Agilent G1978B
Multimode Source for
6500 Series Q-TOF
LC/MS

Set-Up Guide
Notices

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Safety Notices

CAUTION

A CAUTION notice denotes a hazard. It calls attention to an operating procedure, practice, or the like that, if not correctly performed or adhered to, could result in damage to the product or loss of important data. Do not proceed beyond a CAUTION notice until the indicated conditions are fully understood and met.

WARNING

A WARNING notice denotes a hazard. It calls attention to an operating procedure, practice, or the like that, if not correctly performed or adhered to, could result in personal injury or death. Do not proceed beyond a WARNING notice until the indicated conditions are fully understood and met.
In This Guide

This guide explains how to install, maintain and troubleshoot your multimode ion source.

1 Installation

This chapter tells you how to install the multimode source.

2 Set-Up

This chapter describes basic operation and maintenance for the multimode source.
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Installation

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This chapter contains instructions to install the multimode source on a 6510 Series Q-TOF LC/MS system, and also to remove and replace the source.
1 Installation

Step 1. Prepare to install

The Multimode Enablement Kit, G1978-60451, is shipped with the multimode source. This kit needs to be installed before the multimode source is used.

Note that the multimode source and its accessories are to be installed by an Agilent Customer Engineer.

1 Check that the Multimode Enablement Kit contains the following parts:
   • Multimode Bd HV Cable, p/n G1960-60858
   • Multimode HV PCA, p/n G1960-61015
   • Multimode Bd Power/Data Cable, p/n G1960-60873

![Figure 1](image1.png)  
**Figure 1** From left to right: G1960-60858, G1960-61015 and G1960-60873

2 Install the APCI Enablement Kit, G1947-60451, which is shipped with the multimode source.

The APCI Enablement kit contains the following parts:
   • Fast APCI HV Supply, p/n G1946-80058
   • Valve BD-APCI Supply Cable, p/n G1960-60802
   • Valve BD-APCI Needle Interlock Cable, p/n G1960-60856

![Figure 2](image2.png)  
**Figure 2** From left to right: G1946-80058, G1960-60802 and G1960-60856
Step 2. Install the HV control PCA and cables

1. Turn off the system power and remove the system power cord.

The power cord should be kept intact if the vacuum control switch box is used. The switch box is intended to keep the vacuum on while a service engineer works on the electronics. The switch box is for service engineer use only.

2. Remove the CDS cover, top, side, front, and the Aux Module cover.

3. Disconnect the ribbon cable that connects the valve PCA to the Vcap/Vchamber power supply. Then disconnect the Vcap and Vchamber cable from the power supply.

4. Place the multimode HV power supply PCA in the slot between the valve PCA and the Vcap/Vchamber power supply. Secure the board by pressing it down into its slot and then attach it with two screws.

5. Connect the short gray cable from the valve PCA to the multimode HV power supply.

Figure 3  Disconnecting the Vcap/Vchamber power supply from the valve PCA (left) and the Vcap/Vchamber.

Figure 4  Connecting the valve PCA to the multimode HV power supply.
1 **Installation**

**Step 2. Install the HV control PCA and cables**

6 Install the APCI HV power supply. The APCI HV power supply is located at the end of the AUX Module.

7 Connect ribbon cable between the valve PCA and Vcap/Vchamber power supply.

![Figure 5](image1.png)

**Figure 5**     Connecting the valve PCA to the Vcap/Vchamber power supply.

8 Connect the Vcap and Vchamber cables to the Vcap/Vchamber power supply.

![Figure 6](image2.png)

**Figure 6**     Connecting the Vcap and Vchamber cables to the power supply.

9 Connect the long ribbon cable, p/n G1960-60802, from the APCI HV power supply to the valve PCA.
Step 2. Install the HV control PCA and cables

10 Insert one end of the APCI Needle Interlock cable, G1960-60856, through the slot at the front of the system and then plug it to the APCI HV connector. Attach the other end to the chassis with the o-ring and the nut (see Figure 8).

11 Insert the cable, G1960-60858, to the top slot and attach it to the chassis. Plug the other two ends into the multimode HV PCA.

12 Close the AUX Module cover and reconnect all cables.
13 Install the multimode source onto the system and connect all connectors.
1  **Installation**

Step 2. Install the HV control PCA and cables

![Image of multimode source installation](image)

**Figure 10**  Installing the multimode source (left) and connecting all connectors.

14 Put back the side, top, front and CDS cover.
15 Plug the system power cord back on and turn the front switch on.

   The pump down process will start.
16 Start the MassHunter Workstation program and verify that the software recognizes the source.
17 Set the **Context** view to **Tune**, and in **Manual Tune**, verify that the system can generate the proper tune peaks.
To remove the multimode source

Do the following steps to remove the multimode source.

1. Turn off the multimode source temperatures and flows:
   a. Change the Context view to Acquisition.
   b. Click the MS Q-TOF tab.
   c. Turn off all voltages and temperatures in the Source tab.
   d. Wait approximately 20 minutes for the source to cool down.

Warning: Do not touch the multimode source or the capillary cap. They may be very hot. Let the parts cool before you handle them.

Warning: Never touch the source surfaces, especially when you analyze toxic substances or when you use toxic solvents. The source has several sharp pieces which can pierce your skin including the APCI corona needle, vaporizer sensor and counter current electrode.

Warning: Do not insert fingers or tools through the openings on the multimode chamber. When in use, the capillary and capillary cap are at high voltages up to 4 kV.

2. Wait approximately 20 minutes or until the source is cool.
3. Open the CDS door at the front of the MS to access the cables.
4. Disconnect the ESI high voltage charging electrode cable.
5. Disconnect the APCI Needle Interlock, and multimode HV cable.
6. Unscrew the nebulizer gas line from the nebulizer.
7. Unscrew the LC sample tubing from the nebulizer.
8. Open the latch on the source and open the source.
9. Remove the multimode source from the spray chamber mount.
10. Place the source shipping cover on the source.
To convert from multimode to ESI or APCI

**WARNING** Never touch the source surfaces, especially when you analyze toxic substances or when you use toxic solvents. The source has several sharp pieces which can pierce your skin including the APCI corona needle, vaporizer sensor and counter current electrode.

1. Unscrew and remove the multimode spray shield with the field shaping electrodes.
2. Install the new source and the standard spray shield, making sure that the hole in the spray shield is in the 12 o'clock position.
3. For an APCI ion source, connect the vaporizer heater cable and the APCI high voltage cable.
4. For all sources, reconnect the nebulizer gas line tubing and the LC/MS sample tubing.
To convert from ESI or APCI to the multimode source

CAUTION If you are installing this source on this instrument for the first time, follow the steps in “Installation” on page 7.

1 Turn off the multimode source temperatures and flows:
   a Change the Context view to Acquisition.
   b Click the MS Q-TOF tab.
   c Turn off all voltages and temperatures in the Source tab.
   d Wait approximately 20 minutes for the source to cool down.
2 Wait for the source to cool (until temperatures are at least below 100°C).
3 Disconnect the nebulizer gas tubing from the currently installed ion source.
4 Disconnect the LC/MS sample inlet tubing.
5 If the APCI source is installed, remove the APCI vaporizer heater cable and APCI high voltage cable.
6 Remove the currently installed ion source.
7 Unscrew and remove the spray shield. See Figure 11.

WARNING Do not touch the multimode source or the capillary cap. They may be very hot. Let the parts cool before you handle them.

WARNING Do not insert fingers or tools through the openings on the multimode chamber. When in use, the capillary and capillary cap are at high voltages up to 4 kV.
1 Installation
To convert from ESI or APCI to the multimode source

8 Remove the capillary cap. If needed, moisten a clean cloth with isopropyl alcohol and wipe the capillary cap. See Figure 12.

9 Place the capillary cap back on the capillary.

10 Install the new spray shield with field shaping electrodes. See Figure 13.
To convert from ESI or APCI to the multimode source

11 Screw the multimode spray shield into the holder for the spray shield. See Figure 14.

The field shaping electrodes should be in the nine o’clock and the six o’clock position. Loosen the end plate screws on each side to adjust the field shaping electrodes position.

12 Remove the shipping cover from the multimode source spray chamber.
1 Installation
To convert from ESI or APCI to the multimode source

13 Install the spray chamber on the spray chamber mount.

14 Install the nebulizer on the multimode source spray chamber.
Installation 1

To convert from ESI or APCI to the multimode source

15 Connect the 1/8-inch nebulizer gas tubing from the LC/MS mainframe to the nebulizer gas fitting. See Figure 18.
16 Connect the LC/MS sample tubing to the LC/MS diverter valve inlet filter.

**WARNING** The LC/MS Liquid Chromatograph diverter valve is an integral part of the G1978B safety system. The LC mobile phase flow must always be connected to the diverter valve inlet filter. Never bypass the diverter valve and connect directly to the nebulizer. If the diverter valve is used in a manner not specified by Agilent Technologies, the protections provided by the diverter valve may be impaired.

17 If you are installing the multimode source for the first time, follow the steps in “Step 2. Install the HV control PCA and cables” on page 9.
This chapter describes the tasks that you need to operate and maintain the multimode source.
To set up a method to use the multimode source

**WARNING**
The LC/MS diverter valve is an integral part of the G1978B safety system. The LC mobile phase flow must always be connected to the diverter valve inlet filter. Never bypass the diverter valve and connect directly to the nebulizer. If the diverter valve is used in a manner not specified by Agilent Technologies, the protections provided by the diverter valve may be impaired and the system may catch fire.

1. In the MassHunter software, change the Context to Acquisition.
2. In the MS Q-TOF tab, set Ion source to Multimode (see Figure 19 on page 23).
3. In the Sources tab, choose an ionization mode from the Ion Modes (Seg) list. You may set the ionization mode to one of the following:
   - ESI
   - APCI
   - Mixed

   The Ion Mode selection Mixed will specify a method for simultaneous ESI and APCI operation.

   Note that the Ionization Modes selection is only visible if Ion source is set to Multimode.
4. In the Source tab, set the desired source conditions. See “Guidelines” in the *Agilent G1978A/B Multimode Source Maintenance Guide* for suggested source conditions for the multimode source for the different ionization modes.
5. Make any other changes that are necessary for your method.
6. Save the method.
To set up a method to use the multimode source

**Figure 19**  Multimode acquisition settings

<table>
<thead>
<tr>
<th>Multimode (Seg)</th>
<th>Multimode (Expt)</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Gas Temp</strong></td>
<td><strong>Capillary</strong></td>
</tr>
<tr>
<td>325 °C</td>
<td>0.141 uA</td>
</tr>
<tr>
<td><strong>Vaporizer</strong></td>
<td><strong>Corona</strong></td>
</tr>
<tr>
<td>200 °C</td>
<td>110 V</td>
</tr>
<tr>
<td><strong>Drying Gas</strong></td>
<td><strong>Chamber</strong></td>
</tr>
<tr>
<td>5 L/min</td>
<td>3.61 uA</td>
</tr>
<tr>
<td><strong>Nebulizer</strong></td>
<td><strong>Charging Voltage</strong></td>
</tr>
<tr>
<td>30 psig</td>
<td>2000 V</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>MS TOF (Expt)</th>
<th><strong>Ionization Modes (seg)</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Fragmentor</strong></td>
<td><strong>Mixed</strong></td>
</tr>
<tr>
<td>175 V</td>
<td></td>
</tr>
<tr>
<td><strong>Skimmer</strong></td>
<td></td>
</tr>
<tr>
<td>65 V</td>
<td></td>
</tr>
<tr>
<td><strong>OCT 1 RF Vpp</strong></td>
<td></td>
</tr>
<tr>
<td>750 V</td>
<td></td>
</tr>
</tbody>
</table>
To open the multimode source

Open the multimode source to access the end cap and the capillary cap for cleaning and inspection.

**WARNING** Do not touch the multimode source or the capillary cap. They may be very hot. Let the parts cool before you handle them.

**WARNING** Never touch the source surfaces, especially when you analyze toxic substances or when you use toxic solvents. The source has several sharp pieces which can pierce your skin including the APCI corona needle, vaporizer sensor and counter current electrode.

**WARNING** Do not insert fingers or tools through the openings on the multimode chamber. When in use, the capillary and capillary cap are at high voltages up to 4 kV.

1. Turn off the multimode source temperatures and flows:
   a. Change the Context view to Acquisition.
   b. Click the MS Q-TOF tab.
   c. Put the instrument in Standby mode.
   d. Wait approximately 20 minutes for the source to cool down.
2. Open the spray chamber cover by pulling the latch.
   The high voltage automatically turns off when the chamber door is opened so that no high voltages are present within the chamber.
3. Check that the vaporizer temperature sensor is straight and extends 15 mm from back of chamber.
4. Check that the separator is aligned vertically.
5. Check that the APCI corona needle is in and extends approximately 3 mm from the corona guide.
6. Check that the source is clean.
To check tuning with the multimode source

Autotune is currently only available for the G3251B Dual Electrospray source. However, mass calibrations and manual optimization of mass resolution can be done using the G1978B source. To calibrate mass accuracy, do these steps.

1. Run an Autotune with the G3251B Dual Electrospray source installed.
2. Remove the G3251B Dual Electrospray source and install the G1978B multimode source.
3. Uninstall the Electrospray Calibrant Bottle B from the instrument. Cap the calibrant bottle with one of the supplied bottle caps (p/n 9300-2575).
4. Rinse one of the extra calibrant bottles (p/n 9300-2576) that was supplied as part of the Q-TOF Shipping Kit (p/n G2581-60170) with high purity acetonitrile. Pour the contents of the MMI-L Low Concentration Tuning Mix (p/n G1969-85020) into the rinsed calibrant bottle. Install the calibrant bottle on the Q-TOF mainframe in the bottle B location.
5. Set the Context view to Tune in the MassHunter Workstation program.
   a. Load the most recently used autotune file. Change the source type Multimode.
   b. Click the Mass TOF Calibration tab and do a mass calibration.
   c. Adjust the lens voltages and other tune parameters as required to optimize the mass resolution of the instrument. If changes are made to the Mid Mirror, a mass calibration will have to be done again.
   d. Verify that you have sufficient abundance for the tune peaks, that the tune peak at 2122 has greater than 10,000 resolution, and that all mass assignments are with 2 ppm after a mass calibration has been done.
6. Save the tune file and close the tune context.
2  Set-Up
   To check tuning with the multimode source
In this chapter, you create and run methods to check out the system.
Step 1. Auto tune

This step applies to MassHunter Workstation Software - Acquisition for TOF/Q-TOF revision B.01.03 or higher.

- Run autotune with the G1969-85000 ESI-L Low Concentration Tuning Mix. There are no tune specific methods.
  - Tune the 6220 in 2GHz extended dynamic range for both positive and negative.
  - Tune the 6210 in Standard (3200 $m/z$) mode 1GHz.
Step 2. Set up method names and parameters

1. Create six methods from Default.m for the multimode ESI + APCI LC Demo Sample (p/n G1978-85000), using these method names:
   - MMCHECKTOF_EI_POS.m
   - MMCHECKTOF_EI_NEG.m
   - MMCHECKTOF_CI_POS.m
   - MMCHECKTOF_CI_NEG.m
   - MMCHECKTOF_MX_EI_POS_CI_POS.m
   - MMCHECKTOF_MX_EI_NEG_CI_NEG.m

2. Use these parameters for each method:

<table>
<thead>
<tr>
<th>Table 1</th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>Parameter/Tab</th>
<th>Value</th>
</tr>
</thead>
</table>
| Column | Cartridge Hardware, Rapid Resolution, (p/n 820555-901)  
SB-C18 Rapid Res 3.5um, 2.1x30mm, (p/n 873700-902) |
| Sample Tab | Name: MM Demo Sample  
Position 1  
Run Type: Standard  
Acquisition only  
Path D:\PE Sciex Data\Projects\Data |
| ALS Tab | Standard Injection 1μL  
Bin Pump Tab:  
Flow .4mL/min  
Stop time: 3 min  
Solvent A  100.0 % (65%MeOH:35%H₂O + 0.2%acetic acid)  
Run time same as pump |
| Data files (data files for B.01.03 or greater use the suffix .d) | Data File: MM_ESI_POS.wiff  
Data File: MM_ESI_NEG.wiff  
Data File: MM_APCI_POS.wiff  
Data File: MM_APCI_NEG.wiff  
Data File: MM_ESI_APCI_POS.wiff  
Data File: MM_ESI_APCI_NEG.wiff |
Step 3. Create MMCHECKTOF_EI_POS.m

The graphics in this topic differ slightly for MassHunter B.01.03 or higher. For B.01.03, access these tabs from the Acquisition view.

- Set the parameters for MMCHECKTOF_EI_POS.m:

![Figure 20](image1.png) Acquisition parameters

![Figure 21](image2.png) Chromatogram
Ionization Mode: MM-ES
Polarity: Negative

**1100 Binary Pump 1**
Control:
Column flow: 0.400 mL/min
Stop Time: No Limit
Post Time: Off
Solvents:
Solvent A: 100.0% (65%MeOH:35%H₂O + 0.2%acetic acid))
Solvent B: 0.0%
Pressure Limits:
Minimum Pressure: 0 bar
Maximum Pressure: 400 bar

**Spray Chamber**
[MSZones]
Gas Temp: 350 °C (Maximum 350 °C)
Vaporizer: 200 °C (Maximum 250 °C)
Drying Gas: 5.0 L/min (Maximum 13.0 L/min)
Neb Pres: 60 psig (Maximum 60 psig)
VCap (Positive): 1000 V
VCap (Negative): 1000 V
VCharge (Positive): 2000 V
VCharge (Negative): 2000 V
Corona (Positive): 0.0 μA
Corona (Negative): 0.0 μA
3 Installation Verification

Step 4. Create MMCHECKTOF_EI_NEG.m

- Set the parameters for MMCHECKTOF_EI_NEG.m:

![Figure 22 Acquisition](image)

![Figure 23 Chromatogram](image)
**Ionization Mode**
- MM-ES

**Polarity**
- Negative

**1100 Binary Pump 1**
- Control
  - Column flow: 0.400 mL/min
  - Stop Time: No Limit
  - Post Time: Off

**Solvents**
- Solvent A: 100.0 % (65%MeOH:35%H₂O + 0.2%acetic acid))
- Solvent B: 0.0 %

**Pressure Limits**
- Minimum Pressure: 0 bar
- Maximum Pressure: 400 bar

**Spray Chamber**
- [MSZones]
  - Gas Temp: 350 °C
    - Maximum: 350 °C
  - Vaporizer: 200 °C
    - Maximum: 250 °C
  - Drying Gas: 5.0 L/min
    - Maximum: 13.0 L/min
  - Neb Pres: 60 psig
    - Maximum: 60 psig
  - VCap (Positive): 1000 V
  - VCap (Negative): 1000 V
  - VCharge (Positive): 2000 V
  - VCharge (Negative): 2000 V
  - Corona (Positive): 0.0 μA
  - Corona (Negative): 0.0 μA
Step 5. Create MMCHECKTOF_CI_POS.m

- Set the parameters for MMCHECKTOF_CI_POS.m:

Figure 24  Acquisition

Figure 25  Chromatogram
Ionization Mode
Polarity
**1100 Binary Pump 1**
Control
Column flow
Stop Time
Post Time
Solvents
Solvent A
Solvent B
Pressure Limits
Minimum Pressure
Maximum Pressure
**Spray Chamber**
[MSZones]
Gas Temp
Vaporizer
Drying Gas
Neb Pres
VCap (Positive)
VCap (Negative)
VCharge (Positive)
VCharge (Negative)
Corona (Positive)
Corona (Negative)
Step 6. Create MMCHECKTOF_CI_NEG.m

- Set the parameters for MMCHECKTOF_CI_NEG.m:

![Figure 26 Acquisition](image1)

![Figure 27 Chromatogram](image2)
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**Step 6. Create MMCHECKTOF_CI_NEG.m**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Setting and Details</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Ionization Mode</strong></td>
<td>MM-APCI</td>
</tr>
<tr>
<td><strong>Polarity</strong></td>
<td>Negative</td>
</tr>
<tr>
<td><strong>1100 Binary Pump 1</strong></td>
<td><strong>Control</strong></td>
</tr>
<tr>
<td>Column flow</td>
<td>0.400 mL/min</td>
</tr>
<tr>
<td>Stop Time</td>
<td>No Limit</td>
</tr>
<tr>
<td>Post Time</td>
<td>Off</td>
</tr>
<tr>
<td><strong>Solvents</strong></td>
<td></td>
</tr>
<tr>
<td>Solvent A</td>
<td>100.0 % (65%MeOH:35%H2O + 0.2%acetic acid)</td>
</tr>
<tr>
<td>Solvent B</td>
<td>0.0 %</td>
</tr>
<tr>
<td><strong>Pressure Limits</strong></td>
<td></td>
</tr>
<tr>
<td>Minimum Pressure</td>
<td>0 bar</td>
</tr>
<tr>
<td>Maximum Pressure</td>
<td>400 bar</td>
</tr>
<tr>
<td><strong>Spray Chamber</strong></td>
<td></td>
</tr>
<tr>
<td>[MSZones]</td>
<td></td>
</tr>
<tr>
<td>Gas Temp</td>
<td>350 °C</td>
</tr>
<tr>
<td>Vaporizer</td>
<td>200 °C</td>
</tr>
<tr>
<td>Drying Gas</td>
<td>5.0 L/min</td>
</tr>
<tr>
<td>Neb Pres</td>
<td>20 psig</td>
</tr>
<tr>
<td>VCap (Positive)</td>
<td>1000 V</td>
</tr>
<tr>
<td>VCap (Negative)</td>
<td>1000 V</td>
</tr>
<tr>
<td>VCharge (Positive)</td>
<td>2000 V</td>
</tr>
<tr>
<td>VCharge (Negative)</td>
<td>2000 V</td>
</tr>
<tr>
<td>Corona (Positive)</td>
<td>6.0 μA</td>
</tr>
<tr>
<td>Corona (Negative)</td>
<td>6.0 μA</td>
</tr>
</tbody>
</table>
Step 7. Create MMCHECKTOF_MX_EI POS_CI POS.m

- Set the parameters for MMCHECKTOF_MX_EI POS_CI POS.m.

**Figure 28** Acquisition

**Figure 29** Chromatogram
### Installation Verification

#### Step 7. Create MMCHECKTOF_MX_EI POS_CI POS.m

<table>
<thead>
<tr>
<th>Ionization Mode</th>
<th>MM-ES+APCI</th>
</tr>
</thead>
<tbody>
<tr>
<td>Polarity</td>
<td>Positive</td>
</tr>
</tbody>
</table>

**1100 Binary Pump 1**

- **Control**
  - Column flow: 0.400 mL/min
  - Stop Time: No Limit
  - Post Time: Off

- **Solvents**
  - Solvent A: 100.0 % (65%MeOH:35%H₂O + 0.2% acetic acid))
  - Solvent B: 0.0 %

- **Pressure Limits**
  - Minimum Pressure: 0 bar
  - Maximum Pressure: 400 bar

**Spray Chamber [MSZones]**

- **Gas Temp**: 350 °C (Maximum 350 °C)
- **Vaporizer**: 200 °C (Maximum 250 °C)
- **Drying Gas**: 5.0 L/min (Maximum 13.0 L/min)
- **Neb Pres**: 60 psig (Maximum 60 psig)
- **VCap (Positive)**: 1000 V
- **VCap (Negative)**: 1000 V
- **VCharge (Positive)**: 2000 V
- **VCharge (Negative)**: 2000 V
- **Corona (Positive)**: 1.0 μA
- **Corona (Negative)**: 1.0 μA
Step 8. Create MMCHECKTOF_MX_EI NEG_CI NEG.m

- Set the parameters for MMCHECKTOF_MX_EI NEG_CI NEG.m:

![Figure 30 Acquisition](image1.png)

![Figure 31 Chromatogram](image2.png)
<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ionization Mode</td>
<td>MM-ES+APCI</td>
</tr>
<tr>
<td>Polarity</td>
<td>Negative</td>
</tr>
<tr>
<td><strong>1100 Binary Pump 1</strong></td>
<td></td>
</tr>
<tr>
<td>Control</td>
<td></td>
</tr>
<tr>
<td>Column flow</td>
<td>0.400 mL/min</td>
</tr>
<tr>
<td>Stop Time</td>
<td>No Limit</td>
</tr>
<tr>
<td>Post Time</td>
<td>Off</td>
</tr>
<tr>
<td>Solvents</td>
<td></td>
</tr>
<tr>
<td>Solvent A</td>
<td>100.0 % (65% MeOH:35% H₂O + 0.2% acetic acid)</td>
</tr>
<tr>
<td>Solvent B</td>
<td>0.0 %</td>
</tr>
<tr>
<td>Pressure Limits</td>
<td></td>
</tr>
<tr>
<td>Minimum Pressure</td>
<td>0 bar</td>
</tr>
<tr>
<td>Maximum Pressure</td>
<td>400 bar</td>
</tr>
<tr>
<td><strong>Spray Chamber</strong></td>
<td></td>
</tr>
<tr>
<td>[MSZones]</td>
<td></td>
</tr>
<tr>
<td>Gas Temp</td>
<td>350 °C</td>
</tr>
<tr>
<td>Vaporizer</td>
<td>200 °C</td>
</tr>
<tr>
<td>Drying Gas</td>
<td>5.0 L/min</td>
</tr>
<tr>
<td>Neb Pres</td>
<td>60 psig</td>
</tr>
<tr>
<td>VCap (Positive)</td>
<td>1000 V</td>
</tr>
<tr>
<td>VCap (Negative)</td>
<td>1000 V</td>
</tr>
<tr>
<td>VCharge (Positive)</td>
<td>2000 V</td>
</tr>
<tr>
<td>VCharge (Negative)</td>
<td>2000 V</td>
</tr>
<tr>
<td>Corona (Positive)</td>
<td>1.0 μA</td>
</tr>
<tr>
<td>Corona (Negative)</td>
<td>1.0 μA</td>
</tr>
</tbody>
</table>
3 Installation Verification

Step 9. Run each of the methods created

1. Run each of the methods that you just created.
   The real time plot below shows the six runs.

   ![Real time plot of six runs]

   - ESI POS Crystal Violet
   - ESI NEG 1-Hexanesulfonic acid
   - APCI POS Carbazole
   - APCI NEG 9-Phenanthrol
   - ESI +APCI POS Crystal Violet & Carbazole
   - ESI +APCI NEG 1-Hexanesulfonic acid & 9-Phenanthrol

3 View the data in the data analysis program for MM_ESI_Neg. Extract Ion 165-165.4. Record the peak height Example 97,000.
3 Installation Verification

Step 9. Run each of the methods created.

4 View the data in the data analys program for MM_APCI_POS. Extract Ion 168-168.4. Record the peak height. Example 140,000.
5 View the data in the data analysis program for MM_APCI_NEG. Extract Ion 193-193.4. Record the peak height. Example 640,000.
3 **Installation Verification**  
Step 9. Run each of the methods created

6 View the data in the data analysis program for MM_ESI_APCI_POS. Extract Ion 372-372.4. Record the peak height. Example: 57,000.
7 View the data in the data analysis program for MM_ESI_APCI_POS. Extract Ion 168-168.4. Record the peak height. Example: 34,000.
3 Installation Verification
Step 9. Run each of the methods created

8 View the data in the data analysis program for MM_ESI_APCI_NEG. Extract Ion 165-165.4. Record the peak height. Example: 110,000.
9 View the data in the data analysis program for MM_ESI_APCI_NEG. Extract Ion 193-193.4. Record the peak height. Example: 400,000.
Step 10. Calculate the response of Multimode Demo

1. Manually fill in the values in the Multimode Ion Source report.

The values in the example report below have been manually entered from the data collected in the runs from the previous steps. This is an example of how to enter the values from the instrument being installed and verified.

The blank report is on the next page for installed instruments data.

<table>
<thead>
<tr>
<th>Compound</th>
<th>m/z</th>
<th>Polarity</th>
<th>ESI mode</th>
<th>Mixed mode</th>
<th>Mixed:ESI ratio</th>
<th>Result</th>
</tr>
</thead>
<tbody>
<tr>
<td>Crystal violet</td>
<td>372.2</td>
<td>Positive</td>
<td>91k</td>
<td>57k</td>
<td>63%</td>
<td>Pass</td>
</tr>
<tr>
<td>1-Hexanesulfonic acid</td>
<td>165.1</td>
<td>Negative</td>
<td>97k</td>
<td>110k</td>
<td>113%</td>
<td>Pass</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Compound</th>
<th>m/z</th>
<th>Polarity</th>
<th>APCI mode</th>
<th>Mixed mode</th>
<th>Mixed:APCI ratio</th>
<th>Result</th>
</tr>
</thead>
<tbody>
<tr>
<td>Carbazole</td>
<td>168.1</td>
<td>Positive</td>
<td>140k</td>
<td>34k</td>
<td>24%</td>
<td>Pass</td>
</tr>
<tr>
<td>9-Phenanthrol</td>
<td>193.1</td>
<td>Negative</td>
<td>640k</td>
<td>400k</td>
<td>63%</td>
<td>Pass</td>
</tr>
</tbody>
</table>

Passing criteria: Mixed mode response 20% or greater of single-mode response.

2. Run all methods and get the peak heights. Calculate the amount of signal.
Step 11. Fill out Multimode Report for calculation of peak heights

- Use the graphic below to fill out the multimode report for calculation of peak heights.

### Multimode Ion Source Report

<table>
<thead>
<tr>
<th>MSD type: TOF</th>
<th>Instrument name:</th>
<th>Operator name:</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Acquisition date:** 23-Feb-2006

**Datafiles:**
- MM_ESI_pos.wif
- MM_ESI_NEG.wif
- MM_APCI_POS.wif
- MM_APCI_NEG.wif
- MM_ESI_APCI_POS.wif
- MM_ESI_APCI_NEG.wif

#### ESI Compound Results

<table>
<thead>
<tr>
<th>Compound</th>
<th>m/z</th>
<th>Polarity</th>
<th>ESI mode</th>
<th>Mixed mode</th>
<th>Mixed:ESI ratio</th>
<th>Result</th>
</tr>
</thead>
<tbody>
<tr>
<td>Crystal Violet</td>
<td>372.2</td>
<td>Positive</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1-hexanesulfonic acid</td>
<td>165.1</td>
<td>Negative</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

#### APCI Compound Results

<table>
<thead>
<tr>
<th>Compound</th>
<th>m/z</th>
<th>Polarity</th>
<th>APCI mode</th>
<th>Mixed mode</th>
<th>Mixed:APCI ratio</th>
<th>Result</th>
</tr>
</thead>
<tbody>
<tr>
<td>Carbazole</td>
<td>168.1</td>
<td>Positive</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>9-Phenanthrol</td>
<td>193.1</td>
<td>Negative</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Passing criteria:** Mixed mode response 20% or greater of single-mode response.
3 Installation Verification
Step 11. Fill out Multimode Report for calculation of peak heights
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In This Book

This book contains installation, operation, maintenance and troubleshooting instruction for the Multimode Source for 6500 Series Q-TOF LC/MS.