

# 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  $\mu$ m, 0.25  $\mu$ 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/ $\mu$ L, 100 ng/ $\mu$ L, and 100 pg/ $\mu$ L concentrations and are shown in Table 1.

**Table 1** Sample Compound list

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

Prepare the Qualitative Analysis sample by emptying the contents of the 10 ng/ $\mu$ 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><b>a</b> Double-click the <b>Data Acquisition</b> icon on the windows desktop.</p> <p><b>b</b> Click the <b>Inlet and Injection Parameters</b> icon.</p> <p><b>c</b> Select <b>GC</b> for the sample inlet and the installed ALS for the injection source.</p> <p><b>d</b> Select the <b>Use MS</b> check box.</p>	<ul style="list-style-type: none"> <li>The <b>Data Acquisition</b> window shown in Figure 1 is displayed.</li> <li>Hover over an icon to display a tag identifying the icon.</li> <li>The <b>Inlet and Injection Parameters</b> dialog box shown in Figure 2 on page 6 is displayed.</li> </ul>

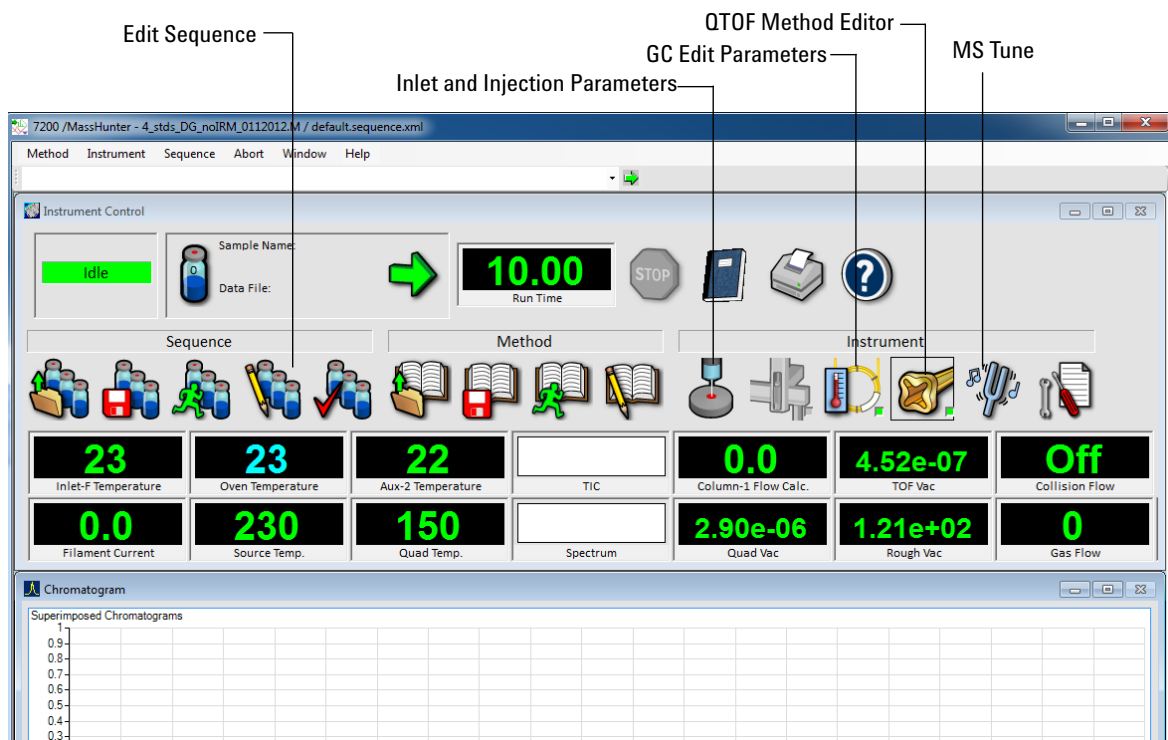
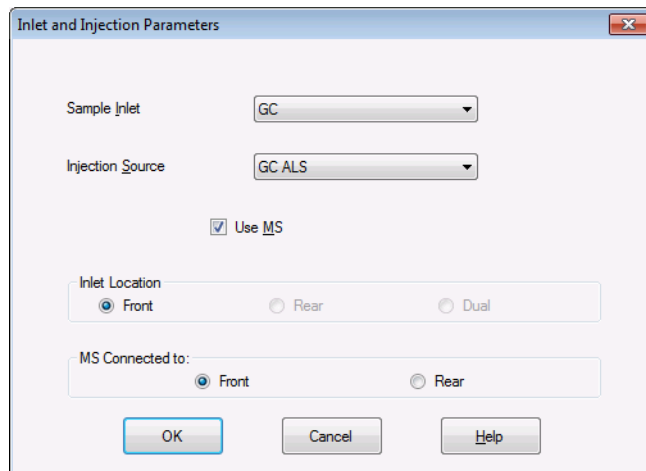


Figure 1 Agilent MassHunter Workstation Software – Data Acquisition window

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

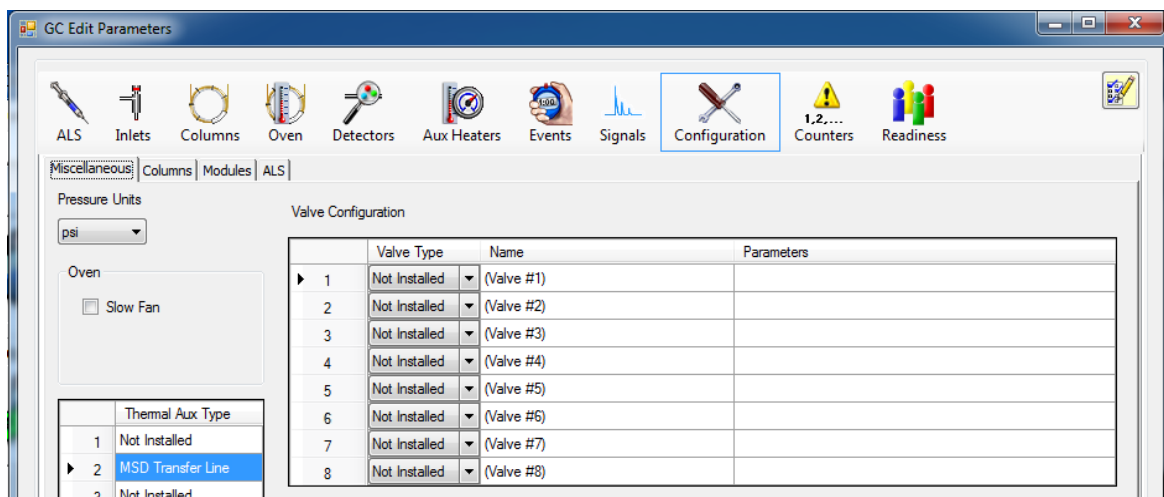


Figure 3 The Configuration Settings

## Exercise – Develop an acquisition method for the 7200

### Task 3. Perform a Mass Calibration

#### Task 3. Perform a Mass Calibration

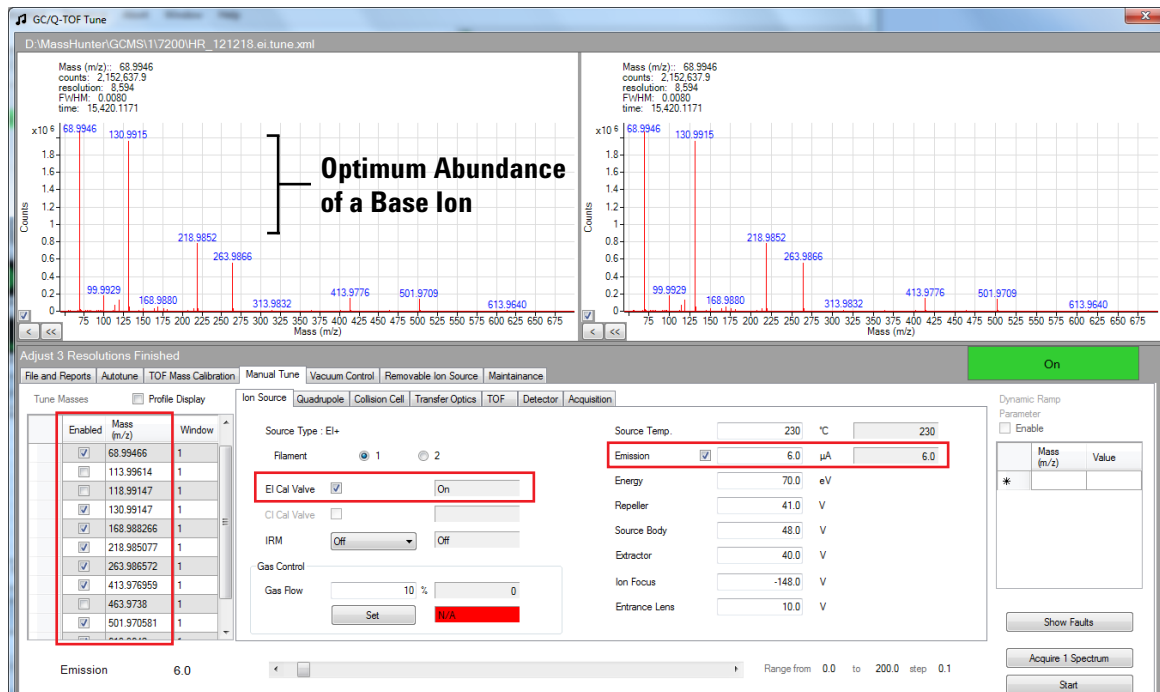
In this exercise you perform a mass calibration from the **TOF Mass Calibration** tab in the **GC/Q-TOF Tune** window. A mass calibration is completed in less than two minutes and it is good practice to calibrate the instrument as often as possible. A sequence table keyword allows automatic mass calibration 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><b>a</b> Click the <b>MS Tune</b> icon.</p> <p><b>b</b> Click the <b>Manual Tune</b> tab, then click the <b>Ion Source</b> tab and enable the <b>Emission</b> and <b>El Cal Valve</b>.</p> <p><b>c</b> In the <b>Tune Masses</b> area, select <b>Enabled</b> for calibrant masses surrounding a base ion of interest.</p> <p><b>d</b> Adjust the <b>Emission</b> current so that the abundance of the ion of interest is between <math>1 \times 10^6</math> and <math>2 \times 10^6</math> counts.</p> <p><b>e</b> Save the tune file as <code>qtofatunes_DG_date.ei.tune.xml</code>.</p> <p><b>f</b> Select the <b>Close</b> button.</p>	<ul style="list-style-type: none"><li>• The <b>GC/Q-TOF Tune</b> window is displayed.</li><li>• To enable calibrant flow ionization. See Figure 4 on page 9.</li><li>• Uncheck the ions that have interferences with selected ions. See Figure 4 on page 9.</li><li>• Higher values will saturate the signal and lower values will not provide sufficient ion statistics for optimal mass accuracy.</li><li>• Where date is today's date.</li><li>• The <b>GC/Q-TOF Tune</b> window closes.</li></ul>
<p>2 Perform a mass calibration.</p>	<p><b>a</b> Select the <b>TOF Mass Calibration</b> tab from the <b>GC/Q-TOF Tune</b> window.</p> <p><b>b</b> Click the <b>Run Calibration</b> button.</p> <p><b>c</b> Select the <b>Close</b> button.</p> <p><b>d</b> Click the <b>File and Reports</b> tab and save the tune file.</p> <p><b>e</b> Select the <b>Close</b> button.</p>	<ul style="list-style-type: none"><li>• See Figure 5 on page 9.</li><li>• When the calibration completes the <b>TOF Mass Calibration Results</b> window displays. <b>Mass Accuracy (PPM)</b> should typically be below 2 PPM for all ions used in calibration. See Figure 6 on page 10.</li><li>• The <b>TOF Mass Calibration Results</b> closes.</li><li>• The <b>GC/Q-TOF Tune</b> window closes.</li></ul>

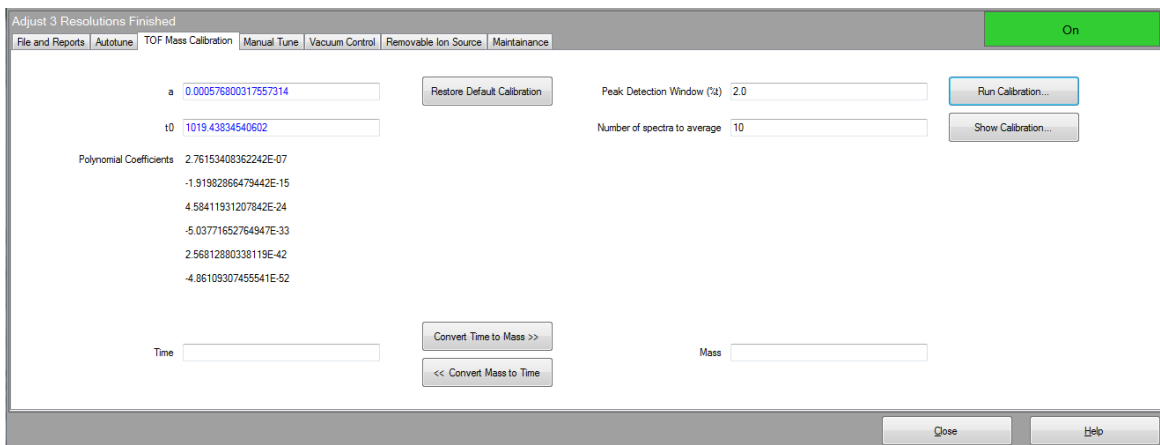


## Exercise – Develop an acquisition method for the 7200

### Task 3. Perform a Mass Calibration



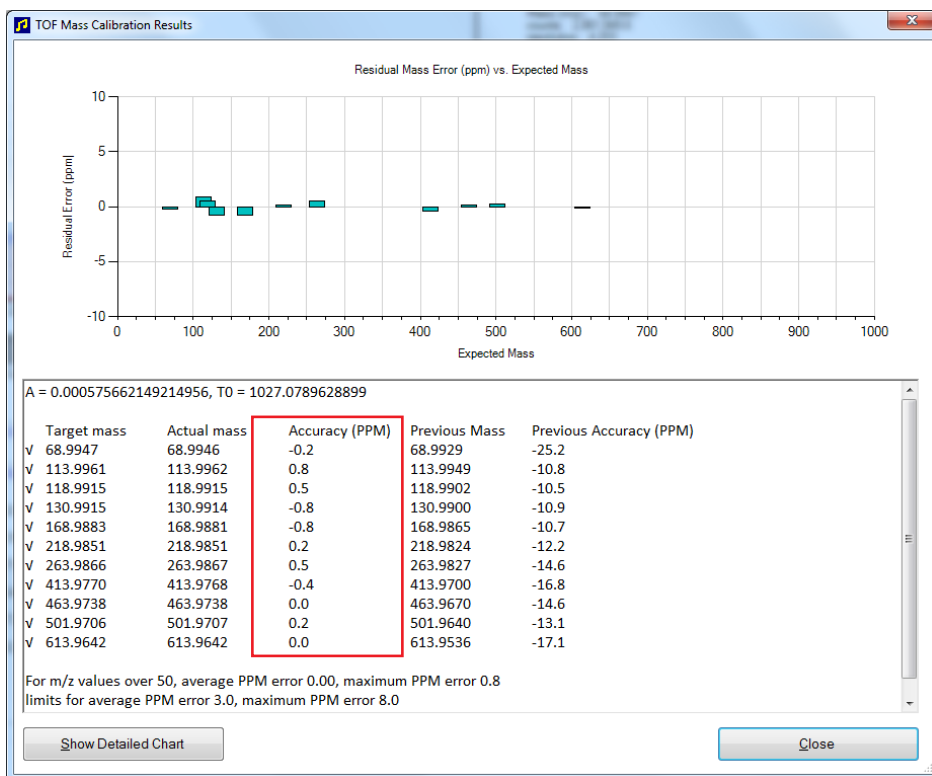
**Figure 4** Optimizing base ion abundance



**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

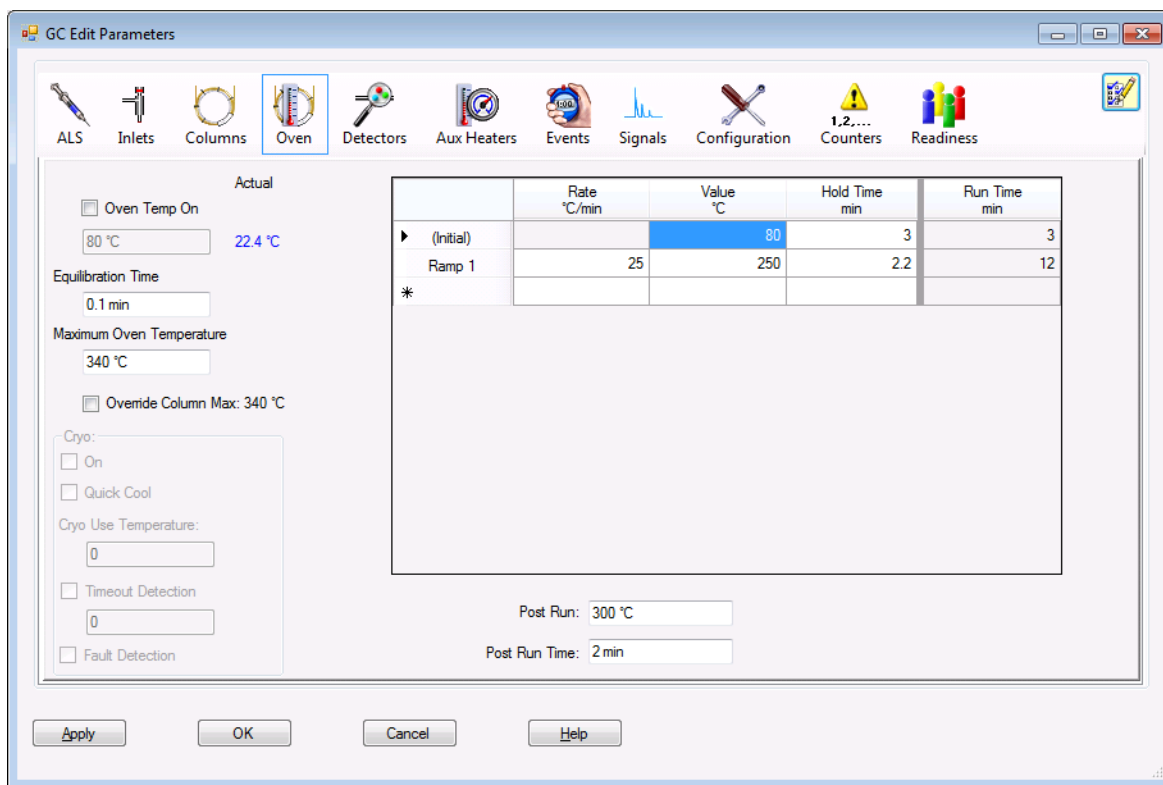
## Task 4. Enter GC acquisition parameters

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

Steps	Detailed instructions	Comments
3 Enter GC parameters appropriate for the sample. See Table 2.	<p><b>a</b> Click the <b>GC Edit Parameters</b> icon (Figure 1).</p> <p><b>b</b> Select the <b>Columns</b> icon then select column <b>1</b> in the <b>Selection</b> column.</p> <p><b>c</b> Select control mode <b>On</b> and then select <b>Constant Flow</b> mode. Enter 1.1 mL/min for the initial <b>Value</b>.</p> <p><b>d</b> Select the <b>Collision Cell EPC</b> in the <b>Selection</b> column and then in the <b>Collision Cell EPC</b> area, set the <b>N2 Collision Gas</b> on at 1.5 mL/min.</p> <p><b>e</b> In the <b>Collision Cell EPC</b> area, uncheck the <b>He Quench Gas</b>.</p> <p><b>f</b> Select the <b>Inlets</b> icon then the <b>SSL</b> tab and enter the inlet parameters listed in Table 2.</p> <p><b>g</b> Select the <b>Oven</b> icon and enter the oven parameters listed in Table 2.</p> <p><b>h</b> Select the <b>ALS</b> icon then the <b>Front Injector</b> tab and enter the injector parameters listed in Table 2.</p> <p><b>i</b> Select the <b>Aux Heaters</b> icon, enable, and set the temperature to 280 °C.</p> <p><b>j</b> Select the <b>OK</b> button.</p>	<ul style="list-style-type: none"> <li>• The <b>GC edit parameters</b> window shown in Figure 7 on page 12 is displayed.</li> <li>• With the window selected, mouse over the icons to identify the icon from the tool tip.</li> <li>• 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.</li> <li>• If your ALS is attached to the <b>Back Inlet</b> select the <b>Back Injector</b> tab.</li> <li>• This is the MSD transfer line heater.</li> <li>• The GC parameters are downloaded to the GC and the window closes.</li> </ul>

## 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
<b>Oven</b>	
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
<b>Front SS Inlet</b>	
	He
Mode	Split
Heater	<b>On</b> 250 °C
Pressure	<b>On</b> Value automatically set with column flow
Septum Purge Flow	<b>On</b> 3 mL/min
Gas Saver	<b>On</b> 20 mL/min after 3 min
Split Flow	220 mL/min
Split Ratio	200:1
<b>Thermal Aux 2 {MSD Transfer Line}</b>	
Heater	<b>On</b>
Temperature	280 °C
<b>Column # 1</b>	
	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	<b>Off</b>
<b>Front Injector</b>	
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

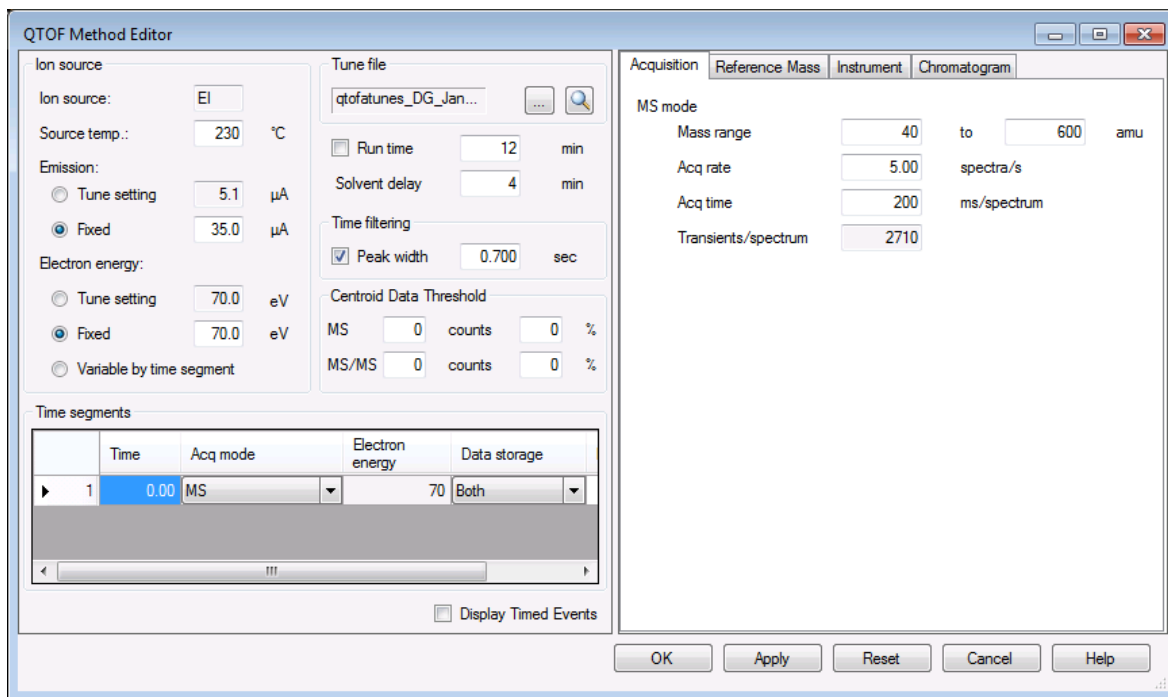
<b>Parameter</b>	<b>Value</b>
Solvent A Washes (PostInj)	2
Solvent A Volume	8 µL
Solvent B Washes (PreInj)	2
Solvent B Washes (PostInj)	2
Solvent B Volume	8
Sample Washes	0
Sample Wash Volume	8 µL
Sample Pumps	4
Dwell Time (PreInj)	0 min
Dwell Time (PostInj)	0 min
Solvent Wash Draw Speed	300 µL/min
Solvent 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
<b>Collision cell EPC Module</b>	
Nitrogen	<b>On</b> 1.5 mL/min
Helium	<b>Off</b>

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

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

## 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   $\mu$ L  
 Override using 1   $\mu$ 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   $\mu$ L  
 Override using   $\mu$ L

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

Method Sections to Run:

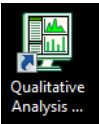
Data Acquisition  Data Analysis

**Figure 9** Start Run dialog box

## Exercise – Analyze data

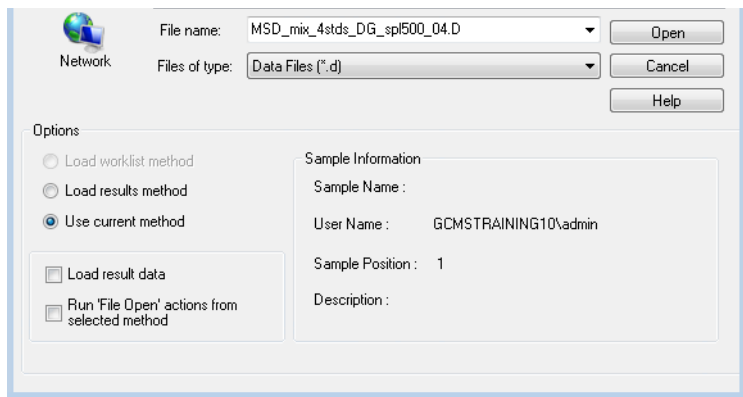
### Task 1. Start the qualitative analysis program

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.

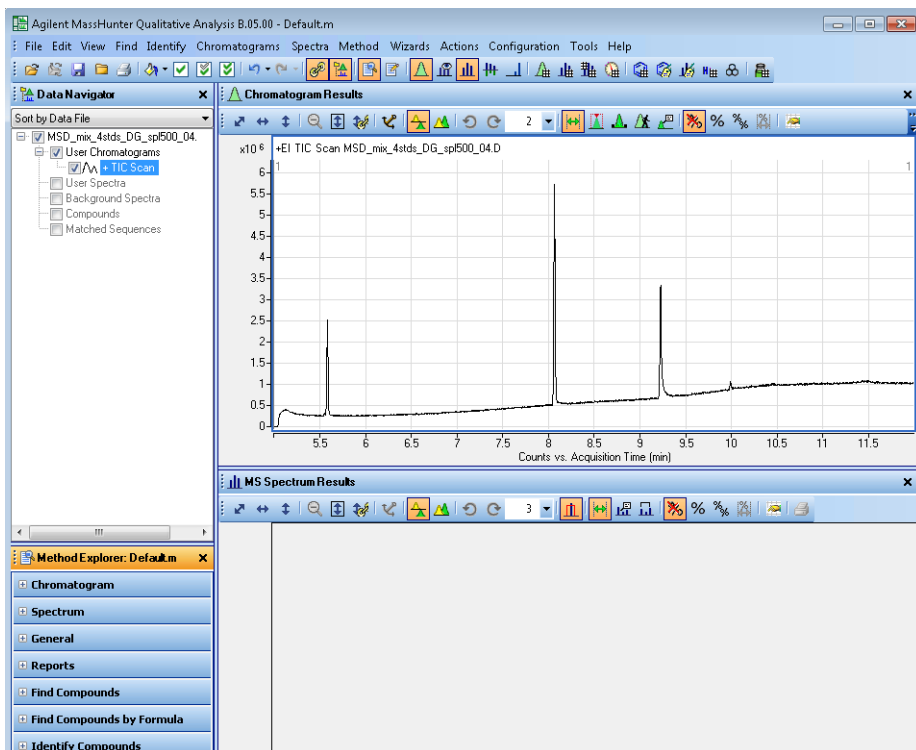
Steps	Detailed instructions	Comments
1 Start the Qualitative Analysis program.	<p><b>a</b> Double-click <b>Qualitative Analysis</b> icon on your desktop.</p> 	<ul style="list-style-type: none"> <li>The system displays the Open Data Files dialog box.</li> </ul> <p>You can get help by:</p> <ul style="list-style-type: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

## Exercise – Analyze data

### Task 1. Start the qualitative analysis program

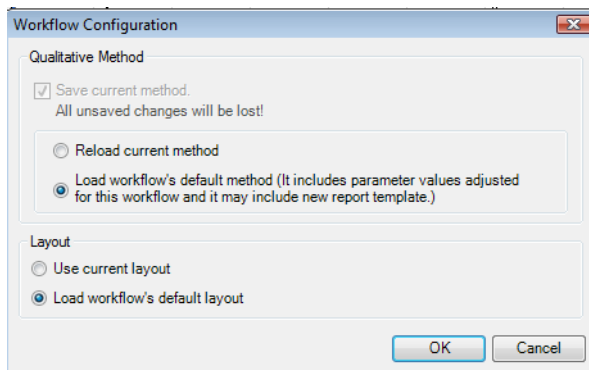


**Figure 10** Opening the data file



**Figure 11** The TIC of the loaded data file

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

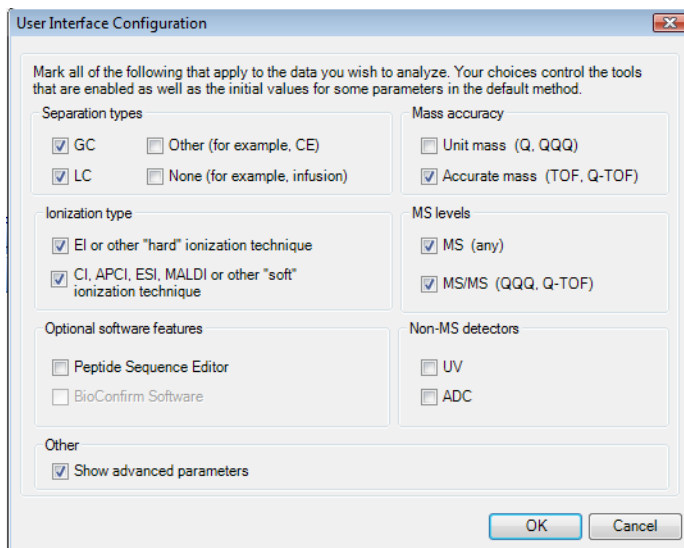


**Figure 12** Configuring the Workflow

## Exercise – Analyze data

### Task 1. Start the qualitative analysis program



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



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

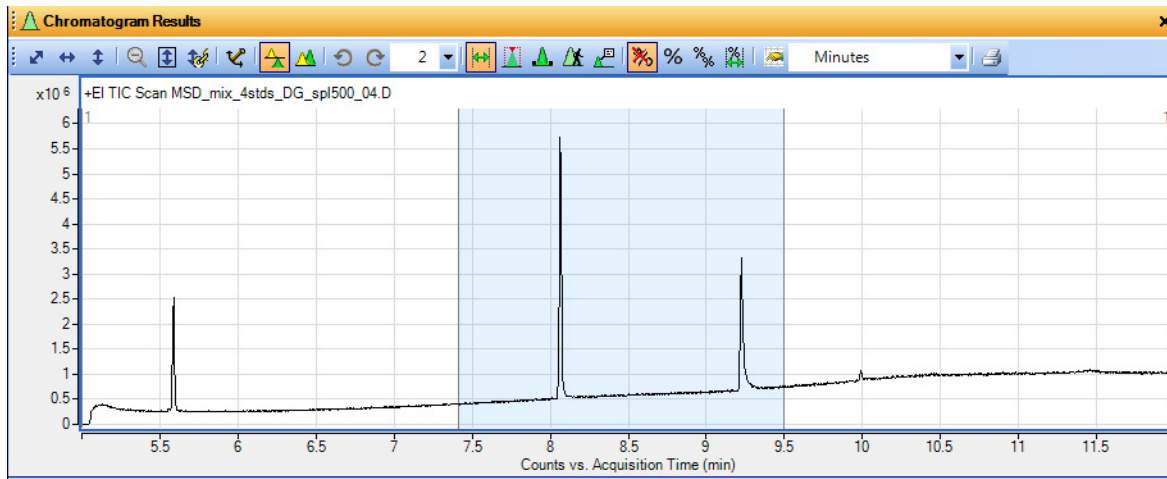


Figure 14 The Chromatogram Results window

## Exercise – Analyze data

### Task 2. Find compounds by deconvolution

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

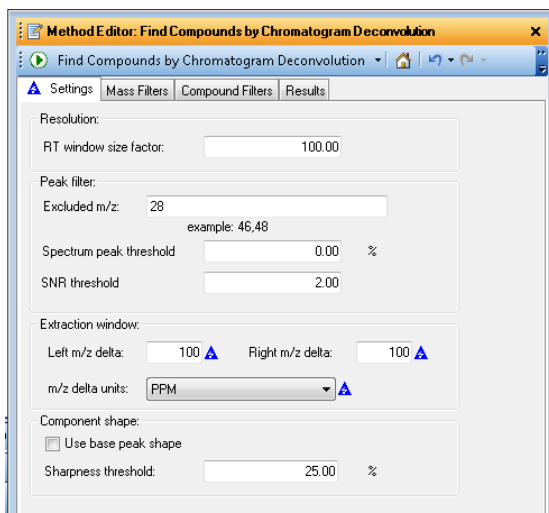
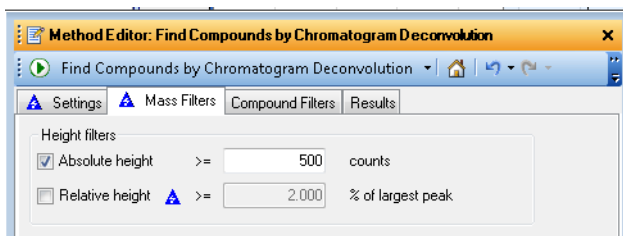


Figure 15 The Settings tab



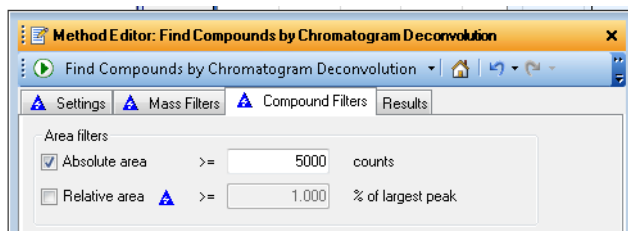
Steps	Detailed instructions	Comments
Step 1 continued.	<p><b>c</b> Set the <b>Mass Filters</b> tab entries as follows:</p> <ul style="list-style-type: none"> <li>• <b>Height Filters</b> area: Absolute height: enabled 500 counts Relative height: disabled</li> </ul> <p><b>d</b> Set the <b>Compound Filters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



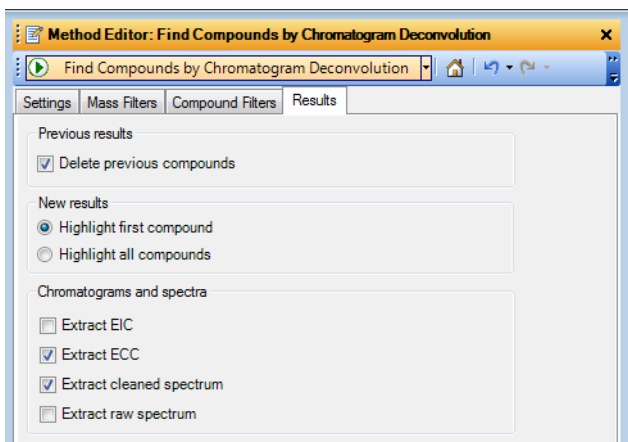
**Figure 16** The **Mass Filters** tab

## Exercise – Analyze data

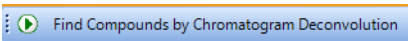
### Task 2. Find compounds by deconvolution



**Figure 17** The **Compound Filters** tab



**Figure 18** The **Results** tab

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

## Exercise – Analyze data

### Task 2. Find compounds by deconvolution

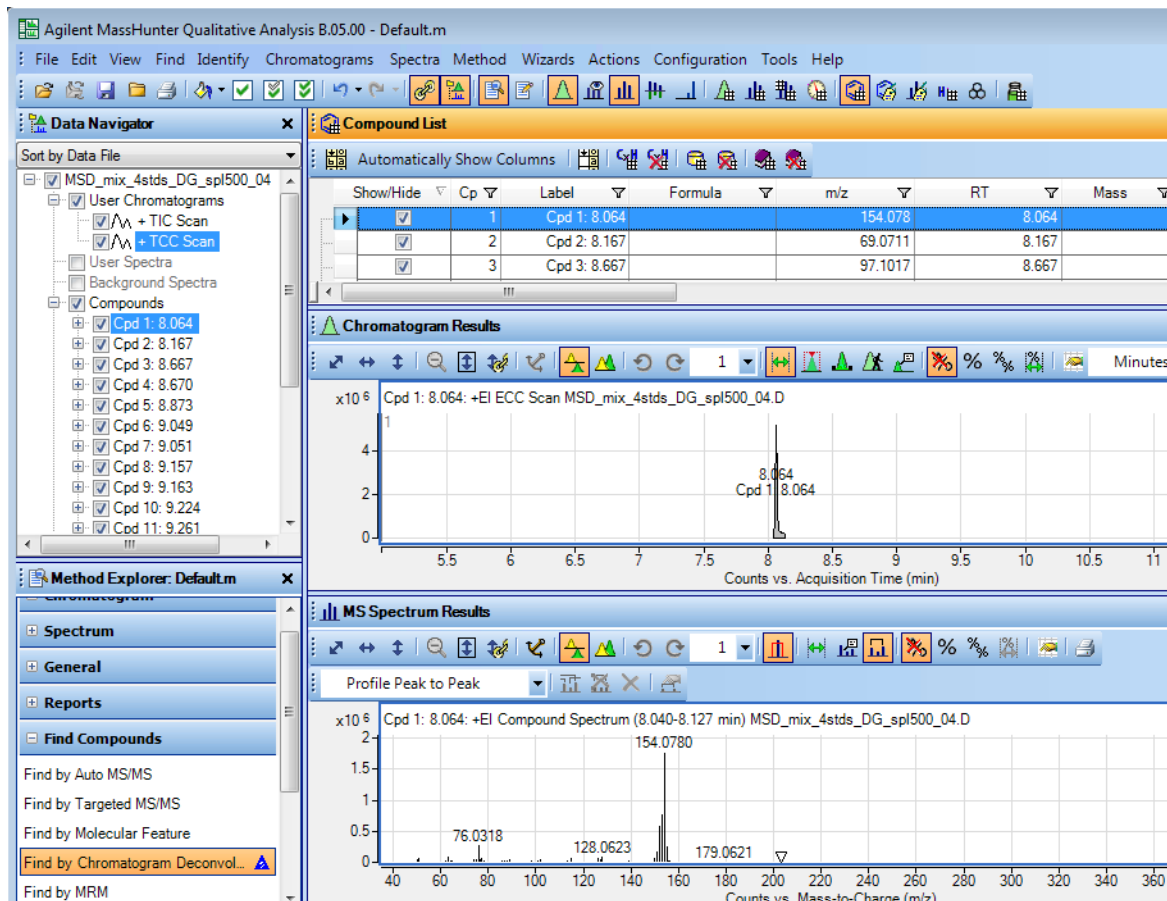
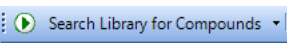


Figure 19 The deconvolution results

## Task 3. Search an accurate mass library

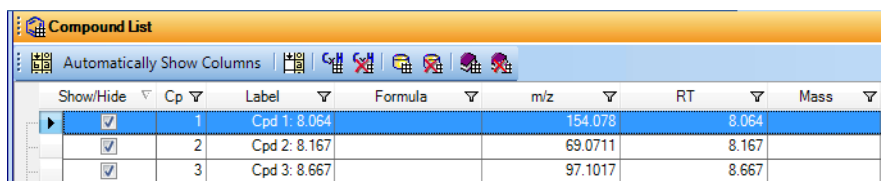
The library used in this exercise is a GCMS accurate mass library stored in an XML data format. This library file is provided by Agilent and stored in the **QTOF\_Familiarization\Library** folder of your Data Acquisition installation disk.

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><b>a</b> In the Compound List window, click in the first row to highlight it.</p>	<ul style="list-style-type: none"> <li>This task begins by selecting a compound from the compound list generated in the last task. See Figure 20 on page 30.</li> </ul>
2 Open Method Editor Search Unit Mass Library dialog box and choose settings.	<p><b>b</b> From the Method Explorer window, select <b>Identify Compounds &gt; Search Unit Mass Library</b>.</p> <p><b>c</b> In the <b>Library selection</b> area of the <b>Settings</b> tab, set the <b>Spectral library path</b> to MSD_mix_lib.mslibrary.xml.</p> <p><b>d</b> In the <b>Search criteria</b> area of the <b>Settings</b> tab, set the <b>Begin spectral matching</b> to 30 m/z, set <b>Enable Screening</b> to disabled, and <b>Adjust score</b> to enabled.</p> <p><b>e</b> In the <b>MS/MS search</b> area of the <b>Settings</b> tab, set the <b>m/z expansion</b> to <b>Symmetric (m/z)</b> at <math>\pm 0.5000</math>.</p> <p><b>f</b> In the <b>Search Results</b> area of the <b>Search Results</b> tab, set the <b>Maximum hits per compound</b> to 2 hits and the <b>Minimum match score</b> to 50.00.</p> <p><b>g</b> Select </p> <p><b>h</b> In the <b>Compound List</b> click the + icon next to the first compound at RT = 8.064 minutes.</p>	<ul style="list-style-type: none"> <li><b>The Method Editor: Search Unit Mass Library</b> dialog box opens.</li> <li>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.</li> <li>See Figure 22 on page 30.</li> <li>After the search is complete the results are shown in the <b>Compound List</b>, <b>Chromatogram Results</b>, and <b>Spectrum Results</b> windows.</li> <li>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.</li> </ul>

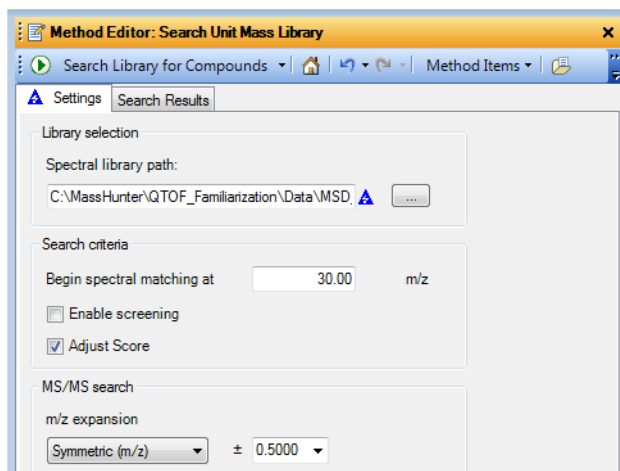
## Exercise – Analyze data

### 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

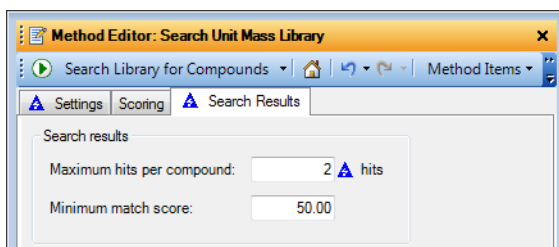
Enable screening

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

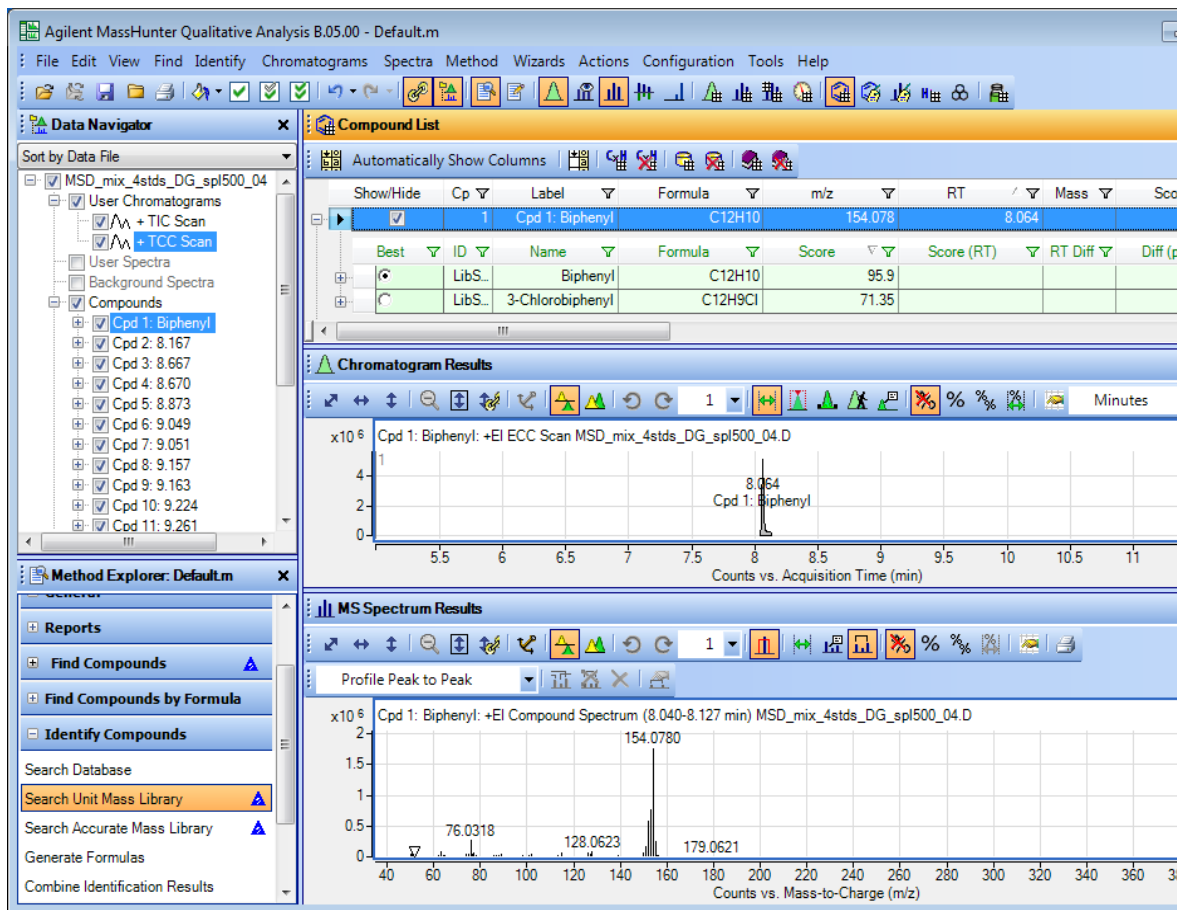




Figure 23 Accurate Mass Library Search Results

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

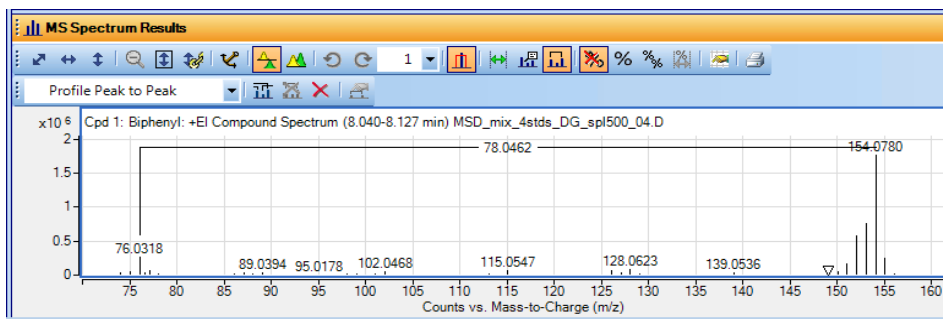
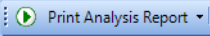


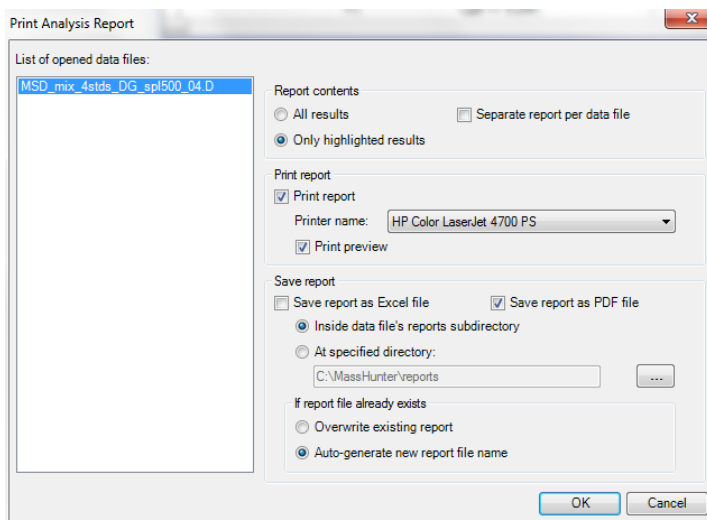
Figure 24 Displaying the peak to peak difference.



## 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.

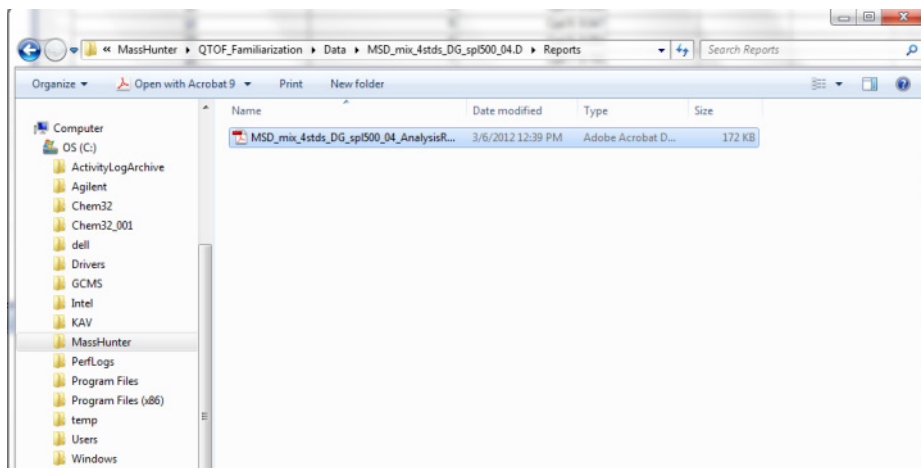
Steps	Detailed instructions	Comments
1 Open <b>Method Editor Analysis Report</b> dialog box and choose settings.	<p><b>a</b> From the <b>Method Explorer</b> window, select <b>Reports &gt; Analysis Reports</b>.</p> <p><b>b</b> For this example, mark all checkboxes.</p>	<ul style="list-style-type: none">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



**Figure 25** Print Analysis Report settings

## Exercise – Analyze data

### Task 5. Print a report



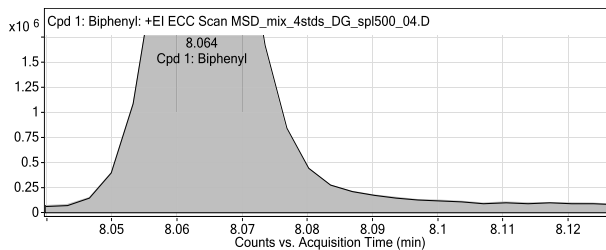
**Figure 26** Location of saved pdf file inside data file's reports subdirectory

### Qualitative Analysis Report

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

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