

Agilent MassHunter Workstation Software – 7200 Accurate-Mass Quadrupole Time of Flight GC/MS

Familiarization Guide

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This guide shows how to use the Agilent 7200 Q-TOF GC/MS System to acquire and analyze sample data. If you want to skip the data acquisition steps in this guide, use the demo data files located in a data directory shipped with the system (in the **QTOF_Familiarization** folder of your Data Acquisition installation disk).



In this guide, you learn how to determine the best acquisition settings for analyzing your compounds of interest. These instructions help you understand not only how to set up a method to optimize instrument parameters for best sensitivity in acquisition, but also how to use the Qualitative Analysis program to identify parameter values producing optimum signal response. You can also learn about the Qualitative Analysis program by using the *Qualitative Analysis Familiarization Guide* and the Quantitative Analysis program by using the *Quantitative Analysis Familiarization Guide*.

See the *Concepts Guide* to learn more about how the 7200 Q-TOF GC/MS System works and see the online Help for detailed information on how the program works.

Each task 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.

Before you begin

Before you begin, you need to check that your system is ready. If you plan to acquire data, you also need to set up the instrument.

Prepare your system

- 1 Check that:
 - MassHunter Acquisition, MassHunter Qualitative Analysis, and MassHunter Quantitative Analysis are installed.
 - Your system uses an Agilent 7890 GC with split/splitless or MultiMode (MMI) inlet and automatic liquid sampler.
 - The acquisition uses a 10 uL ALS syringe tapered, fixed, with 23-26s needle. A suitable syringe may be substituted.
 - The 7200 Q-TOF GC/MS System is configured and has a valid tune.
 - The performance is verified.
 - The system is turned on.
 - A suitable column is installed. The J&W model 122-3832 DB-35MS: 30 m x 250 μ m, 0.25 μ m column is used for the examples in this guide.
- 2 Configure the GC for the installed column.
- 3 Copy the data files to your PC.
- 4 Copy the files in the **QTOF_Familiarization** folder on your Data Acquisition installation disk to any location on your hard disk. This folder contains the data file and accurate mass library file needed for this exercise.

Before you begin

Prepare the samples required for data acquisition

Prepare the samples required for data acquisition

If you do not intend to acquire data but want to learn how to use the Qualitative Analysis program you can skip the sample preparation and actual acquisition and use the data file shipped with this guide. It is recommended that you read the exercise *Develop an acquisition method for the 7200* to understand settings unique to the Agilent instrument.

Materials required for sample preparation:

- Sample (p/n 05970-60045 or p/n 5074-3025 Japan only)
- Isooctane for sample dilution
- Sample vials

The sample compounds are in an isooctane solvent contained in 1 mL ampules of 10 ng/ μ L, 100 ng/ μ L, and 100 pg/ μ L concentrations and are shown in Table 1.

Table 1 Sample Compound list

Compound	MW	Formula
Dodecane	170	C ₁₂ H ₂₆
Biphenyl	154	C ₁₂ H ₁₀
4-Chlorobiphenyl (p/n 05970-60045 only)	188	C ₁₂ H ₉ Cl
Methyl palmitate	270	C ₁₇ H ₃₄ O ₂

Prepare the Qualitative Analysis sample by emptying the contents of the 10 ng/ μ L ampoule into an ALS sample vial and cap the vial.

Fill an ALS wash vial with isooctane.

Exercise – Develop an acquisition method for the 7200

Task 1. Set the inlet and injection parameters

Steps	Detailed instructions	Comments
1 Set up the inlet, injection source, and enable the 7200.	<p>a Double-click the Data Acquisition icon on the windows desktop.</p> <p>b Click the Inlet and Injection Parameters icon.</p> <p>c Select GC for the sample inlet and the installed ALS for the injection source.</p> <p>d Select the Use MS check box.</p>	<ul style="list-style-type: none"> The Data Acquisition window shown in Figure 1 is displayed. Hover over an icon to display a tag identifying the icon. The Inlet and Injection Parameters dialog box shown in Figure 2 on page 6 is displayed.

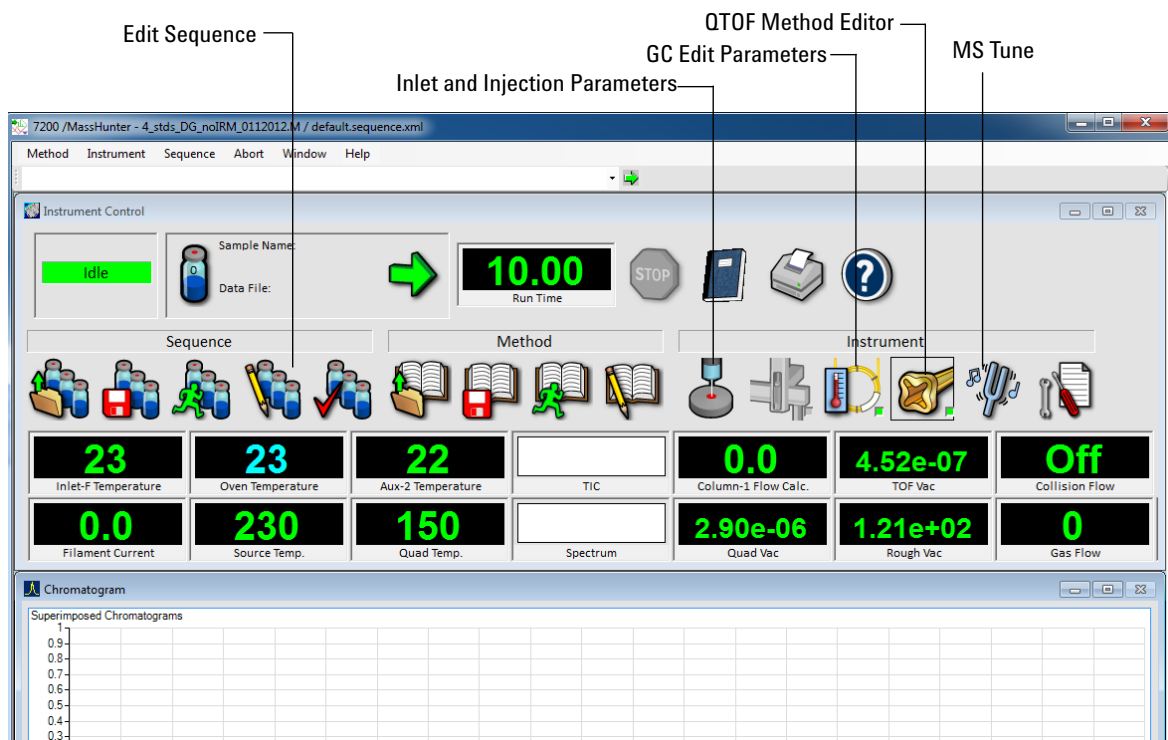


Figure 1 Agilent MassHunter Workstation Software – Data Acquisition window

Exercise – Develop an acquisition method for the 7200

Task 1. Set the inlet and injection parameters

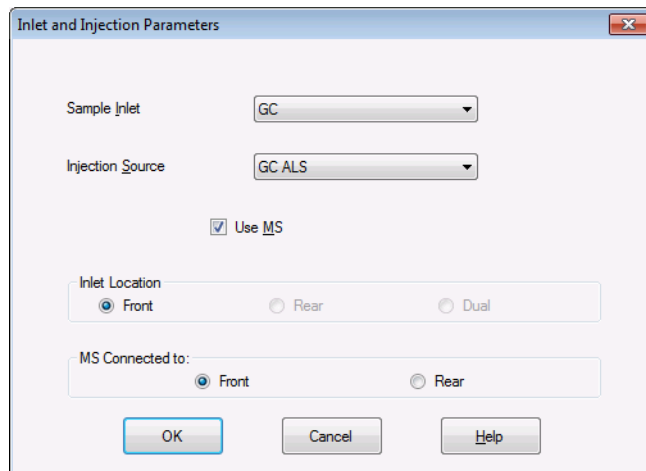


Figure 2 Inlet and Injection Parameters

Task 2. Check the GC Configuration

In this exercise, you review the GC hardware setup for the analysis.

Steps	Detailed instructions	Comments
2	<p>Check that the GC hardware configuration is suitable for the analysis.</p> <ol style="list-style-type: none"> Click the GC Edit Parameters icon. Select the Configuration icon and then the Miscellaneous tab. Set the Pressure Units to psi. In the Oven area the Slow Fan mode is unchecked. Select the Columns tab and set Column 1 to a J&W 122-3832 column or one that is similar. Set the Inlet to Front (or Rear) Inlet and the Outlet to Vacuum. Heated By is set to Oven. Select the Modules tab and set the SS inlet gas to He and the Collision Cell EPC gas to N2. Select the ALS tab and set the Syringe Size to 10 uL and the Solvent Wash Mode to A, B. Select the OK button. 	<ul style="list-style-type: none"> See Figure 1. The GC edit parameters window shown in Figure 3 is displayed. If using a different column you must adjust your GC parameter settings accordingly for acceptable chromatography. 10 uL ALS syringe tapered, fixed, with 23-26s needle. A suitable syringe may be substituted. The GC parameters are downloaded to the GC and the window closes.

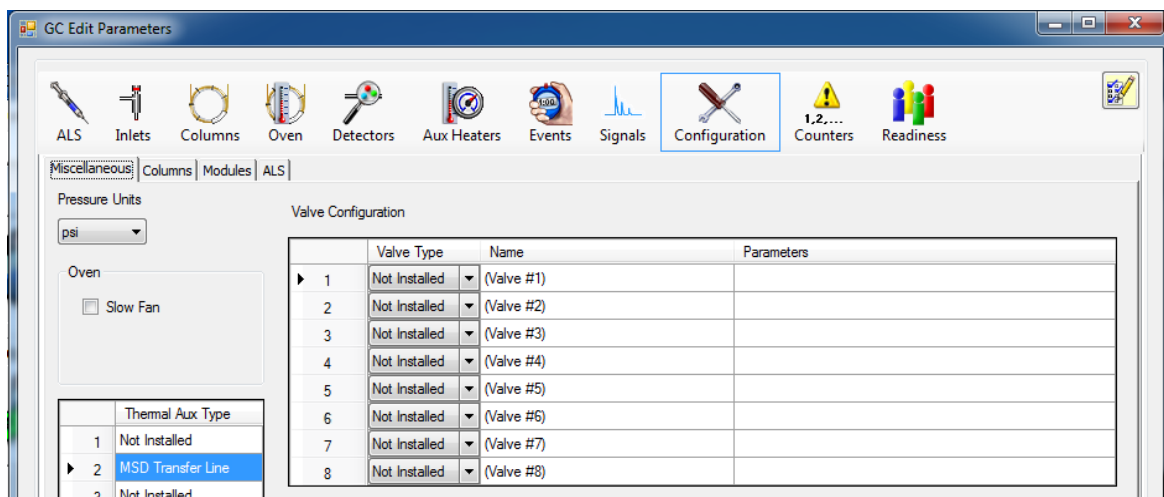


Figure 3 The Configuration Settings

Exercise – Develop an acquisition method for the 7200

Task 3. Perform a Mass Calibration

Task 3. Perform a Mass Calibration

In this exercise you perform a mass calibration from the **TOF Mass Calibration** tab in the **GC/Q-TOF Tune** window. A mass calibration is completed in less than two minutes and it is good practice to calibrate the instrument as often as possible. A sequence table keyword allows automatic mass calibration between samples in a sequence. In addition, you may also use the method's Reference Mass feature to adjust mass accuracy during acquisition or later during data analysis. See the on-line help for more information.

Steps	Detailed instructions	Comments
<p>1 Optimize the base ion abundance.</p> <p>This step is usually done when selecting new calibrant masses surrounding a base ion of interest.</p>	<p>a Click the MS Tune icon.</p> <p>b Click the Manual Tune tab, then click the Ion Source tab and enable the Emission and El Cal Valve.</p> <p>c In the Tune Masses area, select Enabled for calibrant masses surrounding a base ion of interest.</p> <p>d Adjust the Emission current so that the abundance of the ion of interest is between 1×10^6 and 2×10^6 counts.</p> <p>e Save the tune file as <code>qtofatunes_DG_date.ei.tune.xml</code>.</p> <p>f Select the Close button.</p>	<ul style="list-style-type: none">• The GC/Q-TOF Tune window is displayed.• To enable calibrant flow ionization. See Figure 4 on page 9.• Uncheck the ions that have interferences with selected ions. See Figure 4 on page 9.• Higher values will saturate the signal and lower values will not provide sufficient ion statistics for optimal mass accuracy.• Where date is today's date.• The GC/Q-TOF Tune window closes.
<p>2 Perform a mass calibration.</p>	<p>a Select the TOF Mass Calibration tab from the GC/Q-TOF Tune window.</p> <p>b Click the Run Calibration button.</p> <p>c Select the Close button.</p> <p>d Click the File and Reports tab and save the tune file.</p> <p>e Select the Close button.</p>	<ul style="list-style-type: none">• See Figure 5 on page 9.• When the calibration completes the TOF Mass Calibration Results window displays. Mass Accuracy (PPM) should typically be below 2 PPM for all ions used in calibration. See Figure 6 on page 10.• The TOF Mass Calibration Results closes.• The GC/Q-TOF Tune window closes.

Exercise – Develop an acquisition method for the 7200

Task 3. Perform a Mass Calibration

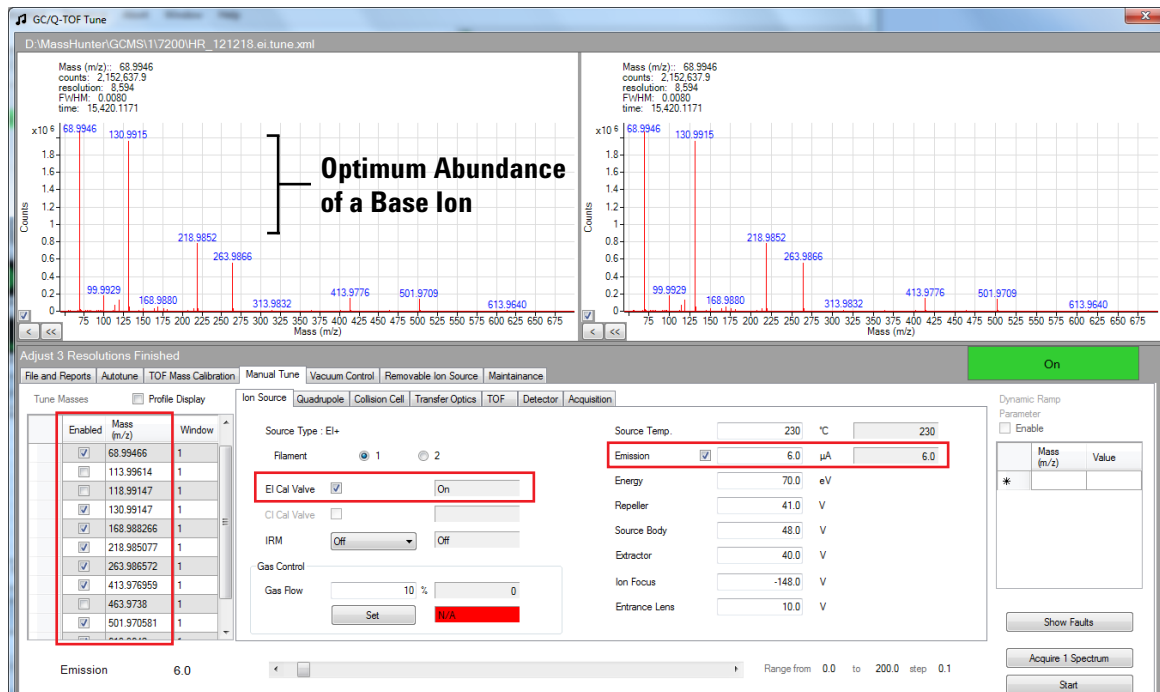


Figure 4 Optimizing base ion abundance

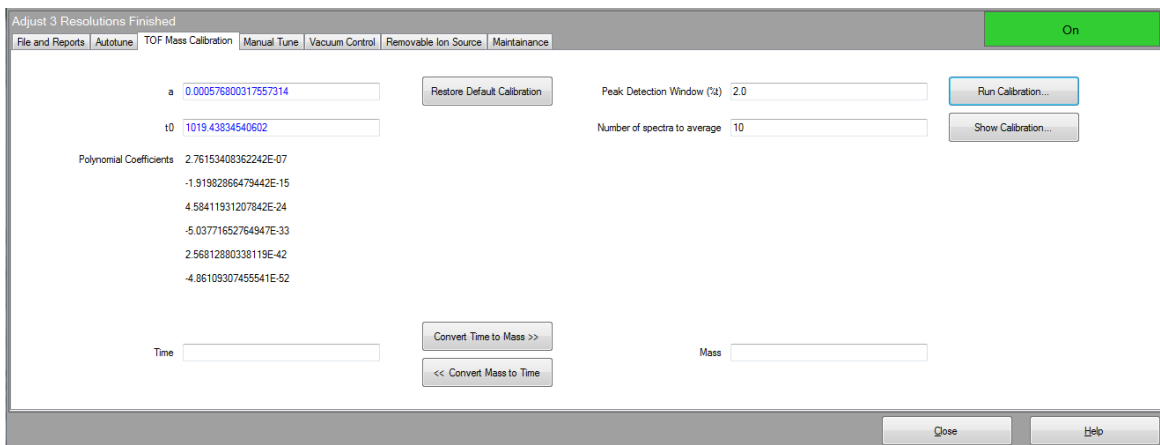


Figure 5 TOF Mass Calibration tab

Exercise – Develop an acquisition method for the 7200

Task 3. Perform a Mass Calibration

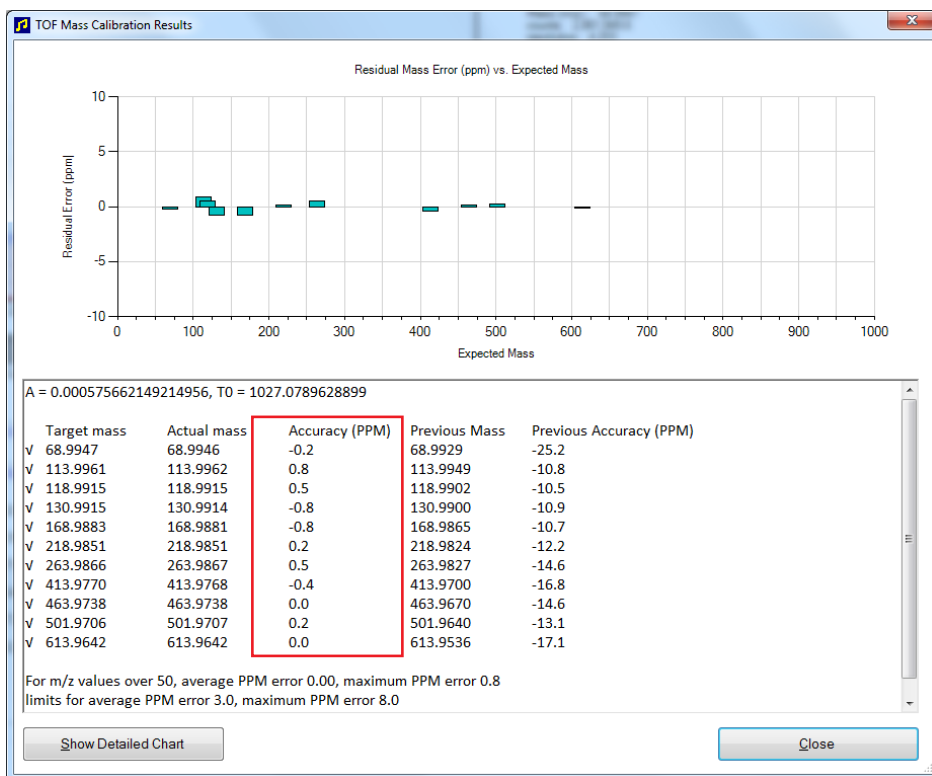


Figure 6 TOF Mass Calibration Results

Task 4. Enter GC acquisition parameters

In this exercise, you enter the GC conditions for the analysis.

Steps	Detailed instructions	Comments
3	<p>Enter GC parameters appropriate for the sample. See Table 2.</p> <p>a Click the GC Edit Parameters icon (Figure 1).</p> <p>b Select the Columns icon then select column 1 in the Selection column.</p> <p>c Select control mode On and then select Constant Flow mode. Enter 1.1 mL/min for the initial Value.</p> <p>d Select the Collision Cell EPC in the Selection column and then in the Collision Cell EPC area, set the N2 Collision Gas on at 1.5 mL/min.</p> <p>e In the Collision Cell EPC area, uncheck the He Quench Gas.</p> <p>f Select the Inlets icon then the SSL tab and enter the inlet parameters listed in Table 2.</p> <p>g Select the Oven icon and enter the oven parameters listed in Table 2.</p> <p>h Select the ALS icon then the Front Injector tab and enter the injector parameters listed in Table 2.</p> <p>i Select the Aux Heaters icon, enable, and set the temperature to 280 °C.</p> <p>j Select the OK button.</p>	<ul style="list-style-type: none"> The GC edit parameters window shown in Figure 7 on page 12 is displayed. With the window selected, mouse over the icons to identify the icon from the tool tip. If the current flow value of the collision cell N2 gas is not 1.5 mL/min and you change it to this value, an autotune will be required. If your ALS is attached to the Back Inlet select the Back Injector tab. This is the MSD transfer line heater. The GC parameters are downloaded to the GC and the window closes.

Exercise – Develop an acquisition method for the 7200

Task 4. Enter GC acquisition parameters

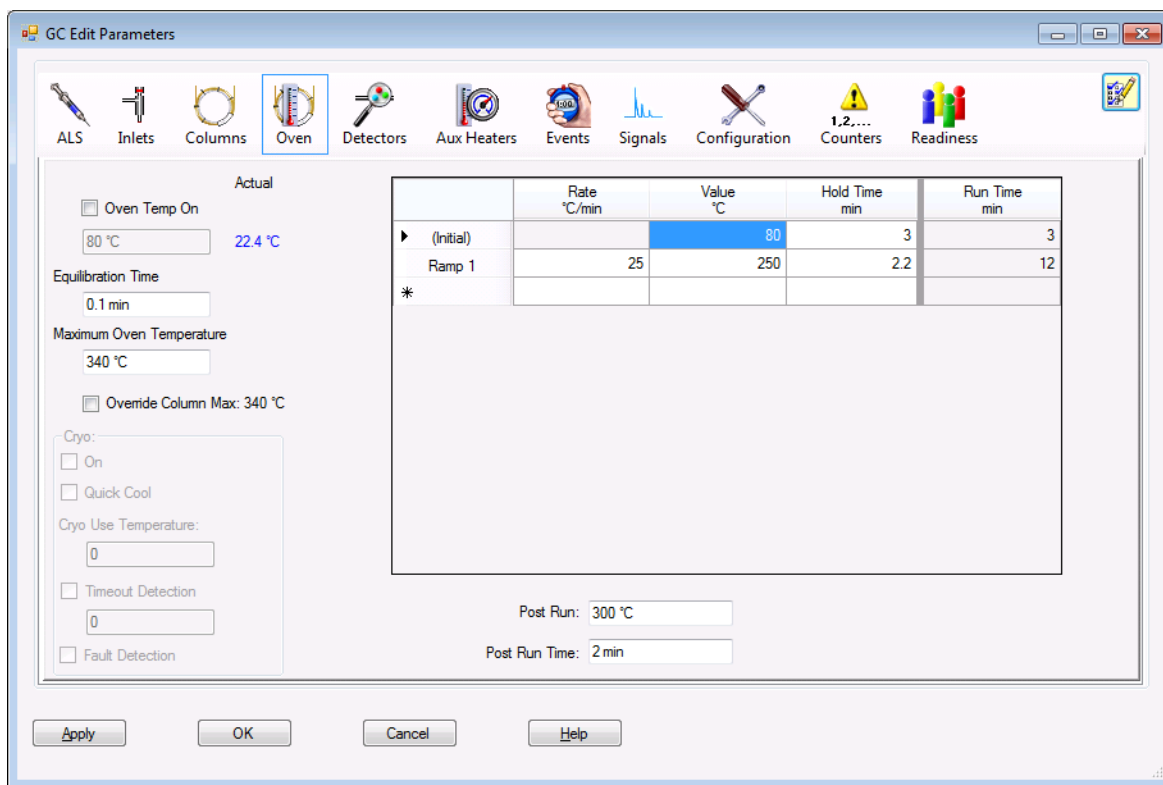


Figure 7 GC Edit Parameters window with **Oven** icon selected

Table 2 GC parameters for data acquisition method

Parameter	Value
Oven	
Equilibration Time	0.1 min
Oven Program	80 °C for 3 min, 25 °C/min to 250 °C, hold for 2.2 min
Run Time	12 min
Front SS Inlet	
	He
Mode	Split
Heater	On 250 °C
Pressure	On Value automatically set with column flow
Septum Purge Flow	On 3 mL/min
Gas Saver	On 20 mL/min after 3 min
Split Flow	220 mL/min
Split Ratio	200:1
Thermal Aux 2 {MSD Transfer Line}	
Heater	On
Temperature	280 °C
Column # 1	
	J&W 122-3832 DB-35ms: 30 m x 250 µm, 0.25 µm
In	Front SS Inlet He
Out	Vacuum
(Initial)	80 °C
Flow	1.1 mL/min
Flow Program	Off
Front Injector	
Syringe Size	10 µL
Injection Volume	1 µL
Solvent A Washes (Prelnj)	2


Exercise – Develop an acquisition method for the 7200

Task 4. Enter GC acquisition parameters

Parameter	Value
Solvent A Washes (PostInj)	2
Solvent A Volume	8 µL
Solvent B Washes (PreInj)	2
Solvent B Washes (PostInj)	2
Solvent B Volume	8
Sample Washes	0
Sample Wash Volume	8 µL
Sample Pumps	4
Dwell Time (PreInj)	0 min
Dwell Time (PostInj)	0 min
Solvent Wash Draw Speed	300 µL/min
Solvent Wash Dispense Speed	6000 µL/min
Sample Wash Draw Speed	300 µL/min
Sample Wash Dispense Speed	6000 µL/min
Injection Dispense Speed	6000 µL/min
Viscosity Delay	0 sec
Sample Depth	Disabled
Collision cell EPC Module	
Nitrogen	On 1.5 mL/min
Helium	Off

Task 5. Create a Qual acquisition method for scanning ions

This exercise starts with the GC parameters entered in the method from Task 4. In this task you will enter the 7200 parameters for ion scanning and save to the method.

Steps	Detailed instructions	Comments
4	<p>Enter MS parameters appropriate for the sample and save the method as <i>iii_MS_Scan.M</i>, where <i>iii</i> are your initials.</p> <p>a Click the QTOF Method Editor icon (Figure 1).</p> <p>b In the Tune file area, click the  icon and select a tune file suitable for this acquisition.</p> <p>c In the Ion Source area, set the Source temperature to 230 °C, set the Emission to Fixed with a value of 35.0 entered, and set the Electron energy to Fixed with a value of 70.0 entered.</p> <p>d Set the Solvent delay to 5 minutes.</p> <p>e In the Time Filtering area select Peak width and set it to 0.7 seconds.</p> <p>f In the Time segment area, select a Scan Type of MS from the Acq mode drop-down list. Select Both for Data stored.</p> <p>g In the MS mode section, for the Mass range enter 40 for the start mass, 600 for the end mass, and 5.00 spectra/s for the Acq rate.</p> <p>h Click OK to close the window.</p> <p>i From the main window select Method > Save Method As and save the method as <i>iii_MS_Scan.M</i>, where <i>iii</i> are your initials.</p>	<ul style="list-style-type: none"> The QTOF Method Editor window shown in Figure 8 on page 16 opens. The 7200 starts collecting data at 5 minutes due to the Solvent delay setting. Selecting Both stores both a peak's profile data and centroid data for data analysis. All data between 40 and 1700 m/z is always acquired but only the data selected here is saved to disk.

Exercise – Develop an acquisition method for the 7200
Task 5. Create a Qual acquisition method for scanning ions

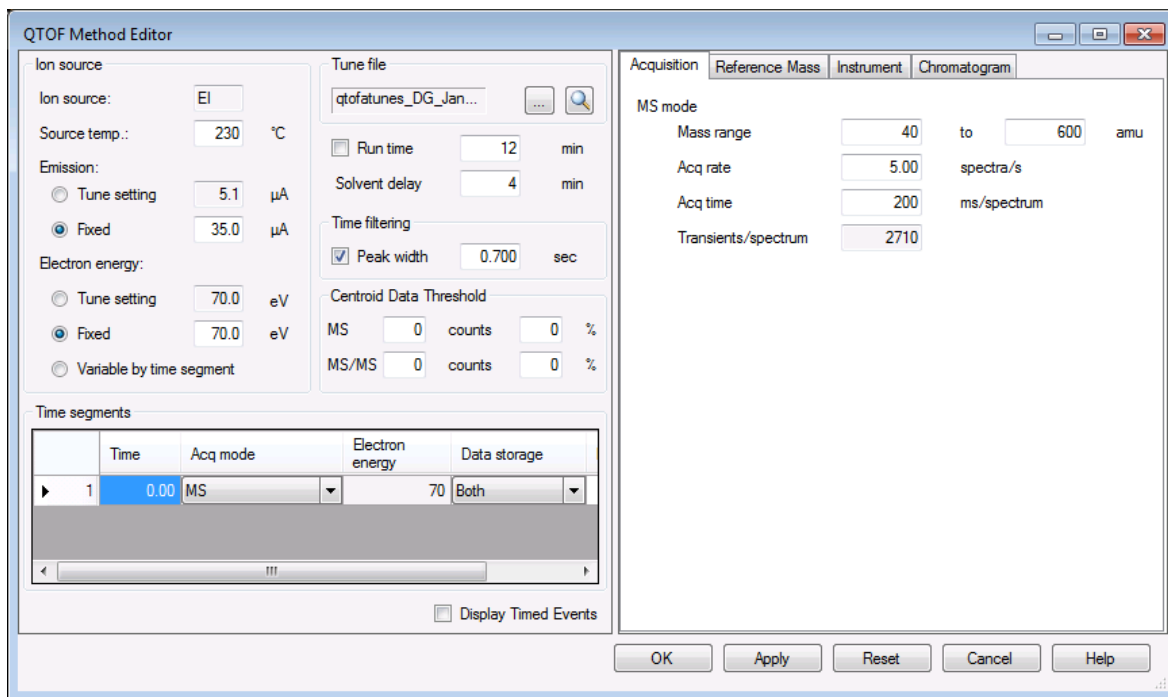


Figure 8 QTOF Method Editor

Task 6. Acquire MS scan data (Optional)

In this task, you acquire the scan data using the method developed in the previous tasks. This task is optional because you can perform the next task with an example data file that comes with the program. However, if you prefer, you can acquire your own data file as described in this task.

Steps	Detailed instructions	Comments
<p>5 Acquire data (optional).</p> <ul style="list-style-type: none"> • Name the data file iii_MS_scan.D, where iii are your initials. • Designate a directory path to hold your data files and method. 	<p>a Click the Start Run (green arrow) icon.</p> <p>b In the Data Path enter the directory to save the data file that is acquired by this run.</p> <p>c In the Front Inlet section, enter iii_MS_scan.D for the Data File Name, where iii are your initials.</p> <p>d Enter the Vial location number in the auto sampler tray.</p> <p>e In the Method Sections to Run section, select Data Acquisition.</p> <p>f Click the OK and Run Method button.</p>	<ul style="list-style-type: none"> • The Start Run dialog box shown in Figure 9 on page 18 is displayed. • If you are using a rear SSL inlet, enter the data file name in the Rear Inlet area. • The method is sent to the GC and the 7200. When the instruments are ready the sample is injected and the data is collected and sent to the data directory specified.

Exercise – Develop an acquisition method for the 7200

Task 6. Acquire MS scan data (Optional)

Start Run

Basic | Advanced

Current Method Injection Style: GC ALS

Inlet Location: Front Rear Dual

MS Connected to: Front Inlet Rear Inlet

Operator Name: TWI/wjt

Data Path: C:\MassHunter\GCMS\2\DATA\

Front Inlet

Data File Name: MSD_mx_4etds_DG_spl500_04.D

Sample Name:

Misc. Info:

Expected Barcode:

Sample Amount: 0

Multiplier: 1

Vial Number: 1

Tray Name: Agilent ALS

Injection Volume: Current Method 1 μ L
 Override using 1 μ L

Rear Inlet

Data File Name: EVALDEMO.D

Sample Name:

Misc. Info:

Expected Barcode:

Sample Amount: 0

Multiplier: 1

Vial Number:

Tray Name: Agilent ALS

Injection Volume: Current Method 0 μ L
 Override using μ L

Data File Name: Enter a data file name or type a ? for a list

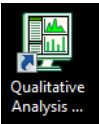
Method Sections to Run: Data Acquisition Data Analysis

Figure 9 Start Run dialog box

Exercise – Analyze data

Task 1. Start the qualitative analysis program

In this exercise, you analyze data acquired from the previous exercises in this manual. For additional details on using the program, see the Familiarization Guide, p/n G3336-90007.

Steps	Detailed instructions	Comments
1 Start the Qualitative Analysis program.	<p>a Double-click Qualitative Analysis icon on your desktop.</p> 	<ul style="list-style-type: none"> The system displays the Open Data Files dialog box. <p>You can get help by:</p> <ul style="list-style-type: none"> Pressing the F1 key when a window is active Selecting Help > Contents in the main menu Selecting the Help button in the active window
	<p>b Navigate to the location where you copied the demo files and select QTOF_Familiarization > Data and then select MSD_mix_4stds_DG_spi500_04.D.</p> <p>c Under Options, select the Use current method checkbox and clear the Run 'File Open' actions from selected method checkbox and the Load result data checkbox.</p> <p>d Click Open.</p>	<ul style="list-style-type: none"> See Figure 10 on page 20.
		<ul style="list-style-type: none"> The data file is loaded and a TIC of the data is displayed. See Figure 11 on page 20.

Exercise – Analyze data

Task 1. Start the qualitative analysis program

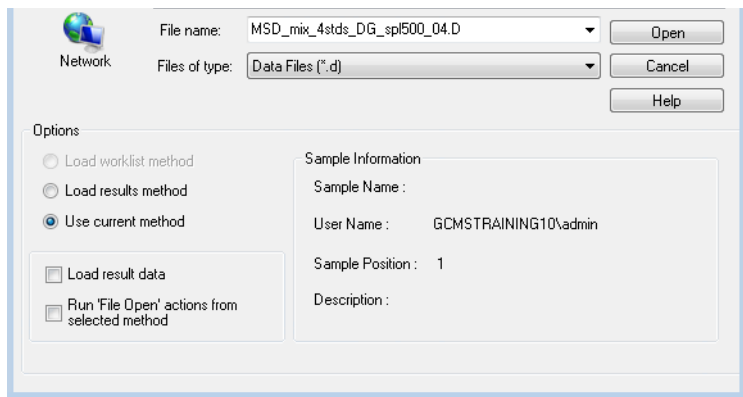


Figure 10 Opening the data file

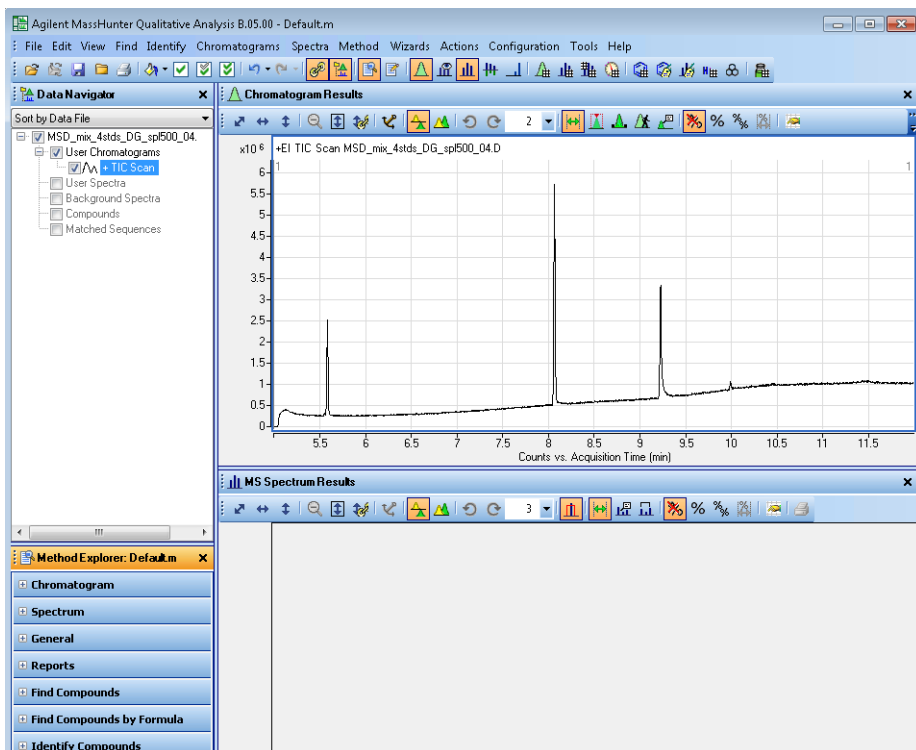


Figure 11 The TIC of the loaded data file

Steps	Detailed instructions	Comments
2 Set the program to use the General workflow.	<p>a From the main menu, select Configuration > Configure for Workflow > General.</p> <p>b Under Qualitative method select Load workflow's default method.</p> <p>c Under Layout select Load workflow's default layout.</p>	<ul style="list-style-type: none">• The Workflow Configuration dialog box opens. See Figure 12. <p>The software has several different workflows. Each workflow loads a different layout. Switching to a different workflow also changes the layout.</p>

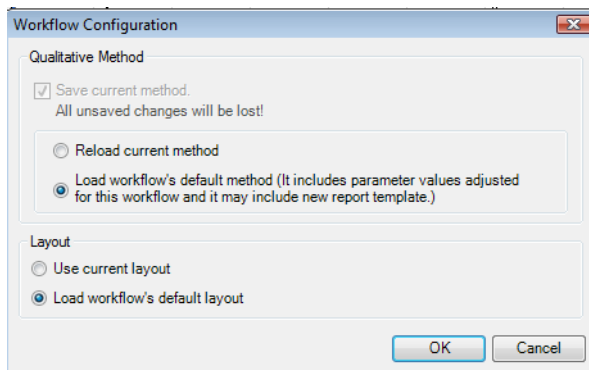


Figure 12 Configuring the Workflow

Exercise – Analyze data

Task 1. Start the qualitative analysis program

Steps	Detailed instructions	Comments
3 Restore the default windows layout.	a From the main menu, select Configuration > Windows Layout > Restore Default Layout.	<ul style="list-style-type: none">• The software has many different layouts created. You can also try loading different layouts.
4 Configure the user interface.	a From the main menu, select Configuration > User Interface Configuration. The User Interface Configuration dialog box opens. b Select the checkboxes for: <ul style="list-style-type: none">• Separation type: GC, LC• Mass accuracy: Unit mass, Accurate mass• Ionization type: EI, CI...• MS levels: MS (any) and MS/MS (QQQ, Q-TOF)• Other: Show advanced parameters c Click OK.	<ul style="list-style-type: none">• The User Configuration dialog box opens. See Figure 13.• You change which commands are available in the user interface through selections in this dialog box.

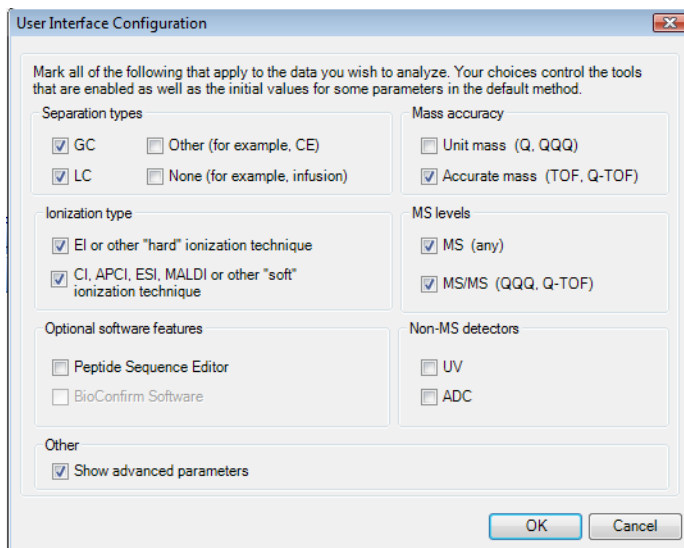




Figure 13 Configuring the User Interface

Task 2. Find compounds by deconvolution

The FindCompounds algorithms identify compounds in MS/MS data. The example presented here uses a simple scan however this function is effective for mining data from more complex scans.

Steps	Detailed instructions	Comments
1 Select the region of the scan to examine.	<p>a In the Chromatogram Results toolbar, select these tools:</p> <ul style="list-style-type: none"> • Range Select  • Auto-scale Y-axis during Zoom  <p>b In the Chromatogram Results window click and drag to select the range from approximately 7.5 to 9.5 minutes.</p>	<ul style="list-style-type: none"> • Continue from previous task. • See Figure 14.

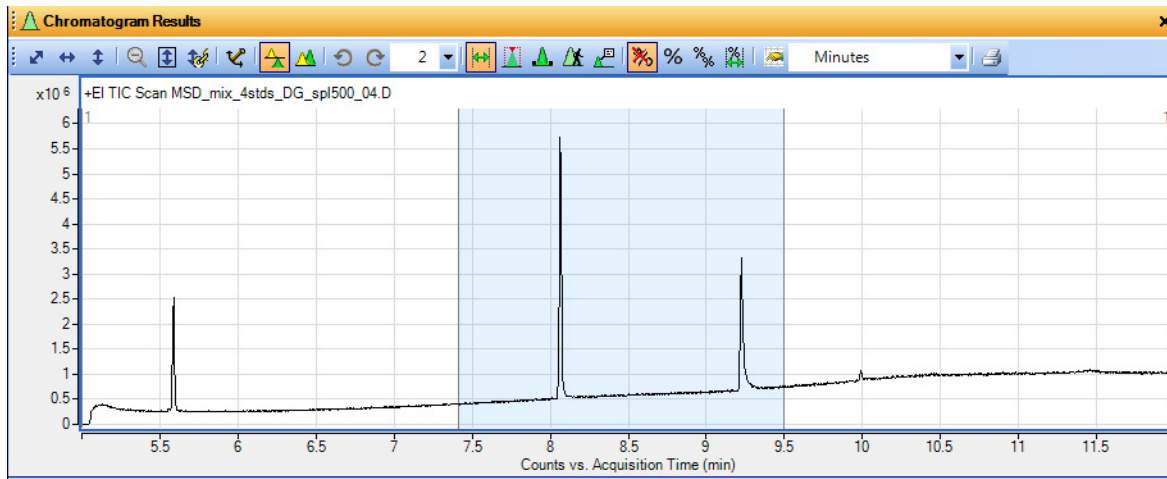


Figure 14 The Chromatogram Results window

Exercise – Analyze data

Task 2. Find compounds by deconvolution

Steps	Detailed instructions	Comments
1 Enter deconvolution settings appropriate for this data.	<p>a From the Method Explorer window, select Find Compounds > Find Compounds by Chromatogram Deconvolution.</p> <p>b Set the Settings tab entries as follows:</p> <ul style="list-style-type: none">• Resolution area: RT window size factor: 100.00• Peak filter area: Excluded m/z: 28 Spectrum peak threshold: 0% SNR threshold 2.00• Extraction window area: Left m/z delta: 100 Right m/z delta: 100 m/z delta units; PPM• Component shape area Use baseline peak shape: disabled Sharpness threshold: 25%	<ul style="list-style-type: none">• The Method Editor: Find Compounds by Chromatogram Deconvolution dialog box opens. See Figure 15.• Enter settings appropriate for this data. See the online help for more information.• If you already have your settings selected, you can also find compounds from the main menu, Find > Find Compounds by Chromatogram Deconvolution > over Selected Ranges.

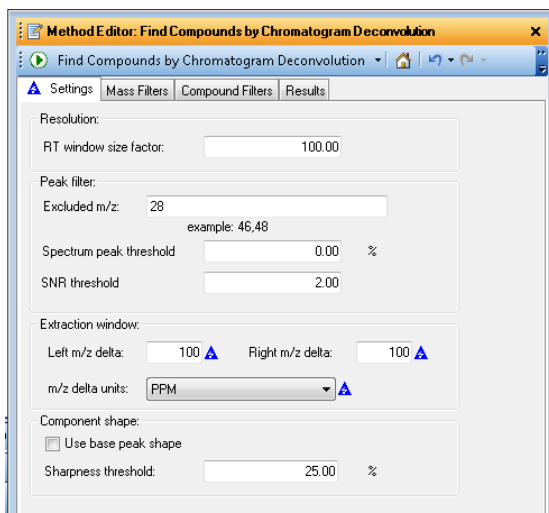


Figure 15 The Settings tab

Steps	Detailed instructions	Comments
Step 1 continued.	<p>c Set the Mass Filters tab entries as follows:</p> <ul style="list-style-type: none"> • Height Filters area: Absolute height: enabled 500 counts Relative height: disabled <p>d Set the Compound Filters tab entries as follows:</p> <ul style="list-style-type: none"> • Area filters area: Absolute area: enabled 5000 counts Relative area: disabled <p>e Set the Results tab entries as follows:</p> <ul style="list-style-type: none"> • Previous results area: Delete previous compounds: enabled • New results area: Highlight first compound • Chromatogram and spectra area: Extract EIC: disabled Extract ECC: enabled Extract cleaned spectrum: enabled Extract raw spectrum: disabled 	<ul style="list-style-type: none"> • See Figure 16. • See Figure 17 on page 26. • See Figure 18 on page 26.

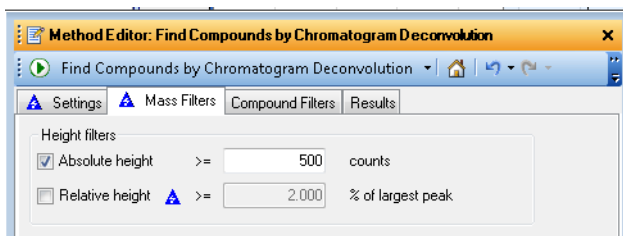


Figure 16 The **Mass Filters** tab

Exercise – Analyze data

Task 2. Find compounds by deconvolution

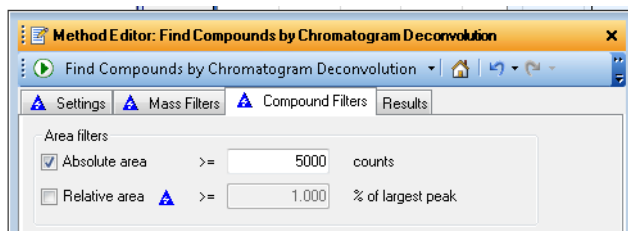


Figure 17 The **Compound Filters** tab

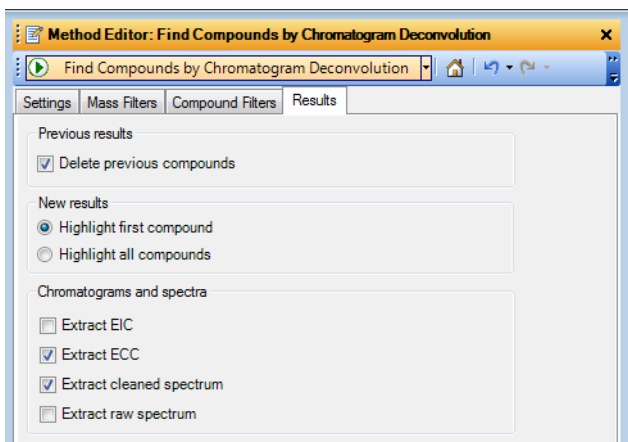
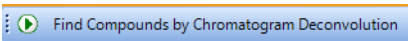


Figure 18 The **Results** tab

Steps	Detailed instructions	Comments
2 Perform the deconvolution.	<p data-bbox="505 322 868 406">a From the Method Editor: Find Compounds by Chromatogram Deconvolution dialog box click</p>  <p data-bbox="505 470 868 579">b After deconvolution is complete the results are shown in the Compound List and MS Spectrum Results windows.</p>	<ul data-bbox="915 322 1233 579" style="list-style-type: none"> <li data-bbox="915 322 1233 348">• See Figure 18 on page 26. <li data-bbox="915 470 1233 522">• The deconvolution takes a long time to complete. <p data-bbox="915 557 1233 579">See Figure 19.</p>

Exercise – Analyze data

Task 2. Find compounds by deconvolution

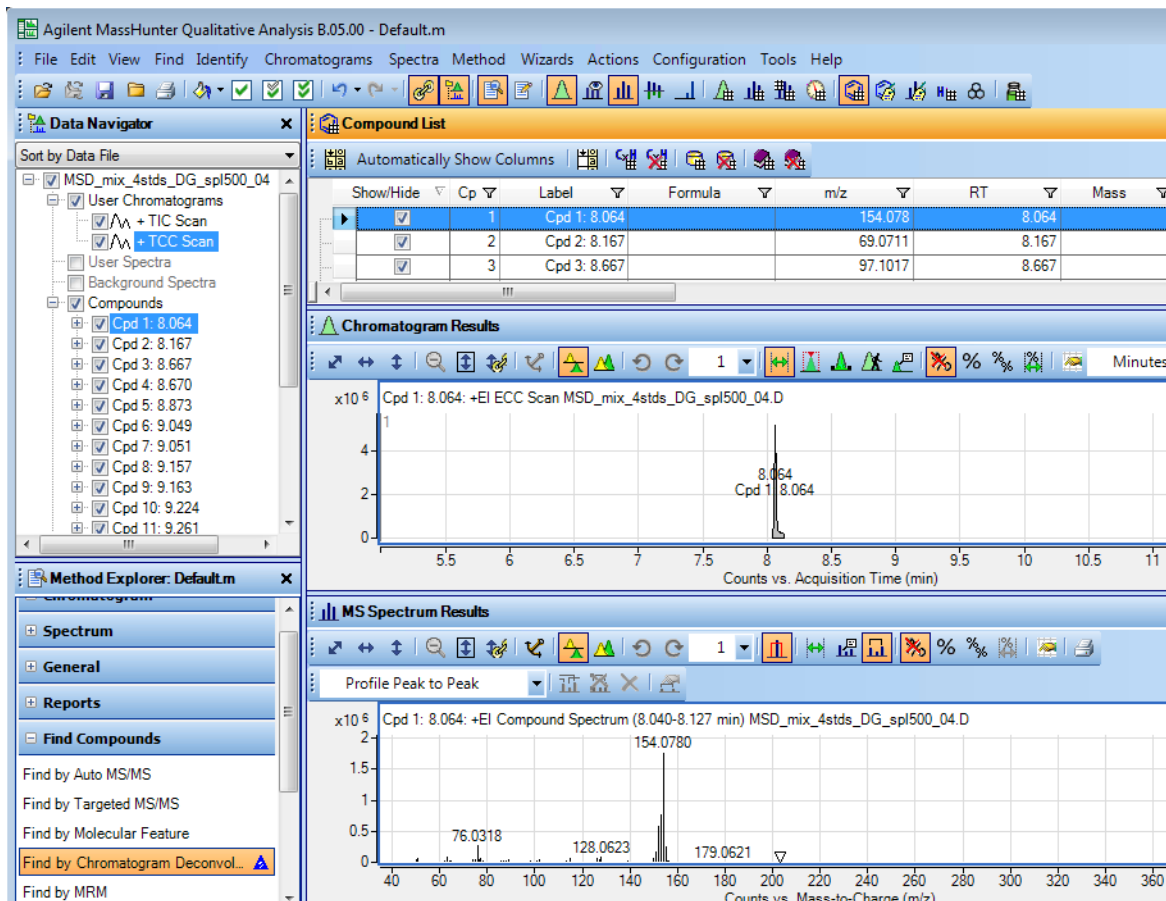
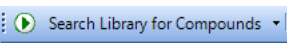


Figure 19 The deconvolution results

Task 3. Search an accurate mass library

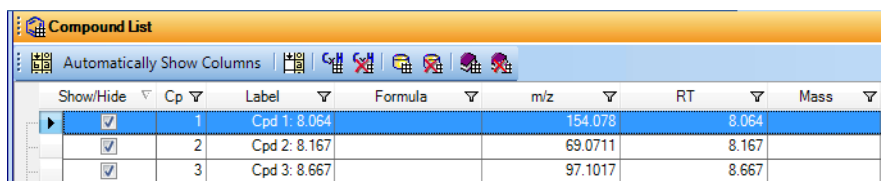
The library used in this exercise is a GCMS accurate mass library stored in an XML data format. This library file is provided by Agilent and stored in the **QTOF_Familiarization\Library** folder of your Data Acquisition installation disk.

The **Search Unit Mass Library** method is used here because it can accommodate this XML accurate mass library file. This method works with both unit mass and accuracy mass XML libraries. The **Search Accurate Mass Library** method can only use a CDB file format and cannot be used here with the example XML library provided.

Steps	Detailed instructions	Comments
1 Select a compound to identify.	<p>a In the Compound List window, click in the first row to highlight it.</p>	<ul style="list-style-type: none"> This task begins by selecting a compound from the compound list generated in the last task. See Figure 20 on page 30.
2 Open Method Editor Search Unit Mass Library dialog box and choose settings.	<p>b From the Method Explorer window, select Identify Compounds > Search Unit Mass Library.</p> <p>c In the Library selection area of the Settings tab, set the Spectral library path to MSD_mix_lib.mslibrary.xml.</p> <p>d In the Search criteria area of the Settings tab, set the Begin spectral matching to 30 m/z, set Enable Screening to disabled, and Adjust score to enabled.</p> <p>e In the MS/MS search area of the Settings tab, set the m/z expansion to Symmetric (m/z) at ± 0.5000.</p> <p>f In the Search Results area of the Search Results tab, set the Maximum hits per compound to 2 hits and the Minimum match score to 50.00.</p> <p>g Select </p> <p>h In the Compound List click the + icon next to the first compound at RT = 8.064 minutes.</p>	<ul style="list-style-type: none"> The Method Editor: Search Unit Mass Library dialog box opens. See Figure 21 on page 30. This library file is provided by Agilent and stored in the QTOF_Familiarization\Library folder of your Data Acquisition installation disk. See Figure 22 on page 30. After the search is complete the results are shown in the Compound List, Chromatogram Results, and Spectrum Results windows. Three possible compounds were identified in the library for the first compound listed. The most probable compound by score is selected and listed first. See Figure 23 on page 31.

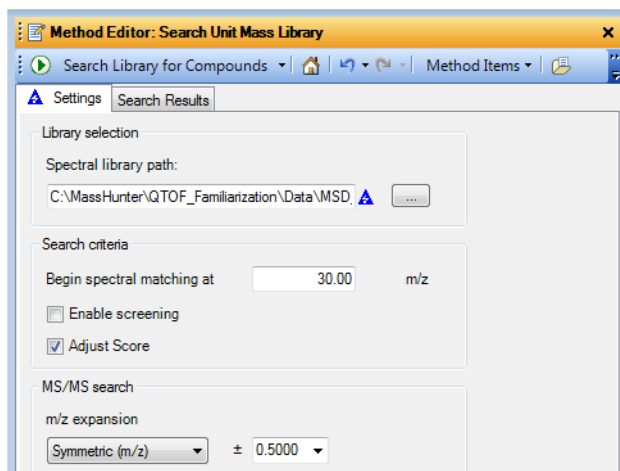
Exercise – Analyze data

Task 3. Search an accurate mass library



Show/Hide	Cp	Label	Formula	m/z	RT	Mass
<input checked="" type="checkbox"/>	1	Cpd 1: 8.064		154.078	8.064	
<input checked="" type="checkbox"/>	2	Cpd 2: 8.167		69.0711	8.167	
<input checked="" type="checkbox"/>	3	Cpd 3: 8.667		97.1017	8.667	

Figure 20 Selecting the compound



Method Editor: Search Unit Mass Library

Search Library for Compounds | Method Items

Settings | Search Results

Library selection

Spectral library path:
C:\MassHunter\QTOF_Familiarization\Data\MSD

Search criteria

Begin spectral matching at: 30.00 m/z

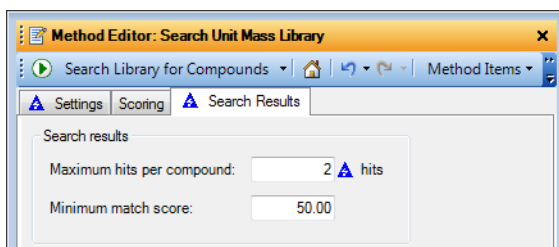
Enable screening

Adjust Score

MS/MS search

m/z expansion:
Symmetric (m/z) ± 0.5000

Figure 21 Search Unit Mass Library **Settings** tab



Method Editor: Search Unit Mass Library

Search Library for Compounds | Method Items

Settings | **Scoring** | Search Results

Search results

Maximum hits per compound: 2 hits

Minimum match score: 50.00

Figure 22 Search Unit Mass Library **Search Results** tab

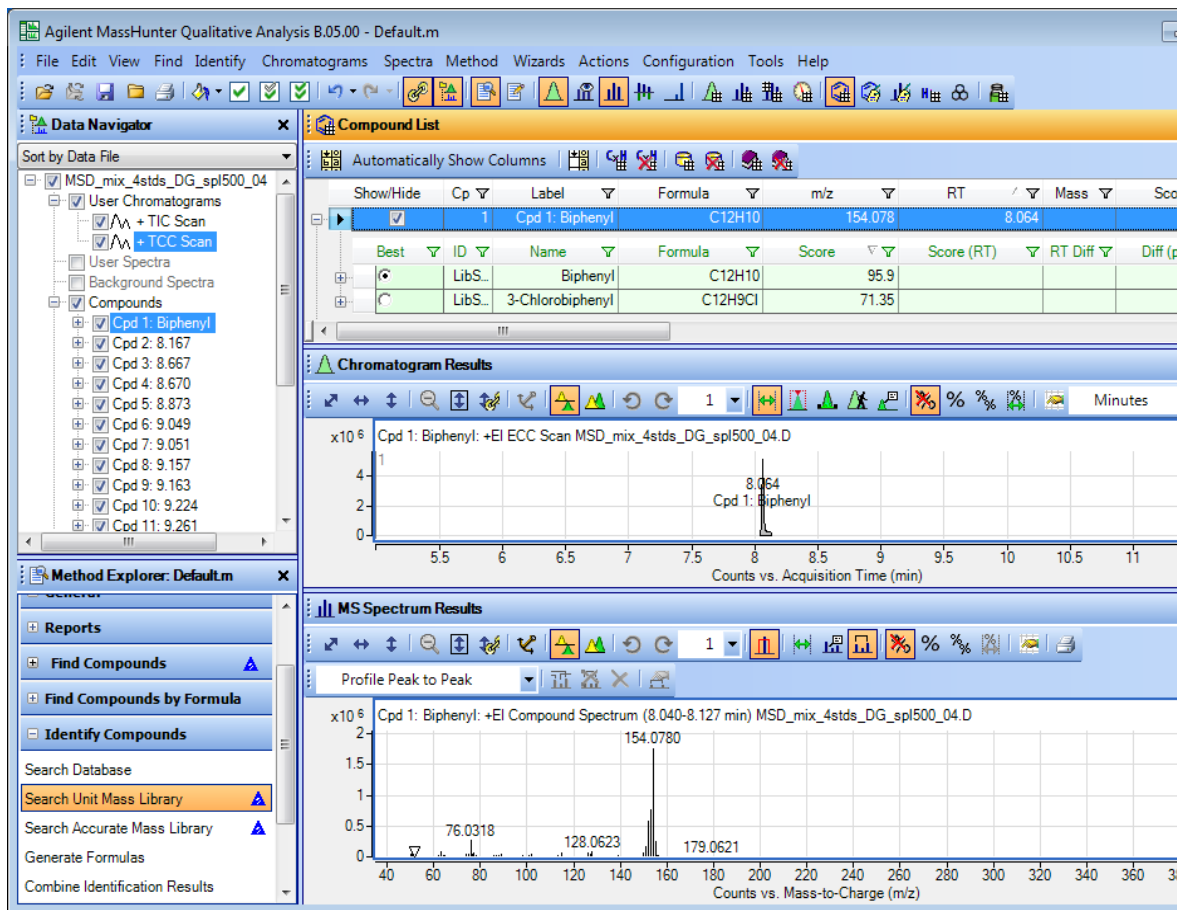




Figure 23 Accurate Mass Library Search Results

Exercise – Analyze data

Task 4. Display the mass difference between two ions.

Task 4. Display the mass difference between two ions.

The mass caliper tool is used to show the difference between two points in a spectrum.

Steps	Detailed instructions	Comments
1	<p>a Place the cursor over the Show/Hide column label in the Compound List and right click to open the context menu. Select Hide > All except highlighted.</p> <p>b Right click and drag the cursor over the m/z scale in the Spectrum Results windows to zoom this scale.</p>	<ul style="list-style-type: none">• Only compound 1 is shown in the Chromatogram Results and MS Spectrum Results windows.• This makes it easier to select the ions with the Delta Mass Caliper tool.
2	<p>Display the mass difference between two ions.</p> <p>a In the MS Spectrum Results window, click the Delta Mass Caliper icon .</p> <p>b Select Profile Peak to Peak for the profile data used in this exercise.</p> 	<ul style="list-style-type: none">• The profile data dropdown menu is displayed in the tool bar and the caliper tool cursor is displayed in the MS Spectrum Results window,• The difference of 78.0462 is displayed on the spectrum. See Figure 24.

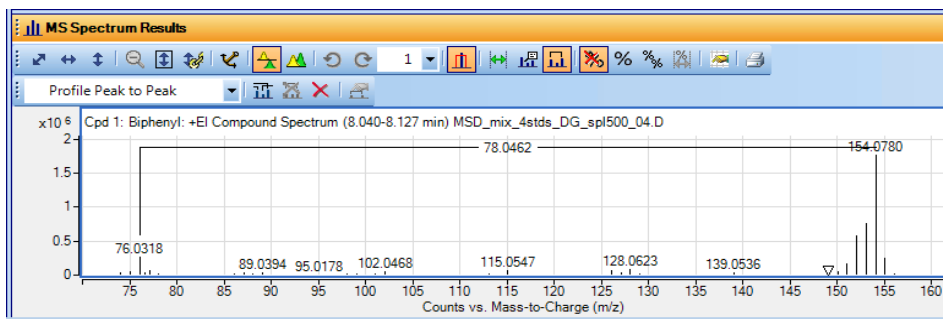
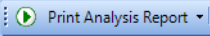


Figure 24 Displaying the peak to peak difference.

Task 5. Print a report

You can print an analysis report after performing any of these tasks. An analysis report can contain the results from extracting and integrating chromatograms, extracting spectra, finding compounds, searching the database for peak spectra or generating formulas from peak spectra.

Steps	Detailed instructions	Comments
1 Open Method Editor Analysis Report dialog box and choose settings.	<p>a From the Method Explorer window, select Reports > Analysis Reports.</p> <p>b For this example, mark all checkboxes.</p>	<ul style="list-style-type: none"> The Method Editor: Analysis Reports dialog box opens.
2 Open Method Editor Search Unit Mass Library dialog box and choose settings.	<p>c Select </p> <p>d Set printing setting for your directory and printer.</p> <p>e Click OK.</p> <p>f Open the report.</p>	<ul style="list-style-type: none"> The Print Analysis Report dialog box opens. See Figure 25. The report is created and saved in the specified directory. See Figure 26 on page 34. See Figure 27 on page 35.

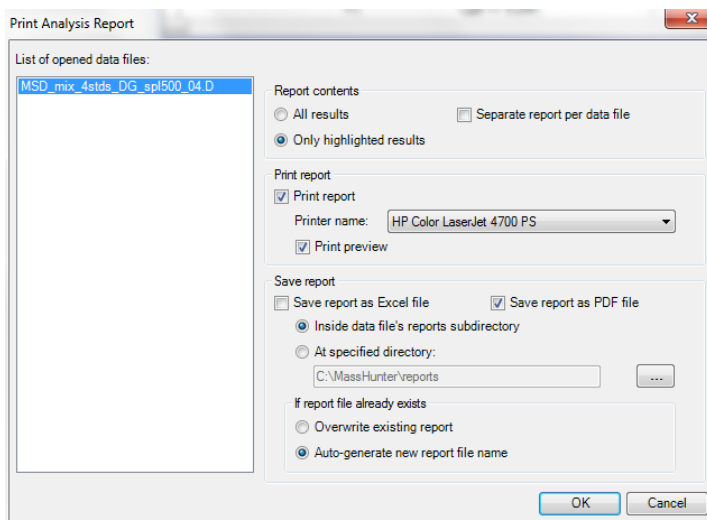


Figure 25 Print Analysis Report settings

Exercise – Analyze data

Task 5. Print a report

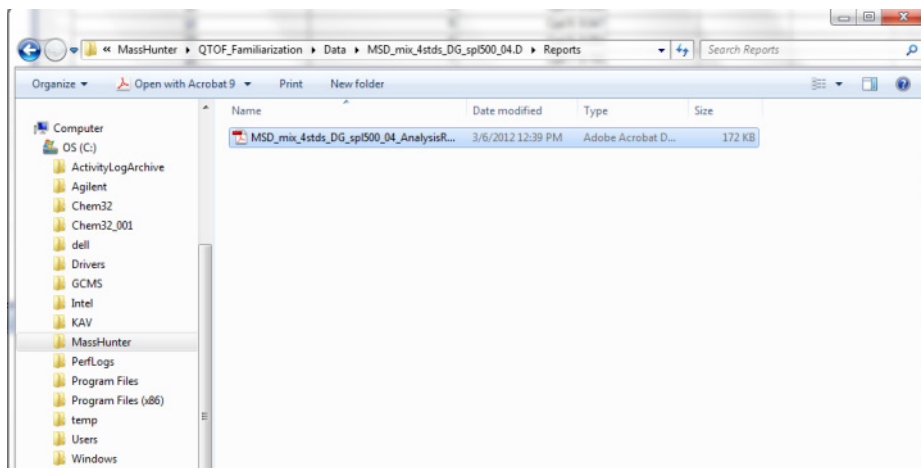


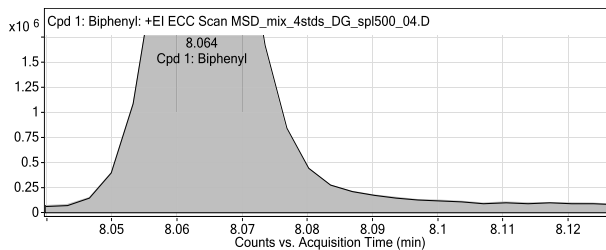
Figure 26 Location of saved pdf file inside data file's reports subdirectory

Qualitative Analysis Report

Data Filename	MSD_mix_4stds_DG_spl500_04.D	Sample Name	
Sample Type		Position	1
Instrument Name	GC QTOF	User Name	GCMSTRAINING10\admin
Acq Method	4_stdsg_DG_noIRM_0112012.M	Acquired Time	1/20/2012 3:15:31 PM
IRM Calibration Status	Success	DA Method	Default.m
Comment			

Expected Barcode		Sample Amount	
Dual Inj Vol	1	TuneName	qtofatuses_DG_Jan20.ei.tune.xml
TunePath	D:\MassHunter\GCMS\1\7200	TuneDateStamp	1/20/2012 5:55:09 PM
OperatorName	GCMSTRAINING10\admin	RunCompletedFlag	True

Compounds



Integration Peak List

Start	RT	End	Height	Area
8.04	8.064	8.127	1767905.03	4764370.15

Figure 27 Qualitative analysis report - page 1 of 2

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