) Click the **Add** button. Select the **NIST11.l** library and click the **OK** button. **e** (optional) Click **Stop at first library match** for the **Multi-library search type**. **f** Click **Identify > Identify All Compounds** from the main menu. You can instead click the **Identify All Compounds** icon to run the algorithm.	• Demo.l and Nist11should be installed in the \MassHunter\ Library folder. • Note that many of the compounds are identified after searching the *NIST11.l* library. • If you do not have the *NIST11.l* library, then select a second library if you have one available. • If you have two or more libraries selected and you select **Stop at first library match**, the library search algorithm searches the first library in the list. If the compound is identified, then it stops. If the compound is not identified, then it searches the next library until the compound is identified or the last library is searched. • You use the Library Editor program to modify **.L** libraries that you use with the Search Library algorithm. This program is installed with the Agilent MassHunter Quantitative Analysis program. You click the  icon to start this program.

Task 12. Identify compounds using the Search Library algorithm

Step	Detailed Instructions	Comments
2 Change the displayed windows.	**a** Click **View > Difference Results**. **b** Click **View > Structure Viewer**. **c** Click the tab of the **Compound Identification Results** window, if necessary to display this window. **d** Highlight a row in the Compound List which has been identified. **e** Click the Hide Empty Columns button ( ) in the Compound List toolbar and in the Compound Identification Results window. **f** Click each compound to review results.	• If a compound is identified, the Formula column has a value.

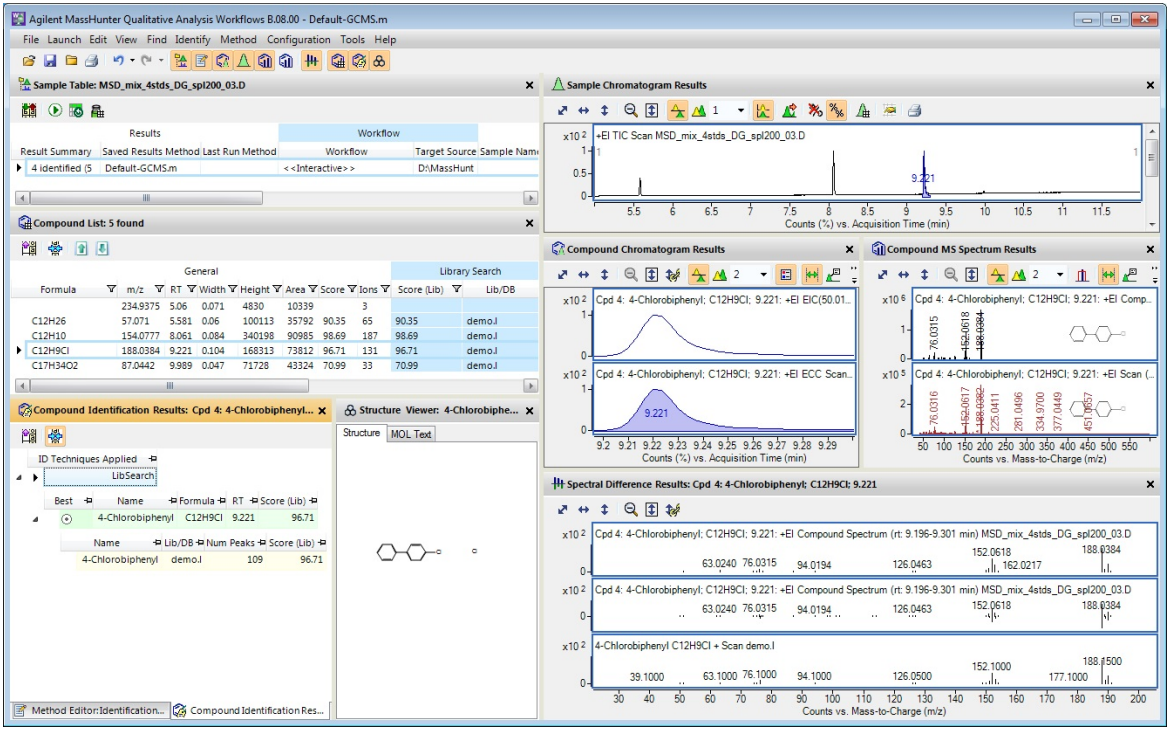


Figure 32 Compounds and the library / database search results

Task 12. Identify compounds using the Search Library algorithm

Step	Detailed Instructions	Comments
3 Close the data file.	**a** Click **File > Close Data File**. **b** Click **No** when you are asked if you want to save results.	• If you want to save these results, see "Task 17. Save results" on page 75.

Task 13. Find Compounds using MRM (MRM only)

The Find Compounds by MRM algorithm identifies compounds in MRM data from a Triple Quadrupole. The algorithm searches for compounds using the MRM transitions. All of the compounds in the acquisition method are extracted and shown in the Compound List. Compounds are not eliminated based on chromatogram integration results. You can only use the Find Compounds by MRM algorithm on data that was acquired using MRM transitions. The MRM algorithm uses information that is found in the data file if the data file is an MRM data file.

Task 13. Find compounds using MRM (MRM only)

Step	Detailed Instructions	Comments
1 Open the TIC for the **Pest - STD 200 MRM.d** data file.	**a** If the program is not open, double-click the **MassHunter Qualitative Workflows icon**. Otherwise, click **File > Open Data File**. **b** Click the **Pest - STD 200 MRM.d** data file in the **GC Pesticides** example data file folder. **c** Clear the **Load result data** check box and click **Open**.	• The user interface is updated automatically to show the appropriate features for the data file which you opened.

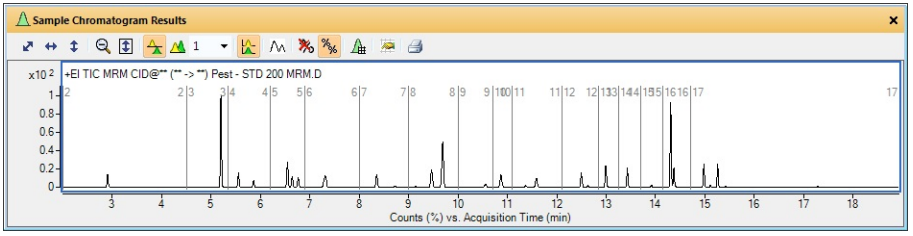


Figure 33 TIC chromatogram from Pest - STD 200 MRM.d

2 Configure the user interface.	**a** Click **Configuration > Window Layouts > Restore Default Layout**. **b** Click **Method > Open**. **c** Select Default-GCMS.m. **d** Click **OK**.	• For these examples, start from the Default-GCMS.m method.

Task 13. Find compounds using MRM (MRM only)

Step	Detailed Instructions	Comments
3 Find compounds using the MRM algorithm.	**a** In the Method Editor window, select **Target/Suspect Screening > Find by MRM.** **b** Review the parameters.	

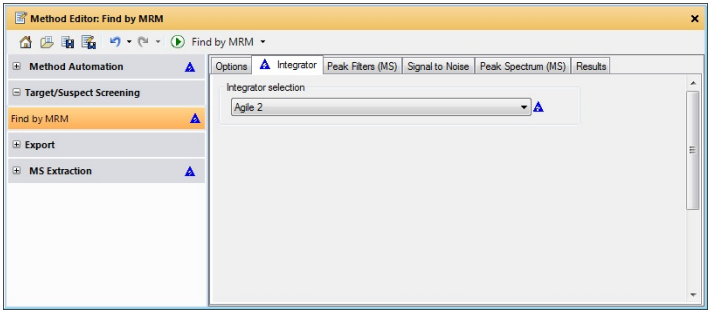


Figure 34 Integrator tab in the Find by MRM section of the Method Editor

	c Click ▶ to run the **Find by MRM** algorithm on the data file. **d** If necessary, click the **View > Compound List** command. **e** If necessary, click the tab for the **Compound Identification Results** window to make it visible. It is tabbed with the Method Editor window.	• The Qualitative Analysis Workflows program finds 28 compounds under these conditions.
4 Examine the compounds. See Figure 35 on page 59.	**a** Select **2** in the **Maximum number of list panes** box in the Compound MS Spectrum Results toolbar. **b** Click the Hide Empty Columns button (🔍) in the Compound List toolbar. **c** Click the first compound in the Compound List window. **d** When the Compound List window is selected, use the arrow keys to switch compounds.	• The "Hide any currently empty columns" algorithm runs on the first level of a table.

Task 13. Find compounds using MRM (MRM only)

Step	Detailed Instructions	Comments
5 Change the visible columns in the Compound Identification Results window.	**a** Right-click a row in the table and click **Add/Remove Columns**. **b** Click **Select All** and click OK. **c** Click the Hide Empty Columns button ( ) in the Compound List toolbar. **d** Click a column that you want to remove. Right-click that column and click **Remove Column** to remove a column. **e** Close some of the windows.	• If you first show all columns and then hide empty columns, then all columns that have values are seen. • The precursor ion is displayed in the **Precursor (Acq)** column, and the product ion is displayed in the **Find by MRM Product Ion** column in the Compound Identification Results window. • The number of compounds is shown in the Sample Table window in the Result Summary column.

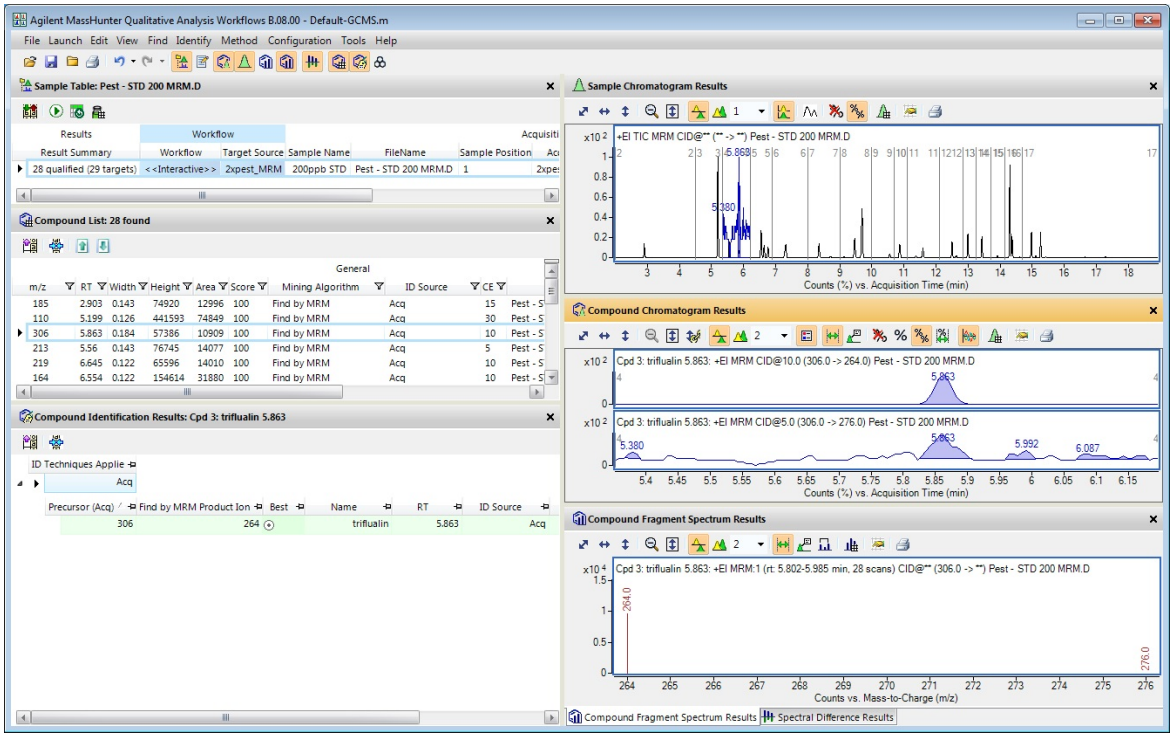


Figure 35 Find by MRM results

Task 13. Find compounds using MRM (MRM only)

Step	Detailed Instructions	Comments
6 Close the data file.	**a** Click **File > Close Data File**. **b** Click **Close**.	• If you want to save these results, see "Task 17. Save results" on page 75.

Task 14. Find Compounds by Integration

The Find Compounds by Integration algorithm identifies compounds based on the integration results. A compound is created for each peak that is identified by the integrator.

Task 14. Find compounds using Integration

Step	Detailed Instructions	Comments
1 Open the TIC for the **MSD_mix_4stds_DG_spl200_03.D** data file.	**a** If the program is not open, double-click the **MassHunter Qualitative Workflows icon**. Otherwise, click **File > Open Data File**. **b** Click the **MSD_mix_4stds_DG_spl200_03.d** data file in the **GC** example data file folder. **c** Clear the **Load result data** check box and click **Open**.	
2 Configure the user interface.	**a** Click **Configuration > Window Layouts > Restore Default Layout**. **b** Click **Method > Open**. **c** Select Default-GCMS.m. **d** Click **OK**.	• For these examples, start from the Default-GCMS.m method.

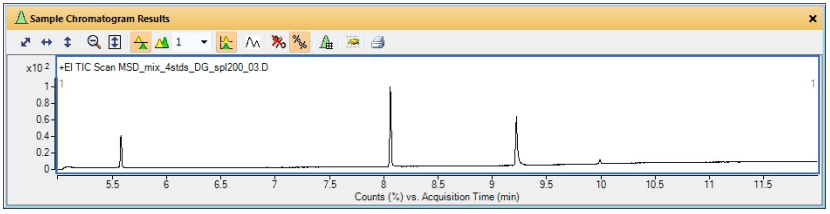


Figure 36 TIC chromatogram from MSD_mix_4stds_DG_spl200_03.d

Task 14. Find compounds using Integration

Step	Detailed Instructions	Comments
3 Find compounds using the Find by Integration algorithm.	**a** In the Method Editor window, select **Compound Discovery > Find by Integration.** **b** Review the parameters.	• You can choose the region of the chromatogram from which you intend to find compounds.

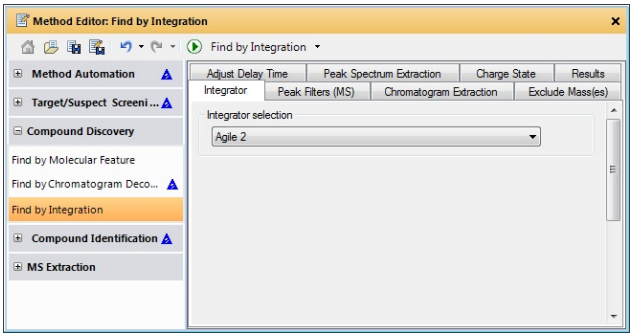


Figure 37 Integrator tab in the Find by Integration section of the Method Editor

	c Click  to run the **Find Compounds by Integration** algorithm on the data file. **d** If necessary, click the **View > Compound List** command.	• The Qualitative Analysis Workflows program finds ten compounds under these conditions.
4 Examine the compounds. See Figure 38 on page 63.	**a** Click the **Hide any currently empty columns** icon in the Compound List window. **b** Click the first compound in the Compound List window.	

Task 14. Find compounds using Integration

Step	Detailed Instructions	Comments
	c When the Compound List window is selected, press the arrow keys to switch compounds.	

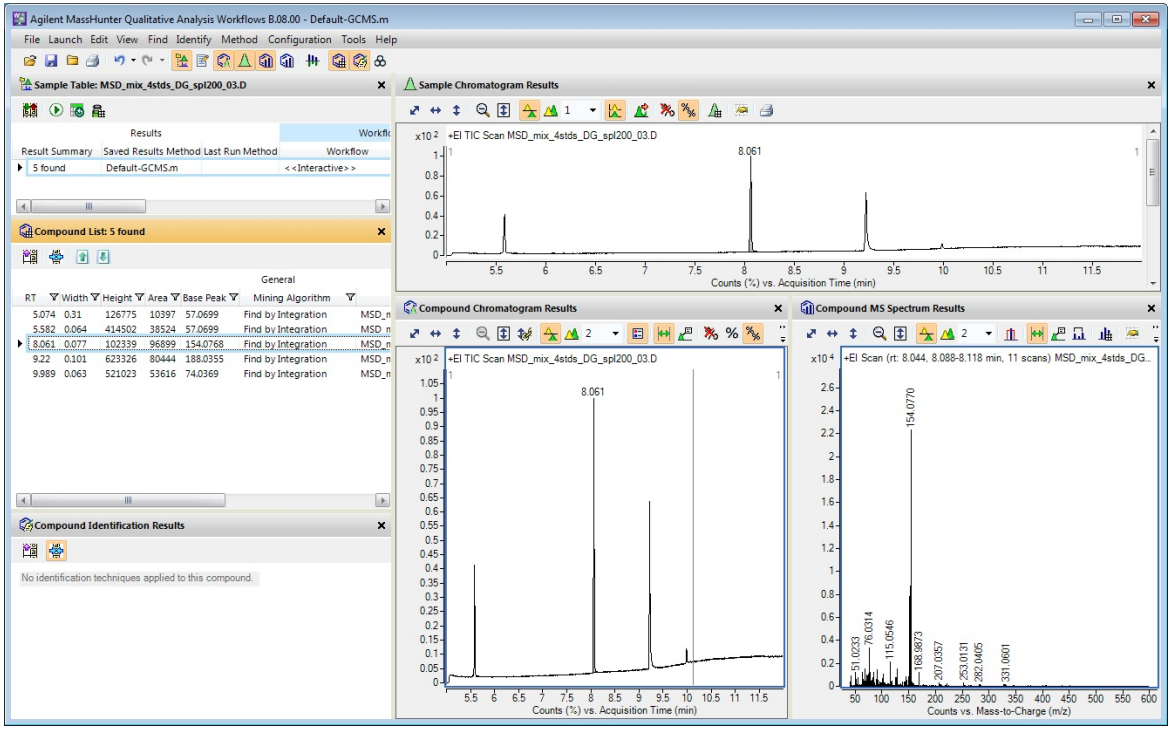


Figure 38 Find by Integration results

5 Close the data file.	**a** Click **File > Close Data File**. **b** Click **No** when asked whether or not to save results. **c** Click **Close**.	• If you want to save these results, see "Task 17. Save results" on page 75.

Task 15. Find by Fragments

For LC/MS data acquired on a TOF or Q-TOF instrument in the All Ions MS/MS mode, the Find by Formula algorithm supports an optional Fragment Confirmation step. In that step, the algorithm tries to confirm the identity of the compounds by looking for fragment ions in the high-energy spectrum that coelute with the molecular ion and that are suggested by the fragments in a library spectrum for that compound.

Find by Fragments is a similar algorithm that is tailored to the characteristics of GC/Q-TOF EI data, which has only high energy spectra that exhibit mostly fragment ions and often do not have an appreciable amount of any molecular ion. The algorithm first selects “n” fragment ions from the EI-MS spectral library based on abundance and *m/z* value (higher *m/z* fragment ions are given preference because they contain more structural information). The algorithm then extracts ion chromatograms of those ions in a time window around the target retention times in the library and creates a list of target chromatographic peaks. It then attempts to find groups of peaks that cluster by RT and selects a reference ion and confirming fragment ions. The reference ion can be the molecular ion if present, but it does not have to be. The algorithm then calculates how well the selected chromatographic peaks co-elute. The target compound is qualified, if a user settable minimum number of ions is found to have a coelution score above a set threshold.

In all cases a "Cleaned HighE Scan" is generated which only shows the reference ion and confirming fragment ions, optionally annotated with their sub formulas.

Task 15. Find by Fragments

Step	Detailed Instructions	Comments
1 Open the TIC for the **Tomato_spiked.D** data file.	**a** If the program is not open, double-click the **MassHunter Qualitative Workflows** icon. Otherwise, click **File > Open Data File**. **b** Click the **Tomato_spiked.d** data file in the **GCMS Pesticide** example data file folder. **c** Clear the **Load result data** check box and click **Open**.	• You use the General Workflow when working with GC/QQQ data. • You can use either the General Workflow or the GC/Q-TOF Compound Screening workflow when working with GC/Q-TOF data.

Task 15. Find by Fragments

Step	Detailed Instructions	Comments

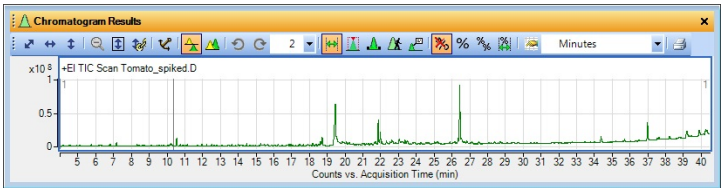



Figure 39 TIC chromatogram from Tomato_spiked.d		
2 Configure the user interface.	• Click **Configuration > Window Layouts > Restore Default Layout**.	• For these examples, start from the Default-GCMS.m method.
3 Load the GCQTOF_Pesticide_Example.m method file.	**a** Click **Method > Open.** **b** Select the **GCQTOF_Pesticide_Example.m** method and click **Open**. **c** Click the **Method Editor** tab which is in the lower left corner of the program. **d** If the **Target Source** on the Target/Suspect Screening > Find by Fragments has an error, fix the path.	• This method is installed in the \\MassHunter\methods\B.08.00 folder. • If you see any blue triangles when you load the method, you can ignore them for now. • If you see any red errors, then fix the problem.
4 Save the method to *iii*_GCQTOF_Pesticide_Example.m, where "*iii*" are your initials.	**a** From the top menu, click **Method > Save As**. **b** Type **iii_GCQTOF_Pesticide_Example.m**. **c** Click the **Save** button.	• Note that saving the method causes all the blue triangles indicating value changes in the opened method to disappear.
5 Verify the parameters for Find by Fragments.	**a** In the Method Editor window, select **Target/Suspect Screening > Find by Fragments.** **b** Click the **Target Source** tab. **c** Select the **Pesticide_Example.cdb** library in the PCDL folder. **d** Click the **Match Tolerance** tab. **e** Select **Symmetric (ppm)** for the **Possible m/z** and review the value. **f** Mark the **Limit EIC extraction range** check box, select **Symmetric**, and type `1.0` for the **Expected retention time**.	• These values are already set in this example method. • The value selected for **Possible m/z** may depend on whether you are running your acquisition method in high resolution mode or dual gain mode.

Task 15. Find by Fragments

Step	Detailed Instructions	Comments

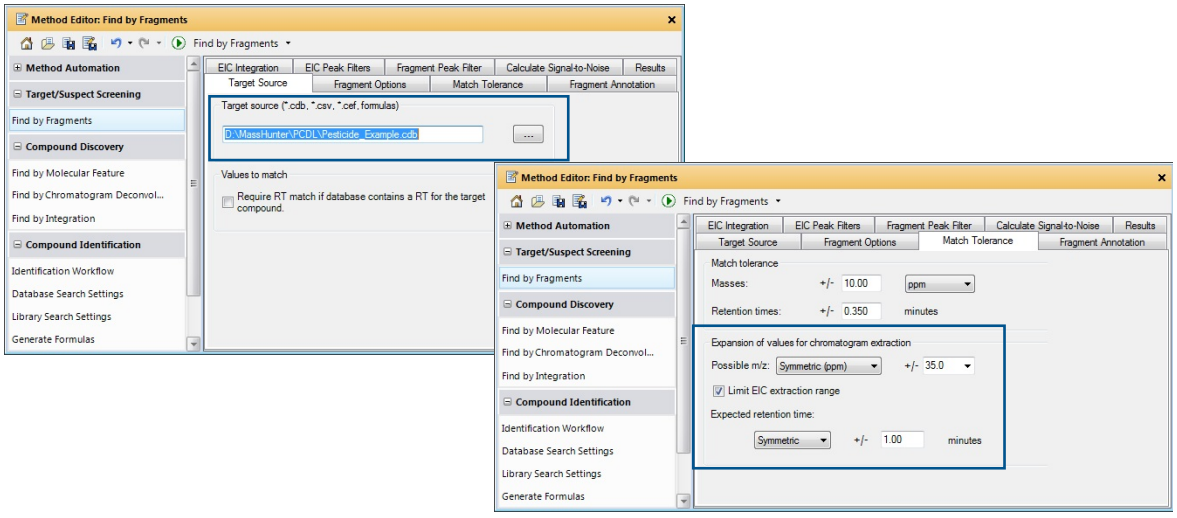


Figure 40 **Target Source** tab and **Match Tolerance** tab in the Find by Fragments section

g Click the **Fragment Options** tab.

h Click **Use spectral library only** and type `7` for the **Number of most specific ions from spectral library**.

i Type `0.2` for the **RT difference**.

- A higher number of ions produces a greater specificity and more confidence in the results; however, a higher number of ions results in a longer program run time.
- The recommended range for the **RT difference** is 0.1 to 0.2 This value is the difference that is allowed for the retention time shift of the reference ion. The reference ion is automatically chosen by the Qualitative Workflows program.

Task 15. Find by Fragments

Step	Detailed Instructions	Comments
	j Clear the **S/N ratio** check box. **k** Type 70 for the **Coelution score**. **l** Click **Minimum number of qualified fragments** and type 1.	• If the **S/N ratio** check box is marked, you have a high probability of producing false negatives (if the ratio is too low). • The recommended starting value is 1 to 3. A setting of 1 requires two qualified ions: a reference ion and a qualified ion. • Leave the values in the other tabs the same.

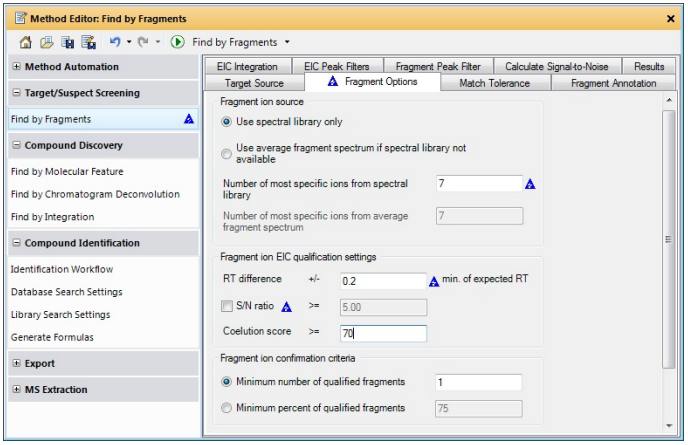


Figure 41 **Fragment Options** tab in the Find by Fragments section

6 Run the Find by Fragments algorithm.	• Click to run the **Find by Fragments** algorithm on the data file. • Click **Find > Find by Fragments**.	• The Qualitative Workflows program finds five compounds under these parameter values.
7 Save the method.	• Save the method in one of three ways: ◦ Click the **Save Method** icon in the Method Editor. ◦ Right-click the Method Editor, and click **Save Method**. ◦ From the top menu click **Method > Save**.	

Task 15. Find by Fragments

Step	Detailed Instructions	Comments
8 Examine the compounds. See Figure 42.	**a** Click the Compound Identification Results tab if it is not visible. **b** Close the Structure Viewer window. **c** Click **View > Compound Fragment Spectrum Results**. **d** In the Compound List window, right-click the header of any column that you want to remove, and click **Remove Column**.	• Selecting a compound in the Compound List window displays results in the other windows.

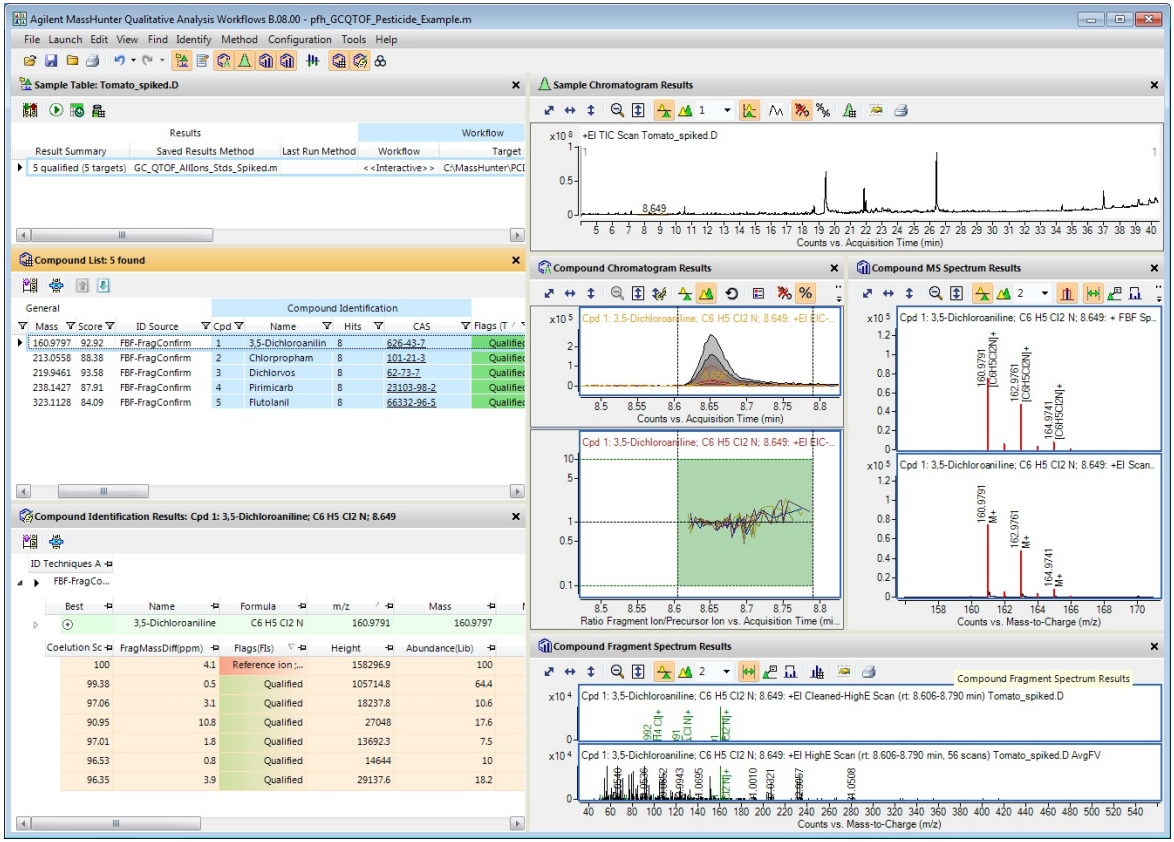


Figure 42 Find by Fragments results

Task 15. Find by Fragments

Step	Detailed Instructions	Comments
	e Click or press the arrow keys to change compounds in the Compound List to review one compound at a time. **f** Review the information in the Compound Identification Results window. **g** Click the **arrow** icon at the beginning of a row to expand a level of the table. When the level of the table is expanded, the icon changes to a - icon.	• The first level of the table shows the summary information for all of the identification algorithms that you ran. • The second level (blue) shows individual scores that were used to create the overall score. This row is only present when a molecular ion is found and reflects how well the molecular ion matches the expected mass, RT, and isotope distribution of the target compound. • The table at the bottom shows the fragment ions and their coelution scores. It also shows whether or not the fragment ion is qualified.

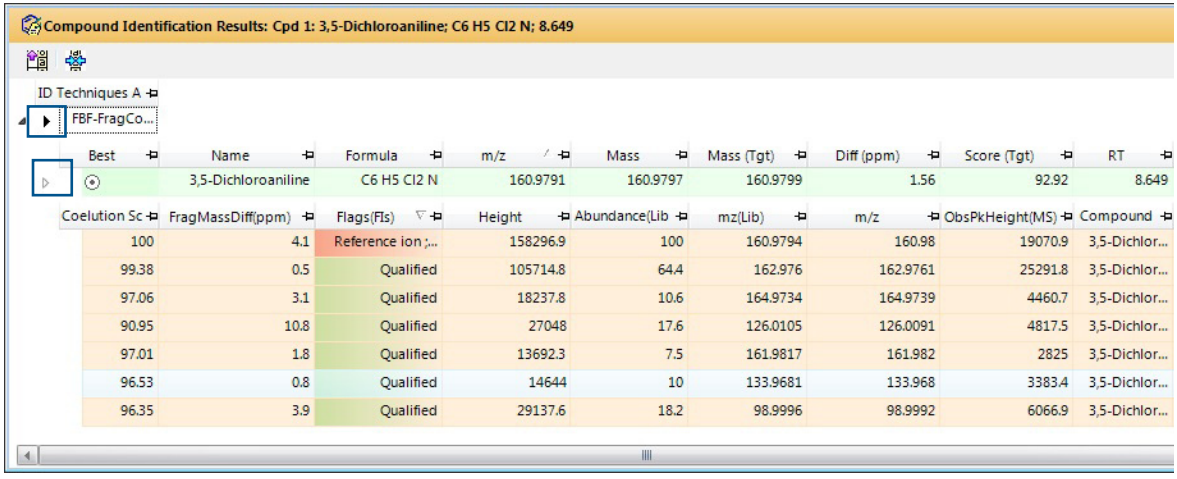


Figure 43 Compound Identification Results window

Task 15. Find by Fragments

Step	Detailed Instructions	Comments
	h Review the results in the Compound Chromatogram Results window. **i** Verify that the Coelution Plot pane is visible. **j** Verify that the chromatograms are overlaid. The icons in the toolbar are set like this: 	• The Compound Chromatogram Results window shows individual ion traces for each fragment ion. • It also shows the Coelution Plot which displays how closely the Fragment ions coelute with the compound. For reference a black line is shown with the y-value of 1. A value of 1 shows the qualifier ions are exactly coeluting with the reference ion chromatogram. As the ratio approaches 1, the qualifier ion is more closely coeluting with the reference ion.

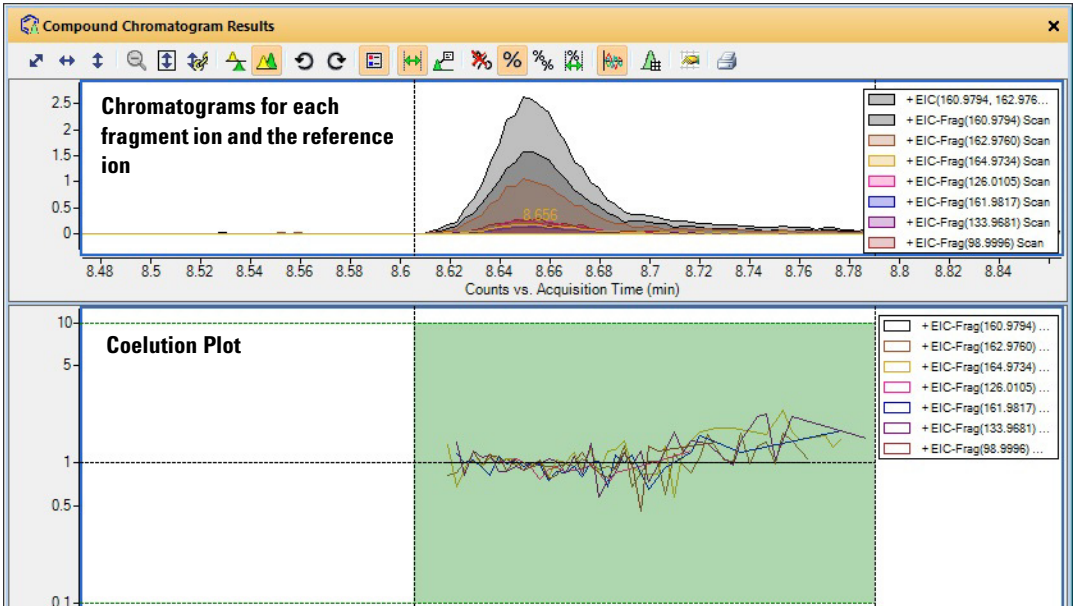


Figure 44 Compound Identification Results window

9 Close the data file.	**a** Click **File > Close Data File**. **b** Click **No** when asked whether or not to save results.	• If you want to save these results, see "Task 17. Save results" on page 75.

Task 16. Search library for mass spectra

In this task, you first integrate and extract peak spectra from a GC/Q-TOF data file. You use the MassHunter Qualitative Analysis Navigator program. Then, you generate possible formulas for each of the peak spectra.

Task 16. Search library for mass spectra

Step	Detailed Instructions	Comments
1 Open the TIC for the **MSD_mix_4stds_DB_spl200_03.d** data file.	**a** If the program is not open, double-click the **MassHunter Qualitative Navigator** icon. Otherwise, click **File > Open Data File**. **b** Click the **MSD_mix_4stds_DB_spl200_03.d** data file in the **GC** example data file folder. **c** Clear the **Load result data** check box and click **Open**.	• If the **Load result data** check box is not available, then no results have been saved in the data file. See "Task 17. Save results" on page 75 for instructions on how to save results. • The General workflow is loaded.
2 Configure the user interface.	**a** Click **Configuration > Window Layouts > Restore Default Layout**. **b** Click **Method > Open**. **c** Select *Default-GCMS.m*. **d** Click **OK**.	• For these examples, start from the Default-GCMS.m method.
3 Integrate and extract peak spectra.	**a** Click View > Method Editor. **b** Click the Chromatograms > Integrate (MS) section in the Method Editor window. **c** Click the **Peak Filters** tab. **d** Click the **Peak height** button. **e** Mark the **Relative height** check box. **f** Click **Chromatograms > Integrate and Extract Peak Spectra**.	

Task 16. Search library for mass spectra

Step	Detailed Instructions	Comments
4 Do a library search for peak spectra 1 to 4.	**a** In the Data Navigator window, click **Spectra**. **b** In the Method Editor window, click **Identify Spectra > Identification Workflow**. **c** Mark the **Identify by - Library / Database search** check box. **d** Type 50 for the Score (rev) for demo.l. **e** Select the **Identify Spectra > Library Search Settings** section. **f** Click the **Peak Filters** tab. **g** Clear the **Absolute Height** check box on the Peak Filters tab. **h** In the Method Editor, click Identify Spectra > Generate Formulas. **i** Click the Fragment Formulas tab. **j** Mark the **Annotate fragment spectrum peaks with formulas** check box. **k** Click **Identify > Search Library/DB for Spectra** in the main menu. **l** Close the Method Editor window.	• You can have multiple libraries and databases in the Identification Workflow. • If you click Search all libraries/databases, then the algorithm returns the matches from all libraries. • If you mark the **Annotate fragment spectrum peaks with formulas** check box in the Fragment Formulas tab in the Identify Spectra > Generate Formulas section, then peak annotations are added to the spectra in the MS Spectrum Results window when you click **Identify > Search Library / DB for Spectra**. • **Score (fwd)** is the minimum value for the forward search score. **Score (rev)** is the minimum value for the reverse search score.
5 Modify the columns that are visible.	**a** Right-click the Spectrum Identification Results window and click **Add/Remove Columns**. In the **Add/Remove Columns** dialog box, mark the columns that you want to display. Click **OK**. **b** Click the Hide any currently empty columns icon,  ,in the Spectrum Identification Results window.	

Task 16. Search library for mass spectra

Step	Detailed Instructions	Comments
6 Review the results.	• Review the Formula & Ion Species that are shown above the peaks in the MS Spectrum Results window.	• When the Data Navigator has the focus, you can press the Up and Down arrow keys to move between spectra. • Note that the two-color display of annotated fragment ions (green) and "other" ions (red in this case) is only seen when fragment annotation is enabled. If you only see green, you can change the spectrum color (click **Edit > Choose Defined Color**) in order to see two colors.

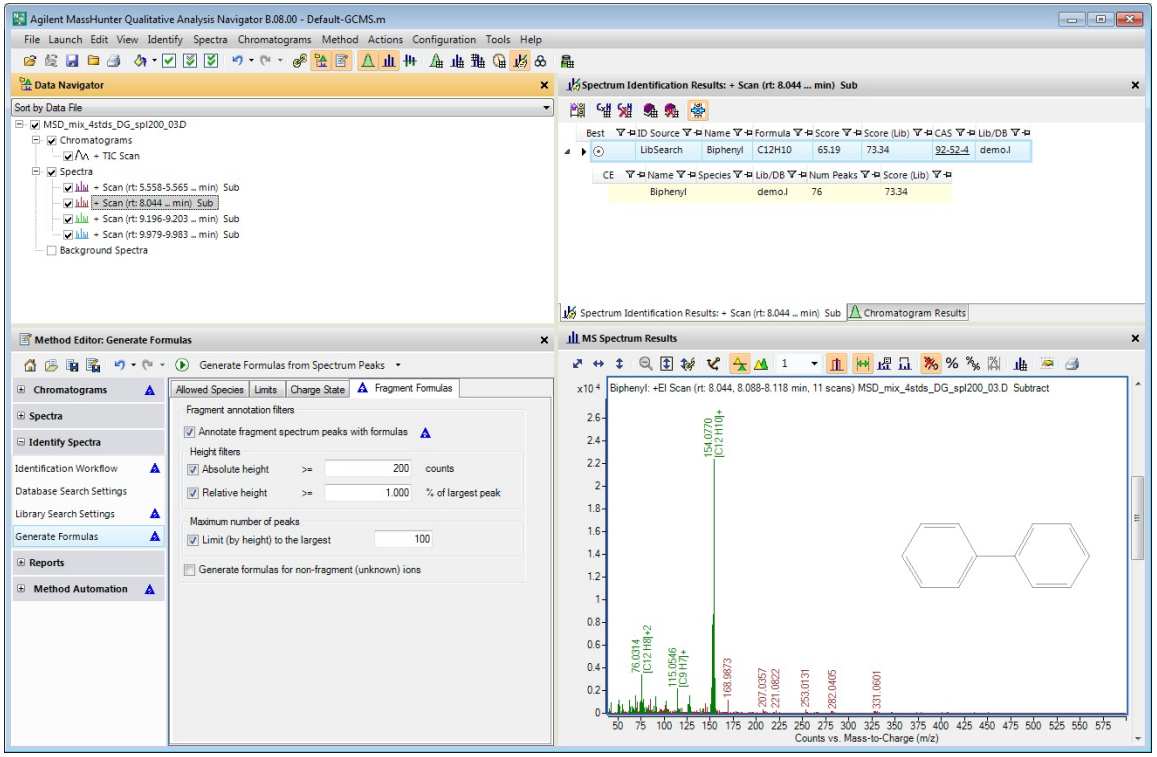
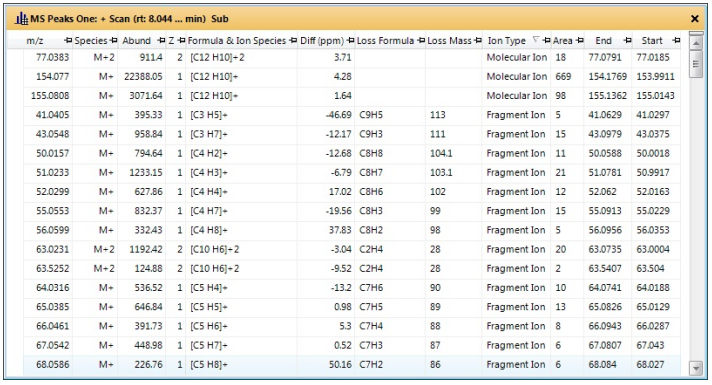


Figure 45 Results for Library Search and Generate Formulas for first peak spectra

Task 16. Search library for mass spectra

Step	Detailed Instructions	Comments
7 Review results for each spectrum in the MS Peaks One window.	**a** Click **View >MS Spectrum Peak List 1**. **b** Right-click and click **Add/Remove Columns**. **c** Verify that the columns shown in Figure 46 are in the **Show these columns** list. **d** Sort by the **Ion Type** column. **e** If the Ion Type is Fragment Ion, then the Formula & Ion Species is shown in green on each peak in the MS Spectrum Results window.	• The **Ion Type** can be Molecular Ion, Fragment Ion or blank. If it is a Fragment Ion, then the Loss Formula and Loss Mass column shows the Formula and Mass that accounts for getting to that ion from the Molecular Ion. The Formula & Ion Species shows the formula and ion species for that ion.



MS Peaks One: + Scan (rt: 8.044 ... min) Sub

m/z	Species	Abund	Z	Formula & Ion Species	Diff (ppm)	Loss Formula	Loss Mass	Ion Type	Area	End	Start
77.0383	M+2	911.4	2	[C12 H10]+2	3.71			Molecular Ion	18	77.0791	77.0185
154.077	M+	22388.05	1	[C12 H10]+	4.28			Molecular Ion	669	154.1769	153.9911
155.0808	M+	3071.64	1	[C12 H10]+	1.64			Molecular Ion	98	155.1362	155.0143
41.0405	M+	395.33	1	[C3 H5]+	-46.69	C9H5	113	Fragment Ion	5	41.0629	41.0297
43.0548	M+	958.84	1	[C3 H7]+	-12.17	C9H3	111	Fragment Ion	15	43.0979	43.0375
50.0157	M+	794.64	1	[C4 H2]+	-12.68	C8H8	104.1	Fragment Ion	11	50.0588	50.0018
51.0233	M+	1233.15	1	[C4 H3]+	-6.79	C8H7	103.1	Fragment Ion	21	51.0781	50.9917
52.0299	M+	627.86	1	[C4 H4]+	17.02	C8H6	102	Fragment Ion	12	52.062	52.0163
55.0553	M+	832.37	1	[C4 H7]+	-19.56	C8H3	99	Fragment Ion	15	55.0913	55.0229
56.0599	M+	332.43	1	[C4 H8]+	37.83	C8H2	98	Fragment Ion	5	56.0956	56.0353
63.0231	M+2	1192.42	2	[C10 H6]+2	-3.04	C2H4	28	Fragment Ion	20	63.0735	63.0004
63.5252	M+2	124.88	2	[C10 H6]+2	-9.52	C2H4	28	Fragment Ion	2	63.5407	63.504
64.0316	M+	536.52	1	[C5 H4]+	-13.2	C7H6	90	Fragment Ion	10	64.0741	64.0188
65.0385	M+	646.84	1	[C5 H5]+	0.98	C7H5	89	Fragment Ion	13	65.0826	65.0129
66.0461	M+	391.73	1	[C5 H6]+	5.3	C7H4	88	Fragment Ion	8	66.0943	66.0287
67.0542	M+	448.98	1	[C5 H7]+	0.52	C7H3	87	Fragment Ion	6	67.0807	67.043
68.0586	M+	226.76	1	[C5 H8]+	50.16	C7H2	86	Fragment Ion	6	68.084	68.027

Figure 46 MS Peaks One table with **Ion Type**, **Loss Formula**, **Loss Mass**, and **Formula & Ion Species** columns

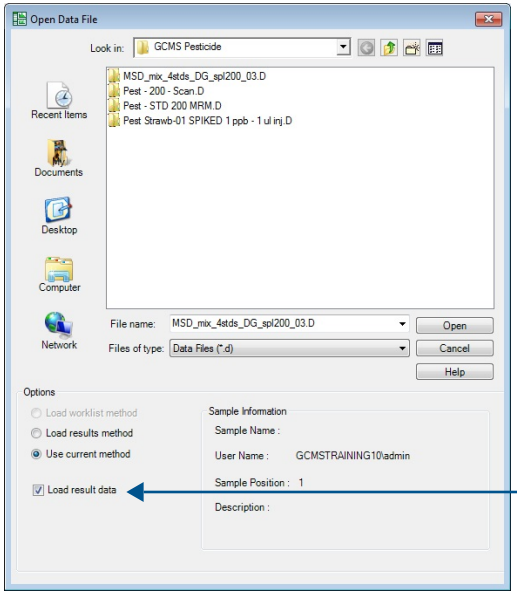
8 (optional) Close the data file. • You can proceed to the next task to learn how to save results.	**a** Click **File > Close Data File**. **b** Click **Close**.	• If you want to save these results, see "Task 17. Save results" on page 75.

Task 17. Save results

In this task, you save the results for the current data file.

Task 17. Save results

Step	Detailed Instructions	Comments
1 Save the results for the current data file and close the data file.	**a** Click **File > Save Results**. **b** Click **File > Close Data File**.	• You can only save one set of results with a data file. If you already have saved results with the current data file, then these results are overwritten when you click **File > Save Results**.
2 Open the data file and load the results.	**a** Click **File > Open Data File**. The **Open Data File** dialog box opens. **b** Select a data file. For this example, select the data file MSD_mix_4stds_DG_spl200_03.d. **c** Mark the **Load result data** check box. **d** Click the **Open** button.	



The Load result data check box is marked.

Figure 47 Open Data File dialog box

Task 17. Save results

Step	Detailed Instructions	Comments
3 Examine the results.	**a** Click the **Spectrum Identification Results** window. **b** Review the results.	

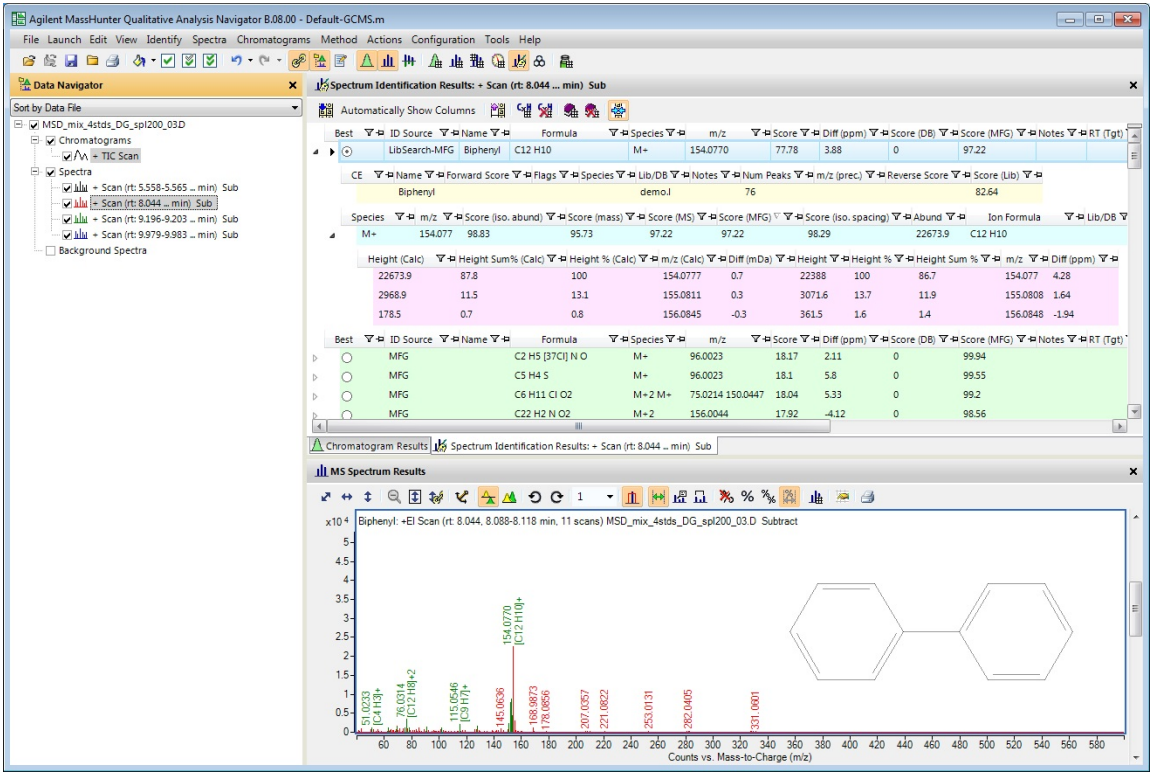


Figure 48 Results for Library Search and Generate Formulas for first peak spectra

4 Close the data file.	**a** Click **File > Close Data File**. **b** Click **No** when asked whether or not to save results.	

Task 17. Save results

Step	Detailed Instructions	Comments
5 Open the data file again and do not load the results.	**a** Click **File > Open**. The **Open Data File** dialog box opens. **b** Select a data file. For this example, select the data file MSD_mix_4stds_DG_spl200_03.d. **c** Clear the **Load result data** check box. **d** Click the **Open** button.	• If you do not load results, then by default a TIC is opened when you open a data file.

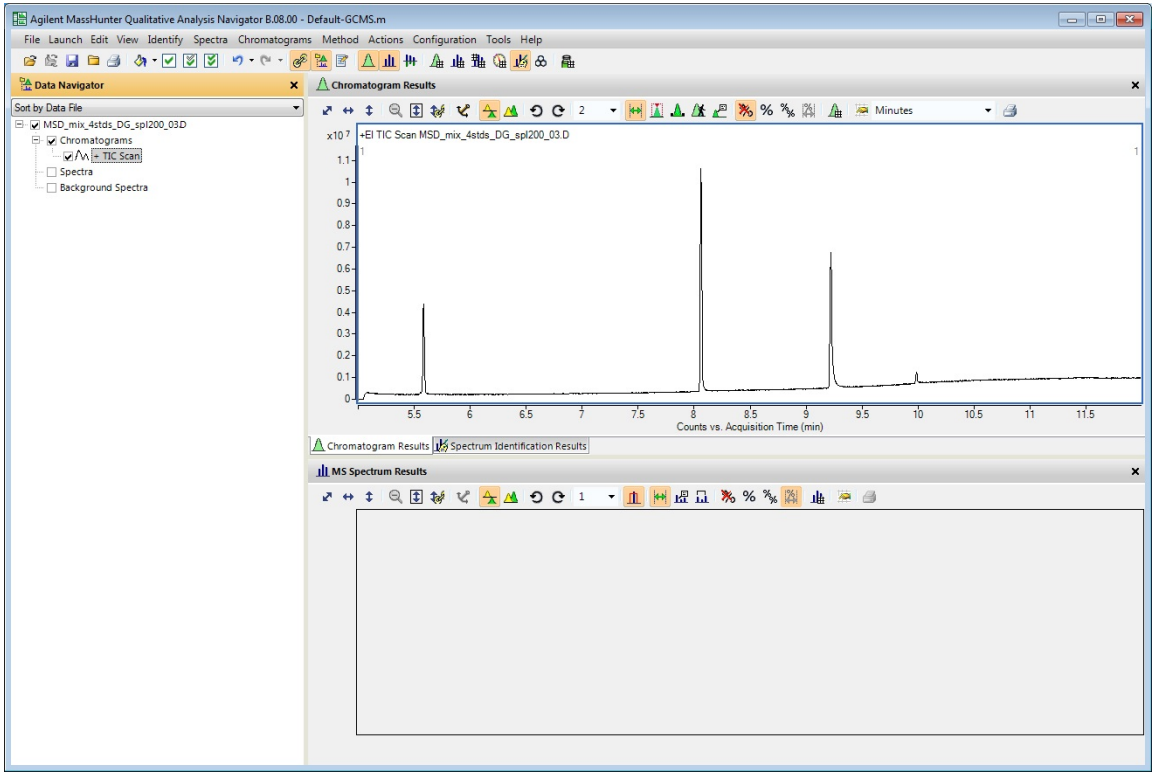


Figure 49 Results for Library Search and Generate Formulas for first peak spectra

6 Close the data file.	**a** Click **File > Close Data File**. **b** Click **No**.	

Exercise 3
Use workflows, export and print

In these tasks, you learn to set up and run a workflow.

Each exercise is presented in a table with three columns:

- Steps – Use these general instructions to proceed on your own to explore the program.
- Detailed Instructions – Use these if you need help or prefer to use a step-by-step learning process.
- Comments – Read these to learn tips and additional information about each step in the exercise.

Task 18. Set up and run a Target/Suspect Screening workflow

When you first start to use the Qualitative Analysis Workflows program, the method default.m is loaded. For GC/MS, a better starting point is the Default-GCMS.m method. You can make changes to the opened method and save it, or open a new method, make changes and save the method. You cannot overwrite the method Default.m or Default-GCMS.m.

In the Qualitative Analysis Navigator program, you can only run the Custom Workflow. In the Qualitative Analysis Workflows program, you can run any of the workflows, but some of the actions in a Custom workflow cannot be executed. You can only edit the parameters for compound mining in the Qualitative Workflows program. You use the Qualitative Workflows program in this task.

Task 18. Set up and run a Target/Suspect Screening workflow

Steps	Detailed Instructions	Comments
1 Open the TIC for the **Tomato_spiked.d** data file.	**a** If the program is not open, double-click the **MassHunter Qualitative Workflows icon**. Otherwise, click **File > Open Data File**. **b** Click the **Tomato_spiked.d** data file in the **GCMS Pesticide** example data file folder. **c** Clear the **Load result data** check box, and click **Open**.	• For GC/MRM data files, you can use the **Target/Suspect Screening** or **Custom** workflow. • For GC/TOF and GC/Q-TOF files, you can use the **Target/Suspect Screening**, **Compound Discovery**, or **Custom** workflow. • If you select **Custom**, some actions cannot be executed in the Qualitative Workflows program.
2 Configure the user interface.	**a** Click **Configuration > Window Layouts > Restore Default Layout**. **b** Click **Method > Open**. **c** Select **Default-GCMS.m**. **d** Click **OK**.	• For these examples, start from the Default-GCMS.m method.
3 Set up the method to run the Target/Suspect Screening workflow. • Select default_GC.csv as the target.	**a** In the Method Editor window, select **Method Automation > Workflow**. **b** Select **Target/Suspect Screening** as the Workflow. **c** If necessary, select the **Compound mining** algorithm. In this example, **Find by Fragments** is the only option. **d** Select **Pesticide_Example.cdb** as the **Target source**. **e** Mark the **Only report qualified compounds** check box.	• When only GC/Q-TOF or GC/TOF data files are open, **Find by Fragments** is the only option for the Compound Mining algorithm for the **Target/Suspect Screening** workflow. • When only MRM data files are open, then Find by MRM is the only option for the **Compound Mining** algorithm for the Target/Suspect Screening Workflow. • When you update the **Target source** on the **Method Automation > Workflow** section, the **Target source** on the **Target/Suspect Screening > Find by Fragments > Target Source** tab is also updated.

Task 18. Set up and run a Target/Suspect Screening workflow

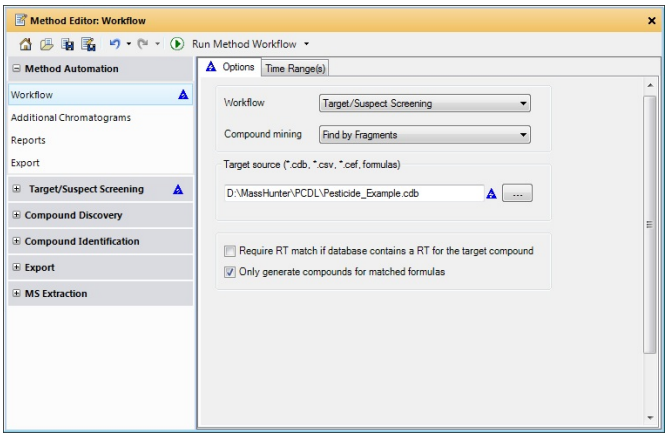
Steps	Detailed Instructions	Comments
		**You can modify the parameters in the Target/Suspect Screening section.** **You can click the Save Method icon to save the current method.**

Figure 50 The Method Automation > Workflow section

4 Test the workflow to make sure that five compounds are found and qualified.	• Click the **Run Method Workflow** icon . You can instead click Method > Run Method Workflow.	• If you click **Method > Run Method Automation (Workflow + Reports)**, then first the method workflow is run, and then a report is generated.
5 Save the method to *iii*_GCexercise1, where "*iii*" are your initials.	**a** From the top menu, click **Method > Save As**. **b** Type **iii_GCexercise1.m**. **c** Click the **Save** button.	• Note that saving the method causes all the blue triangles indicating value changes in the opened method to disappear. • You can click the Save Method icon to save the current method.

Task 18. Set up and run a Target/Suspect Screening workflow

Steps	Detailed Instructions	Comments
6 Review the results.	**a** Close the Structure Viewer window. **b** Click **View > Compound Fragment Spectrum Results**. **c** If necessary, click the Overlaid icon in the Compound Chromatogram Results toolbar. **d** Click the second compound in the Compound List window. **e** Review the other compounds to explore the results. **f** Close the data file.	• The Compound Overlay mode is on. The red chromatogram in the Sample Chromatogram Results window is the compound chromatogram for the second compound.

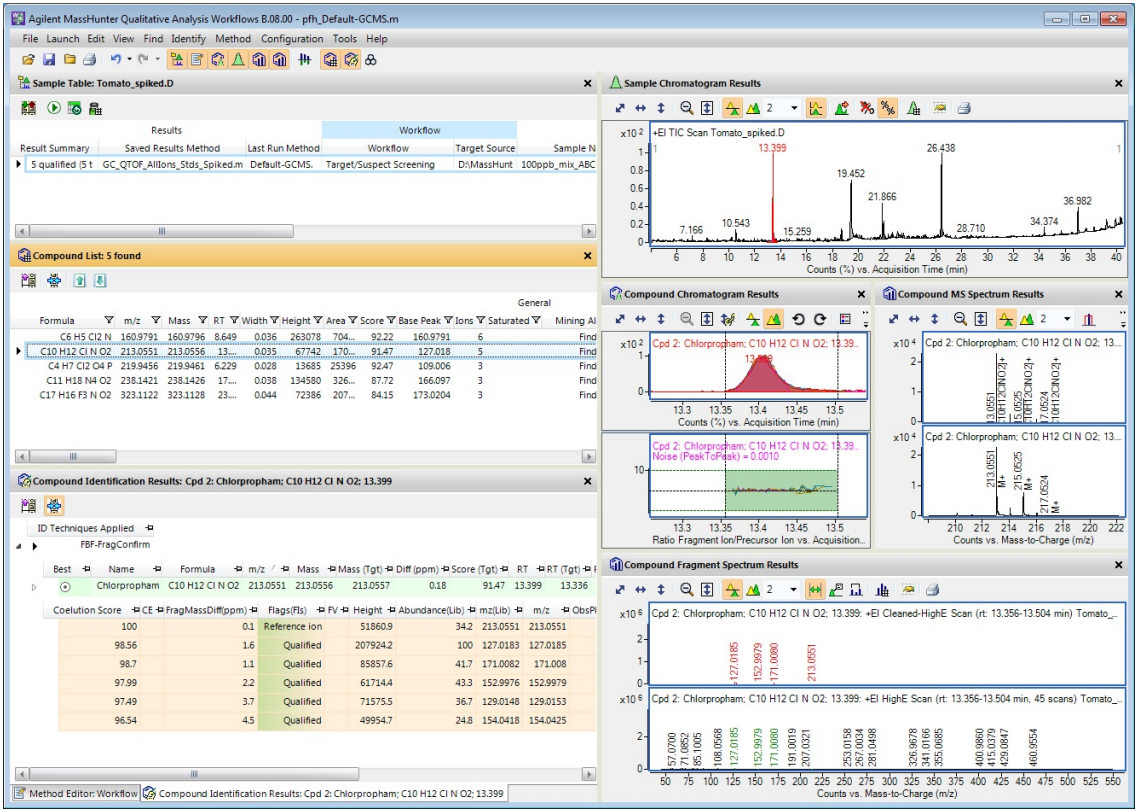


Figure 51 After running the Target/Suspect Screening workflow

Task 19. Set up and run a method using the Compound Discovery workflow

In this task you set up a qualitative analysis method that runs the Compound Discovery workflow. This workflow runs the selected compound mining algorithm and the identification algorithms that you mark.

In the Qualitative Analysis Navigator program, you can only run the Custom Workflow. In the Qualitative Analysis Workflows program, you can run any of the workflows, but some of the actions in a Custom workflow cannot be executed. You can only edit the parameters for compound mining in the Qualitative Workflows program. You use the Qualitative Workflows program in this task.

Task 19. Set up and run a method using the GC/Q-TOF Compound Screening workflow

Steps	Detailed Instructions	Comments
1 Open the TIC for the **MSD_mix_4stds_DG_spl200_03.d** data file.	**a** If the program is not open, double-click the **MassHunter Qualitative Analysis icon**. Otherwise, click **File > Open Data File**. **b** Click **MSD_mix_4stds_DG_spl200_03.d** in the **GCMS Pesticide** example data file folder. **c** Clear the **Load result data** check box and click **Open**.	
2 Configure the user interface.	**a** Click **Configuration > Window Layouts > Restore Default Layout**. **b** Click **Method > Open**. **c** Select **Default-GCMS.m**. **d** Click **OK**.	• For these examples, start from the Default-GCMS.m method.

Task 19. Set up and run a method using the GC/Q-TOF Compound Screening workflow

Steps	Detailed Instructions	Comments
3 Set up the method to run the Compound Discovery workflow.	**a** In the Method Editor window, click **Method Automation > Workflow**. **b** Select **Compound Discovery** as the Workflow. By default, the **Compound mining** algorithm is **Auto-Select Compound Mining**, and **Identify by Library/Database search** is marked. By default, **Identify by - Formula generation** is cleared.	• Auto-Select Compound Mining selects the best of the available compound mining algorithms based on the type of data file that is being analyzed. • Two library/database files are listed in the table in this method.

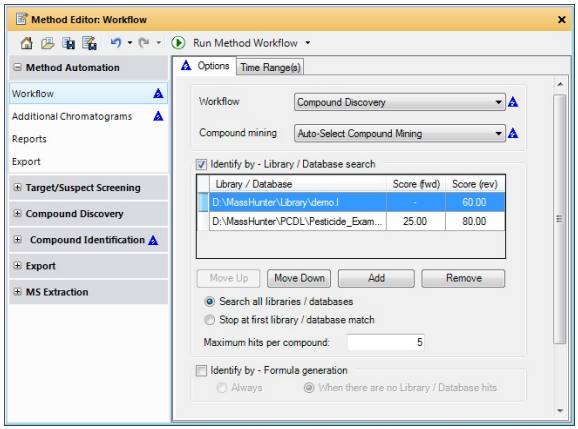


Figure 52 Method Automation > Workflow section when the Workflow is Compound Discovery

4 Save the method to *iii*_GCexercise2, where "*iii*" are your initials.	**a** From the top menu, click **Method > Save As**. **b** Type **iii_GCexercise2**. **c** Click the **Save** button.	

Task 19. Set up and run a method using the GC/Q-TOF Compound Screening workflow

Steps	Detailed Instructions	Comments
5 Test the workflow.	**a** Click the **Run Method Workflow** icon to run the workflow. You can instead click **Method > Run Method Workflow** or click **Method > Run Method Automation (Workflow and Reports)**. **b** Review the results. 26 compounds were found, and the four most abundant compounds were identified. This information is provided in the **Result Summary** column in the Sample Table.	• When you run the method as part of an acquisition workflow, the workflow is run, and the report is generated. • Once the method is set up, you just click the Run button. The system runs the compound mining algorithm, and it also tries to identify all of the compounds using a combination of accurate mass database search and spectral library matching.

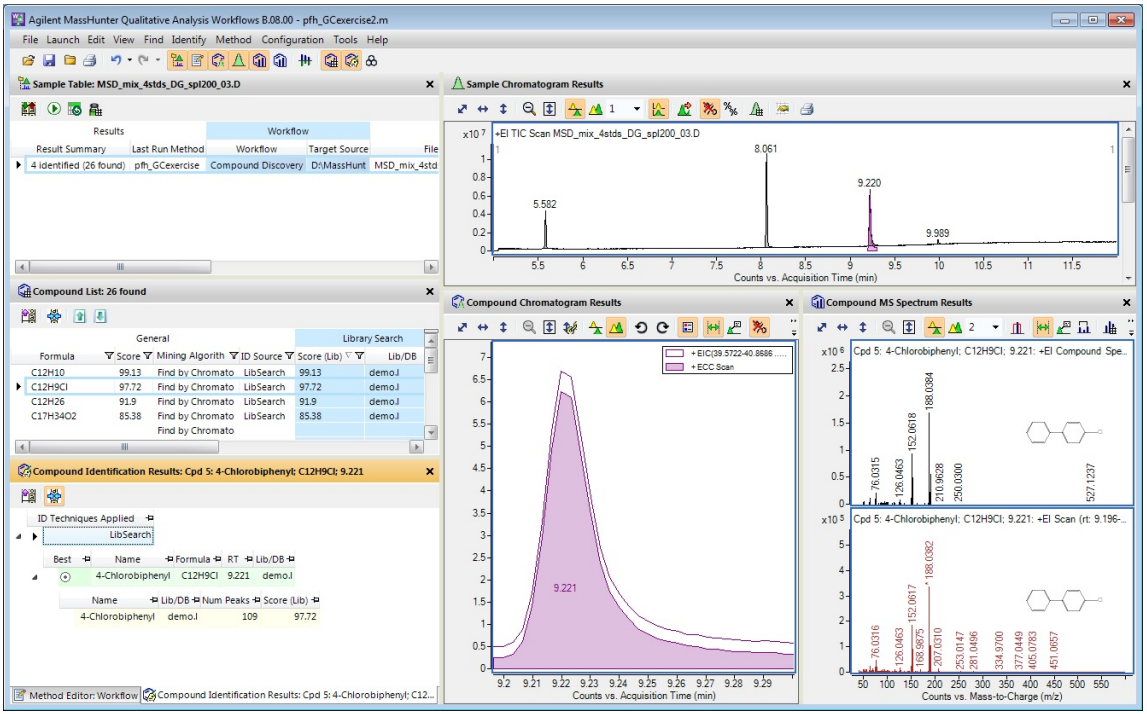


Figure 53 Results from running Compound Screening Workflow

Task 19. Set up and run a method using the GC/Q-TOF Compound Screening workflow

Steps	Detailed Instructions	Comments
6 Close the data file without saving results.	**a** Click **File > Close Data File**. **b** Click **No** when asked to save results.	

Task 20. Set up and run a method using the Custom workflow

In this task you set up a qualitative analysis method that contains a list of analysis actions to run in a specific order. The list of actions is different in the Qualitative Navigator program and the Qualitative Workflows program.

In the Qualitative Analysis Navigator program, you can only run the Custom Workflow. In the Qualitative Analysis Workflows program, you can run any of the workflows, but some of the actions in a Custom workflow cannot be executed. You can only edit the parameters for compound mining in the Qualitative Workflows program. You use the Qualitative Analysis Navigator program in this task.

Task 20. Set up and run a method using the Custom workflow

Steps	Detailed Instructions	Comments
1 Open the TIC for the **MSD_mix_4stds_DG_spl200_03.d** data file.	**a** If the program is not open, double-click the **MassHunter Qualitative Navigator** icon. Otherwise, click **File > Open Data File**. **b** Click the **MSD_mix_4stds_DG_spl200_03.d** data file in the **GC** example data file folder. **c** Clear the **Load result data** check box and click **Open**.	
2 Configure the user interface.	**a** Click **Configuration > Window Layouts > Restore Default Layout**. **b** Click **Method > Open**. **c** Select **Default-GCMS.m**. **d** Click **OK**.	• For these examples, start from the Default-GCMS.m method.
3 Add actions to the Custom Workflow.	**a** If necessary, click **View > Method Editor**. **b** In the Method Editor window, select **Method Automation > Workflow**. **c** Select **Custom** for the **Workflow**. By default, the custom workflow extracts additional chromatograms, integrates and extracts peak spectra, and identifies the selected spectra.	• The actions are run in the order that they are listed in the Actions to be run list. You can change the order of the items in the list using the arrow buttons in the Options tab.

Task 20. Set up and run a method using the Custom workflow

Steps	Detailed Instructions	Comments
4 Review parameters for the Identify Selected Spectra action.	**a** Click the **Identify Spectra > Identification Workflow** section in the Method Editor window. **b** Review the parameters. **c** Click the **Database Search Settings** tab. **d** Review the parameters. **e** Click the **Library Search Settings** tab. **f** Review the parameters.	• Note that blue triangles appear in other sections of Method Explorer. These indicate that the same parameter values have been changed elsewhere as well.
5 Save the method to *iii*_GCexercise3, where "*iii*" are your initials.	**a** From the top menu, click **Method > Save As**. **b** Type **iii_GCexercise3**. **c** Click the **Save** button.	
6 Test the custom workflow.	**a** Click the **Method Automation > Workflows** section in the Method Editor window. **b** Click the **Run Method Workflow** icon  to run the workflow on the data file. You can instead click **Method > Run Method Workflow**.	

Task 20. Set up and run a method using the Custom workflow

Steps	Detailed Instructions	Comments
7 Review the results.	**a** Click the Spectrum Identification Results tab to show the Spectrum Identification Results window. This window is tabbed with the Chromatogram Results window. **b** Click the spectra at 9.2 minutes. **c** Click **View > Difference Results**. **d** Click **View > Structure Viewer**. **e** Review the results.	• When you run a custom workflow, a report is generated if you click **Run Method Automation (Workflow + Reports)**. • The Spectral Difference Results window is tabbed with the MS Spectrum Results window.

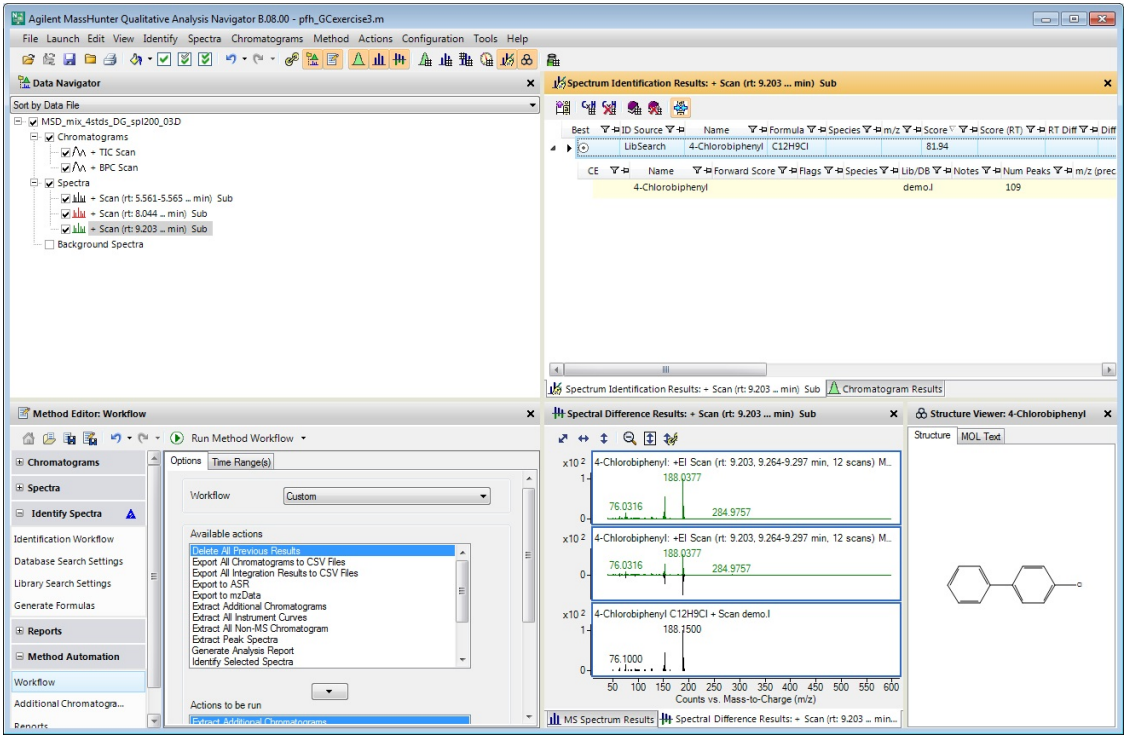


Figure 54 Results from running a custom workflow in the Qualitative Analysis Navigator program

8 Close the data file without saving results.	**a** Click **File > Close Data File**. **b** Click **No** when asked to save results.	

Task 21. Export a CEF file

You can export a CEF file containing compound information. This CEF file can be imported into other programs such as MassHunter Mass Profiler and Mass Profiler Professional. You can only export a CEF file from the MassHunter Qualitative Workflows program.

Task 21. Export a CEF file

Steps	Detailed Instructions	Comments
1 Open the **MSD_mix_4stds_DG_spl200_03.d** data file.	**a** If the program is not open, double-click the **MassHunter Qualitative Workflows** icon. Otherwise, click **File > Open Data File**. **b** Click **MSD_mix_4stds_DG_spl200_03.d** in the **GCMS Pesticide** folder. **c** Clear the **Load result data** check box. **d** Click **Open**.	• You can export a CEF file interactively or when you run **Method Automation (Workflow + Reports)**.
2 Configure the user interface.	**a** Click **Configuration > Window Layouts > Restore Default Layout**. **b** Click **Method > Open**. **c** Select **Default-GCMS.m**. **d** Click **OK**.	• For these examples, start from the Default-GCMS.m method.
3 Find compounds.	• Run any compound mining algorithm. For example, click **Find > Find by Molecular Feature.**	• A CEF file is used to export compounds.

Task 21. Export a CEF file (continued)

Steps	Detailed Instructions	Comments
4 Export a CEF file.	**a** To interactively export the file, click **File > Export > as CEF.** **b** Click the **All results** option. **c** Select the location of the export file. **d** Click **OK**.	• You can import a CEF file in the Mass Profiler Professional software and the MassHunter Mass Profiler software.

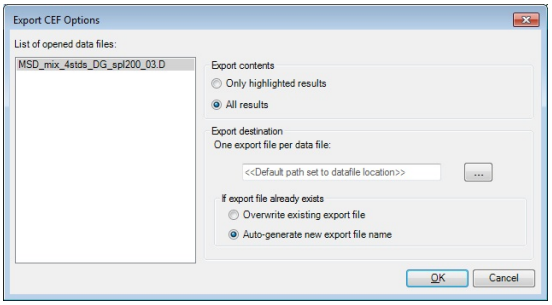


Figure 55 Export CEF Options dialog box

5 Edit the method to export a CEF file.	**a** Click the Method Editor tab to see the Method Editor window. It is tabbed with the Compound Identification Results window by default. **b** Click Method Automation > Export. **c** Mark the **CEF** check box. **d** Review the other parameters in this section.	• You can export results in multiple formats. • You can modify Export parameters for some algorithms. You do not specify additional parameters when you export a CEF file.

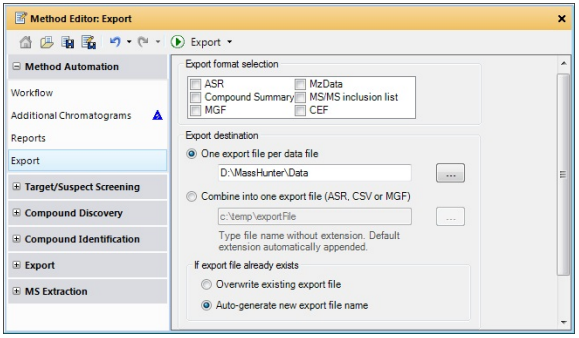


Figure 56 Method Automation > Export section in the Method Editor window

Task 21. Export a CEF file (continued)

Steps	Detailed Instructions	Comments
6 Run the Method Automation (Workflow + Reports) algorithm.	**a** Click **Method Automation > Workflow**. **b** Click **Method > Run Method Automation (Workflow + Reports)**. You can instead click the arrow next to the run icon to run the workflow on the data file.	• When you run Method Automation (Workflow + Reports), the following algorithms are run: ◦ Method Workflow ◦ Extract additional chromatograms ◦ Generate a report ◦ Export results

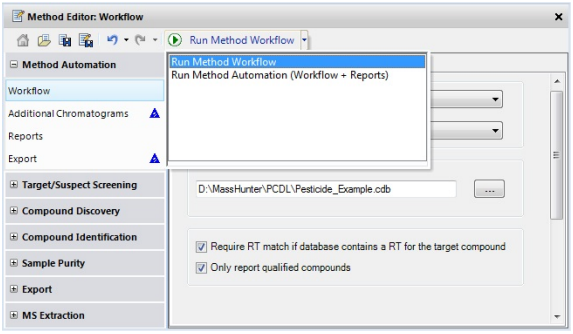


Figure 57 Method Automation > Workflow section showing run options.

7 Save the method to *iii*_GCexercise4, where "*iii*" are your initials.	**a** From the top menu, click **Method > Save As**. **b** Type **iii_GCexercise4**. **c** Click the **Save** button.	

Task 22. Print an analysis report

Whenever you want to print an analysis report in the Qualitative Analysis Navigator program, use these instructions.

An analysis report can contain the results from extracting and integrating chromatograms, extracting spectra, searching the database for peak spectra, or generating formulas from peak spectra.

Task 22. Print an analysis report

Steps	Detailed Instructions	Comments
1 If the **MSD_mix_4stds_DG_spl200_03.d** data file is not loaded, then open this data file and run the workflow for the method iii_GCexercise3.m which was created in "Task 20. Set up and run a method using the Custom workflow" on page 87.	**a** If the program is not open, double-click the **MassHunter Qualitative Navigator icon**. Otherwise, click **File > Open Data File**. **b** Click the **MSD_mix_4stds_DG_spl200_03.d** data file in the **GC** example data file folder. **c** Clear the **Load result data** check box. **d** Click the **Use current method** button and click **Open**. **e** Click **Method > Run Method Workflow**.	• If you finished "Task 20. Set up and run a method using the Custom workflow" on page 87, then the current method is iii_GCexercise3.m. This method is set up to extract additional chromatograms, integrate and extract peak spectra, and identify selected spectra. • An analysis report contains integration information, and spectral information. If you identify the spectra, then this report can include that information.
2 Change the analysis report selections in the method: • Mark the check boxes for the chromatograms, spectra or tables you want to print. • Clear the check boxes for the chromatograms, spectra or tables which you do not want to print.	**a** Click View > Method Editor. **b** In the Method Editor window, click **Reports > Analysis Report**. **c** Mark the check boxes for any additional selections you want to print. **d** Clear any check boxes for items which you do not want to print.	• The Analysis report only contains the information that you mark in this section. • You can instead click Method Automation > Reports to set up the reporting parameters. Changes made there are reflected in the Reports section, and vice versa. • If some results are not available, then those results are not included, even if those results are marked in this section. For example, if you have not integrated the chromatogram, then the peak table is not included.

Task 22. Print an analysis report (continued)

Steps	Detailed Instructions	Comments

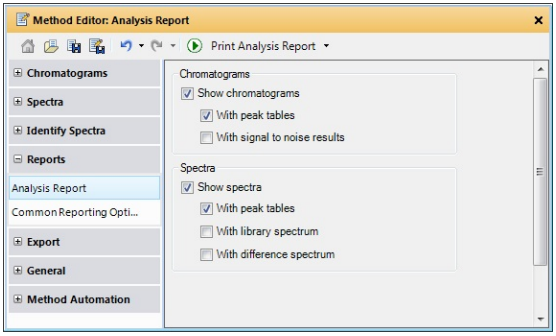
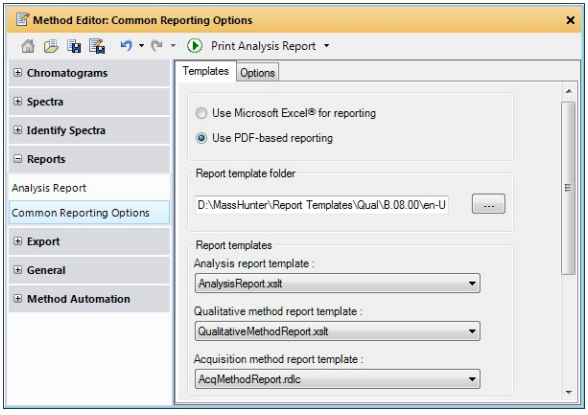


Figure 58 Analysis Report section in the Method Editor window

3 Review the Templates parameters.	**a** In the Method Editor window, click **Reports > Common Reporting Options**. **b** (optional) Select a different Analysis report template.	• Different report templates are available. These templates contain different information.



You can select whether to use Microsoft Excel for reporting or to use PDF-based reporting.

If you click Use Microsoft Excel for reporting, then a different set of templates is available to select. You can use Excel to modify the selected template. See the online Help for the Report Designer to learn more about modifying a template.

Figure 59 Common Reporting Options > Templates tab in the Method Editor window

Task 22. Print an analysis report (continued)

Steps	Detailed Instructions	Comments
4 Print the report.	**a** Print the report in one of these ways: • From the main menu, click **File > Print > Analysis Report.** • From the main toolbar, click the Printer icon. • Click the **Print Analysis Report** icon,  in the Method Editor toolbar when the Analysis Report section is selected. • Right-click the Analysis Report section in the Method Editor, and click **Print Analysis Report**. • From the data file shortcut menu in the Data Navigator, click **Analysis Report**. **b** Click one of the options under **Report contents**. **c** (optional) Mark the **Separate report per data file** check box. **d** Mark the **Print report** check box and select a printer. **e** Mark the **Print preview** check box. **f** Click the **OK** button.	• The Run icon  in the Method Editor toolbar sometimes allows you to choose an action from a set of possible actions. For example, if you switch to the Reports > Common Reporting Options section of the Method Editor window, four different actions are possible when you click the Run icon. If you click the arrow, a list of possible actions is shown, and you can choose which action to do. Choosing a different action from the list changes the default action. If you simply click the Run button, the current default action is performed. • When you click **Method > Run Method Automation (Workflow + Reports),** the method workflow is run. Then, any additional chromatograms are extracted, and the report is printed. Finally, export files may be generated if marked in the Method Automation > Export section.

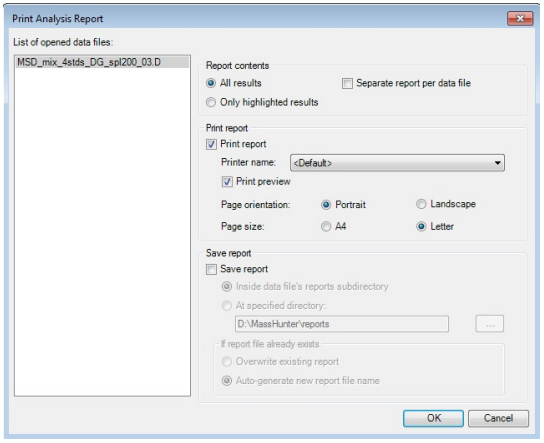


Figure 60 Print Analysis Report dialog box

Task 22. Print an analysis report (continued)

Steps	Detailed Instructions	Comments
	g Review the report. **h** Click the **Close Print Preview** icon in the toolbar.	

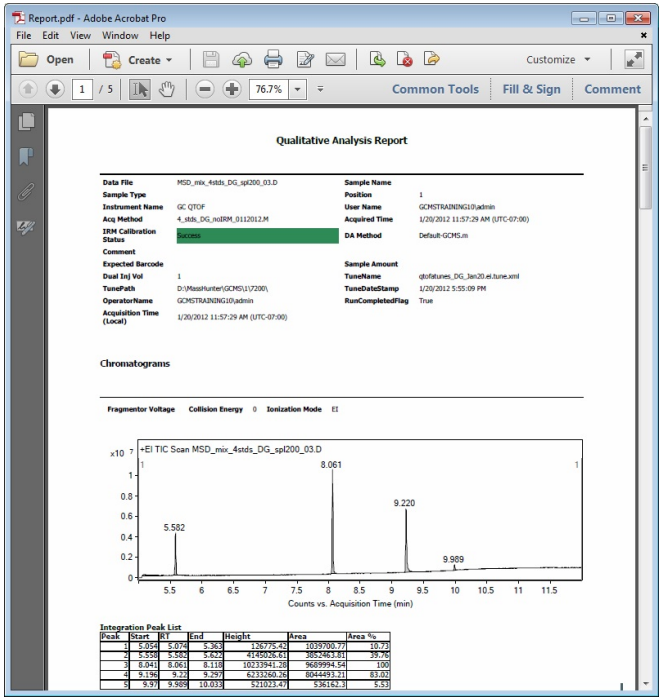


Figure 61 Preview of the Analysis Report

Task 23. Print a compound report

Whenever you want to print a compound report, use these instructions. You print a compound report from the Qualitative Workflows program.

Task 23. Print a compound report

Step	Detailed Instructions	Comments
1 If the **MSD_mix_4stds_DG_spl200_03.d** data file is not loaded, then open this data file and run the workflow for the method iii_GCexercise2.m which was created in "Task 19. Set up and run a method using the Compound Discovery workflow" on page 83.	**a** If the program is not open, double-click the **MassHunter Qualitative Workflows** icon. Otherwise, click **File > Open Data File**. **b** Click the **MSD_mix_4stds_DG_spl200_03.d** data file in the **GC** example data file folder. **c** Clear the **Load result data** check box. **d** Click the **Use current method** button and click **Open**.	• If you finished "Task 19. Set up and run a method using the Compound Discovery workflow" on page 83, then the current method is iii_GCexercise2.m. The workflow for this method is Compound Discovery. The Compound mining algorithm is automatically selected, and the Identify by - Library/Database search option is marked.
2 Run the workflow. • A compound report includes a compound table.	• Click **Method > Run Method Workflow**.	• The compound mining algorithm is automatically selected. • The Library/Database search algorithm is run on the compounds.
3 Review the template selected. • If you want to choose a different template, then you need to know the workflow selected to know which report template parameter to modify. • If you click **Use Microsoft Excel for reporting**, you can use Excel and the Report Designer add-in to customize any of the templates that have the extension XLTX. You cannot customize the acquisition method report.	**a** In Method Editor, click **Method Automation > Reports**. **b** Click the **Templates** tab. **c** (optional) Select a different report template for the **Target screening report template**. **d** (optional) Select a different report template for the **Compound Discovery report template**. **e** (optional) Select a different report template for the **Sample purity report template**. **f** (optional) Select a different report template for the **Compound report template**.	• The report template that is used when you print a compound report depends on the current workflow. • The Target screening report template is used with the **Target/Suspect Screening** workflow. • The Compound Discovery report template is used with the **Compound Discovery** workflow. • The Compound report template is used with the **Custom** workflow. • The current workflow is selected on the **Method Automation > Workflow** section.

Task 23. Print a compound report

Step	Detailed Instructions	Comments
4 Change some of the selections in the method for compound reports: • Turn off viewing the MS spectra zoomed in on special peaks. • Turn off the MS/MS options in the report.	**a** Click the **Contents** tab. **b** Clear the **Show MS spectrum (zoomed in on special peaks)** check box. **c** If visible, clear the **Show MS/MS spectrum** check box. **d** If visible, clear the **Show MS/MS peak table** check box.	• These check boxes allow you to specify what information to include in a report if it is available. If the information is not available, that section is automatically skipped. For example, MS/MS results are never included when the data file only has MS data. • The **Compound spectrum (MS/MS)** section is not visible when the opened data files only contain MS data. • For GC/MS data, clear the **Overlay compound chromatograms** check box.

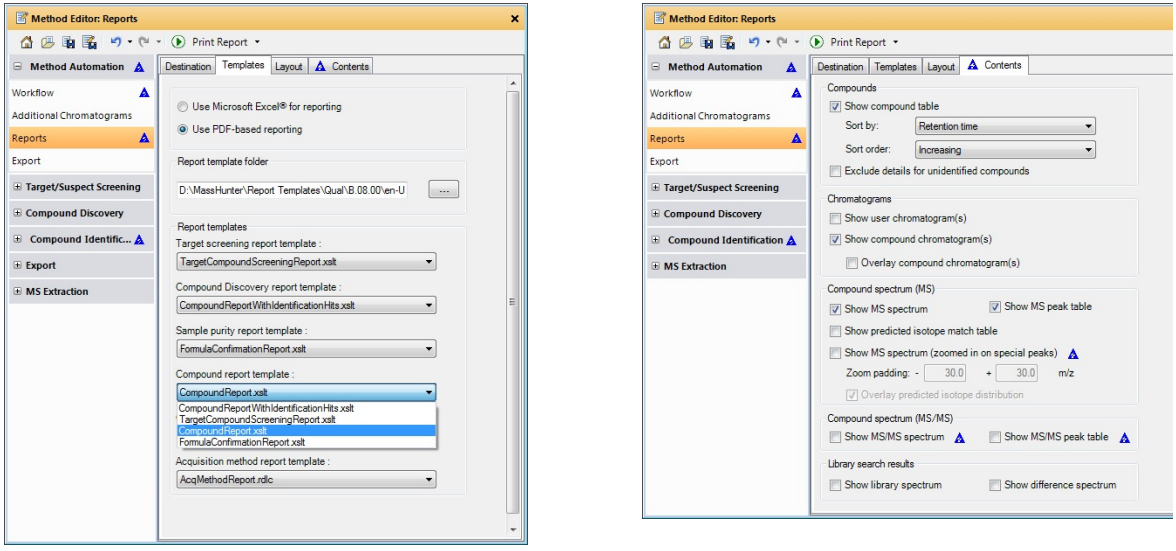


Figure 62 Compound Report section in the Method Editor

Task 23. Print a compound report

Step	Detailed Instructions	Comments
5 Print the report.	**a** Click **File > Print > Compound Report.** If you click the **Print Report** icon to print the compound report, it is printed immediately. **b** Mark the **Print preview** check box. **c** Click **OK**. Examine the report. **d** Click the **Close Print Preview** icon.	• In the Print Compound Report dialog box, you can select a different printer, select to save the report to a PDF or Excel file, select whether to print all results or only the highlighted results, and whether or not to combine different data files into one report.

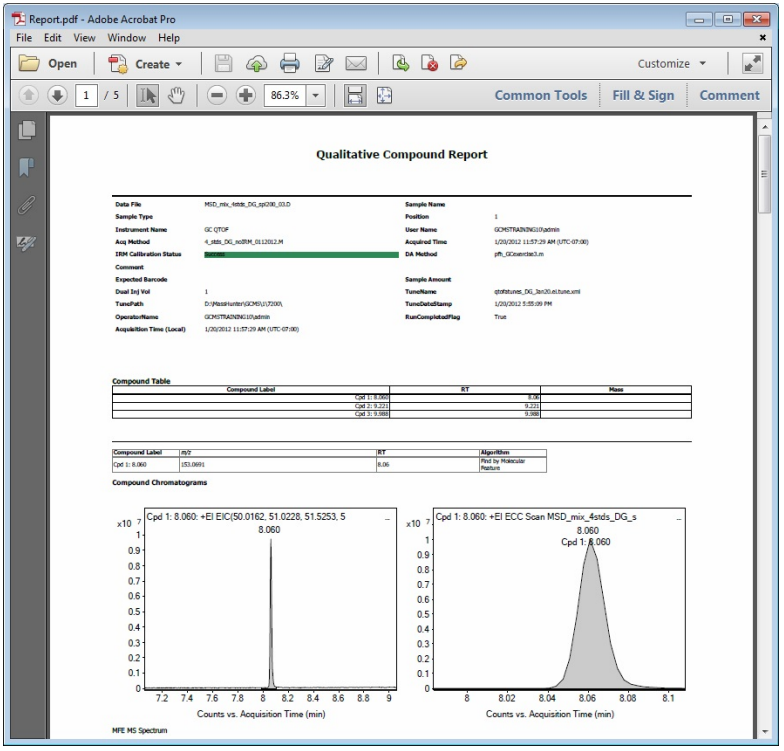


Figure 63 Print Preview window with the Compound Report

6 Close the data file without saving results.	**a** Click **File > Close Data File**. **b** Click **No** when asked if you want to save the results.	

Reference

Qualitative Analysis Navigator Program

Main Functional Areas

When you first open the Qualitative Analysis navigator program, you see three parts: (1) the Menu Bar, (2) the Toolbar, and (3) the Main Window. The main functional areas are shown in Figure 64.

Figure 64 Overview of the Qualitative Analysis Navigator program

1. Menu Bar

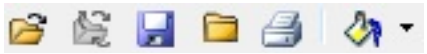
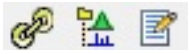
The menu bar (Figure 65) provides actions that are used for extracting chromatograms and spectra and identifying the spectra, printing and exporting reports, and launching the Qualitative Analysis Workflows program or the BioConfirm program. The online Help describes each menu.

Figure 65 The menu bar for the Qualitative Analysis Navigator program

2. Toolbar

The toolbar provides actions that are used for opening and closing data files. You can also open and save methods, print a compound report, and toggle whether a window is visible or not.

Figure 66 The toolbar for the Qualitative Analysis Navigator program

Toolbar Icon	Action
	File > Open Data File File > Refresh Data File File > Save Results File > Close Data File File > Print > Analysis Report Edit > Choose Defined Color
	Edit > Show > Highlighted Edit > Show > Only Highlighted Edit > Show > All Items Edit > Undo Edit > Redo
	View > Linked Navigation View > Data Navigator View > Method Editor

Toolbar Icon	Action
	Chromatogram Results window MS Spectrum Results window Difference Results window UV Spectrum Results window
	Integration Peak List window MS Spectrum Peak List 1 window MS Spectrum Peak List 2 window MS Actuals window
	Spectrum Identification Results window Structure Viewer window Sample Information window

3. Main window

The main window (see Figure 64 on page 102) is further divided into up to 17 windows:

- Data Navigator
- Method Editor
- Chromatogram Results
- Spectrum Preview
- MS Spectrum Results
- Recalibration
- Difference Results
- UV Spectrum Results
- Integration Peak List
- MS Spectrum Peak List 1
- MS Spectrum Peak List 2
- MS Actuals
- Spectrum Identification Results
- Structure Viewer
- Sample Information
- Formula Calculator
- Mass Calculator

Two of these windows (Spectrum Preview and Recalibration) are started from one of the other windows, and two of these windows (Formula Calculator and Mass Calculator) are started from the Tools menu. When you first open the Qualitative Analysis navigator program, you see three windows in the default layout: Data Navigator, Chromatogram Results, and MS Spectrum Results.

Windows - Qualitative Analysis Navigator Program

Data Navigator The Data Navigator organizes all the results of extraction and spectrum selection either by data file or by data type. When sorting by data file, all of the extracted chromatograms are listed under Chromatograms for each data file. All of the extracted spectra are listed under either Spectra or Background Spectra.

When you click a chromatogram or spectrum, the plot is automatically highlighted in the plot window, and the windows containing tables are updated. When Linked Navigation is activated (**View > Linked Navigation**), additional linking of a chromatogram to spectra extracted from that chromatogram (and vice versa) is active. Highlighting a chromatogram in Data Navigator also highlights the corresponding spectra. The corresponding chromatogram and spectrum graphic results are also highlighted. Linked Navigation only works if you have used the **Integrate and Extract Peak Spectra** command from the Chromatograms Menu.

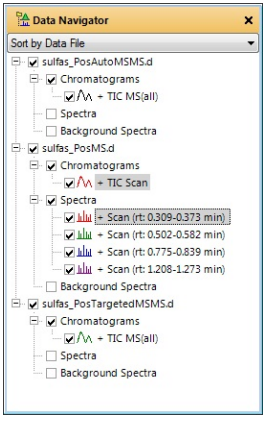


Figure 67 Data Navigator window with three data files opened

Method Editor This window allows you to edit method parameters. These parameters are separated into different tabs, and related tabs are grouped together in different sections. The left-hand side of the window shows the different sections. You can get help on the currently viewed tab of the current section when you press the **F1** key.

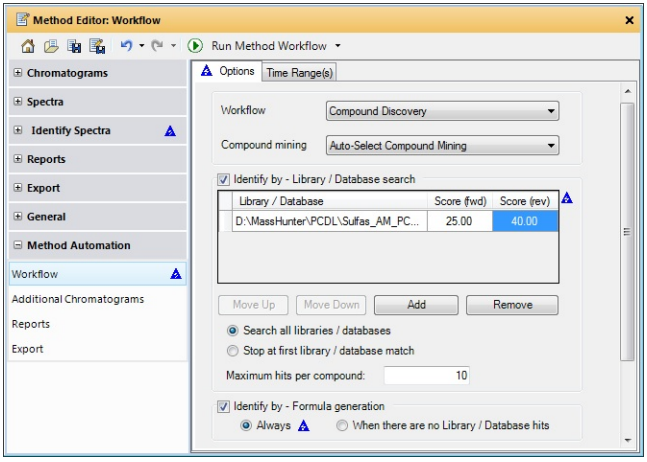


Figure 68 Method Editor window

Chromatogram Results You view any chromatogram in this window. You can view multiple chromatograms from different files at the same time. You can show these chromatograms overlaid or in list mode. Figure 69 shows the chromatograms in list mode.

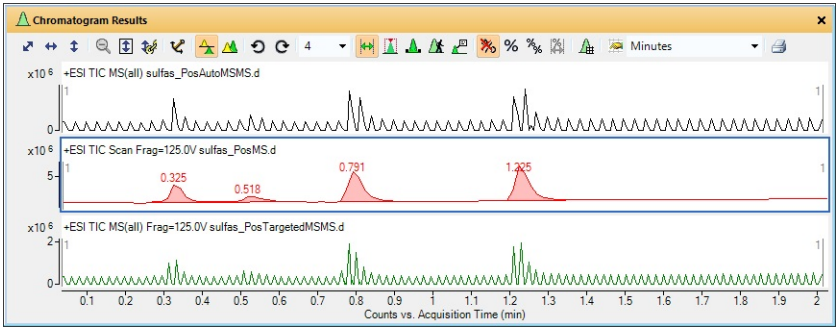


Figure 69 Chromatogram Results window showing three chromatograms in List Mode

Perform operations on the chromatogram

You can perform many operations on chromatograms.

- You can change the appearance of the plots in the window via icons in the Chromatogram Results toolbar.
- You can extract additional chromatograms or mass spectra, or process chromatograms via the **Chromatograms** menu.
- You can initiate many operations via the shortcut menu. When you right-click a chromatogram in the Chromatogram Results window, you see the shortcut menu.

See the online Help for more information. The following table shows some possible operations.

Action	How to do it
Change peak labels in chromatogram	Click  in the Chromatogram Results toolbar
Extract a chromatogram	Chromatograms > Extract Chromatograms
Extract additional chromatograms	Chromatograms > Extract Additional Chromatograms
Integrate the chromatogram	Chromatograms > Integrate Chromatogram
Integrate and extract peak spectra	Chromatograms > Integrate and Extract Peak Spectra
Smooth the chromatogram	Chromatograms > Smooth Chromatogram
Calculate Signal-to-Noise	Chromatograms > Calculate Signal-to-Noise

Spectrum Preview You use this window to quickly scan the spectra in a data file. You start this window in the Chromatogram Results window when you select the “Walk Chromatogram” tool ( ). The spectra displayed in this window are not kept in the Data Navigator window unless you copy a spectrum to the Spectra section.

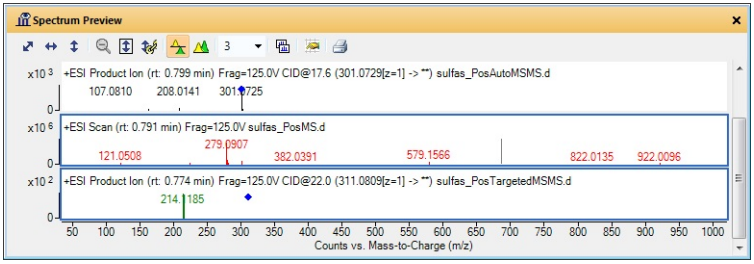


Figure 70 Spectrum Preview window showing spectra from 3 data files

MS Spectrum Results You display MS and MS/MS spectra in this window. You can add annotations and calipers to these spectra. You can change the peak labels and the font in the **MS and MS/MS Spectra Display Options** dialog box. If you performed a library search and identified the spectrum, a structure may also be visible in the pane for that spectrum. You can also see predicted isotope distributions (from formula generation) and custom text or graphic annotations, including “calipers” to measure mass differences.

You can perform many operations on spectra.

- You can change the appearance of the plots in the window via icons in the MS Spectrum Results toolbar. You can also add annotations and calipers via the toolbar.
- You can add or subtract spectra, send spectra to PCDL, and recalibrate a spectrum via the **Spectra** menu.
- You can initiate many operations via the shortcut menu. When you right-click a spectrum in the MS Spectrum Results window, you see the shortcut menu.

See the online Help for more information on toolbars, menus, and shortcut menus.

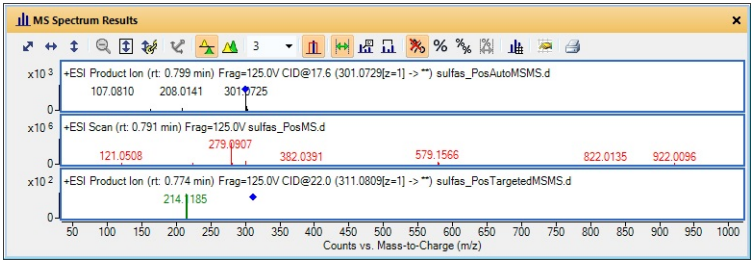


Figure 71 MS Spectrum Results window showing three MS spectra

Recalibration You refine the mass calibration for TOF or Q-TOF data from this window. You specify the reference mass list, and the system finds matches to the reference masses in the spectrum from which you start the window. You can apply these values to a data file. You start this window from the shortcut menu in the MS Spectrum Results window.

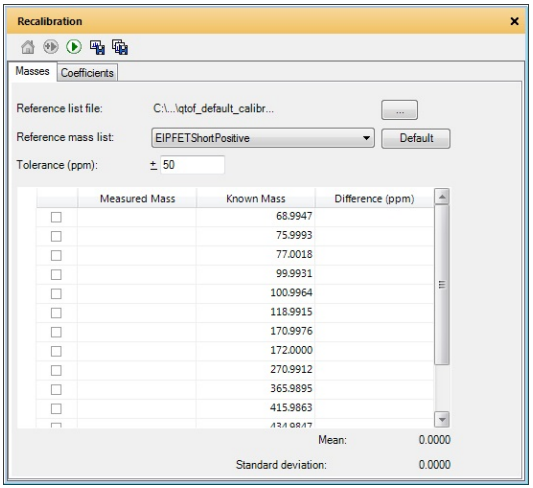


Figure 72 Recalibrate window

Spectral Difference Results After you run the Search Library algorithm and identify the spectrum with library search, this window shows three spectra. The first spectrum is the spectrum that was searched. The second spectrum is a difference spectrum. The spectra from the library is subtracted from the user spectrum to create the difference spectrum. The third spectrum is the spectrum from the library that is currently selected in the Spectrum Identification Results window.

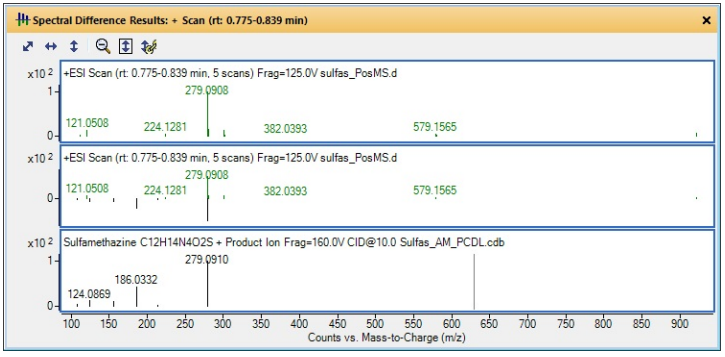


Figure 73 Spectral Difference Results window

UV Spectrum Results This window shows UV spectra. You can extract a UV spectrum from either an MS chromatogram or a UV chromatogram if you acquired UV data. You can add annotations to a UV spectrum.

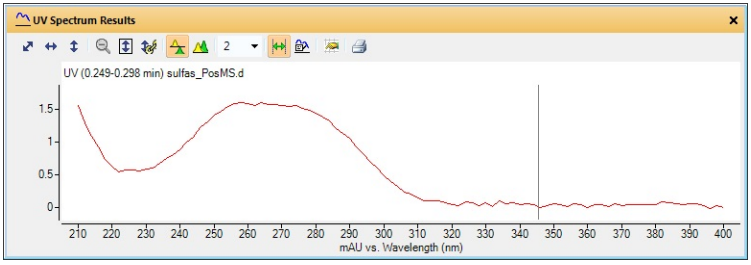


Figure 74 UV Spectrum Results

Integration Peak List This window contains a table of the integration results for the selected chromatogram. Each peak in the chromatogram is listed on a separate row in the table. If you have more than one chromatogram highlighted, the first chromatogram in the Data Navigator window that is highlighted is shown in the Integration Peak List table. You can sort the contents of the table and change the columns that are displayed using the commands in the shortcut menu. You can drag columns to a different location in the table. Column headers and other cells have different shortcut menus.

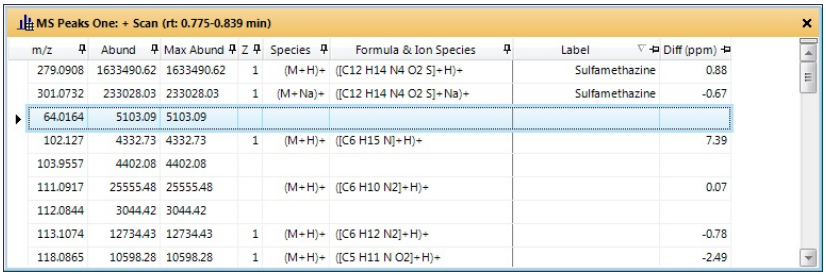
Peaks: + TIC Scan

Peak	RT	Area	Area %	Height	Max Y	Base Peak	Width	Symmetry	FWHM
1	0.325	6620637.37	48.22	2518629.43	3714626.75	271.0316	0.193	1.93	0.037
2	0.518	2989417.09	21.77	805897.31	2046221.12	285.0203	0.171	2.92	0.058
3	0.791	12361740.51	90.03	4415680.64	5718803.5	279.0899	0.166	2.14	0.041
4	1.225	13731361.99	100	5097321.16	6556291	311.0796	0.244	2.31	0.038

Figure 75 Integration Peak List window

MS Spectrum Peak List 1 and MS Spectrum Peak List 2 This table shows the peaks that are part of a spectrum. Each point in a spectrum is listed on a separate row in the table. If you have more than one spectrum highlighted, the first spectrum is shown in this table, and the other spectrum can be seen in the MS Spectrum Peak List 2 window. You can sort the contents of the table

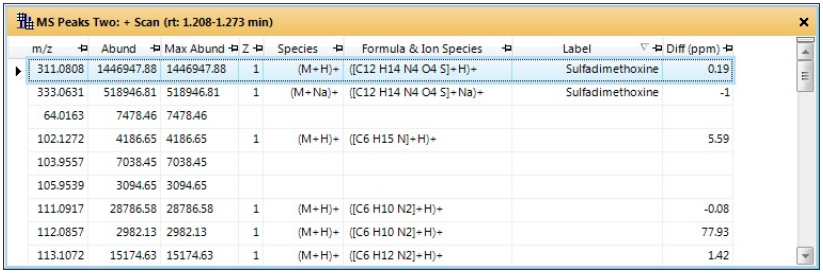
and change the columns that are displayed using the commands in the shortcut menu. You can drag columns to a different location in the table. Column headers and other cells have different shortcut menus.



MS Peaks One: + Scan (rt: 0.775-0.839 min)

m/z	Abund	Max Abund	Z	Species	Formula & Ion Species	Label	Diff (ppm)
279.0908	1633490.62	1633490.62	1	(M+H)+	([C12 H14 N4 O2 S]+H)+	Sulfamethazine	0.88
301.0732	233028.03	233028.03	1	(M+Na)+	([C12 H14 N4 O2 S]+Na)+	Sulfamethazine	-0.67
64.0164	5103.09	5103.09					
102.127	4332.73	4332.73	1	(M+H)+	([C6 H15 N]+H)+		7.39
103.9557	4402.08	4402.08					
111.0917	25555.48	25555.48		(M+H)+	([C6 H10 N2]+H)+		0.07
112.0844	3044.42	3044.42					
113.1074	12734.43	12734.43	1	(M+H)+	([C6 H12 N2]+H)+		-0.78
118.0865	10598.28	10598.28	1	(M+H)+	([C5 H11 N O2]+H)+		-2.49

Figure 76 MS Peaks One window

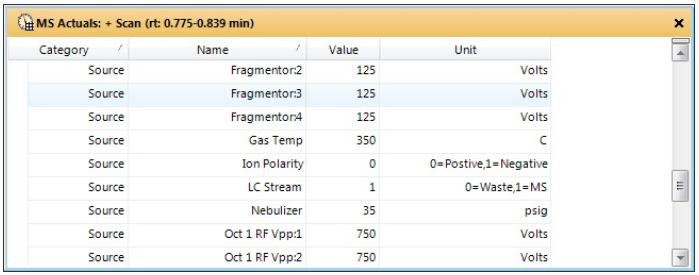


MS Peaks Two: + Scan (rt: 1.208-1.273 min)

m/z	Abund	Max Abund	Z	Species	Formula & Ion Species	Label	Diff (ppm)
311.0808	1446947.88	1446947.88	1	(M+H)+	([C12 H14 N4 O4 S]+H)+	Sulfadimethoxine	0.19
333.0631	518946.81	518946.81	1	(M+Na)+	([C12 H14 N4 O4 S]+Na)+	Sulfadimethoxine	-1
64.0163	7478.46	7478.46					
102.1272	4186.65	4186.65	1	(M+H)+	([C6 H15 N]+H)+		5.59
103.9557	7038.45	7038.45					
105.9539	3094.65	3094.65					
111.0917	28786.58	28786.58	1	(M+H)+	([C6 H10 N2]+H)+		-0.08
112.0857	2982.13	2982.13	1	(M+H)+	([C6 H10 N2]+H)+		77.93
113.1072	15174.63	15174.63	1	(M+H)+	([C6 H12 N2]+H)+		1.42

Figure 77 MS Peaks Two window

MS Actuals This window shows acquisition information for the highlighted spectrum. Closing the MS Actuals window will increase performance. Only four columns are possible in this table: **Category**, **Name**, **Value**, and **Unit**.



Category	Name	Value	Unit
Source	Fragmentor:2	125	Volts
Source	Fragmentor:3	125	Volts
Source	Fragmentor:4	125	Volts
Source	Gas Temp	350	C
Source	Ion Polarity	0	0=Postive,1=Negative
Source	LC Stream	1	0=Waste,1=MS
Source	Nebulizer	35	psig
Source	Oct 1 RF Vpp:1	750	Volts
Source	Oct 1 RF Vpp:2	750	Volts

Figure 78 MS Actuals window showing instrument parameters for current spectrum

Spectrum Identification Results This window shows the results from using the identification algorithms on a spectrum. If you run the Generate Formulas (MFG) or Search Library/DB, then those results are shown in this window. The results for one spectrum are shown in this window. When you highlight a different spectrum, the results in this window are changed to show any results from the new spectrum. This table has up to three levels. The first level shows the overall results for the spectrum. The second level shows the individual scores which were used to create the overall score for an algorithm. The third level of the table shows height and m/z values (both calculated and actual). This level is available for the Generate Formulas algorithm and the Search Database algorithm.

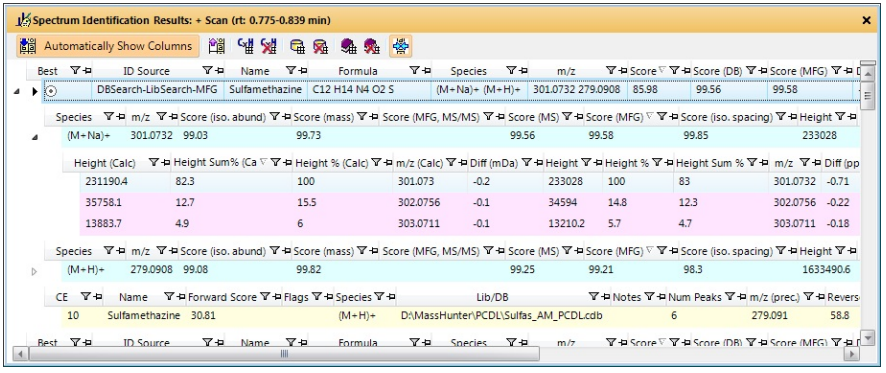


Figure 79 Spectrum Identification Results window

Structure Viewer Structures can be attached to a spectrum when you run the Search Library/DB algorithm, and the database or library contains a structure for the best hit. A structure can also be attached when you add or edit a manual identification to the spectrum. The Structure Viewer contains two tabs. The Structure tab shows a graphical representation of the structure. The MOL Text tab contains text that describes the structure.

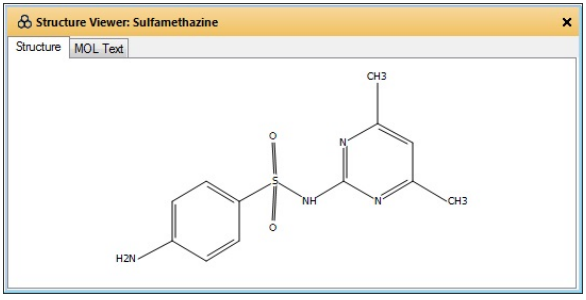


Figure 80 Structure Viewer window

Formula Calculator This tool calculates possible empirical formulas corresponding to the mass or mass-to-charge value which you enter. The results may be viewed interactively, and printed or exported.

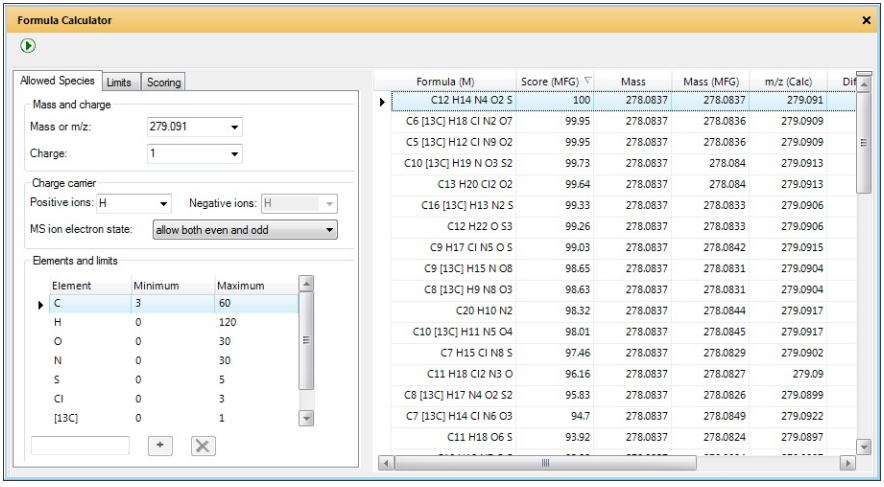


Figure 81 Formula Calculator window

Mass Calculator This tool allows you to enter a base formula and a list of ion species (positive or negative ions). When you run the Mass Calculator algorithm, the Mass Calculator table contains a row for each ion species and calculates the mass for each species.

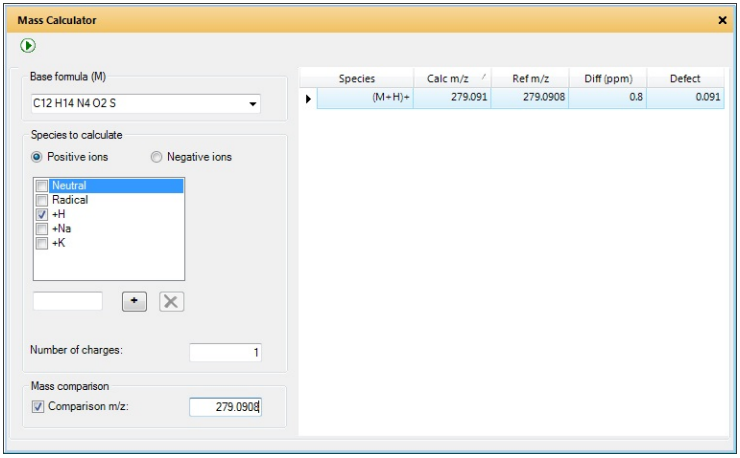


Figure 82 Mass Calculator window

Qualitative Analysis Workflows program

Main Functional Areas

When you first open the Qualitative Analysis Workflows program, you see three parts: (1) the Menu Bar, (2) the Toolbar, and (3) the Main Window. The main functional areas are shown in Figure 83.

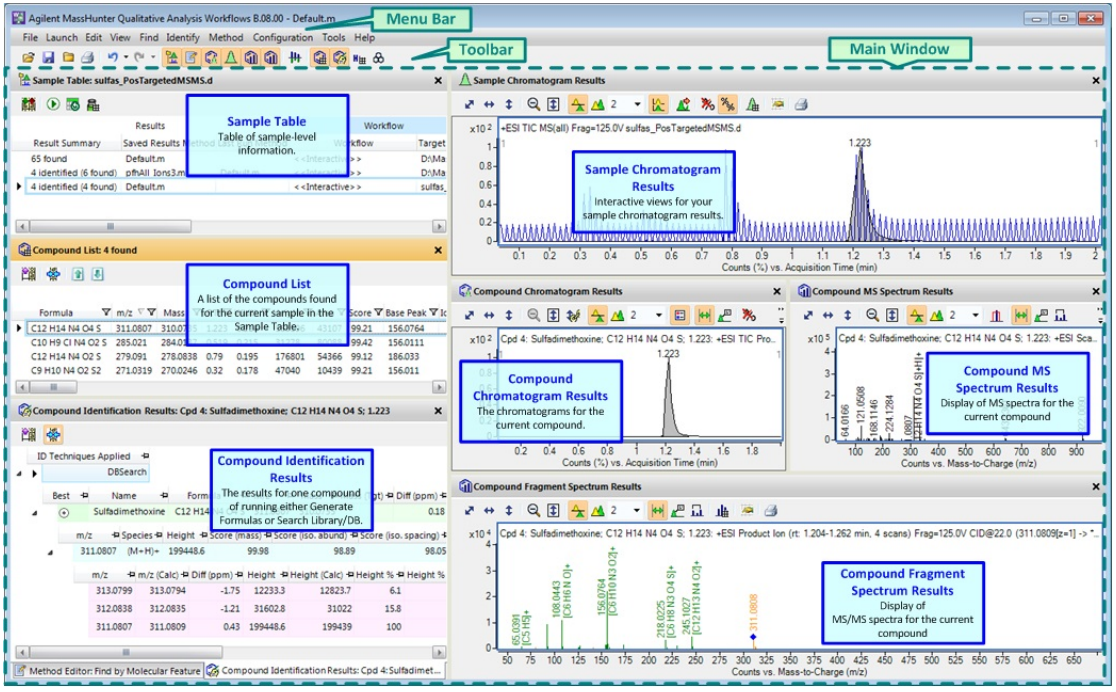


Figure 83 Overview of the Qualitative Analysis Workflows program

1. Menu Bar

The menu bar (Figure 84) provides actions that are used for finding and identifying compounds, printing and exporting reports, and launching the Qualitative Analysis Navigator program. The online Help contains detailed information on each menu.

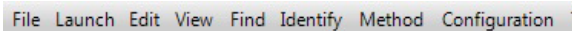


Figure 84 The menu bar for the Qualitative Analysis Workflows program

2. Toolbar

The toolbar provides actions that are used for opening and closing data files. You can also open and save methods, print a compound report, and toggle whether a window is visible or not.

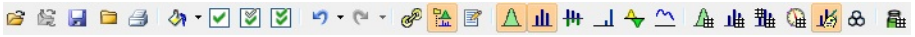


Figure 85 The toolbar for the Qualitative Analysis Workflows program

Toolbar Icon	Action
	File > Open Data File File > Save Results File > Close Data File File > Print > Compound Report Edit > Undo Edit > Redo
	View > Sample Table View > Method Editor
	View > Compound Chromatogram Results View > Sample Chromatogram Results View > Compound MS Spectrum Results View > Compound Fragment Spectrum Results View > Difference Results
	View > Compound List View > Compound Identification Results View > MS/MS Formula Details View > Structure Viewer

3. Main window

The main window (see Figure 83 on page 116) is further divided into up to 13 windows. When you first open the Qualitative Analysis Workflows program, you see a subset of the windows in the default layout:

- Sample Table
- Compound List
- Compound Identification Results
- Method Editor
- Structure Viewer
- Sample Chromatogram Results
- Compound Chromatogram Results
- Compound MS Spectrum Results.
- Compound Fragment Spectrum Results
- Difference Results
- MS/MS Formula Details
- Formula Calculator
- Mass Calculator.

Windows - Qualitative Analysis Workflows

Sample Table The Sample Table shows information for each sample (data file) that is opened. Data from the sample or samples which you select in this window are displayed in the other windows. You can reprocess a selected sample.

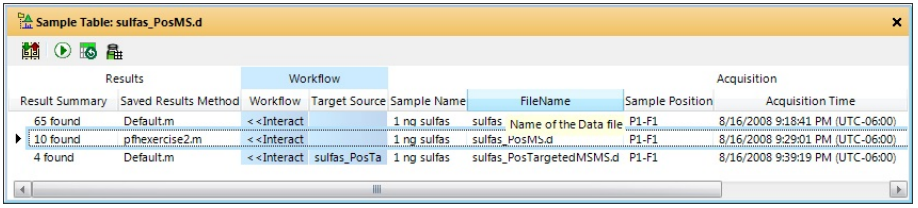


Figure 86 Sample Table

Compound List This windows shows all of the compounds which were found for the selected sample files. You can add and remove columns from this table, and you can change the order of the columns within a category.

Columns in the Compound List window are separated into categories. You can change the order of the columns within a category. These columns are also shown in the **Add/Remove Columns** dialog box. The categories are

- General
- Compound Identification
- Formula Generation
- Molecular Feature Extraction
- Database Search
- Library Search
- Sample Purity
- Target/Suspect Screening

Compound List Toolbar

Toolbar Icon	Action
	• Hides any currently empty columns
	• Toggles whether to auto size all columns. When On, the width of columns is automatically changed to show the information in that column.
	• Switches to the previous compound. If the first compound is selected, this icon is not available. • Switches to the next compound. If the last compound is selected, this icon is not available.

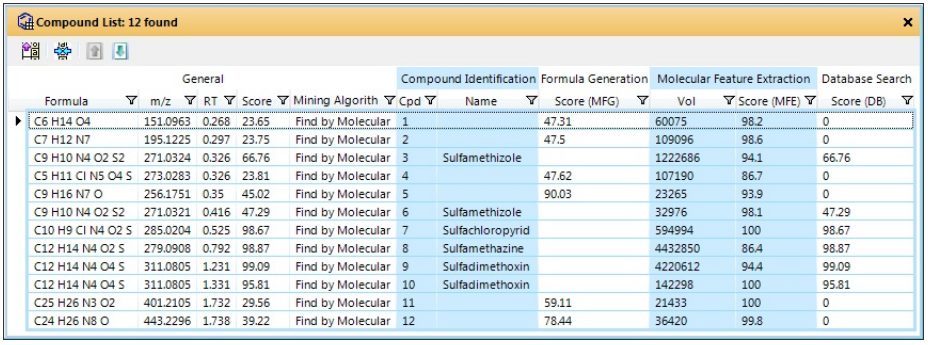


Figure 87 Compound List window showing columns in five categories

Method Editor A method is a set of parameters that are associated with the different algorithms that you can run. Methods containing these parameters can be saved using unique file names.

You select the section of the method to display in the left pane. The right pane contains either a single section or multiple tabs. You can get help for the currently selected tab or section in the Method Editor when you press **F1**.

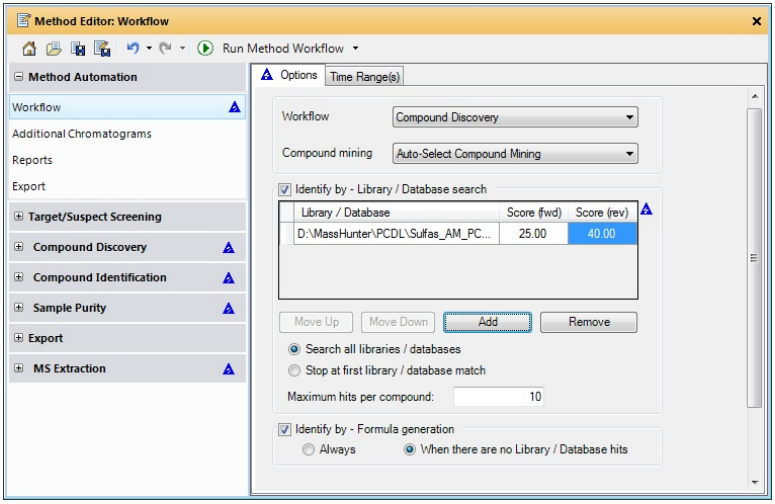


Figure 88 Method Editor window

Compound Chromatogram Results This window shows the chromatograms associated with the compound (or compounds) selected in the Compound List window including an Extracted Ion Chromatogram (EIC). You can display a legend in the upper right corner of the graphic if you select Overlaid mode for the chromatograms. You can add annotations to the graphic. You can also export or print the graphic.

Perform operations on the chromatogram

You can perform many operations on chromatograms.

- You can change the appearance of the plots in the window via icons in the Compound Chromatogram Results toolbar.
- You can add annotations to a chromatogram via the Annotation tool.
- You can initiate many operations via the shortcut menu. When you right-click a chromatogram in the Compound Chromatogram Results window, you see the shortcut menu.

See the online Help for more information.

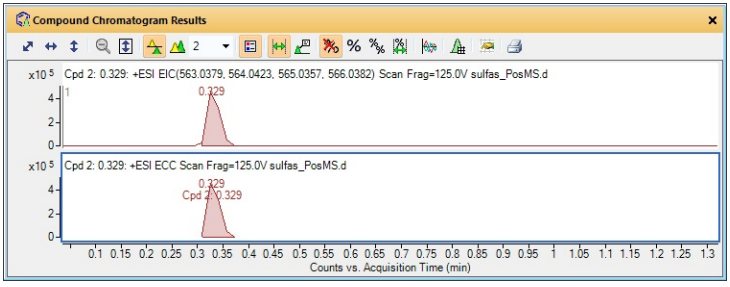
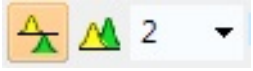
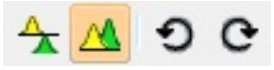
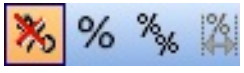


Figure 89 Compound Chromatogram Results window

Compound Chromatogram Results Tools

Toolbar Icon	Action
Zoom tools 	• Autoscale X-axis and Y-axis • Autoscale X-axis • Autoscale Y-axis • Unzoom • Autoscale Y-axis during Zoom • Linked Y-axis mode
 or 	• **List mode** - chromatograms are drawn with each chromatogram having a separate Y-axis. • **Overlay mode** - chromatograms are drawn with the same X-axis and the same Y-axis • **Number of chromatograms to show** at the same time before adding a scroll bar. This option is shown when you click **List mode**. • **Cycle to Previous Plot** or **Cycle to next plot**. These options are shown when you click **Overlay** mode.
	• **Show legend in Overlay mode** - If you select Overlay mode, you can select whether or not to show a legend. If you show the coelution plot, this option also controls whether that legend is visible. • **Range Select** – When On, you can draw a range for chromatogram, for which you can perform actions. • **Annotation** – When On, you can add image and text annotations to the chromatograms.
Scaling tools 	• Stops scaling chromatograms • Scales all chromatograms to the largest peak in any of the chromatograms • Scales all chromatograms to the largest peak in itself • Scales each chromatogram to the highest peak within the selected range

Toolbar Icon	Action
Other tools 	• Toggles whether or not the Coelution Plot is visible • Toggles whether the Integration Peak List is visible • Opens **Chromatogram Display Options** dialog box • Prints the displayed chromatograms

Sample Chromatogram Results This window shows the chromatograms for each sample that is selected in the Sample Table window. This chromatogram may be a Total Ion Chromatogram (TIC) or a Base Peak Chromatogram (BPC). You can also overlay compound chromatograms. UV chromatograms that are extracted as part of the Find by Formula algorithm also are displayed in this window. You can export or print the graphic.

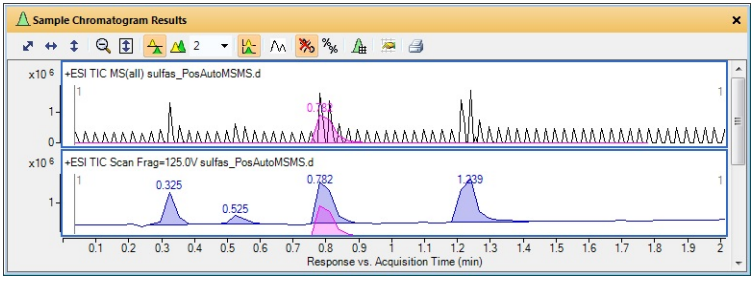
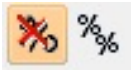
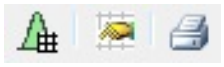


Figure 90 Sample Chromatogram Results window

Sample Chromatogram Results Tools

Toolbar Icon	Action
Zoom tools 	• Autoscale X-axis and Y-axis • Autoscale X-axis • Autoscale Y-axis • Unzoom • Autoscale Y-axis during Zoom

Toolbar Icon	Action
 or 	• **List mode** - chromatograms are drawn with each chromatogram having a separate Y-axis. • **Overlay mode** - chromatograms are drawn with the same X-axis and the same Y-axis • **Number of chromatograms to show** at the same time before adding a scroll bar. This option is shown when you click **List mode**. • **Cycle to Previous Plot** or **Cycle to next plot**. These options are shown when you click **Overlay** mode.
	• **Compound Overlay mode** - compound chromatograms are also shown in the Sample Chromatogram Results window. • **Extract Chromatograms** - the **Extract Chromatograms** dialog box is opened.
Scaling tools 	• Stops scaling chromatograms • Scales all chromatograms to the largest peak in itself
Other tools 	• Displays the peak list table for the chromatogram • Opens **Chromatogram Display Options** dialog box • Prints the displayed chromatograms

Compound MS Spectrum Results This window shows the mass spectra associated with the selected compound(s) if one or two compounds are selected. When you select more than two compounds, then only the spectra of the first two highlighted compounds are shown. MS/MS spectra are displayed in the Compound Fragment Spectrum window. You can add annotations and calipers to a spectrum in this window. You can display the peak list which is displayed in a table on the right-side of this window. A tab is added for each spectrum that is displayed. You can send the spectra to PCDL, export, and print a spectrum.

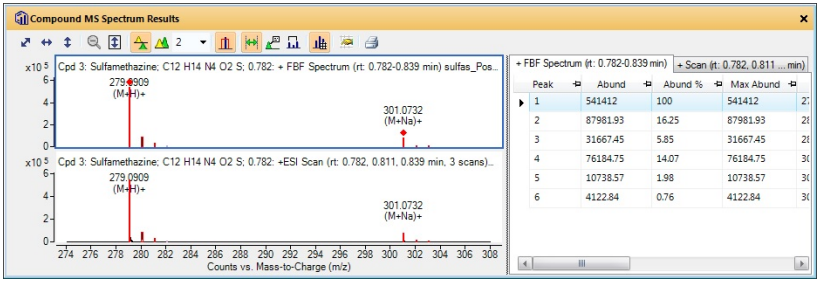
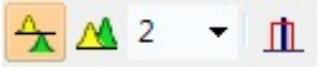
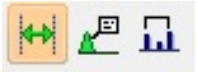


Figure 91 Compound MS Spectrum Results window

Compound MS Spectrum Results Tools

Toolbar Icon	Action
Zoom tools 	• Autoscale X-axis and Y-axis • Autoscale X-axis • Autoscale Y-axis • Unzoom • Autoscale Y-axis during Zoom
 or 	• **List mode** - spectra are drawn with each spectrum having a separate Y-axis • **Overlay mode** - spectra are drawn with the same X-axis and the same Y-axis • **Number of spectra to show** at the same time before adding a scroll bar. This option is shown when you click **List mode**. • **Cycle to Previous Plot** or **Cycle to next plot**. These options are shown when you click **Overlay** mode. • **Show Predicted Isotope Distribution**
Select tools in order  One of these tools always has to be selected. The Range Select tool is selected in this image. The selected tool has an orange background.	• **Range Select** – When **On**, you can draw a range for spectra, for which you can perform actions • **Annotation** – When **On**, you can add image and text annotations to the spectra. • **Calipers** – When **On**, you can add a Delta Mass caliper to the selected spectrum. See the online Help for more information.

Toolbar Icon	Action
Other tools 	• Displays the peak list table for the spectrum • Opens **MS and MS/MS Spectra Display Options** dialog box • Prints the displayed spectra

Compound Fragment Spectrum Results This window shows the MS/MS spectra associated with the selected compound(s) if one or two compounds are selected. When you select more than two compounds, then only the MS/MS spectra for the first two highlighted compounds are shown. MS spectra are displayed in the Compound MS Spectrum window. You can also annotate and add calipers to a Compound Fragment Spectrum.

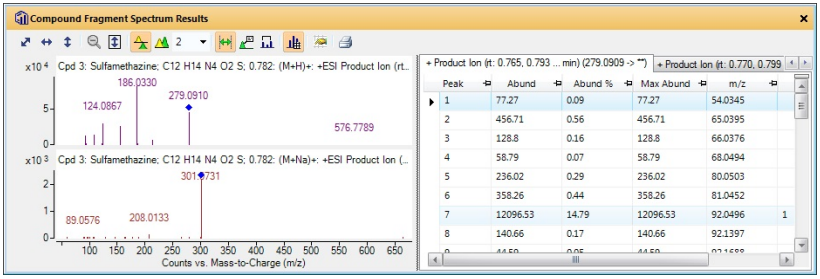
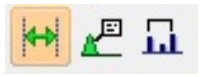


Figure 92 Compound Fragment Spectrum Results window with corresponding peak list

Compound Fragment Spectrum Results Tools

Toolbar Icon	Action
Zoom tools 	• Autoscale X-axis and Y-axis • Autoscale X-axis • Autoscale Y-axis • Unzoom • Autoscale Y-axis during Zoom

Toolbar Icon	Action
 or 	• **List mode** - spectra are drawn with each spectrum having a separate Y-axis • **Overlay mode** - spectra are drawn with the same X-axis and the same Y-axis • **Number of spectra to show** at the same time before adding a scroll bar. This option is shown when you click **List mode**. • **Cycle to Previous Plot** or **Cycle to next plot**. These options are shown when you click **Overlay** mode.
Select tools in order  One of these tools always has to be selected. The Range Select tool is selected in this image. The selected tool has an orange background.	• **Range Select** – When **On**, you can draw a range for spectra, for which you can perform actions • **Annotation** – When **On**, you can add image and text annotations to the spectra. • **Calipers** – When **On**, you can add a Delta Mass caliper to the selected spectrum. See the online Help for more information.
Other tools 	• Displays the peak list table for the spectrum • Opens **MS and MS/MS Spectra Display Options** dialog box • Prints the displayed spectra

Difference Results After you run the Search Library algorithm and identify the compound with library search, this window shows three spectra. The first spectrum is the spectrum that was searched. The second spectrum is a difference spectrum. The spectra from the library is subtracted from the user spectrum to create the difference spectrum. The third spectrum is the spectrum from the library that is currently selected in the Spectrum Identification Results window.

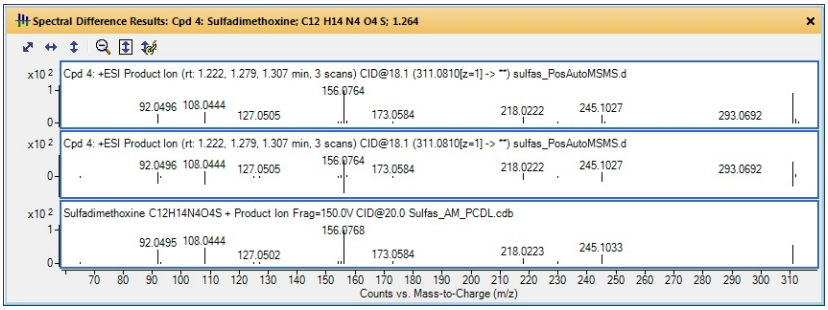


Figure 93 Difference Results window

Compound Identification Results This window shows the results of running an identification algorithm such as Generate Formulas or Search Library/DB.

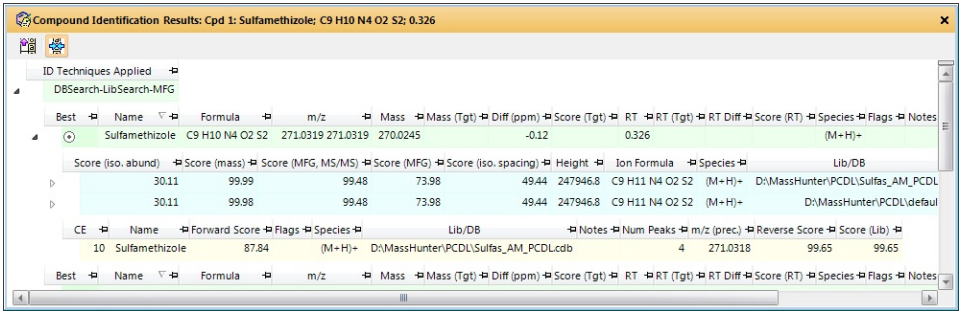
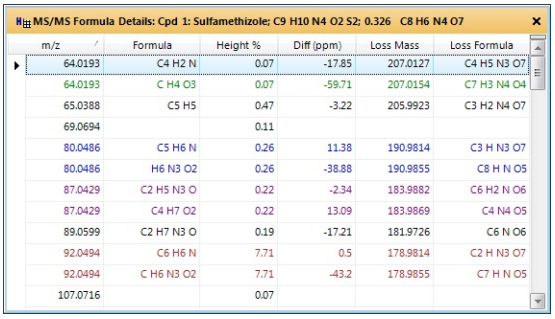


Figure 94 Compound Identification Results window

MS/MS Formula Details This window contains a table that shows possible formulas calculated for fragments seen in an MSMS spectrum that are consistent with a proposed formula. Its contents are the results that are related to the currently-selected formula row in the Compound Identification Results table. The data in this table is used to compute the Score (MFG, MS/MS) column in the Compound Identification Results table.



m/z	Formula	Height %	Diff (ppm)	Loss Mass	Loss Formula
64.0193	C4 H2 N	0.07	-17.85	207.0127	C4 H5 N3 O7
64.0193	C H4 O3	0.07	-59.71	207.0154	C7 H3 N4 O4
65.0388	C5 H5	0.47	-3.22	205.9923	C3 H2 N4 O7
69.0694		0.11			
80.0486	C5 H6 N	0.26	11.38	190.9814	C3 H N3 O7
80.0486	H6 N3 O2	0.26	-38.88	190.9855	C8 H N O5
87.0429	C2 H5 N3 O	0.22	-2.34	183.9882	C6 H2 N O6
87.0429	C4 H7 O2	0.22	13.09	183.9869	C4 N4 O5
89.0599	C2 H7 N3 O	0.19	-17.21	181.9726	C6 N O6
92.0494	C6 H6 N	7.71	0.5	178.9814	C2 H N3 O7
92.0494	C H6 N3 O2	7.71	-43.2	178.9855	C7 H N O5
107.0716		0.07			

Figure 95 MS/MS Formula Details window

Structure Viewer Structures can be attached to a spectrum when you run the Search Library/DB algorithm, and the database or library contains a structure for the best hit. A structure can also be attached when you add or edit a manual identification to the spectrum. The Structure Viewer window has two tabs. The Structure tab shows a graphical representation of the structure. The MOL Text tab contains text that describes the structure.

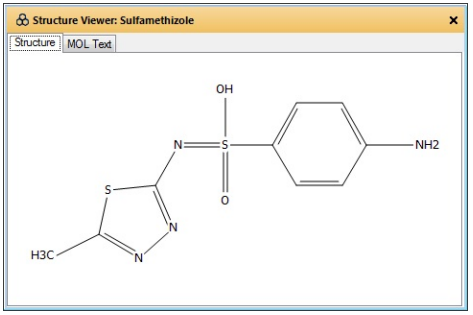


Figure 96 Structure Viewer window

Qualitative Analysis Navigator and Workflows Programs

Layouts

You can open and save different layouts. You can modify any of the following attributes, and they are saved in the layout. Two default layouts are shipped with the software: default.xml (for the Qualitative Analysis Workflows program) and CDN_Default.xml (for the Qualitative Analysis Navigator program).

A layout consists of the following:

- Each window's position and size
- Which windows are tabbed
- Which windows are floating
- Which tabbed window is on top
- Which windows are visible by default
- Whether the status bar is visible

For each plot window (in Qualitative Analysis Navigator: the Chromatogram Results window, the Spectrum Preview window, the MS Spectrum Results window, the Difference Results window, and the UV Results window; in Qualitative Analysis Workflows: the Sample Chromatogram Results window, the Compound Chromatogram Results window, the Compound MS Spectrum Results window, the Compound Fragment Spectrum Results window, and the Difference Results window), the following are saved:

- Whether or not the graphics are overlaid
- Whether or not the Autoscale Y-Axis during Zoom mode is on
- Whether or not the Linked Y-Axis mode is on

For each table window, the following are saved

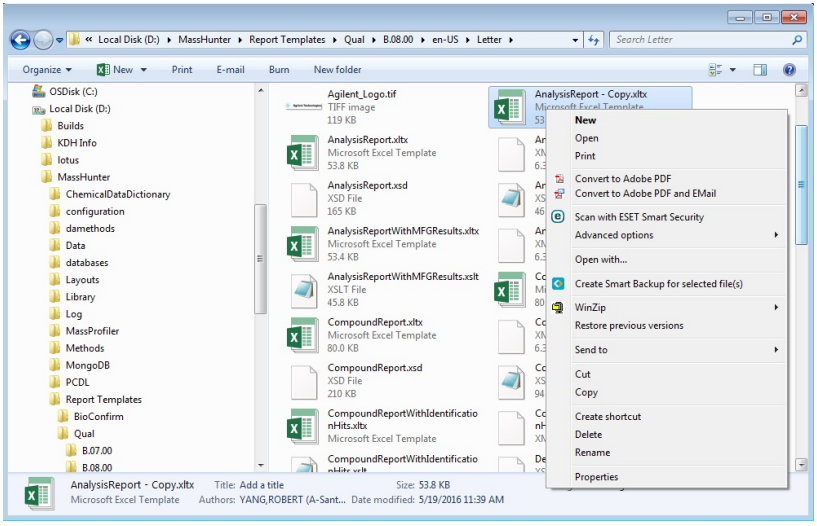
- Which columns are visible
- The order of the columns
- The width of each column

- Any filter that has been added to the table (only available for the Compound List table, the Compound Identification Results table, and the Spectrum Identification Results window).

Customize a report template

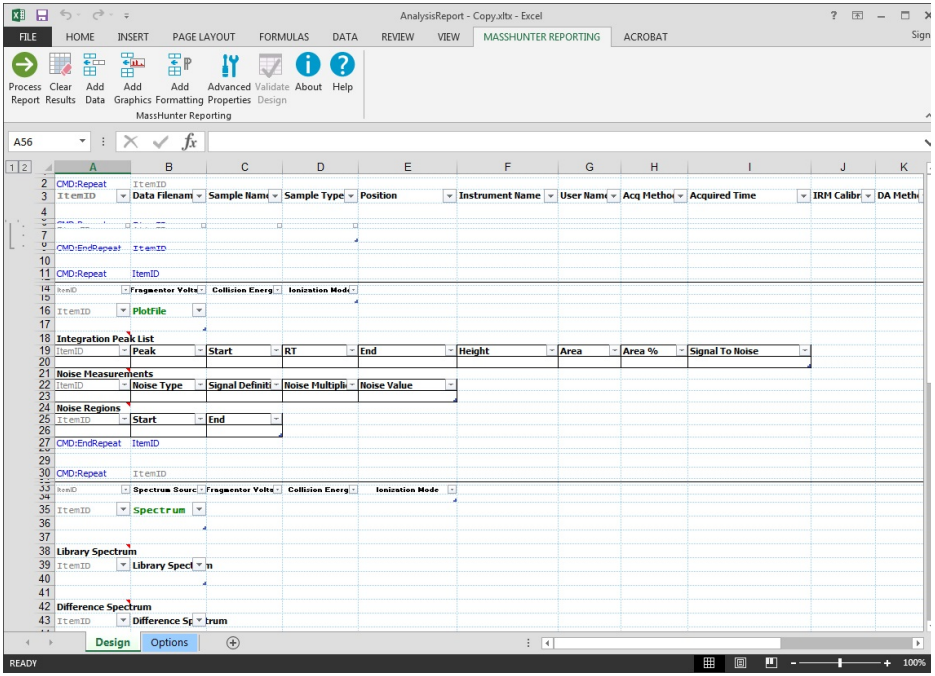
Please refer to either the online Help for the MassHunter Report Designer Add-in, the Report Designer Familiarization Guide or the Reporting Training DVD for detailed information on how to modify a report template. The following steps give you a quick look at what it means to customize a template. These instructions apply to a Microsoft Excel report template only.

1. Go to the folder that contains the report templates. By default, this folder is **\MassHunter\Report Templates\Qual\B.08.00\en-US\Letter**. You can select a different folder in the Method Editor in the Method Automation > Reports > Templates tab.
2. Make a copy of the template which you intend to modify.
3. Right-click the copy and click **Properties**. If necessary, clear the **Read-only** check box. Then, right-click the copy and click **Open** from the shortcut menu.



When the template is open, you can modify headers and footers. You can also add, remove or move parameter columns. You can refer to the online Help for more information.

Many templates are installed with the Qualitative Analysis program.



4 Make the changes you want to make.

For more information on how to modify a template, see either the online Help for the MassHunter Report Designer add-in, or the *Agilent MassHunter Reporting - Training DVD*.

5 To save the new template, either click **Save** or click **Save As > Other Formats** from the Microsoft Office button.

6 Type an identifying name, and click **Save**.

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In This Book

This guide contains information to learn to use your Agilent MassHunter Workstation Software - Qualitative Analysis with LC/MS data. Qualitative Analysis has two main programs.This guide contains information to learn to use your Agilent MassHunter Workstation Software - Qualitative Analysis with GC/MS data. Qualitative Analysis has two main programs.

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